Cobalt-Catalyzed Intermolecular [2+2+2] Cycloaddition of Nitriles and Alkynes: Facile Synthesis of Polyarylpyridines and Their Mechanochemical Cyclodehydrogenation to Nitrogen-Containing Polyaromatics

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Simple, inexpensive and robust cobalt-based catalytic systems for the [2+2+2] cycloaddition between unactivated nitriles and diarylacetylenes are reported. The present systems tolerate a broad range of aryl and alkyl nitriles and cyanamides as well as various di(hetero)arylacetylenes, allowing for the facile preparation of diverse polyarylated pyridines. Mechanochemistry-enabled multifold cyclodehydrogenation of tetra- and pentaarylpyridine is demonstrated to achieve the synthesis of nitrogen-containing polycyclic aromatic compounds having hitherto unprecedented skeletons.

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Cobalt-Catalyzed Intermolecular [2+2+2] Cycloaddition of Nitriles and Alkynes: Facile Synthesis of Polyarylpiperidines and Their Mechanochemical Cyclodehydrogenation to Nitrogen-Containing Polyaromatics

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Abstract

Transition metal-catalyzed [2+2+2] cycloaddition of nitriles and alkynes has been extensively developed as a straightforward and atom-economical synthetic approach to piperidines over the last several decades using various transition metal catalysts, both precious and non-precious. Despite this long history, cycloadditions of this type have often relied on the use of tethered diyne or cyanoalkyne as one of the reactants. Thus, examples of efficient, fully intermolecular catalytic [2+2+2] piperidine synthesis, especially those employing unactivated nitriles and internal alkynes leading to pentasubstituted piperidines, remain scarce. Herein, we report on simple and inexpensive catalytic systems based on cobalt(II) iodide, 1,3-bis(diphenylphosphino)propane, and Zn that promote [2+2+2] cycloaddition of various nitriles and diarylacetylenes without using a large excess of the nitrile. The present systems allow for the synthesis of broad range of polyarylated piperidines, many of which have not been previously accessed by the [2+2+2] manifold. Computational studies have supported a reaction pathway involving oxidative coupling of two alkynes, insertion of the nitrile into cobaltacyclopentadiene, and C–N reductive elimination, while shedding light on stepwise nature of the oxidative coupling and insertion processes. We also demonstrate that tetra- and pentaarylpiperidines can serve as precursors to hitherto unprecedented nitrogen-containing polycyclic aromatic hydrocarbons via mechanochemically assisted multifold reductive cyclodehydrogenation.

Introduction

Transition metal-catalyzed [2+2+2] cycloaddition between a nitrile and two alkynes represents a straightforward and atom-economical approach to the synthesis of multisubstituted pyridines,^[1] which has found a number of applications in the synthesis of pyridine-containing complex natural products,^[2] bioactive molecules,^[3] and extended π -conjugated materials,^[4] to name a few. Since the pioneering work of Wakatsuki and Yamazaki on CpCo complex-mediated/catalyzed reactions,^[5] this cycloaddition has been extensively explored with the aid of various transition metal catalysts including cobalt,^[6,7] nickel,^[8] iron,^[9] ruthenium,^[10] rhodium,^[11] and iridium,^[12] in addition to stoichiometric variants using zirconium^[13] and titanium^[14] reagents. Despite the tremendous developments in the last decades, the majority of efficient catalytic [2+2+2] pyridine formations take advantage of using tethered diyne or cyanoalkyne as one of the starting materials to reduce the entropic penalty as well as to address the issues of chemoselectivity (e.g., competition with alkyne [2+2+2] cycloaddition to form benzene derivatives) and regioselectivity (Scheme 1a). Except for the stoichiometric variants involving the reaction between preformed zircona-^[13] and titanacycles,^[14] examples of fully intermolecular [2+2+2] pyridine synthesis from unactivated nitriles and unactivated internal alkynes are surprisingly scarce. This problem, especially with respect to the cycloaddition involving diarylacetylenes, warrants attention in light of the significant interest in polyarylated pyridines for their optical/electronic properties and relevant applications.^[15] For example, literature reports on the synthesis of pentarylpriidines through catalytic [2+2+2] cycloaddition of aryl nitrile and diarylacetylene have been limited to those promoted by Cp*Co(η^3 -allyl)^[16] or palladium catalysts,^[17] with only one or two examples for each catalyst (Scheme 1b). During the preparation of this manuscript, Wang and coworkers reported a catalytic system comprised of iron and cobalt complexes for such cycloaddition, albeit using only diphenylacetylene and a limited scope of aryl nitriles.^[18]

As a part of our continuing pursuit of low-valent cobalt–diphosphine catalyzed synthetic transformations^[19,20] we report herein that cobalt(II) iodide, 1,3-bis(diphenylphosphino)propane (dppp), and Zn in appropriate polar solvents give rise to simple, inexpensive, and highly robust catalytic systems for the fully intermolecular [2+2+2] cycloaddition of various aryl and alkyl nitriles with diarylacetylenes (Scheme 1c). The present systems allow for the synthesis of a diverse range of polyarylated pyridines without using large excess of the nitrile with respect to the alkyne (nitrile:alkyne = 1:1 to 1.5:1). Computational studies have suggested that the present [2+2+2] cycloaddition is initiated by oxidative coupling of two alkynes on cobalt, followed by nitrile insertion into cobaltacyclopentadiene and C–N

reductive elimination. We have also demonstrated, for the first time, multifold cyclodehydrogenation of tetra- and pentaarylpyridines enabled under mechanochemical conditions to form hitherto unprecedented types of nitrogen-containing polycyclic aromatic hydrocarbons (PAHs).

(a) [2+2+2] Pyridine synthesis using tethered substrates

(b) Fully intermolecular [2+2+2] pentaarylpyridine synthesis

(c) This work

- Simple, inexpensive and robust catalyst
- Broad range of nitriles ($\text{R} = \text{aryl}, \text{alkyl}, \text{NR}_2$)
- Various diarylacetylenes
- DFT calculations
- Mechanochemical cyclodehydrogenation to aza-PAHs

Scheme 1. Transition metal-catalyzed [2+2+2] cycloaddition of nitrile and alkynes.

Results and Discussion

The present study commenced with screening of reaction conditions for the cycloaddition of benzonitrile (**1a**, 0.5 mmol) with diphenylacetylene (**2a**, 0.2 mmol). In the initial attempts, a catalytic system comprised of CoI_2 (10 mol%), dppp (10 mol%), and Zn dust (50 mol%) was found to promote the desired cycloaddition in NMP at 120 °C to afford, after 24 h, pentaphenylpyridine (**3aa**) in 53% yield (Table 1, entry 1), along with a small amount (4%) of competitive cyclotrimerization product of **2a** (i.e. hexaphenylbenzene). The reaction also took place in DMF to give **3aa** in a comparable yield, which was accompanied by a small amount of byproduct arising from the addition of DMF to **2a** via carbamoyl C–H activation (entry 2).^[20f] No pyridine formation was observed in toluene (entry 3). Lowering the temperature to 80 °C improved the yield of **3aa** to 82% (80% isolated yield; entry 4). The use of CoCl_2 or CoBr_2 as the precatalyst in place of CoI_2 led to a substantial drop in the yield of **3aa** (entries 5 and 6). A well-defined Co^{I} complex, $\text{CoCl}(\text{PPh}_3)_3$, also served as a viable precatalyst under otherwise identical conditions (entry 7). However, this complex did not promote the reaction at all when Zn was omitted (entry 8), implying that reduction of Co^{I} to Co^0 was necessary for the catalytic activity. Screening of various ligands in combination with CoI_2 revealed that the present catalytic activity is unique to dppp. Thus, common diphosphine ligands such as dppm, dppe, dppb, and dppbz as well as monophosphine ligands such as PPh_3 barely promoted either pyridine-forming cycloaddition or benzene-forming cycloaddition (entries 9-13; see Table S1 for additional results). It was particularly surprising to us that the $\text{CoI}_2/\text{dppe}/\text{Zn}$ system was completely ineffective (entry 10), as it is rather similar to the $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}/\text{dppe}/\text{Zn}$ system developed by Okamoto for the cycloaddition between tethered diynes and nitriles.^[7b,c] With the $\text{CoI}_2/\text{dppp}/\text{Zn}$ system, we were able to reduce the ratio of **1a** and **2a** to 1:1 without apparent decrease in the yield of **3aa** (79% isolated yield; entry 14), while further reduction to 1:2 (which corresponds to the theoretical stoichiometry) led to a drop to 52% yield (entry 15).

Table 1. [2+2+2] Cycloaddition of Benzonitrile (**1a**) and Diphenylacetylene (**2a**)^[a]

<div style="text-align: center;"><div style="display: flex; align-items: center; justify-content: center;"><div style="text-align: center;">$\text{Ph}-\text{CN}$ 1a</div><div style="margin: 0 10px;">+</div><div style="text-align: center;">$\text{Ph}-\text{C}\equiv\text{C}-\text{Ph}$ 2a</div></div><div style="display: flex; align-items: center; justify-content: center; margin-top: 10px;"><div style="text-align: center;">$\xrightarrow[\text{solvent, } T, 24 \text{ h}]{\begin{array}{c} \text{CoX}_n \text{ (10 mol\%)} \\ \text{ligand (10 mol\%)} \\ \text{Zn (50 mol\%)} \end{array}}$</div><div style="margin: 0 10px;">$\longrightarrow$</div><div style="text-align: center;"><div style="text-align: center;"> 3aa</div></div></div></div>					
Entry	CoX _n	Ligand	Solvent	T [°C]	Yield [%] ^[b]
1	CoI ₂	dppp	NMP	120	53
2	CoI ₂	dppp	DMF	120	47 ^[c]
3	CoI ₂	dppp	toluene	120	0
4	CoI ₂	dppp	NMP	80	82 (80)
5	CoCl ₂	dppp	NMP	80	25
6	CoBr ₂	dppp	NMP	80	54
7	CoCl(PPh ₃) ₃	dppp	NMP	80	45
8 ^[d]	CoCl(PPh ₃) ₃	dppp	NMP	80	0
9	CoI ₂	dppm	NMP	80	4
10	CoI ₂	dppe	NMP	80	0
11	CoI ₂	dppb	NMP	80	0
12	CoI ₂	dppbz	NMP	80	2
13 ^[e]	CoI ₂	PPh ₃	NMP	80	0
14 ^[f]	CoI ₂	dppp	NMP	80	81 (79)
15 ^[g]	CoI ₂	dppp	NMP	80	52

[a] Unless otherwise noted, the reaction was performed using **1a** (0.5 mmol), **2a** (0.2 mmol), CoX_n (10 mol%), ligand (10 mol%), and Zn (50 mol%) in 0.3 mL of solvent for 24 h. dppp = 1,3-bis(diphenylphosphino)propane; dppm = bis(diphenylphosphino)methane; dppe = 1,2-bis(diphenylphosphino)ethane; dppb = 1,4-bis(diphenylphosphino)butane; dppbz = 1,2-bis(diphenylphosphino)benzene. [b] Determined by GC using *n*-tridecane as an internal standard. Isolated yield is shown in the parentheses. [c] The hydrocarbamylation product (addition of DMF to **2a**) was obtained in 13% yield. [d] The reaction was performed without Zn. [e] 20 mol% of PPh₃ was used. [f] 0.2 mmol of **1a** and 0.2 mL of NMP were used. [g] 0.1 mmol of **1a** and 0.2 mL of NMP were used.

With the optimized catalytic system (Table 1, entry 14) in hand, we set out to explore the scope of the [2+2+2] cycloaddition. First, a variety of aryl nitriles were subjected to the reaction with **2a** (Table 2). The reaction of parent benzonitrile (**1a**) could be performed on a 3 mmol scale to afford the desired pyridine **3aa** in 83% yield (entry 1). Benzonitriles bearing various electron-donating or -withdrawing substituents (**1b–1f**) participated in the reaction to

We next explored the reaction of benzonitrile (**1a**) with various alkynes (Table 3). Symmetrical diarylacetylenes bearing a series of electron-donating (alkyl, OMe) or -withdrawing (F, CO₂Et, COMe) substituents at the *para*-positions took part in the cycloaddition with **1a** to afford the corresponding products **3ab–3ag** in moderate to good yields (entries 1–6), where only a small amount of the alkyne cyclotrimerization product was indicated by TLC analysis of the reaction mixture. Among these substituents, electron-donating *t*-butyl and methoxy groups made the reaction somewhat sluggish, necessitating an increase in the nitrile/alkyne ratio to 1.5:1 and a prolonged reaction time of 72 h (entries 2 and 3). The reaction also tolerated diarylacetylenes bearing *meta*-substituents (**2h–2k**), affording pentaarylpyridines **3ah–3ak** in moderate to high yields (entries 7–10), while those bearing *ortho*-substituents such as 1,2-di-*o*-tolylethyne failed to undergo the cycloaddition. The reaction of an unsymmetrical diarylacetylene such as ethyl 4-((4-methoxyphenyl)ethynyl)benzoate afforded an inseparable mixture of multiple pyridine regioisomers, despite the electronic difference between the two aryl groups (see Figure S2). The CoI₂/dppp system failed to engage a dialkylacetylene such as 4-octyne (**2l**) in the cycloaddition with **1a**. However, a modified catalytic system employing bis(dicyclohexylphosphino)methane (dcypm) and 1,2-dimethoxyethane (DME) instead of dppp and NMP, respectively, promoted the reaction to afford the desired pyridine **3al** in 63% yield (entry 11; see Table S2 for the optimization).

Table 3. [2+2+2] Cycloaddition of **1a** with Various Alkynes^[a]

$ \begin{array}{c} \text{Ph-CN} + \text{R} \equiv \text{R} \xrightarrow[\text{NMP, 80 } ^\circ\text{C, 24 h}]{\text{CoI}_2 \text{ (10 mol\%)} \\ \text{dppp (10 mol\%)} \\ \text{Zn (50 mol\%)}} \\ \textbf{1a} \qquad \qquad \textbf{2b-2l} \qquad \qquad \qquad \textbf{3ab-3al} \end{array} $			
Entry	R	Product	Yield [%] ^[b]
1	4-MeC ₆ H ₄ (2b)	3ab	65
2 ^[c]	4- <i>t</i> BuC ₆ H ₄ (2c)	3ac	67
3 ^[c]	4-MeOC ₆ H ₄ (2d)	3ad	57
4	4-FC ₆ H ₄ (2e)	3ae	71
5	4-EtO ₂ CC ₆ H ₄ (2f)	3af	63
6	4-Me(O)CC ₆ H ₄ (2g)	3ag	41
7	3-MeC ₆ H ₄ (2h)	3ah	51

8	3-MeOC ₆ H ₄ (2i)	3ai	84
9	3-Me ₂ NC ₆ H ₄ (2j)	3aj	66
10	3,5-(MeO) ₂ C ₆ H ₃ (2k)	3ak	86
11 ^[d]	Pr (2l)	3al	63

[a] Unless otherwise noted, the reaction was performed using **1a** (0.4 mmol), alkyne **2** (0.4 mmol), CoI₂ (10 mol%), dppp (10 mol%), and Zn (50 mol%) in 0.4 mL of NMP at 80 °C for 24 h. [b] Isolated yield. [c] The reaction was performed using 0.6 mmol of **1a** for 72 h. [d] The reaction was performed using bis(dicyclohexylphosphino)methane (dcypm) and DME in place of dppp and NMP, respectively.

The present catalytic system also proved effective for the cycloaddition of di(heteroaryl)acetylenes, as demonstrated by the synthesis of structurally interesting, symmetric penta(heteroaryl)pyridines (Scheme 2). Thus, the cycloaddition of 2-cyanothiophene (**1l**) and di(2-thienyl)ethyne (**2m**) afforded penta(2-thienyl)pyridine (**3lm**) in 80% yield, which was previously synthesized via sequential Stille couplings^[15a] or fivefold Suzuki–Miyaura coupling of pentachloropyridine.^[15c] Penta(3-pyridyl)pyridine (**3nn**), which remains unknown in the literature, could also be prepared from 3-cyanopyridine (**1n**) and di(3-pyridyl)ethyne (**2n**) albeit in a modest yield.

Scheme 2. Synthesis of penta(heteroaryl)pyridines.

The scope of the [2+2+2] cycloaddition was further extended to alkyl nitriles (Table 4). We noted that the above catalytic system was only moderately effective for the reaction of MeCN (**1o**) and **2a**. With further optimization (see Table S3), a modified catalytic system

comprised of CoI_2 (5 mol%), dppp (5 mol%), and Zn (25 mol%) in DMA was found to efficiently promote the reaction, at the expense of large excess MeCN (**1o**:**2a** = 5:1), affording the desired product **3oa** in 90% yield. MeCN could also be coupled with *para*-substituted diphenylacetylenes, affording **3ob** and **3oc** in good yields. The reaction using CD_3CN in place of MeCN was equally efficient and afforded **3oa-*d*₃** in 92% yield. The reaction of propionitrile (**1p**) and **2a** was subjected to additional optimization (see Table S4) and was achieved in high yield (89%) at a lower nitrile/alkyne ratio of 1.5:1. This ratio was effective for a variety of other alkyl nitriles. Sterically unhindered alkyl and benzyl nitriles, including those bearing an olefin moiety, participated in the reaction with **2a** to afford the desired pyridine derivatives **3qa–3ua** in high yields. The reaction also tolerated sterically hindered secondary alkyl nitriles (see **3va** and **3wa**) as well as nitriles containing dialkylamino, ester, and pyridyl groups (see **3xa–3za**). Note that, among these 2-alkyl-3,4,5,6-tetraarylpyridines, only **3oa**, **3pa**, and **3qa** are known in the literature, reflecting the scarcity of relevant [2+2+2] cycloadditions.^[16,18] A cyanamide derivative such as morpholine-4-carbonitrile (**1aa**) also participated in the reaction with **2a** to afford the 2-aminopyridine derivative **3aaa** in an excellent yield. As we observed for the reaction of PhCN (**1a**) and 4-octyne (**2l**; Table 3, entry 11), the reaction of **1p** and **2l** was achieved using the $\text{CoI}_2/\text{dcypm}$ system in DME in a moderate yield.

Table 4. [2+2+2] Cycloaddition of Alkyl Nitriles^[a]

R^1-CN 1o–1aa	+	$R^2-C\equiv C-R^2$ 2a–2c, 2l	$\xrightarrow[\text{DMA, 80 } ^\circ\text{C, 24 h}]{\text{CoI}_2 \text{ (5 mol\%)}, \text{dppp (5 mol\%)}, \text{Zn (25 mol\%)}}$	 3
<hr/>				
3oa (Ar = Ph), 90% ^[b]		[D₃]-3oa , 92% ^[b]		3pa , 89%
3ob (Ar = 4-MeC ₆ H ₄), 82% ^[b]				
3oc (Ar = 4- <i>t</i> BuC ₆ H ₄), 74% ^[b]				
3qa , 89%		3ra , 85%		3sa , 80%
3ta , 79%		3ua , 91%		3va , 51% ^[c]
3wa , 41% ^[c]		3xa , 50% ^[d]		3ya , 39% ^[d]
3za , 42% ^[d]		3aaa , 92% ^[d]		3pl , 55% ^[e]

[a] Unless otherwise noted, the reaction was performed using nitrile **1** (0.6 mmol), alkyne **2** (0.4 mmol), CoI₂ (5 mol%), dppp (5 mol%), and Zn (25 mol%) in 0.4 mL of DMA at 80 °C for 24 h. The yields refer to isolated yields. [b] 2 mmol of nitrile was used. [c] The reaction was performed for 72 h. [d] CoI₂ (10 mol%), dppp (10 mol%), and Zn (50 mol%) were used. [e] The reaction was performed using propionitrile (2 mmol), 4-octyne (0.4 mmol), CoI₂ (10 mol%), dcypm (10 mol%), and Zn (50 mol%) in DME at 100 °C.

The applicability of the present catalytic system to the cycloaddition of tethered substrates was briefly examined (Scheme 3). A diyne substrate capped with phenyl groups (**4**) underwent efficient cycloaddition with benzonitrile (**1a**) to afford the pentasubstituted pyridine

5 in 89% yield. Note that, despite the extensive previous studies, bicyclic pyridines bearing 2,3,6-triaryl substituents such as **5** have not been synthesized by bimolecular [2+2+2] cycloaddition between diyne and nitrile. The reaction between a tethered cyanoalkyne **6** and diphenylacetylene (**2a**) also proved feasible, affording the 2,3,4-triarylpyridine derivative **7** albeit in a modest yield. This type of bimolecular cycloaddition leading to a bicyclic 2,3,4-triaryl-5,6-dialkylpyridine framework is also rare.^[8c]

Scheme 3. [2+2+2] Cycloaddition using tethered substrates.

To gain insight into the reaction pathway of the present [2+2+2] cycloaddition, we turned to density functional theory (DFT) calculations. The [2+2+2] pyridine formation promoted by CpCo^{I} catalysts has been studied computationally, and reaction pathways initiated by oxidative coupling of two alkyne molecules on Co^{I} have been identified.^[7f,21] The resulting cobaltacyclopentadiene may undergo [4+2] cycloaddition with nitrile to form the pyridine skeleton directly or go through stepwise bond formation processes involving nitrile insertion and C–N reductive elimination. On the other hand, the working mode of cobalt–diphosphine catalysts has not been studied computationally, while oxidative cyclization of a bis-alkyne complex has been proposed to be operative.^[7b,c]

In light of the above background, we explored the cycloaddition of **1a** and **2a** on two model low-valent cobalt complexes, namely, $[(\text{dppp})\text{Co}^0]$ and $[(\text{dppp})\text{Co}^{\text{I}}]^+$.^[22] In short, these studies have shown the following points. Firstly, both the Co^0 and Co^{I} complexes can promote the reaction via oxidative coupling of two molecules of **2a** as the initial step, followed by insertion of **1a** into the cobaltacyclopentadiene and C–N reductive elimination. The potentially competing oxidative coupling of **1a** and **2a** requires a much higher activation barrier than that of the alkyne/alkyne oxidative coupling and is unlikely to operate. Secondly, the activation

barrier for the alkyne/alkyne oxidative coupling is distinctly lower for the Co^0 complex than for the Co^{I} complex, suggesting that a Co^0 species is more likely to serve as the active species for the present cycloaddition. We describe the reaction pathways for the Co^0 complex below (Figure 1), and leave the detail of the Co^{I} -mediated reaction pathways in the Supporting Information (Figures S12 and S13).

Among a series of $(\text{dppp})\text{Co}^0$ complexes of **1a** and/or **2a**, the monoalkyne complex **CP_A** (spin state: doublet) was calculated to be the most stable (Figure S8). Note that the quartet spin state was found to be much higher in energy than the doublet state for a series of key intermediates and transition states along the reaction pathway (Figure S9). Note that the quartet spin state was found to be much higher in energy than the doublet state for a series of key intermediates along the reaction pathway (Figure S8). Coordination of the second molecule of **2a** to **CP_A** forms a tetrahedral bisalkyne complex **CP_{2A}** ($\Delta G = 7.8 \text{ kcal mol}^{-1}$), where the two alkyne ligands take twisted arrangement to avoid steric repulsion between the phenyl groups on the nearby carbons (C2 and C3). Subsequent oxidative coupling via **TS1**, with an activation energy of $24.7 \text{ kcal mol}^{-1}$ (from **CP_A**), leads to a metastable cobaltacycle intermediate **INT1** ($\Delta G = 13.4 \text{ kcal mol}^{-1}$). Reflecting the twisted orientation of the two alkyne ligands, **INT1** adopts a half-chair-like conformation (Figure 2). Notably, the metallacycle core of **INT1** is unsymmetrical, the Co–C1 bond ($1.82 \text{ \AA}$) being distinctly shorter than the Co–C4 bond ($1.97 \text{ \AA}$), which is also in line with higher Mayer bond order of the former (0.529) than the latter (0.332). The Co–C2 ($1.96 \text{ \AA}$) and Co–C3 ($2.04 \text{ \AA}$) distances are also unequal. These parameters, together with typical Co–C bond lengths ($1.92\text{--}1.99 \text{ \AA}$) in known cobaltacyclopentadiene complexes,^[23] suggest that the Co–C1 bond has a partial carbene-like character.^[24] **INT1** then undergoes facile bond reorganization and rearrangement via **TS2** ($\Delta G = 17.1 \text{ kcal mol}^{-1}$) to generate another, significantly more stable cobaltacycle **INT2** ($\Delta G = -5.7 \text{ kcal mol}^{-1}$). **INT2** has a distorted tetrahedral geometry and shows a clear structural feature of metallacyclopentadiene (Figure 2).^[25] Importantly, the potentially competing alkyne/nitrile oxidative coupling (**CP_A** to **TS6**) was found to require an activation energy ($29.9 \text{ kcal mol}^{-1}$) distinctly higher than that of the alkyne/alkyne oxidative coupling, producing an azacobaltacycle **INT7** ($\Delta G = 20.7 \text{ kcal mol}^{-1}$) in a significantly endergonic manner. As such, further reaction pathway of **INT7** was not considered.

The cobaltacyclopentadiene **INT2** accepts either side-on or end-on coordination of **1a** to form **INT3** ($\Delta G = 9.0 \text{ kcal mol}^{-1}$) or **INT3'** ($\Delta G = -4.8 \text{ kcal mol}^{-1}$), respectively, which features square-pyramidal geometry with C4 at the apical site. The former complex is connected to an insertion transition state **TS3** with an overall activation barrier of 19.1 kcal

mol⁻¹ (from **INT2**), leading to a metastable intermediate **INT4** ($\Delta G = 4.3$ kcal mol⁻¹). **INT4** features a fused azametallabicyclic structure,^[7f,10d,21a,b] with the Co–C1 bond (2.05 Å) at the junction. Partial carbene-like nature of the Co–C4 bond is suggested from the geometry around Co and C2–C4 (Figure 2). **INT4** undergoes a rearrangement involving Co–C1 bond cleavage via **TS4** with a small activation barrier (2.0 kcal mol⁻¹), affording a more stable azacobaltacycloheptadiene **INT5** ($\Delta G = -4.3$ kcal mol⁻¹). Note that all attempts to locate a transition state for direct [4+2] cycloaddition between **INT2** and **1a** failed, converging to the transition state of nitrile insertion. Finally, C–N reductive elimination of **INT5** occurs via **TS5** with a relatively small activation energy (8.3 kcal mol⁻¹) to give an η^4 -type product complex **INT6**, followed by ligand exchange with **2a** to release **3aa** and regenerate **CP_A**.

While the overall reaction pathway described above conforms to the commonly proposed mechanistic framework involving alkyne/alkyne oxidative coupling and nitrile insertion into cobaltacyclopentadiene,^[7b,c] the present calculations have revealed nontrivial stepwise nature of the elementary steps (i.e., oxidative coupling and nitrile insertion). Given that nitrile/alkyne oxidative coupling has been proposed as a plausible operative mechanism for some of the previously reported nickel- and iron-catalyzed [2+2+2] pyridine synthesis,^[8a,9a] the difference among the neighboring first-row transition metal triad (i.e., Fe/Co/Ni) would deserve further theoretical investigation.

Figure 1. Gibbs free energy diagram of the [2+2+2] cycloaddition of benzonitrile (**1a**) and diphenylacetylene (**2a**) on [(dppp)Co⁰] calculated at the SMD(NMP)-M06L/6-311++G(2df,2p)-SDD(Co)//M06L/6-31G(d)-SDD(Co) level.

Figure 2. Structures of selected cobaltacycle intermediates. The phenyl groups of dppp are truncated for clarity. The distances are in Å.

In light of Scholl-type cyclodehydrogenation of polyarylbenzenes as a well-established and widely practiced strategy to construct polycyclic aromatic hydrocarbons (PAHs),^[26] it appears a natural idea to use tetra- and pentaarylpyridines as precursors to aza-PAHs^[27] via analogous cyclodehydrogenation. However, to our best knowledge, no single example of such a transformation has been reported to date. This is somewhat surprising but understandable, because the electron-deficient nature and the basicity of a pyridine ring would prevent the oxidative Scholl reaction typically employing Lewis or Brønsted acid. In this context, the reductive cyclodehydrogenation using potassium metal,^[28] which has recently been utilized by

Ito, Itami and coworkers for the conversion of azine-containing polyaromatic systems to aza-PAHs,^[29] appeared attractive.

Adopting the reductive cyclodehydrogenation strategy powered by mechanochemistry,^[30-32] we have successfully converted some of the tetra- and pentaarylpyridines described above into the corresponding aza-PAH derivatives (Scheme 4). The threefold cyclodehydrogenation of 2,3,4,5-tetraaryl-6-alkylpyridines **3oa**, **3pa**, and **3ob** in the presence of potassium (20 equiv) proceeded under ball milling (30 Hz, 2 h) to afford the corresponding aza-PAHs **8a–8c** as poorly soluble light-yellow solids in 19–37% yields (Scheme 4a). Importantly, the reaction of **3oa** in toluene afforded **8a** in only 14% yield (NMR), which could not be isolated in a pure form due to accompanying byproducts arising from incomplete (single and twofold) cyclodehydrogenations. Curiously, the mechanochemical reaction of analogous tetraarylpyridine **3oc** afforded cyclodehydrogenation/demethylation product **9** as the only isolable compound (Scheme 4b). Finally, the fourfold cyclodehydrogenation of pentaarylpyridine **3ac** afforded the corresponding aza-PAH **10** in 27% yield (Scheme 4c). Note that the reaction of **3ac** in toluene failed to give **10** in a detectable amount. We speculate that the failure of the solution-phase syntheses of the aza-PAHs is mainly ascribed to the inhomogeneity of the reaction mixture and the decreased solubility of partially cyclodehydrogenated intermediates, which represent problems that can be effectively addressed under mechanochemical conditions.

Scheme 4. Mechanochemically assisted cyclodehydrogenation of tetra- and pentaarylpiperidines to nitrogen-containing PAHs.

The planarized structure of the novel aza-PAH **10** was unambiguously confirmed by X-ray crystallographic analysis (Figure 3a).^[33] The C–C bonds connecting the pyridine ring and the peripheral benzene rings (bonds **a–e**) have average length of 1.444 Å, which is shorter than that of the corresponding bonds in the known structure of penta(*p*-tolyl)pyridine (1.494 Å),^[15c] reflecting the extended π -conjugation. Meanwhile, as expected from the Clar structure^[34] of **10**, these and the newly formed C–C bonds (bonds **f–i**; average length 1.469 Å) are distinctly longer than that of the C–C bonds in the rings **A–E** (average 1.400 Å). The molecular packing of **10** displayed a face-to-face antiparallel π - π stacked pair with a distance between the C4 positions of the pyridine rings of 3.31 Å, which is sandwiched by two other molecules of **10** through C–H/ π interactions (Figure 3b and Figure S4).

Figure 3. (a) ORTEP representation of **10** (thermal ellipsoids at the 50% probability). Solvent molecule (THF) is omitted for clarity. (b) Molecular packing in single crystal X-ray structure of **10**. Distances are in Å.

Figure 4 shows the UV-vis absorption and emission spectra of the aza-PAHs **8a** and **10**. Similar to their known hydrocarbon analogues,^[35] **8a** and **10** displayed the absorption spectra featuring high degree of fine structure in the ranges of 290–402 nm and 304–430 nm, respectively, where the absorption peaks may be designated as α , β , or para-bands. With TD-DFT calculations of the optimized structures, the lowest transition energies of **8a** and **10** were calculated to be 379 nm and 405 nm, respectively (see Tables S7 and S8). The emission spectra of **8a** and **10** were characterized by multiple peaks (407, 432, and 457 nm for **8a**; 435, 462, and 494 nm for **10**) with rather small Stokes shift (< 10 nm), reflecting their rigid molecular structures. The emission quantum yields were determined to be 0.27 and 0.47 for **8** and **10**, respectively. Mechanochemical synthesis of a greater variety of aza-PAHs from polyarylpyridines and exploration of their optical and electronic properties are currently underway.

Figure 4. UV-vis absorption (solid lines) and emission (dashed lines) spectra of **8a** and **10** in CH₂Cl₂ (excitation wavelengths: 301 nm for **8a** and 331 nm for **10**).

Conclusion

In summary, we have developed highly robust cobalt-based catalytic systems for the fully intermolecular [2+2+2] cycloaddition of nitrile and internal alkynes for the synthesis of pentasubstituted pyridines. Thus, simple and inexpensive catalysts generated from CoI₂, dppp, and Zn have enabled the preparation of monocyclic tetra- and pentarylpyridines with an unprecedented level of structural diversity. DFT calculations supported the often-proposed reaction pathway involving oxidative coupling of two alkyne molecules, insertion of nitrile into cobaltacyclopentadiene, and C–N reductive elimination, while providing insight into the mechanistic subtlety of each of the elementary steps. Furthermore, we have also demonstrated the power of mechanochemistry in forging hitherto unknown types of aza-PAHs through multifold reductive cyclodehydrogenation of polyarylated pyridines. Taken together, the present studies would stimulate further development and mechanistic study of intermolecular [2+2+2] pyridine formation as well as the use of polyarylated pyridines as precursors to nitrogen-doped nanographenes.

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Supporting Information
Cobalt-Catalyzed Intermolecular [2+2+2] Cycloaddition of Nitriles and
Alkynes: Facile Synthesis of Polyarylpyridines and Their
Mechanochemical Cyclodehydrogenation to Nitrogen-Containing
Polyaromatics

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1. Materials and Methods

General. All reactions dealing with air- or moisture-sensitive compounds were performed by standard Schlenk techniques in oven-dried reaction vessels under nitrogen atmosphere or in an argon-filled glove box. Analytical thin-layer chromatography (TLC) was performed on Merck 60 F254 silica gel plates. Flash column chromatography was performed using 40-63 μm silica gel (Si 60, Merck). ^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on Bruker AV-300 (300 MHz), AV-400 (400 MHz), AV-500 (500 MHz) or BBFO-400 (400 MHz) NMR spectrometers. ^1H and ^{13}C NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm) and CHCl_3 (77.0 ppm), respectively. Gas chromatography (GC) analysis was performed on a Shimadzu GC-2010 system equipped with an FID detector and a glass capillary column, DB-5 (Agilent J&W, 0.25 mm i.d. x 30 m, 0.25 μm film thickness). High-resolution mass spectra (HRMS) were obtained with a Q-ToF Premier LC HR mass spectrometer. Melting points were determined using a capillary melting point apparatus and are uncorrected.

Materials. Unless otherwise noted, commercial reagents were purchased from Sigma-Aldrich, Alfa Aesar, and other commercial suppliers and were used as received. NMP and DMA were distilled over CaH_2 and stored under N_2 . Anhydrous CoI_2 (99%), CoCl_2 (99%), CoBr_2 (99%), $\text{Co}(\text{PPh}_3)_3\text{Cl}$ (99%), $\text{Co}_2(\text{CO})_8$ (99%), CoF_2 (99%), and $\text{Co}(\text{acac})_3$ (99%) were purchased from Alfa Aesar. Phosphine ligands were purchased from Sigma-Aldrich or Alfa Aesar. Zinc (-100 mesh, 97+%) was purchased from Alfa Aesar, and preactivated by the treatment with 1 M HCl, washed successively with diethyl ether and acetone, dried under vacuum, and stored under argon. Nitriles except 2-(pyridin-2-yl)propanenitrile (prepared according to the patent procedure¹¹) were purchased from Sigma-Aldrich, Alfa Aesar, or other commercial suppliers and used as received. Diphenylacetylene (**2a**) and oct-4-yne (**2l**) was purchased from Sigma-Aldrich and used as received. Symmetrical diarylalkynes except **2a** were prepared according to the literature procedures.^{2,3} Spectral data for **2b–2d**,² **2e**,⁴ **2f**,⁵ **2g**,² **2h**,⁶ **2i**,⁷ **2j**,⁸ **2k**,⁹ and **2m–2n**² showed good agreement with the literature data. Ethyl 4-((4-methoxyphenyl)ethynyl)benzoate (**2o**) was prepared according to the literature procedure.¹⁰ The tethered diyne **4**¹¹ and cyanoalkyne **6**¹² were prepared according to the literature procedure.

Figure S1. Starting materials used in this study.

2. Optimization of Reaction Conditions

Table S1. [2+2+2] Cycloaddition of PhCN and Diphenylacetylene

$ \begin{array}{c} \text{Ph-CN} + \text{Ph}-\text{C}\equiv\text{C}-\text{Ph} \xrightarrow[\text{Zn (50 mol\%)}]{\text{CoX}_n \text{ (10 mol\%)} \\ \text{ligand (10 mol\%)}} \\ \text{1a} \quad \quad \quad \text{2a} \\ 0.5 \text{ mmol} \quad \quad 0.2 \text{ mmol} \\ \text{solvent (0.3 mL)} \\ T, 24 \text{ h} \end{array} $

Entry	CoX _n	Ligand	T [°C]	Solvent	Yield [%] ^[a]	
					3aa	C ₆ Ph ₆
1	CoI ₂	dppp	120	NMP	53	4
2	CoI ₂	dppp	120	DMF	47 ^[b]	2
3	CoI ₂	dppp	120	DMA	43	2
4	CoI ₂	dppp	120	DMSO	6	0
5	CoI ₂	dppp	120	toluene	0	0
6	CoI ₂	dppp	120	DCE	0	0
7	CoI ₂	dppp	120	DME	0	0
8	CoI ₂	dppp	100	NMP	70	5
9	CoI ₂	dppp	80	NMP	82(80)	3
10	CoI ₂	dppp	50	NMP	0	0
11	CoCl ₂	dppp	80	NMP	25	3
12	CoBr ₂	dppp	80	NMP	54	5
13	Co(acac) ₃	dppp	80	NMP	0	0
14	CoF ₂	dppp	80	NMP	0	0
15	CoCl(PPh ₃) ₃	dppp	80	NMP	45	<1
16 ^[c]	CoCl(PPh ₃) ₃	dppp	80	NMP	0	0
17	CoI ₂	dppm	80	NMP	4	<1
18	CoI ₂	dppe	80	NMP	0	0
19	CoI ₂	dppb	80	NMP	0	0
20	CoI ₂	dppf	80	NMP	0	0
21	CoI ₂	dppbz	80	NMP	2	1
22 ^[d]	CoI ₂	PPh ₃	80	NMP	0	0
23 ^[d]	CoI ₂	PCy ₃	80	NMP	0	0
24 ^[e]	CoI ₂	dppp	80	NMP	81(79)	3
25 ^[f]	CoI ₂	dppp	80	NMP	62	2
26 ^[g]	CoI ₂	dppp	80	NMP	52	2

[a] Determined by GC using *n*-tridecane as an internal standard. Isolated yield is shown in the parentheses. [b] The hydrocarbamylation product (addition of DMF to **2a**) was obtained in 13% yield. [c] Zn was omitted. [d] 20 mol% of ligand was used. [e] 0.2 mmol of **1a** and 0.2 mL of NMP were used. [f] 0.15 mmol of **1a** and 0.2 mL of NMP were used. [g] 0.1 mmol of **1a** and 0.2 mL of NMP were used.

Table S2. [2+2+2] Cycloaddition of PhCN and Oct-4-yne

$\text{Ph-CN} + \text{Pr}\equiv\text{Pr} \xrightarrow[\text{solvent (0.2 mL), 80 }^\circ\text{C, 24 h}]{\text{CoI}_2 \text{ (10 mol \%), ligand (10 mol \%), Zn (50 mol \%)}}$

$\text{1a (0.2 mmol)} + \text{2l (0.2 mmol)} \rightarrow \text{3al} + \text{C}_6\text{Pr}_6$

Entry	Ligand	Solvent	Yield [%] ^[a]	
			3al	C ₆ Pr ₆
1	dppp	NMP	0	6
2	dppm	NMP	0	24
3	dppe	NMP	0	12
4	dppb	NMP	0	13
5	dppf	NMP	9	7
6	dppbz	NMP	7	5
7	dcypm	NMP	38	8
8	dcype	NMP	0	0
9	dcypm	DMA	46	8
10	dcypm	DMSO	0	0
11	dcypm	DCE	0	0
12	dcypm	DME	67(63)	3
13	dcypm	2-MeTHF	56	2
14	dcypm	THF	0	0
15	dcypm	toluene	30	5

[a] Determined by GC using *n*-tridecane as an internal standard. Isolated yield is shown in the parentheses.

Table S3. [2+2+2] Cycloaddition of MeCN and Diphenylacetylene

$\text{MeCN} + \text{Ph}\equiv\text{Ph} \xrightarrow[\text{solvent (0.2 mL), 80 }^\circ\text{C, 24 h}]{\text{CoI}_2 \text{ (10 mol \%), dppp (10 mol \%), Zn (50 mol \%)}}$

$\text{1o (x mmol)} + \text{2a (0.2 mmol)} \rightarrow \text{3oa} + \text{C}_6\text{Ph}_6$

Entry	x	Solvent	Yield [%] ^[a]	
			3oa	C ₆ Ph ₆
1	0.2	NMP	42	2
2	0.2	DMA	62	2
3	0.3	DMA	83	1
4	0.5	DMA	86	< 1
5	1.0	DMA	97	< 1
6 ^[b]	1.0	DMA	94 (90)	< 1

[a] Determined by GC using *n*-tridecane as an internal standard. Isolated yield is shown in the parentheses. [b] The amounts of CoI₂, dppp, and Zn were reduced by half.

Table S4. [2+2+2] Cycloaddition of EtCN and Diphenylacetylene

Entry	x	Solvent	Yield [%] ^[a]	
			3pa	C₆Ph₆
1	1.0	NMP	77	2
2	1.0	DMA	81	< 1
3	0.3	DMA	95	< 1
4	0.2	DMA	86	< 1
5 ^[b]	0.3	DMA	93 (89)	< 1

[a] Determined by GC using *n*-tridecane as an internal standard. Isolated yield is shown in the parentheses. [b] The amounts of CoI_2 , dppp, and Zn were reduced by half.

3. [2+2+2] Cycloaddition of Nitriles and Alkynes

General Procedure A: [2+2+2] Cycloaddition of Aryl Nitriles and Diarylalkynes.

In an argon-filled glove box, a 4-mL vial equipped with a magnetic stir bar was charged sequentially with CoI_2 (6.3 mg, 0.020 mmol), dppp (8.3 mg, 0.020 mmol), Zn (6.5 mg, 0.10 mmol), diarylalkyne (0.40 mmol), and aryl nitriles (0.40 mmol), followed by the addition of NMP (0.4 mL). The vial was closed and removed from the glove box, and the mixture was stirred at 80 °C for 24 h. Upon cooling to room temperature, the reaction mixture was diluted with ethyl acetate (3 mL) and filtered through a pad of silica gel with additional ethyl acetate (10 mL) as an eluent. The organic solution was concentrated under reduced pressure, and the residue was purified by flash chromatography on silica gel to afford the desired pentaarylpyridine.

General Procedure B: [2+2+2] Cycloaddition of Alkyl Nitrile and Diarylacetylene.

In an argon-filled glove box, a 4-mL vial equipped with a magnetic stir bar was charged sequentially with CoI_2 (3.1 mg, 0.010 mmol), dppp (4.1 mg, 0.010 mmol), Zn (3.3 mg, 0.050 mmol), diarylacetylene (0.40 mmol), and alkyl nitrile (0.60 mmol), followed by the addition of DMA (0.4 mL). The vial was closed and removed from the glove box, and the mixture was stirred at 80 °C for 24 h. Upon cooling to room temperature, the reaction mixture was diluted with ethyl acetate (3 mL) and filtered through a pad of silica gel with additional ethyl acetate (10 mL) as an eluent. The organic solution was concentrated under reduced pressure, and the residue was purified by flash chromatography on silica gel to afford the desired 2-alkyl-3,4,5,6-tetraphenylpyridine.

2,3,4,5,6-Pentaphenylpyridine (3aa):¹³ The reaction was performed according to the general procedure A to afford the title compound as a white solid (72.7 mg, 79%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 244-246 °C; ^1H NMR (500 MHz, CDCl_3): δ 7.43-7.39 (m, 4H), 7.19-7.17 (m, 6H), 7.02-6.99 (m, 6H), 6.94-6.90 (m, 7H), 6.79-6.76 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.4, 150.2, 140.9, 138.4, 138.2, 133.7, 131.3, 130.4, 130.2, 127.5, 127.4, 127.3, 126.9, 126.2, 126.1; HRMS (ESI) Calcd for $\text{C}_{35}\text{H}_{26}\text{N}$ [$\text{M} + \text{H}$]⁺ 460.2065, found 460.2065.

Procedure for a gram-scale reaction: In an argon-filled glove box, a 25 mL Schlenk tube equipped with a magnetic stir bar was charged sequentially with CoI_2 (93.6 mg, 0.30 mmol), dppp (123.6 mg, 0.30 mmol), Zn (97.5 mg, 1.5 mmol), diphenylacetylene (1.10 g, 6.0 mmol), and benzonitrile (0.62 g, 6.0 mmol), followed by the addition of NMP (6.0 mL). The Schlenk tube was closed and removed from the glove box, and the mixture was stirred at 80 °C for 24 h. Upon cooling to room temperature, the reaction mixture was diluted with ethyl acetate (20 mL) and filtered through a pad of silica gel with additional ethyl acetate (50 mL) as an eluent. The organic solution was concentrated under reduced pressure, and the residue was purified by flash chromatography on silica gel to afford **3aa** as a white solid (1.14 g, 83%; eluent: hexane/EtOAc = 30/1).

2,3,4,5-Tetraphenyl-6-(*p*-tolyl)pyridine (3ba): The reaction was performed according to the general procedure **A** to afford the title compound as a white solid (68.1 mg, 72%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 235-237 °C; ^1H NMR (300 MHz, CDCl_3): δ 7.45-7.38 (m, 2H), 7.31 (d, J = 8.1 Hz, 2H), 7.20-7.16 (m, 3H), 7.03-6.98 (m, 8H), 6.94-6.89 (m, 7H), 6.80-6.74 (m, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.3, 150.2, 141.0, 138.7, 138.5, 138.3, 138.0, 137.0, 133.5, 133.4, 131.3 (two signals overlapped), 130.4, 130.2, 130.1, 128.2, 127.4 (two signals overlapped), 127.3 (two signals overlapped), 126.9, 126.2 (two signals overlapped), 126.1, 21.2; HRMS (ESI) Calcd for $\text{C}_{36}\text{H}_{28}\text{N}$ $[\text{M} + \text{H}]^+$ 474.2222, found 474.2224.

2-(4-Methoxyphenyl)-3,4,5,6-tetraphenylpyridine (3ca): The reaction was performed according to the general procedure **A** to afford the title compound as a white solid (59.7 mg, 61%; eluent: hexane/EtOAc = 20/1); R_f 0.2 (hexane/EtOAc = 20/1); m.p. 200-202 °C; ^1H NMR (500 MHz, CDCl_3): δ 7.44-7.41 (m, 2H), 7.39-7.36 (m, 2H), 7.21-7.16 (m, 3H), 7.06-6.98 (m, 6H), 6.95-6.89 (m, 7H), 6.80-6.76 (m, 2H), 6.74-6.71 (m, 2H), 3.76 (s, 3H); ^{13}C

NMR (100 MHz, CDCl₃): δ 159.0, 156.3, 155.8, 150.2, 141.0, 138.7, 138.6, 138.3, 133.4, 133.2 (two signals overlapped), 131.6, 131.3 (two signals overlapped), 130.4, 130.2, 127.5 (two signals overlapped), 127.4, 127.3, 127.2, 126.9, 126.2 (two signals overlapped), 126.1, 113.0, 55.1; HRMS (ESI) Calcd for C₃₆H₂₈NO [M + H]⁺ 490.2171, found 490.2174.

2,3,4,5-Tetraphenyl-6-(4-(trifluoromethyl)phenyl)pyridine (3da): ¹⁴ The reaction was performed according to the general procedure A to afford the title compound as a white solid (65.3 mg, 62%; eluent: hexane/EtOAc = 30/1); *R_f* 0.3 (hexane/EtOAc = 30/1); m.p. 188-190 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.53 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.40-7.38 (m, 2H), 7.22-7.17 (m, 3H), 7.06-6.99 (m, 6H), 6.95-6.93 (m, 3H), 6.91-6.89 (m, 4H), 6.79-6.76 (m, 2H); ¹³C NMR (100 MHz, C₆D₆): δ 157.3, 155.4, 150.7, 145.0, 141.3, 138.9, 138.5 (two signals overlapped), 134.6, 134.2, 131.9, 131.7, 131.6, 131.3, 130.9, 130.8, 129.7 (q, ²*J*_{C-F} = 32.0 Hz), 128.2, 128.0, 127.9, 127.5, 127.0, 126.8, 126.7, 125.0 (q, ¹*J*_{C-F} = 270.4 Hz), 124.8 (q, ³*J*_{C-F} = 3.7 Hz); ¹⁹F NMR (282 MHz, CDCl₃): δ -62.5; HRMS (ESI) Calcd for C₃₆H₂₅F₃N [M + H]⁺ 528.1939, found 528.1940.

1-(4-(3,4,5,6-Tetraphenylpyridin-2-yl)phenyl)ethan-1-one (3ea): The reaction was performed according to the general procedure A to afford the title compound as a white solid (76.2 mg, 76%; eluent: hexane/EtOAc = 20/1); *R_f* 0.3 (hexane/EtOAc = 20/1); m.p. 192-194 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.79 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.44-7.39 (m, 2H), 7.23-7.17 (m, 3H), 7.06-6.99 (m, 6H), 6.96-6.91 (m, 7H), 6.82-6.77 (m, 2H), 2.55 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 197.9, 156.7, 155.1, 150.5, 145.6, 140.6, 138.2, 138.0, 137.9, 135.8, 134.3, 134.0, 131.2 (two signals overlapped), 130.4 (two signals overlapped), 130.2, 127.6 (two signals overlapped), 127.5 (two signals overlapped), 127.1,

126.6, 126.4, 126.3, 26.6; HRMS (ESI) Calcd for $C_{37}H_{28}NO$ $[M + H]^+$ 502.2171, found 502.2170.

4-(3,4,5,6-Tetraphenylpyridin-2-yl)benzonitrile (3fa): The reaction was performed with modification of the general procedure **A** using terephthalonitrile **1f** (0.20 mmol) and **2a** (0.60 mmol). Flash chromatography of the crude product (eluent: hexane/EtOAc = 50/3 to 10/1) afforded the title compound (58.9 mg, 61%) and the twofold cycloadduct (see below; 11.0 mg, 7%), both as white solids; R_f 0.2 (Hexane/EtOAc = 10/1); m.p. 215-218 °C; 1H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 8.5 Hz, 2H), 7.40-7.38 (m, 2H), 7.22-7.17 (m, 3H), 7.09-6.99 (m, 6H), 6.97-6.93 (m, 3H), 6.92-6.88 (m, 4H), 6.79-6.76 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.9, 154.2, 150.7, 145.5, 140.5, 138.0, 137.7, 137.6, 134.7, 134.0, 131.3, 131.2, 131.1, 130.8, 130.3, 130.1, 127.7, 127.6, 127.5, 127.1, 126.8, 126.5, 126.4, 118.9, 111.0; HRMS (ESI) Calcd for $C_{36}H_{25}N_2$ $[M + H]^+$ 485.2018, found 485.2021.

1,4-Bis(3,4,5,6-tetraphenylpyridin-2-yl)benzene (3fa'): R_f 0.2 (Hexane/EtOAc = 10/1); m.p. 367-370 °C; 1H NMR (500 MHz, $CDCl_3$): δ 7.42-7.38 (m, 4H), 7.24 (s, 4H), 7.19-7.17 (m, 6H), 7.00-6.95 (m, 12H), 6.92-6.90 (m, 6H), 6.89-6.87 (m, 4H), 6.87-6.84 (m, 4H), 6.76-6.73 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.4, 156.1, 150.2, 141.0, 139.7, 138.5, 138.4, 138.2, 133.7 (two signals overlapped), 131.4, 131.3, 130.4, 130.2, 129.5, 127.5, 127.4, 127.3 (two signals overlapped), 126.9, 126.2, 126.1; HRMS (ESI) Calcd for $C_{64}H_{45}N_2$ $[M + H]^+$ 841.3583, found 841.3579.

2,3,4,5-Tetraphenyl-6-(*m*-tolyl)pyridine (3ga): The reaction was performed according to the general procedure A to afford the title compound as a white solid (60.5 mg, 64%; eluent: hexane/EtOAc = 50/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 208-210 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.43-7.41 (m, 2H), 7.32 (s, 1H), 7.20-7.18 (m, 3H), 7.12 (d, J = 7.2 Hz, 1H), 7.05-7.01 (m, 8H), 6.94-6.91 (m, 7H), 6.80-6.78 (m, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.6, 156.4, 150.2, 141.0, 140.8, 138.6, 138.5, 138.3, 137.0, 133.7, 133.6, 131.3 (two signals overlapped), 131.0, 130.5, 130.2, 128.1, 127.5, 127.3 (four signals overlapped), 127.2, 126.9, 126.2 (two signals overlapped), 126.1, 21.3; HRMS (ESI) Calcd for $\text{C}_{36}\text{H}_{28}\text{N}$ $[\text{M} + \text{H}]^+$ 474.2222, found 474.2223.

2-(3-Methoxyphenyl)-3,4,5,6-tetraphenylpyridine (3ha): The reaction was performed according to the general procedure A to afford the title compound as a white solid (76.3 mg, 78%; eluent: hexane/EtOAc = 20/1); R_f 0.3 (hexane/EtOAc = 20/1); m.p. 184-186 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.46-7.44 (m, 2H), 7.21-7.20 (m, 3H), 7.15-7.09 (m, 2H), 7.05-7.02 (m, 6H), 6.97-6.94 (m, 8H), 6.83-6.80 (m, 2H), 6.77 (d, J = 7.6 Hz, 1H), 3.59 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.8, 156.4, 156.1, 150.3, 142.1, 140.9, 138.6, 138.4, 138.1, 133.8, 133.6, 131.3, 131.2, 130.4, 130.2, 128.5, 127.4 (three signals overlapped), 127.3, 126.9, 126.2 (three signals overlapped), 122.9, 115.2, 114.0, 55.1; HRMS (ESI) Calcd for $\text{C}_{36}\text{H}_{28}\text{NO}$ $[\text{M} + \text{H}]^+$ 490.2171, found 490.2171.

2,3,4,5-Tetraphenyl-6-(*o*-tolyl)pyridine (3ia): The reaction was performed according to the general procedure A to afford the title compound as a white solid (40.7 mg, 43%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 220-222 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.38-7.33 (m, 2H), 7.17-7.13 (m, 4H), 7.10-7.06 (m, 2H), 7.02-6.97 (m, 4H), 6.96-6.90 (m, 8H), 6.87-6.84 (m, 2H), 6.83-6.78 (m, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.9, 156.2, 149.9, 140.9, 140.7, 138.5, 138.2, 138.0, 136.0, 134.7, 133.7, 131.4,

130.9, 130.5, 130.3, 130.2, 129.8, 127.5, 127.4, 127.3, 127.2, 127.0, 126.9, 126.2 (two signals overlapped), 126.1, 124.8, 20.3; HRMS (ESI) Calcd for $C_{36}H_{28}N$ $[M + H]^+$ 474.2222, found 474.2221.

2-(2-Fluorophenyl)-3,4,5,6-tetraphenylpyridine (3ja): The reaction was performed according to the general procedure A to afford the title compound as a white solid (49.6 mg, 52%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 235-237 °C; 1H NMR (500 MHz, $CDCl_3$): δ 7.44 (td, J = 7.5, 1.7 Hz, 1H), 7.38-7.35 (m, 2H), 7.21-7.16 (m, 4H), 7.06 (td, J = 7.5, 1.0 Hz, 1H), 7.02-6.99 (m, 3H), 6.96-6.90 (m, 10H), 6.86-6.82 (m, 1H), 6.81-6.78 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6 (d, $^1J_{C-F}$ = 245.7 Hz), 156.7, 152.8, 149.8, 140.7, 138.3, 137.9, 137.7, 135.5, 134.4, 131.9 (d, $^3J_{C-F}$ = 3.5 Hz), 131.3, 130.8, 130.4, 130.2, 129.5 (d, $^3J_{C-F}$ = 7.9 Hz), 129.3, 127.5 (d, $^2J_{C-F}$ = 16.1 Hz), 127.3, 127.0, 126.9, 126.3 (three signals overlapped), 123.6 (d, $^4J_{C-F}$ = 3.4 Hz), 115.2 (d, $^2J_{C-F}$ = 22.1 Hz); ^{19}F NMR (377 MHz, $CDCl_3$): δ -113.5; HRMS (ESI) Calcd for $C_{35}H_{25}FN$ $[M + H]^+$ 478.1971, found 478.1971.

2-(Naphthalen-1-yl)-3,4,5,6-tetraphenylpyridine (3ka): The reaction was performed according to the general procedure A to afford the title compound as a white solid (69.2 mg, 68%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 216-218 °C; 1H NMR (400 MHz, $CDCl_3$): δ 7.95-7.92 (m, 1H), 7.79-7.75 (m, 1H), 7.69 (d, J = 7.8 Hz, 1H), 7.45-7.36 (m, 4H), 7.34-7.26 (m, 2H), 7.17-7.14 (m, 3H), 7.05-7.03 (m, 3H), 7.00-6.98 (m, 2H), 6.95-6.93 (m, 3H), 6.86-6.78 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.9, 156.4, 150.1, 140.8, 138.6, 138.4, 138.1, 138.0, 135.7, 134.0, 133.5, 132.3, 131.4, 130.6, 130.5, 130.2, 128.2, 128.0, 127.8, 127.5, 127.4, 127.2, 127.0, 126.8, 126.4, 126.3, 126.2, 126.0, 125.7, 125.4, 124.7; HRMS (ESI) Calcd for $C_{39}H_{28}N$ $[M + H]^+$ 510.2222, found 510.2223.

2,3,4,5-Tetraphenyl-6-(thiophen-2-yl)pyridine (3la): The reaction was performed according to the general procedure A to afford the title compound as a white solid (50.2 mg, 54%; eluent: hexane/EtOAc = 30/1); R_f 0.2 (hexane/EtOAc = 30/1); m.p. 216-219 °C; ^1H NMR (300 MHz, CDCl_3): δ 7.49-7.46 (m, 2H), 7.24-7.20 (m, 7H), 7.15-7.10 (m, 2H), 7.03-6.98 (m, 3H), 6.93-6.88 (m, 5H), 6.79-6.75 (m, 3H), 6.35 (dd, J = 3.8, 0.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.9, 150.9, 149.0, 145.7, 140.4, 138.4, 137.9, 133.1, 131.6, 131.3, 130.7, 130.3, 130.2, 128.2, 127.9, 127.8, 127.5 (two signals overlapped), 127.4 (two signals overlapped), 127.2, 126.9, 126.3, 126.2; HRMS (ESI) Calcd for $\text{C}_{33}\text{H}_{24}\text{NS}$ $[\text{M} + \text{H}]^+$ 466.1629, found 466.1630.

3,4,5,6-Tetraphenyl-2,2'-bipyridine (3ma):¹⁵ The reaction was performed according to the general procedure A to afford the title compound as a white solid (59.8 mg, 65%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 221-223 °C; ^1H NMR (500 MHz, CDCl_3): δ 8.46 (dq, J = 4.8, 0.8 Hz, 1H), 7.53 (tt, J = 7.7, 1.8 Hz, 1H), 7.42 (dt, J = 7.9, 1.1 Hz, 1H), 7.40-7.36 (m, 2H), 7.18-7.15 (m, 3H), 7.09 (ddd, J = 7.5, 4.9, 1.1 Hz, 1H), 7.01-6.98 (m, 3H), 6.98-6.95 (m, 3H), 6.94-6.87 (m, 7H), 6.80-6.76 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.9, 156.7, 155.7, 150.3, 148.7, 140.7, 138.2, 137.9, 137.8, 135.5, 134.8, 134.3, 131.2, 131.0, 130.4, 130.2, 127.5, 127.3 (two signals overlapped), 127.1, 127.0, 126.3, 126.2, 126.1, 124.8, 122.0; HRMS (ESI) Calcd for $\text{C}_{34}\text{H}_{25}\text{N}_2$ $[\text{M} + \text{H}]^+$ 461.2018, found 461.2017.

3,4,5,6-Tetraphenyl-2,3'-bipyridine (3na): The reaction was performed according to the general procedure **A** to afford the title compound as a white solid (69.9 mg, 76%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 240-242 °C; ^1H NMR (300 MHz, CDCl_3): δ 8.64 (d, J = 1.7 Hz, 1H), 8.42 (dd, J = 4.8, 1.5 Hz, 1H), 7.71 (dt, J = 7.9, 1.9 Hz, 1H), 7.44-7.38 (m, 2H), 7.22-7.18 (m, 3H), 7.11 (dd, J = 7.8, 4.9 Hz, 1H), 7.06-7.00 (m, 6H), 6.95-6.90 (m, 7H), 6.81-6.76 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.9, 153.3, 151.0, 150.6, 148.2, 140.5, 138.1, 137.7 (two signals overlapped), 137.3, 136.6, 134.4, 134.2, 131.2 (two signals overlapped), 130.3, 130.1, 127.7, 127.6, 127.5, 127.4, 127.0, 126.8, 126.4 (two signals overlapped), 122.4; HRMS (ESI) Calcd for $\text{C}_{34}\text{H}_{25}\text{N}_2$ $[\text{M} + \text{H}]^+$ 461.2018, found 461.2016.

2-Phenyl-3,4,5,6-tetra-*p*-tolylpyridine (3ab): The reaction was performed according to the general procedure **A** to afford the title compound as a white solid (66.9 mg, 65%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 245-247 °C; ^1H NMR (500 MHz, CDCl_3): δ 7.41-7.37 (m, 2H), 7.29 (d, J = 8.1 Hz, 2H), 7.18-7.15 (m, 3H), 6.98 (d, J = 8.0 Hz, 2H), 6.82-6.73 (m, 10H), 6.64 (d, J = 8.1 Hz, 2H), 2.28 (s, 3H), 2.20 (s, 3H), 2.19 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.2, 150.3, 141.3, 138.3, 136.8, 135.7, 135.6, 135.5, 135.4, 135.3, 133.6, 133.5, 131.2, 131.1, 130.3, 130.2, 130.1, 128.2, 128.1, 128.0, 127.6, 127.4, 127.0, 21.2, 21.1 (three signals overlapped); HRMS (ESI) Calcd for $\text{C}_{39}\text{H}_{34}\text{N}$ $[\text{M} + \text{H}]^+$ 516.2691, found 516.2692.

2,3,4,5-Tetrakis(4-(*tert*-butyl)phenyl)-6-phenylpyridine (3ac): The reaction was performed with modification of the general procedure A, using 0.6 mmol of **1a** and prolonging the reaction time to 72 h. The title compound was obtained as a white solid (91.4 mg, 67%; eluent: hexane/EtOAc = 100/1); R_f 0.6 (hexane/EtOAc = 10/1); m.p. 201-203 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.46-7.43 (m, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.17-7.15 (m, 5H), 6.99-6.96 (m, 4H), 6.87 (d, J = 8.3 Hz, 2H), 6.81-6.77 (m, 4H), 6.62 (d, J = 8.3 Hz, 2H), 1.26 (s, 9H), 1.18 (s, 9H), 1.17 (s, 9H), 1.12 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.0, 155.8, 150.8, 149.9, 148.8 (two signals overlapped), 148.5, 141.2, 138.2, 135.8, 135.7, 135.5, 133.8, 133.6, 130.9 (two signals overlapped), 130.3, 130.1, 129.8, 127.3, 127.0, 124.3, 124.0, 123.9, 123.4, 34.4, 34.3 (two signals overlapped), 34.2, 31.3, 31.2 (three signals overlapped); HRMS (ESI) Calcd for $\text{C}_{51}\text{H}_{58}\text{N}$ $[\text{M} + \text{H}]^+$ 684.4569, found 684.4568.

2,3,4,5-Tetrakis(4-methoxyphenyl)-6-phenylpyridine (3ad): The reaction was performed with modification of the general procedure A, using 0.6 mmol of **1a** and prolonging the reaction time to 72 h. The title compound was obtained as a white solid (66.1 mg, 57%; eluent: hexane/EtOAc = 5/1); R_f 0.3 (hexane/EtOAc = 5/1); m.p. 227-229 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.41-7.38 (m, 2H), 7.34 (d, J = 8.6 Hz, 2H), 7.20-7.16 (m, 3H), 6.80 (d, J = 9.0 Hz, 2H), 6.77 (d, J = 9.4 Hz, 2H), 6.72 (d, J = 8.7 Hz, 2H), 6.65 (d, J = 8.5 Hz, 2H), 6.58 (d, J = 8.6 Hz, 2H), 6.55 (d, J = 8.6 Hz, 2H), 6.50 (d, J = 8.5 Hz, 2H), 3.76 (s, 3H), 3.71 (s, 3H), 3.69 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.8, 157.7, 157.6, 156.3, 155.9, 150.2, 141.3, 133.7, 133.2, 133.1, 132.4, 132.3, 131.6, 131.5, 131.2, 131.0, 130.8, 130.2, 127.4, 127.0, 113.0, 112.9 (two signals overlapped), 112.6, 55.1, 55.0 (two signals overlapped), 54.9; HRMS (ESI) Calcd for $\text{C}_{39}\text{H}_{34}\text{NO}_4$ $[\text{M} + \text{H}]^+$ 580.2488, found 580.2484.

2,3,4,5-Tetrakis(4-fluorophenyl)-6-phenylpyridine (3ae): The reaction was performed according to the general procedure A to afford the title compound as a white solid (75.5 mg, 71%; eluent: hexane/EtOAc = 25/1); R_f 0.2 (hexane/EtOAc = 10/1); m.p. 272-275 °C; ^1H NMR (300 MHz, CDCl_3): δ 7.39-7.32 (m, 4H), 7.24-7.19 (m, 3H), 6.93-6.66 (m, 14H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.4 (d, $^1J_{\text{C-F}} = 246.3$ Hz), 161.5 (d, $^1J_{\text{C-F}} = 245.5$ Hz, two signals overlapped), 161.3 (d, $^1J_{\text{C-F}} = 245.7$ Hz), 157.0, 155.7, 149.6, 140.4, 136.5 (d, $^4J_{\text{C-F}} = 3.4$ Hz), 134.1 (d, $^4J_{\text{C-F}} = 3.5$ Hz, two signals overlapped), 133.8 (d, $^4J_{\text{C-F}} = 3.5$ Hz), 132.9, 132.7 (d, $^3J_{\text{C-F}} = 7.9$ Hz, two signals overlapped), 131.94 (d, $^3J_{\text{C-F}} = 7.8$ Hz), 131.87 (d, $^3J_{\text{C-F}} = 7.5$ Hz), 130.1, 127.7, 127.6, 114.9 (d, $^2J_{\text{C-F}} = 21.4$ Hz), 114.7 (d, $^2J_{\text{C-F}} = 21.4$ Hz), 114.6 (d, $^2J_{\text{C-F}} = 21.3$ Hz), 114.5 (d, $^2J_{\text{C-F}} = 21.4$ Hz); ^{19}F NMR (282 MHz, CDCl_3): -114.2, -114.8, -114.9, -115.1; HRMS (ESI) Calcd for $\text{C}_{35}\text{H}_{22}\text{NF}_4$ $[\text{M} + \text{H}]^+$ 532.1688, found 532.1688.

Tetraethyl 4,4',4'',4'''-(6-phenylpyridine-2,3,4,5-tetrayl)tetrabenzoate (3af): The reaction was performed according to the general procedure A to afford the title compound as a white solid (94.9 mg, 63%; eluent: hexane/EtOAc = 5/1); R_f 0.2 (hexane/EtOAc = 5/1); m.p. 255-258 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.87 (d, $J = 8.4$ Hz, 2H), 7.71 (d, $J = 8.2$ Hz, 4H), 7.64 (d, $J = 8.3$ Hz, 2H), 7.44 (d, $J = 8.4$ Hz, 2H), 7.37-7.35 (m, 2H), 7.24-7.17 (m, 3H), 6.98 (d, $J = 8.4$ Hz, 2H), 6.97 (d, $J = 8.3$ Hz, 2H), 6.86 (d, $J = 8.2$ Hz, 2H), 4.37-4.26 (m, 8H), 1.38-1.32 (m, 12 H); ^{13}C NMR (100 MHz, CDCl_3): δ 166.2, 166.1, 166.0, 165.9, 157.0, 155.8, 149.1, 144.3, 142.5, 142.2, 141.9, 139.7, 133.0, 132.7, 131.0 (two signals overlapped), 130.1, 130.0 (two signals overlapped), 129.6, 128.9 (two signals overlapped), 128.8, 128.6 (two

signals overlapped), 127.9, 127.7, 60.9 (four signals overlapped), 14.2, 14.1 (three signals overlapped); HRMS (ESI) Calcd for $C_{47}H_{42}NO_8$ $[M + H]^+$ 748.2910, found 748.2908.

1,1',1'',1'''-((6-Phenylpyridine-2,3,4,5-tetrayl)tetrakis(benzene-4,1-diyl))tetrakis(ethan-1-one) (3ag): The reaction was performed according to the general procedure A to afford the title compound as a white solid (51.2 mg, 41%; eluent: hexane/EtOAc = 3/2); R_f 0.3 (hexane/EtOAc = 1/1); m.p. 307-310 °C; 1H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.3 Hz, 2H), 7.62 (d, J = 8.2 Hz, 2H), 7.56 (d, J = 8.3 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.36-7.34 (m, 2H), 7.24-7.18 (m, 3H), 7.01 (d, J = 8.2 Hz, 4H), 6.89 (d, J = 8.3 Hz, 2H), 2.55 (s, 3H), 2.50 (s, 3H), 2.49 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.7, 197.4 (two signals overlapped), 197.3, 157.3, 155.8, 149.1, 144.6, 142.8, 142.5, 142.2, 139.7, 136.3, 135.6, 135.5, 135.4, 133.0, 132.6, 131.4, 131.3, 130.4 (two signals overlapped), 130.1, 128.1, 127.9 (two signals overlapped), 127.8 (two signals overlapped), 127.5, 26.6, 26.4 (three signals overlapped); HRMS (ESI) Calcd for $C_{43}H_{34}NO_4$ $[M + H]^+$ 628.2488, found 628.2484.

2-Phenyl-3,4,5,6-tetra-*m*-tolylpyridine (3ah): The reaction was performed according to the general procedure A to afford the title compound as a white solid (52.3 mg, 51%; eluent: hexane/EtOAc = 100/1); R_f 0.4 (hexane/EtOAc = 10/1); m.p. 137-140 °C; 1H NMR (500 MHz, $CDCl_3$): δ 7.45-7.42 (m, 2H), 7.34 (s, 1H), 7.19-7.17 (m, 3H), 7.12 (d, J = 7.5 Hz, 1H), 7.02 (t, J = 7.5 Hz, 1H), 6.99 (d, J = 7.5 Hz, 1H), 6.88 (t, J = 7.6 Hz, 2H), 6.80 (s, 2H), 6.79

(s, 1H), 6.74-6.69 (m, 5H), 6.62-6.57 (m, 2H), 2.24 (s, 3H), 2.08 (s, 3H), 2.07 (s, 3H), 2.03 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.3, 156.0, 150.4, 141.2, 140.9, 138.5, 138.4, 138.2, 136.9, 136.6, 136.5, 136.0, 133.8, 133.7, 132.2 (two signals overlapped), 131.3, 131.0, 130.2, 128.4 (two signals overlapped), 127.9, 127.5, 127.4, 127.3, 127.1 (two signals overlapped), 127.0 (two signals overlapped), 126.8, 126.7, 126.6 (two signals overlapped), 21.3, 21.1 (two signals overlapped), 21.0; HRMS (ESI) Calcd for $\text{C}_{39}\text{H}_{34}\text{N}$ $[\text{M} + \text{H}]^+$ 516.2691, found 516.2692.

2,3,4,5-Tetrakis(3-methoxyphenyl)-6-phenylpyridine (3ai): The reaction was performed according to the general procedure A to afford the title compound as a white solid (96.9 mg, 84%; eluent: hexane/EtOAc = 20/3); R_f 0.3 (hexane/EtOAc = 5/1); m.p. 134-136 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.45-7.43 (m, 2H), 7.22-7.19 (m, 3H), 7.12 (t, J = 7.8 Hz, 1H), 7.07 (dt, J = 7.6, 1.4 Hz, 1H), 6.97-6.91 (m, 3H), 6.88 (t, J = 7.9 Hz, 1H), 6.76 (dq, J = 7.9, 1.2 Hz, 1H), 6.60-6.52 (m, 5H), 6.50 (s, 1H), 6.47 (s, 1H), 6.43-6.37 (m, 2H), 3.60 (s, 3H), 3.51 (s, 3H), 3.49 (s, 3H), 3.48 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.9 (two signals overlapped), 158.8, 158.6, 156.4, 156.1, 149.8, 142.1, 140.9, 139.8, 139.6, 139.4, 133.4, 133.3, 130.1 (two signals overlapped), 128.5, 128.4 (two signals overlapped), 128.0, 127.5 (two signals overlapped), 127.4, 124.0, 123.9, 123.1, 122.8, 116.6, 116.5, 115.7, 115.1, 114.1, 112.9, 55.1 (four signals overlapped); HRMS (ESI) Calcd for $\text{C}_{39}\text{H}_{34}\text{NO}_4$ $[\text{M} + \text{H}]^+$ 580.2488, found 580.2486.

3,3',3'',3'''-(6-Phenylpyridine-2,3,4,5-tetrayl)tetrakis(*N,N*-dimethylaniline) (3aj): The reaction was performed according to the general procedure A to afford the title compound as

a light yellow solid (83.0 mg, 66%; eluent: hexane/EtOAc = 4/1); R_f 0.3 (hexane/EtOAc = 3/1); m.p. 167-169 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.49-7.47 (m, 2H), 7.20-7.16 (m, 3H), 7.11 (t, J = 7.9 Hz, 1H), 6.99 (d, J = 7.6 Hz, 1H), 6.86 (td, J = 7.9, 4.6 Hz, 2H), 6.82-6.78 (m, 2H), 6.61 (dd, J = 8.1, 2.1 Hz, 1H), 6.43 (s, 1H), 6.41 (s, 1H), 6.38-6.32 (m, 5H), 6.24 (s, 2H), 2.71 (s, 6H), 2.62 (s, 6H), 2.61 (s, 6H), 2.59 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.7, 155.9, 150.5, 150.3, 150.1, 150.0, 149.9, 141.9, 141.6, 139.7, 139.3, 139.2, 134.1, 134.0, 130.2 (two signals overlapped), 128.1, 127.8, 127.7, 127.4, 127.3 (two signals overlapped), 126.9, 120.9 (two signals overlapped), 120.2, 119.4, 117.6, 116.9, 115.8, 112.2, 111.2, 111.1, 40.9 (three signals overlapped), 40.8; HRMS (ESI) Calcd for $\text{C}_{43}\text{H}_{46}\text{N}_5$ $[\text{M} + \text{H}]^+$ 632.3753, found 632.3750.

2,3,4,5-Tetrakis(3,5-dimethoxyphenyl)-6-phenylpyridine (3ak): The reaction was performed according to the general procedure A to afford the title compound as a white solid (120.3 mg, 86%; eluent: hexane/EtOAc = 2/1); R_f 0.2 (hexane/EtOAc = 3/1); m.p. 173-175 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.47-7.44 (m, 2H), 7.23-7.20 (m, 3H), 6.67 (d, J = 2.3 Hz, 2H), 6.34 (t, J = 2.3 Hz, 1H), 6.18 (s, 3H), 6.16 (t, J = 2.3 Hz, 1H), 6.13-6.12 (m, 3H), 6.06 (d, J = 2.2 Hz, 2H), 3.61 (s, 6H), 3.52 (s, 6H), 3.49 (s, 12H); ^{13}C NMR (100 MHz, CDCl_3): δ 160.0 (two signals overlapped), 159.9, 159.7, 156.3, 155.9, 149.6, 142.6, 140.8, 140.3, 140.0, 139.8, 133.3, 133.2, 129.9, 127.5, 127.4, 109.6, 109.5, 108.8, 108.1, 100.9, 99.7, 99.6, 55.3, 55.2 (three signals overlapped); HRMS (ESI) Calcd for $\text{C}_{43}\text{H}_{42}\text{NO}_8$ $[\text{M} + \text{H}]^+$ 700.2910, found 700.2906.

Reaction of benzonitrile (1a) and ethyl 4-((4-methoxyphenyl)ethynyl)benzoate (2o): The reaction was performed according to the general procedure A to afford a mixture of pyridine isomers (81 mg, 61%). ¹H NMR analysis of the mixture indicated the presence of all the four possible isomers, as judged from the number of the characteristic singlet peaks of the methoxy groups (Figure S2). Based on the integrations, the ratio of the four isomers was assumed to be 36:26:20:18, while separation and assignment of individual isomers were not possible.

Figure S2. ¹H NMR spectrum (500 MHz, CDCl₃) of the pyridine mixture obtained from **1a** and **2o**.

2-Phenyl-3,4,5,6-tetrapropylpyridine (3al): ¹⁶ The reaction was performed using bis(dicyclohexylphosphino)methane (10 mol%) and 1,2-dimethoxyethane as the ligand and the solvent, respectively, according to otherwise the same procedure as the general procedure A. The title compound was obtained as a yellow oil (40.7 mg, 63%; eluent: hexane/EtOAc = 30/1); *R_f* 0.3 (hexane/EtOAc = 30/1); ¹H NMR (400 MHz, CDCl₃): δ 7.39-7.30 (m, 5H), 2.77-2.73 (m, 2H), 2.63-2.58 (m, 4H), 2.50-2.46 (m, 2H), 1.78-1.69 (m, 2H), 1.62-1.50 (m,

4H), 1.42-1.32 (m, 2H), 1.08 (t, $J = 7.3$ Hz, 6H), 1.00 (t, $J = 7.4$ Hz, 3H), 0.78 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.1, 156.5, 148.2, 142.5, 132.3, 131.2, 128.9, 127.9, 127.1, 37.4, 31.5, 31.4, 31.0, 24.5 (three signals overlapped), 23.6, 14.9, 14.8, 14.5, 14.3; HRMS (ESI) Calcd for $\text{C}_{23}\text{H}_{34}\text{N}$ $[\text{M} + \text{H}]^+$ 324.2691, found 324.2690.

2,3,4,5,6-Penta(thiophen-2-yl)pyridine (3lm):¹⁷ The reaction was performed according to the general procedure A to afford the title compound as a light yellow solid (78.4 mg, 80%; eluent: hexane/DCM = 1/1); R_f 0.5 (hexane/EtOAc = 10/1); m.p. 311-313 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.34 (t, $J = 4.8$ Hz, 4H), 7.11 (d, $J = 5.0$ Hz, 1H), 6.96 (dd, $J = 4.9, 3.6$ Hz, 2H), 6.89-6.87 (m, 4H), 6.70 (dd, $J = 4.9, 3.7$ Hz, 1H), 6.63 (d, $J = 3.3$ Hz, 2H), 6.60 (d, $J = 2.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.1, 148.0, 144.3, 138.2, 137.1, 129.4, 129.2, 128.9, 128.4, 127.7, 127.3, 127.1, 126.6, 125.8, 124.6; HRMS (ESI) Calcd for $\text{C}_{25}\text{H}_{16}\text{NS}_5$ $[\text{M} + \text{H}]^+$ 489.9886, found 489.9882.

4',5',6'-Tri(pyridin-3-yl)-3,2':3',3''-terpyridine (3nn): The reaction was performed according to the general procedure A to afford the title compound as a white solid (33.9 mg, 36%; eluent: DCM/MeOH = 20/3); R_f 0.2 (DCM/MeOH = 10/1); m.p. 259-261 °C; ^1H NMR (400 MHz, CDCl_3): δ 8.60 (s, 2H), 8.50 (dd, $J = 4.9, 1.7$ Hz, 2H), 8.36 (d, $J = 4.0$ Hz, 2H), 8.28 (d, $J = 4.1$ Hz, 1H), 8.20 (s, 2H), 8.08 (s, 1H), 7.70 (dt, $J = 7.9, 2.0$ Hz, 2H), 7.28-7.26 (m, 2H), 7.20 (dd, $J = 7.9, 4.9$ Hz, 2H), 7.16-7.10 (m, 1H), 7.06 (dd, $J = 7.4, 5.0$ Hz, 2H), 6.99 (dd, $J = 7.7, 4.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.4, 151.1, 150.8 (two signals overlapped), 150.1, 149.2 (two signals overlapped), 148.7 (two signals overlapped), 148.1, 138.1, 137.2 (two signals overlapped), 135.0, 132.6, 132.4, 131.6, 123.0, 122.8 (two signals overlapped); HRMS (ESI) Calcd for $\text{C}_{30}\text{H}_{21}\text{N}_6$ $[\text{M} + \text{H}]^+$ 465.1828, found 465.1825.

2-Methyl-3,4,5,6-tetraphenylpyridine (30a): ¹⁸ The reaction was performed with modification of the general procedure **B** using 2.0 mmol of acetonitrile (**1o**). The title compound was obtained as a white solid (71.5 mg, 90%; eluent: hexane/EtOAc = 30/1); *R_f* 0.3 (hexane/EtOAc = 30/1); m.p. 164-166 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.36-7.33 (m, 2H), 7.22-7.13 (m, 6H), 7.07-7.05 (m, 2H), 6.99-6.94 (m, 3H), 6.91-6.88 (m, 3H), 6.86-6.83 (m, 2H), 6.76-6.72 (m, 2H), 2.49 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 156.1, 155.3, 149.3, 141.0, 138.8, 138.4, 138.1, 134.7, 132.6, 131.4, 130.2, 130.0, 129.9, 127.8, 127.6, 127.3, 127.2, 126.9, 126.6, 126.1, 126.0, 24.2; HRMS (ESI) Calcd for C₃₀H₂₄N [M + H]⁺ 398.1909, found 398.1910.

2-Methyl-3,4,5,6-tetra-*p*-tolylpyridine (30b): The reaction was performed with modification of the general procedure **B** using 2.0 mmol of acetonitrile (**1o**). The title compound was obtained as a white solid (74.3 mg, 82%; eluent: hexane/EtOAc = 30/1); *R_f* 0.3 (hexane/EtOAc = 30/1); m.p. 203-205 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.21 (d, *J* = 8.1 Hz, 2H), 6.99 (d, *J* = 7.6 Hz, 2H), 6.98 (d, *J* = 7.7 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.71-6.69 (m, 4H), 6.59 (d, *J* = 8.1 Hz, 2H), 2.44 (s, 3H), 2.28 (s, 3H), 2.27 (s, 3H), 2.18 (s, 3H), 2.12 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 156.0, 155.1, 149.4, 138.4, 136.6, 136.1, 135.8, 135.7, 135.4, 135.3, 135.2, 134.6, 132.5, 131.2, 130.1, 129.9, 129.8, 128.5, 128.3, 128.0, 127.6, 24.3, 21.2 (two signals overlapped), 21.1 (two signals overlapped); HRMS (ESI) Calcd for C₃₄H₃₂N [M + H]⁺ 454.2535, found 454.2535.

2,3,4,5-Tetrakis(4-(*tert*-butyl)phenyl)-6-methylpyridine (30c): The reaction was performed with modification of the general procedure **B** using 2.0 mmol of acetonitrile (**1o**). The title compound was obtained as a white solid (91.9 mg, 74%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 222-224 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.27 (d, J = 7.9 Hz, 2H), 7.18 (d, J = 8.2 Hz, 2H), 7.16 (d, J = 8.1 Hz, 2H), 6.96-6.93 (m, 4H), 6.84 (d, J = 8.3 Hz, 2H), 6.74 (d, J = 8.3 Hz, 2H), 6.57 (d, J = 8.3 Hz, 2H), 2.51 (s, 3H), 1.25 (s, 9H), 1.24 (s, 9H), 1.16 (s, 9H), 1.11 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.9, 154.9, 149.8 (two signals overlapped), 149.1, 148.6, 148.4, 138.3, 136.0, 135.7, 135.4, 134.6, 132.6, 131.0, 129.9, 129.8, 129.5, 124.4, 124.3, 123.9, 123.3, 34.4, 34.3, 34.2, 34.1, 31.3 (two signals overlapped), 31.2, 31.1, 24.3; HRMS (ESI) Calcd for $\text{C}_{46}\text{H}_{56}\text{N}$ $[\text{M} + \text{H}]^+$ 622.4413, found 622.4416.

2-(Methyl- d_3)-3,4,5,6-tetraphenylpyridine ([D_3]-30a): The reaction was performed with modification of the general procedure **B** using 2.0 mmol of [D_3]-**1o**. The title compound was obtained as a white solid (73.6 mg, 92%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 164-166 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.39-7.35 (m, 2H), 7.23-7.13 (m, 6H), 7.09-7.06 (m, 2H), 6.99-6.96 (m, 3H), 6.92-6.86 (m, 5H), 6.78-6.74 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.2, 155.2, 149.3, 141.0, 138.8, 138.4, 138.2, 134.7, 132.6, 131.4, 130.2, 130.1, 129.9, 127.8, 127.6, 127.3, 127.2, 126.9, 126.6, 126.1, 126.0, 23.4 (septet, J = 19.2 Hz); HRMS (ESI) Calcd for $\text{C}_{30}\text{H}_{21}\text{D}_3\text{N}$ $[\text{M} + \text{H}]^+$ 401.2097, found 401.2099.

2-Ethyl-3,4,5,6-tetraphenylpyridine (3pa):¹⁹ The reaction was performed according to the general procedure **B** to afford the title compound as a white solid (73.2 mg, 89%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 178-180 °C; ^1H NMR (500 MHz, CDCl_3): δ 7.38-7.34 (m, 2H), 7.21-7.17 (m, 5H), 7.16-7.13 (m, 1H), 7.08-7.06 (m, 2H), 6.99-6.94 (m, 3H), 6.91-6.83 (m, 5H), 6.75-6.71 (m, 2H), 2.76 (q, J = 7.5 Hz, 2H), 1.26 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 159.8, 156.1, 149.4, 141.1, 138.6, 138.5, 138.3, 134.2, 132.3, 131.4, 130.3, 130.2, 130.0, 127.6, 127.5, 127.3, 127.2, 126.8, 126.5, 126.0 (two signals overlapped), 29.5, 14.0; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{26}\text{N}$ $[\text{M} + \text{H}]^+$ 412.2065, found 412.2068.

2-Benzyl-3,4,5,6-tetraphenylpyridine (3qa):²⁰ The reaction was performed according to the general procedure **B** to afford the title compound as a white solid (84.2 mg, 89%; eluent: hexane/EtOAc = 20/1); R_f 0.4 (hexane/EtOAc = 10/1); m.p. 168-170 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.38-7.36 (m, 2H), 7.22-7.15 (m, 9H), 7.10 (d, J = 7.0 Hz, 2H), 6.98-6.94 (m, 5H), 6.88-6.84 (m, 5H), 6.72-6.70 (m, 2H), 4.17 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.1, 156.1, 149.9, 141.0, 140.0, 138.4, 138.2, 138.1, 134.8, 132.8, 131.3, 130.6, 130.2, 130.1, 129.2, 127.9, 127.6, 127.5, 127.3, 127.2, 126.8, 126.7, 126.1, 126.0, 125.8, 42.5; HRMS (ESI) Calcd for $\text{C}_{36}\text{H}_{28}\text{N}$ $[\text{M} + \text{H}]^+$ 474.2222, found 474.2227.

2-(Cyclopropylmethyl)-3,4,5,6-tetraphenylpyridine (3ra): The reaction was performed according to the general procedure **B** to afford the title compound as a white solid (74.1 mg, 85%; eluent: hexane/EtOAc = 100/3); R_f 0.4 (hexane/EtOAc = 10/1); m.p. 168-170 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.38-7.36 (m, 2H), 7.19-7.11 (m, 6H), 7.08-7.05 (m, 2H), 6.98-6.96 (m, 3H), 6.89-6.85 (m, 5H), 6.75-6.73 (m, 2H), 2.68 (d, J = 6.8 Hz, 2H), 1.18-1.08 (m, 1H), 0.44-0.39 (m, 2H), 0.10 (q, J = 4.9 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.4, 156.1, 149.4, 141.1, 138.6, 138.4, 134.3, 132.4, 131.4, 130.5, 130.3, 130.1, 127.6, 127.5, 127.3, 127.2, 126.8, 126.6, 126.1, 126.0, 40.7, 11.0, 4.7; HRMS (ESI) Calcd for $\text{C}_{33}\text{H}_{28}\text{N}$ $[\text{M}$

+ H]⁺ 438.2222, found 438.2227.

2-(Pent-4-en-1-yl)-3,4,5,6-tetraphenylpyridine (3sa): The reaction was performed according to the general procedure **B** to afford the title compound as a white solid (72.2 mg, 80%; eluent: hexane/EtOAc = 100/3); *R_f* 0.4 (hexane/EtOAc = 10/1); m.p. 107-110 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.37-7.35 (m, 2H), 7.21-7.12 (m, 6H), 7.08-7.05 (m, 2H), 6.99-6.94 (m, 3H), 6.91-6.83 (m, 5H), 6.76-6.72 (m, 2H), 5.77-5.67 (m, 1H), 4.96-4.90 (m, 1H), 4.89-4.86 (m, 1H), 2.78-2.74 (m, 2H), 2.04 (q, *J* = 7.1 Hz, 2H), 1.88-1.81 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 158.6, 156.1, 149.4, 141.1, 138.7, 138.6, 138.5, 138.3, 134.5, 132.4, 131.4, 130.3 (two signals overlapped), 130.1, 127.6, 127.5, 127.3, 127.2, 126.8, 126.6, 126.0 (two signals overlapped), 114.3, 35.7, 33.6, 28.8; HRMS (ESI) Calcd for C₃₄H₃₀N [M + H]⁺ 452.2378, found 452.2375.

2-(Cyclohex-1-en-1-ylmethyl)-3,4,5,6-tetraphenylpyridine (3ta): The reaction was performed according to the general procedure **B** to afford the title compound as a white solid (75.4 mg, 79%; eluent: hexane/EtOAc = 30/1); *R_f* 0.3 (hexane/EtOAc = 30/1); m.p. 178-180 °C; ¹H NMR (500 MHz, CD₂Cl₂): δ 7.34-7.30 (m, 2H), 7.20-7.11 (m, 6H), 7.07-7.05 (m, 2H), 7.00-6.96 (m, 3H), 6.92-6.87 (m, 5H), 6.81-6.78 (m, 2H), 5.08-5.06 (m, 1H), 3.34 (s, 2H), 1.94-1.90 (m, 2H), 1.86-1.83 (m, 2H), 1.59-1.54 (m, 2H), 1.53-1.48 (m, 2H); ¹³C NMR (100 MHz, CD₂Cl₂): δ 156.9, 155.7, 149.7, 141.4, 138.8, 138.6, 136.4, 135.2, 132.7, 131.6, 130.6, 130.5, 130.2, 127.5 (two signals overlapped), 127.4, 127.2, 126.9, 126.6, 126.2, 126.1, 123.2, 44.9, 29.0, 25.5, 23.2, 22.6; HRMS (ESI) Calcd for C₃₆H₃₂N [M + H]⁺ 478.2535, found 478.2535.

2-Cyclopropyl-3,4,5,6-tetraphenylpyridine (3ua): The reaction was performed according to the general procedure **B** to afford the title compound as a white solid (77.1 mg, 91%; eluent: hexane/EtOAc = 100/1); R_f 0.6 (hexane/EtOAc = 10/1); m.p. 168-170 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.38-7.33 (m, 2H), 7.23-7.15 (m, 8H), 6.99-6.95 (m, 3H), 6.92-6.90 (m, 3H), 6.87-6.84 (m, 2H), 6.76-6.74 (m, 2H), 1.92-1.85 (m, 1H), 1.32-1.29 (m, 2H), 0.87-0.82 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.5, 155.6, 148.8, 141.2, 138.8, 138.5, 138.4, 133.9, 131.4, 130.8, 130.3, 130.1, 127.6, 127.3 (two signals overlapped), 127.1, 126.8, 126.5, 126.0, 15.1, 10.3; HRMS (ESI) Calcd for $\text{C}_{32}\text{H}_{26}\text{N}$ $[\text{M} + \text{H}]^+$ 424.2065, found 424.2064.

2-Cyclohexyl-3,4,5,6-tetraphenylpyridine (3va): The reaction was performed according to the general procedure **B** with a prolonged reaction time of 72 h, affording the title compound as a white solid (47.5 mg, 51%; eluent: hexane/EtOAc = 100/1); R_f 0.5 (hexane/EtOAc = 10/1); m.p. 209-211 °C; ^1H NMR (400 MHz, CDCl_3): δ 7.41-7.37 (m, 2H), 7.20-7.11 (m, 6H), 7.06-7.03 (m, 2H), 7.00-6.94 (m, 3H), 6.89-6.85 (m, 5H), 6.74-6.70 (m, 2H), 2.61 (tt, J = 11.4, 3.4 Hz, 1H), 1.97-1.87 (m, 2H), 1.81-1.73 (m, 4H), 1.64-1.60 (m, 1H), 1.35-1.24 (m, 1H), 1.19-1.07 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.4, 155.6, 149.3, 141.4, 138.9, 138.7 (two signals overlapped), 133.6, 131.9, 131.4, 130.3 (three signals overlapped), 127.5, 127.3 (two signals overlapped), 127.1, 126.8, 126.4, 126.0, 125.8, 42.8, 32.6, 26.5, 26.0; HRMS (ESI) Calcd for $\text{C}_{35}\text{H}_{32}\text{N}$ $[\text{M} + \text{H}]^+$ 466.2535, found 466.2536.

2-Isopropyl-3,4,5,6-tetraphenylpyridine (3wa): The reaction was performed according to the general procedure **B** with a prolonged reaction time of 72 h, affording the title compound as a white solid (34.9 mg, 41%; eluent: hexane/EtOAc = 100/1); R_f 0.5 (hexane/EtOAc =

10/1); m.p. 194-196 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.40-7.37 (m, 2H), 7.20-7.12 (m, 6H), 7.07-7.05 (m, 2H), 6.99-6.95 (m, 3H), 6.90-6.83 (m, 5H), 6.74-6.70 (m, 2H), 3.01 (septet, *J* = 6.7 Hz, 1H), 1.30 (d, *J* = 6.8 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 163.1, 155.71, 149.3, 141.3, 140.6, 140.3, 138.8, 138.8, 138.6, 133.4, 132.0, 131.4, 131.4, 130.3, 127.6, 127.4, 127.3, 127.1, 126.8, 126.6, 126.4, 126.0, 125.9, 125.2, 32.4, 22.7. HRMS (ESI) Calcd for C₃₂H₂₈N [M + H]⁺ 426.2222, found 426.2224.

N,N-dimethyl-2-(3,4,5,6-tetraphenylpyridin-2-yl)ethan-1-amine (3xa): The reaction was performed with modification of the general procedure **B**, using CoI₂ (10 mol %), dppp (10 mol %) and Zn (50 mol %), to afford the title compound as a white solid (45.5 mg, 50%; eluent: DCM/MeOH = 10/1); *R_f* 0.2 (DCM/MeOH = 10/1); m.p. 232-235 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.34-7.31 (m, 2H), 7.24-7.14 (m, 6H), 7.12-7.10 (m, 2H), 6.98-6.93 (m, 3H), 6.90-6.86 (m, 5H), 6.78-6.74 (m, 2H), 3.42 (t, *J* = 7.3 Hz, 2H), 3.14 (t, *J* = 7.4 Hz, 2H), 2.64 (s, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 156.5, 153.0, 150.4, 140.6, 137.9, 137.6, 137.4, 135.3, 134.0, 131.3, 130.1, 130.0, 129.9, 128.2, 127.6, 127.5, 127.4, 127.2, 126.9, 126.3 (two signals overlapped), 57.1, 43.5, 30.6; HRMS (ESI) Calcd for C₃₃H₃₁N₂ [M + H]⁺ 455.2487, found 455.2489.

Methyl 2-(3,4,5,6-tetraphenylpyridin-2-yl)acetate (3ya): The reaction was performed with modification of the general procedure **B**, using CoI₂ (10 mol %), dppp (10 mol %) and Zn (50 mol %), to afford the title compound as a white solid (35.3 mg, 39%; eluent: hexane/EtOAc = 20/3); *R_f* 0.4 (hexane/EtOAc = 5/1); m.p. 148-151 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.35-7.32 (m, 2H), 7.20-7.13 (m, 6H), 7.08-7.06 (m, 2H), 6.99-6.96 (m, 3H), 6.90-6.85 (m, 5H), 6.75-6.72 (m, 2H), 3.85 (s, 2H), 3.63 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 171.5, 156.4, 151.5, 149.9, 140.6, 138.2, 137.9, 137.8, 135.4, 133.7, 131.3, 130.2, 130.1 (two signals overlapped), 127.8, 127.5, 127.4, 127.3, 127.0, 126.9, 126.2 (two signals overlapped), 51.8,

42.6; HRMS (ESI) Calcd for $C_{32}H_{26}NO_2$ $[M + H]^+$ 456.1964, found 456.1966.

2,3,4,5-Tetraphenyl-6-(1-(pyridin-2-yl)ethyl)pyridine (3za): The reaction was performed with modification of the general procedure **B**, using CoI_2 (10 mol %), dppp (10 mol %) and Zn (50 mol %), to afford the title compound as a white solid (41.2 mg, 42%; eluent: hexane/EtOAc = 20/3); R_f 0.3 (hexane/EtOAc = 5/1); m.p. 152-155 °C; 1H NMR (500 MHz, $CDCl_3$): δ 8.44 (d, J = 4.1 Hz, 1H), 7.54 (td, J = 7.7, 1.6 Hz, 1H), 7.39-7.37 (m, 3H), 7.19-7.15 (m, 4H), 7.11-7.02 (m, 4H), 6.99-6.97 (m, 3H), 6.87-6.83 (m, 5H), 6.75-6.73 (m, 2H), 6.69-6.68 (m, 1H), 4.47 (q, J = 7.0 Hz, 1H), 1.76 (d, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 159.4, 155.5, 149.8, 148.6, 141.1, 138.7, 138.4, 138.0, 135.8, 134.9, 132.5, 131.4, 130.8, 130.3, 130.0, 127.6, 127.5, 127.4, 127.2, 126.8, 126.6, 126.1, 126.0, 122.7, 120.8, 46.7, 21.1; HRMS (ESI) Calcd for $C_{36}H_{29}N_2$ $[M + H]^+$ 489.2331, found 489.2332.

4-(3,4,5,6-Tetraphenylpyridin-2-yl)morpholine (3aaa): The reaction was performed with modification of the general procedure **B**, using CoI_2 (10 mol %), dppp (10 mol %) and Zn (50 mol %), to afford the title compound as a white solid (86.1 mg, 92%; eluent: hexane/EtOAc = 30/1); R_f 0.3 (hexane/EtOAc = 30/1); m.p. 207-209 °C; 1H NMR (400 MHz, $CDCl_3$): δ 7.42-7.38 (m, 2H), 7.19-7.07 (m, 8H), 6.98-6.95 (m, 3H), 6.92-6.88 (m, 3H), 6.85-6.82 (m, 2H), 6.72-6.68 (m, 2H), 3.55 (t, J = 4.6 Hz, 4H), 3.16 (t, J = 4.6 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 153.8, 151.2, 141.1, 138.9, 138.6, 138.1, 131.6, 130.8, 130.5, 130.1, 128.8, 127.8, 127.4, 127.3, 127.2, 126.8, 126.4, 125.9 (two signals overlapped), 124.5, 66.9, 49.6; HRMS (ESI) Calcd for $C_{33}H_{29}N_2O$ $[M + H]^+$ 469.2280, found 469.2282.

2-Ethyl-3,4,5,6-tetrapropylpyridine (3pl): The reaction was performed using **1p** (2 mmol), **2o** (0.40 mmol), CoI₂ (10 mol %), bis(dicyclohexylphosphino)methane (10 mol %), and Zn (50 mol %) in DME at 100 °C for 24 h. The title compound was obtained as a colorless oil (30.3 mg, 55%; eluent: hexane/EtOAc = 50/1); *R_f* 0.3 (hexane/EtOAc = 30/1); ¹H NMR (400 MHz, CDCl₃): δ 2.74 (q, *J* = 7.5 Hz, 2H), 2.70-2.66 (m, 2H), 2.53-2.49 (m, 6H), 1.74-1.66 (m, 2H), 1.55-1.44 (m, 6H), 1.25 (t, *J* = 7.5 Hz, 3H), 1.07-0.98 (m, 12H); ¹³C NMR (100 MHz, CDCl₃): δ 157.8, 156.9, 147.5, 130.8, 130.5, 37.4, 31.4, 30.9 (two signals overlapped), 28.3, 24.5 (two signals overlapped), 24.4, 23.5, 14.9, 14.8 (two signals overlapped), 14.4 (two signals overlapped); HRMS (ESI) Calcd for C₁₉H₃₄N [M + H]⁺ 276.2691, found 276.2692.

Dimethyl 1,3,4-triphenyl-5,7-dihydro-6H-cyclopenta[c]pyridine-6,6-dicarboxylate (5):

The reaction of **1a** (0.4 mmol) and tethered diyne **4** (0.2 mmol) was performed according to the general procedure A to afford the title compound as a white solid (82.5 mg, 89%; eluent: hexane/EtOAc = 8/1); *R_f* 0.3 (hexane/EtOAc = 5/1); m.p. 188-191 °C; ¹H NMR (500 MHz, CDCl₃): δ 7.89 (d, *J* = 7.2 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.40-7.36 (m, 2H), 7.33-7.27 (m, 3H), 7.20-7.17 (m, 5H), 3.93 (s, 2H), 3.73 (s, 6H), 3.52 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 171.5, 155.9, 152.4, 150.8, 140.1, 139.4, 137.8, 131.7, 131.1, 130.1, 129.7, 128.6, 128.4 (two signals overlapped), 128.3, 127.5, 127.4, 127.2, 60.1, 53.1, 40.5, 40.4; HRMS (ESI) Calcd for C₃₀H₂₆NO₄ [M + H]⁺ 464.1862, found 464.1858.

Dimethyl 2,3,4-triphenyl-5,7-dihydro-6H-cyclopenta[b]pyridine-6,6-dicarboxylate (7):

The reaction of tethered cyanoalkyne **6** (0.2 mmol) and **2a** (0.2 mmol) was performed according to the general procedure A to afford the title compound as a white solid (33.0 mg, 36%; eluent: hexane/EtOAc = 5/1); *R_f* 0.2 (hexane/EtOAc = 5/1); m.p. 144-147 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.25-7.18 (m, 5H), 7.17-7.13 (m, 3H), 7.02-6.95 (m, 5H), 6.83-6.80 (m, 2H), 3.87 (s, 2H), 3.77 (s, 6H), 3.51 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 171.8, 159.6, 158.0, 146.4, 140.9, 137.9, 137.4, 133.1, 131.4, 130.8, 129.8, 129.0, 128.0, 127.6, 127.4,

127.2 (two signals overlapped), 126.3, 57.9, 53.1, 42.3, 38.5; HRMS (ESI) Calcd for $\text{C}_{30}\text{H}_{26}\text{NO}_4$ $[\text{M} + \text{H}]^+$ 464.1862, found 464.1859.

4. Mechanochemical Cyclodehydrogenation of Polyarylpyridines

General Procedure: In an argon-filled glove box, a 15 mL stainless milling jar equipped with two 10 mm stainless steel balls was charged sequentially with polyarylpyridine (0.10 mmol) and potassium (78.0 mg, 2.0 mmol). The jar was closed, taken out of the glove box, and placed onto Retsch Mixer Mill MM400 machine. The mixture was subjected to 30 Hz milling for 2 h. The reaction mixture was carefully quenched by the slow addition of *tert*-amyl alcohol followed by water. The organic phase was extracted with dichloromethane (30 mL x 3). The combined organic layer was dried over Na₂SO₄ and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the cyclodehydrogenation product.

16-Methyldibenzo[*c,i*]phenanthro[1,10,9,8-*klmna*]phenanthridine (8a): Light yellow solid (14.5 mg, 37%; eluent: hexane/EtOAc = 30/1); *R_f* 0.4 (hexane/EtOAc = 30/1); m.p. 264–266 °C; ¹H NMR (400 MHz, CDCl₃): δ 9.60–9.58 (m, 1H), 8.92–8.78 (m, 7H), 8.11–8.03 (m, 2H), 7.85–7.84 (m, 2H), 7.76–7.75 (m, 2H), 3.62 (s, 3H); ¹³C NMR (100 MHz, CDCl₃/CS₂): δ 152.7, 141.8, 131.4, 131.2 (three signals overlapped), 131.0, 130.0, 129.5, 129.3, 129.1, 128.6, 128.1 (two signals overlapped), 127.6, 127.1, 126.7, 126.6, 125.7, 123.7, 123.4, 123.3, 122.8, 122.1, 121.9, 121.7, 121.5, 121.2, 114.7, 30.7; HRMS (ESI) Calcd for C₃₀H₁₈N [M + H]⁺ 392.1439, found 392.1442.

16-Ethyldibenzo[*c,i*]phenanthro[1,10,9,8-*klmna*]phenanthridine (8b): Light yellow solid (10.5 mg, 26%; eluent: hexane/EtOAc = 30/1); *R_f* 0.4 (hexane/EtOAc = 30/1); m.p. 268–270 °C; ¹H NMR (400 MHz, CDCl₃): δ 9.61–9.59 (m, 1H), 8.87–8.83 (m, 3H), 8.80–8.73 (m,

4H), 8.02 (t, $J = 7.9$ Hz, 1H), 7.99 (t, $J = 7.9$ Hz, 1H), 7.86-7.79 (m, 2H), 7.75-7.69 (m, 2H), 3.87 (q, $J = 7.3$ Hz, 2H), 1.83 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, $\text{CDCl}_3/\text{CS}_2$): δ 156.9, 141.6, 131.3, 131.2, 131.1, 131.0, 130.9, 129.5, 129.3, 129.0, 128.9, 128.4, 128.3, 127.9, 127.5, 127.0, 126.6, 126.3, 125.7, 123.6, 123.2 (two signals overlapped), 122.7, 121.9, 121.8, 121.5, 121.0, 120.9, 114.1, 33.7, 14.3; HRMS (ESI) Calcd for $\text{C}_{31}\text{H}_{20}\text{N}$ $[\text{M} + \text{H}]^+$ 406.1596, found 406.1594.

3,6,9,12,16-Pentamethyldibenzo[*c,i*]phenanthro[1,10,9,8-*klmna*]phenanthridine (8c):

Light yellow solid (8.5 mg, 19%; eluent: hexane/EtOAc = 50/1); R_f 0.3 (hexane/EtOAc = 50/1); m.p. 320-322 °C; ^1H NMR (400 MHz, CDCl_3): δ 9.35 (d, $J = 8.1$ Hz, 1H), 8.66 (d, $J = 8.3$ Hz, 1H), 8.52-8.41 (m, 6H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.48 (d, $J = 8.3$ Hz, 1H), 3.52 (s, 3H), 2.76 (s, 3H), 2.74 (s, 3H), 2.70 (s, 3H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.9, 141.2, 138.0, 137.5, 136.4, 135.7, 131.2, 131.0, 130.9, 130.8, 129.2, 128.9, 128.8 (two signals overlapped), 128.6, 127.9, 127.8 (two signals overlapped), 125.4, 123.6, 122.7, 122.5, 122.4, 122.2, 121.6, 121.5, 121.4, 120.9, 114.2, 30.9, 22.6 (two signals overlapped), 22.2, 21.8; HRMS (ESI) Calcd for $\text{C}_{34}\text{H}_{26}\text{N}$ $[\text{M} + \text{H}]^+$ 448.2065, found 448.2065.

3,6,9,12-Tetra-*tert*-butyldibenzo[*c,i*]phenanthro[1,10,9,8-*klmna*]phenanthridine (9):

Light yellow solid (7.2 mg, 12%; eluent: hexane/EtOAc = 100/1); R_f 0.3 (hexane/EtOAc = 100/1); m.p. 336-338 °C; ^1H NMR (400 MHz, CDCl_3): δ 10.43 (s, 1H), 9.51 (d, $J = 8.6$ Hz, 1H), 9.17 (s, 2H), 9.10 (d, $J = 0.6$ Hz, 1H), 9.05 (s, 1H), 8.96 (d, $J = 8.6$ Hz, 1H), 8.89 (d, $J =$

1.6 Hz, 1H), 8.88 (d, $J = 1.5$ Hz, 1H), 7.95 (dd, $J = 8.6, 1.7$ Hz, 1H), 7.91 (dd, $J = 8.6, 1.8$ Hz, 1H), 1.76 (s, 9H), 1.75 (s, 9H), 1.62 (s, 9H), 1.60 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.5, 151.1, 150.6, 149.6, 143.2, 142.4, 131.5, 131.3, 131.2, 130.2, 130.0, 129.6, 129.3, 127.2, 126.9, 126.2, 125.9, 125.3, 122.8, 121.9, 121.3, 120.9, 119.5, 119.1, 118.9, 118.8, 118.7, 118.5, 116.3, 35.9, 35.8, 35.4, 35.3, 32.0, 31.9, 31.5 (two signals overlapped); HRMS (ESI) Calcd for $\text{C}_{45}\text{H}_{48}\text{N}$ $[\text{M} + \text{H}]^+$ 602.3787, found 602.3787.

3,6,9,12-Tetra-*tert*-butyldibenzo[*c,h*]benzo[5,6]tetraceno[1,12,11,10-*jklmna*]acridine

(10): Light yellow solid (18.2 mg, 27%; eluent: hexane/EtOAc = 200/1); R_f 0.3 (hexane/EtOAc = 200/1); m.p. 362–364 °C; ^1H NMR (400 MHz, CDCl_3): δ 9.84 (dd, $J = 7.6, 1.6$ Hz, 1H), 9.81 (d, $J = 8.5$ Hz, 1H), 9.10 (s, 1H), 9.09 (s, 1H), 9.08 (s, 1H), 9.06 (s, 1H), 9.03 (s, 1H), 8.97 (s, 1H), 8.86 (d, $J = 1.1$ Hz, 1H), 8.79–8.77 (m, 1H), 8.01 (dd, $J = 8.5, 1.6$ Hz, 1H), 7.89–7.81 (m, 2H), 1.79 (s, 18H), 1.75 (s, 9H), 1.67 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ 151.5, 150.8, 149.1 (two signals overlapped), 143.2, 143.1, 132.0 (two signals overlapped), 131.6 (two signals overlapped), 131.5, 129.9, 129.8, 129.7, 129.2, 128.8, 128.6, 127.3, 126.9, 126.1, 126.0, 125.6, 122.8, 122.2, 122.0, 121.9, 119.3, 119.1, 118.7 (five signals overlapped), 115.0 (two signals overlapped), 35.9, 35.8, 35.7, 35.4, 32.0 (three signals overlapped), 31.6; HRMS (ESI) Calcd for $\text{C}_{51}\text{H}_{50}\text{N}$ $[\text{M} + \text{H}]^+$ 676.3943, found 676.3942.

Recrystallization from THF/pentane afforded single crystals of **10** (with a THF molecule) suitable for X-ray diffraction analysis, which unambiguously confirmed its molecular structure (Table S5, Figure S3).²¹

Table S5. Crystal data and structure refinement for yoshi106m (**10**•THF)

Identification code	Yoshi106m	
Chemical formula	C ₅₅ H ₅₇ NO	
Formula weight	748.01 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.180 x 0.240 x 0.260 mm	
Crystal habit	brown block	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 16.0821(8) Å	α = 90°
	b = 24.6181(13) Å	β = 103.4078(16)°
	c = 10.9053(4) Å	γ = 90°
Volume	4199.8(3) Å ³	
Z	4	
Density (calculated)	1.183 g/cm ³	
Absorption coefficient	0.069 mm ⁻¹	
F(000)	1608	
Theta range for data collection	2.54 to 28.00°	
Index ranges	-21<=h<=19, -27<=k<=32, -12<=l<=14	
Reflections collected	26638	
Independent reflections	9873 [R(int) = 0.0575]	
Coverage independent reflections	97.3%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.9880 and 0.9820	
Structure solution technique	direct methods	
Structure solution program	XT, VERSION 2014/5	
Refinement method	Full-matrix least-squares on F ²	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	Σ w(F _o ² - F _c ²) ²	
Data / restraints / parameters	9873 / 317 / 603	
Goodness-of-fit on F ²	1.060	
Δ/σ _{max}	0.001	
Final R indices	7397 data; I>2σ(I)	R1 = 0.0891, wR2 = 0.2388
	all data	R1 = 0.1118, wR2 = 0.2574
Weighting scheme	w=1/[σ ² (F _o ²)+(0.0983P) ² +6.2258P]	
Largest diff. peak and hole	0.582 and -0.626 eÅ ⁻³	
R.M.S. deviation from mean	0.065 eÅ ⁻³

Figure S3. ORTEP diagram of **10** (a THF molecule is omitted for clarity). Thermal ellipsoids drawn at 50% probability.

Figure S4. Molecular packing diagrams of **10**. Molecules with four distinct orientations are color-coded in light blue, pink, light green, and orange, respectively, with nitrogen atoms colored in blue.

5. Absorption and Emission Spectra of **8a** and **10** and Relevant DFT Calculations

The UV-vis absorption and emission spectra of **8a** and **10** were recorded on Shimadzu UV-1800 spectrophotometer and Cary Eclipse spectrophotofluorometer, respectively. The samples were prepared in CH₂Cl₂ at the concentrations of 2×10^{-5} M (for absorption spectra) and 2×10^{-6} M (for emission spectra). The emission spectra were recorded at the excitation wavelengths of 301 nm and 331 nm for **8a** and **10**, respectively. The emission quantum yields were determined using anthracene as a reference material.

Figure S5. UV-vis absorption (a) and emission (b) spectra of **8a** and **10**.

Table S6. Summary of UV-vis absorption and emission data of **8a** and **10**

Cmpd	λ_{abs} [nm] ($\log \epsilon$)	λ_{em} [nm]	Φ_F
8a	290 (4.79), 302 (4.84), 347 (4.25), 360 (4.33), 381 (4.18), 402 (4.30)	407, 432, 457	0.27
10	304 (4.73), 332 (4.83), 362 (4.51), 375 (4.08), 383 (3.95), 405 (4.17), 430 (4.45)	435, 462, 494	0.47

Figure S6. Pictorial representations of the frontier MOs of **8a** (optimized at B3LYP/6-311++G(d,p))

Figure S7. Pictorial representations of the frontier MOs of **10** (optimized at B3LYP/6-311++G(d,p))

Table S7. TD-DFT vertical one-electron excitations (4 states) calculated for the conformation of optimized **8a**.

Exited State	Energy(eV)	Wavelength(nm)	Oscillator Strength
1	3.2679	379.39	0.1987
2	3.3942	365.29	0.0431
3	3.5976	344.63	0.0326
4	3.9099	317.10	0.1852

Table S8. TD-DFT vertical one-electron excitations (4 states) calculated for the conformation of optimized **10**.

Exited State	Energy(eV)	Wavelength(nm)	Oscillator Strength
1	3.0608	405.07	0.1309
2	3.2025	387.15	0.0532
3	3.4636	357.96	0.1138
4	3.5812	346.21	0.5896

6. DFT Calculations of Reaction Pathways

All the density functional theory (DFT) calculations were performed using Gaussian 09 program.²² Geometry optimizations were performed with the M06-L functional²³ using a combined basis set B1 (i.e. the SDD effective core potential²⁴ for cobalt and the 6-31G(d) basis set for all other atoms). Harmonic frequency calculations were performed for each stationary point to ensure that it is either an energy minimum (no imaginary frequency) or a transition state (only one imaginary frequency). For each transition state, intrinsic reaction coordinate (IRC) analysis was performed to ensure that it connects the correct reactant and product. The single-point energy calculations were further performed with the M06-L functional and a combined basis set B2 (i.e. the SDD effective core potential for cobalt and the 6-311++G(2df,2p) basis set for all other atoms), using the SMD model²⁵ (solvent = NMP) to obtain energies in solution. Note that NMP is not defined in Gaussian 09, and thus the keyword `scrf=solvent=generic` along with several parameters (`eps = 32.7`,²⁶ `epsinf = 2.187`,²⁷ `HBondAcidity = 0`,²⁸ `HBondBasicity = 0.88`,²⁸ `SurfaceTensionAtInterface = 58.7`,²⁹ `CarbonAromaticity = 0`, `ElectronegativeHalogenicity = 0`) were used to customize it. The single-point energies corrected by the thermal correction to Gibbs free energies (TCG, obtained from frequency calculations) were used as the Gibbs free energies reported in this work, corresponding to the reference state of 1 mol/L, 298.15 K. The minimum energy crossing points (MECP) between the singlet and triplet states were located with the `sobMECP` software³⁰ at the M06-L/B1 level. For each MECP, the electronic energy gap between it and its precursor was added to the free energy of the precursor to estimate its free energy.³¹ The Mayer bond orders³² were calculated at the M06-L/B1 level using `Multiwfn` program.³³ The 3-D structures were drawn using `CYLview` software.³⁴

[(dppp)Co⁰] System

Among possible (dppp)Co⁰–substrate complexes (all at the doublet spin state), the one bearing one molecule of diphenylacetylene, **CP_A**, was calculated to be the most stable (Figure S8).

Figure S8. Relative stability of (dppp)Co⁰–substrate complexes. All the complexes have doublet spin states.

The feasibility of the quartet spin state was briefly probed for selected key intermediates and transition states, which revealed that the quartet state is uniformly and significantly less favored than the doublet state (Figure S9).

Figure S9. Relative free energies of selected intermediates and transition states at the quartet state with respect to their doublet counterparts.

Figure S10. Structures of selected doublet and quartet intermediates and transition states. The phenyl groups of dppp are truncated for clarity. The suffix q of the structure numbers refers to the quartet state. The distances are in Å.

Figure S11. Structures of selected cobaltacycle intermediates. The phenyl groups of dppp are truncated for clarity. The distances are in Å. The values in the parentheses are Mayer bond orders.

[(dppp)Co]⁺ System

Complexation of [(dppp)Co]⁺, the alternative model catalyst species, with substrates **1a** and/or **2a** was explored (Figure S12). For each complex, the triplet state was calculated to be more stable than the singlet state.

Figure S12. Relative stability of [(dppp)Co]⁺-substrate complexes. The suffixes s and t of the structure numbers refer to the singlet and triplet states, respectively.

Exploration of possible reaction pathways for the [(dppp)Co]⁺-mediated [2+2+2] cycloaddition revealed the following points (Figure S13):

- (1) Regardless of the spin state, oxidative coupling of two alkynes (**TS1_t**, **TS1_s**) is energetically much more favorable than the oxidative coupling of alkyne and nitrile (**TS4_t**, **TS4_s**).
- (2) The oxidative coupling of two alkynes may proceed via either **TS1_t** or **TS1_s** (upon spin crossover), in light of their comparable free energies.
- (3) The nitrile insertion into cobaltacyclopentadiene would preferentially occur at the singlet state (compare **INT3_s/TS2_s** vs **INT3_t/TS2_t**).
- (4) The C–N reductive elimination of azacobaltacycloheptadiene would preferentially occur at the triplet state (compare **INT4_t/TS3_t** and **INT4_s/TS3_s**).
- (5) The oxidative coupling of two alkynes requires the highest activation energies in the entire reaction coordinate (32.6 kcal mol⁻¹ for triplet and 31.0 kcal mol⁻¹ for singlet), which are much higher than that of the corresponding oxidative coupling on [(dppp)Co⁰].

Figure S13. Gibbs free energy diagram of the [2+2+2] cycloaddition of benzonitrile (**1a**) and diphenylacetylene (**2a**) on $[(dppp)Co]^+$ calculated at the SMD(NMP)-M06L/6-311++G(2df,2p)-SDD(Co)/M06L/6-31G(d)-SDD(Co) level. Energies are in kcal mol⁻¹. The suffixes s and t of the structure numbers refer to the singlet and triplet states, respectively.

Table S9. Energies (hartree) of optimized structures. The data for the $[(dppp)Co]^+$ model are shown with gray shading.

Structure	E(M06-L/B1)	TCG	E(M06-L/B2)	TCG+ E(M06-L/B2)	Imaginary Frequency
1a	-324.446777	0.069019	-324.5562536	-324.4872346	
2a	-539.378974	0.152570	-539.5554866	-539.4029166	
CP _A	-2412.392558	0.569388	-2412.974513	-2412.405125	
CP _{2A}	-2951.80137	0.750394	-2952.542969	-2951.792575	
CP _N	-2197.411553	0.478694	-2197.926604	-2197.44791	
CP _N '	-2197.437702	0.482065	-2197.953988	-2197.471923	
CP _{2N}	-2521.899596	0.571983	-2522.514427	-2521.942444	
CP _{2N} '	-2521.912128	0.574253	-2522.519339	-2521.945086	
CP _{2N} ''	-2521.910381	0.572579	-2522.523377	-2521.950798	
CP _{AN}	-2736.865083	0.660891	-2737.547518	-2736.886627	
CP _{AN} '	-2736.865407	0.663765	-2737.540044	-2736.876279	
TS ₁	-2951.773272	0.750941	-2952.51652	-2951.765579	-244.95i
INT ₁	-2951.795428	0.752501	-2952.536174	-2951.783673	

TS2	-2951.791023	0.751865	-2952.529609	-2951.777744	-57.39i
INT2	-2951.81857	0.754479	-2952.568615	-2951.814136	
INT3	-3276.287237	0.84965	-3277.124537	-3276.274887	
INT3'	-3276.297878	0.846749	-3277.143552	-3276.296803	
TS3	-3276.278204	0.848834	-3277.116725	-3276.267891	-288.67i
INT4	-3276.299241	0.854026	-3277.136411	-3276.282385	
TS4	-3276.29803	0.853252	-3277.132501	-3276.279249	-45.66i
INT5	-3276.305917	0.848519	-3277.144634	-3276.296115	
TS5	-3276.296424	0.85074	-3277.133528	-3276.282788	-284.65i
INT6	-3276.354306	0.855713	-3277.187895	-3276.332182	
3aa	-1403.36794	0.432259	-1403.804115	-1403.371856	
TS6	-2736.824301	0.664884	-2737.506625	-2736.841741	-336.75i
INT7	-2736.842552	0.666779	-2737.523153	-2736.856374	
CP_A_q	-2412.337804	0.567589	-2412.921752	-2412.354163	
CP_{2A}_q	-2951.75766	0.744023	-2952.505638	-2951.761615	
INT2_q	-2951.811184	0.750160	-2952.55699	-2951.80683	
INT5_q	-3276.29676	0.845245	-3277.138371	-3276.293126	
TS1_q	-2951.74108	0.747816	-2952.487831	-2951.740015	-168.28i
TS3_q	-3276.255298	0.844678	-3277.098014	-3276.253336	-297.57i
TS5_q	-3276.266073	0.846054	-3277.110481	-3276.264427	-329.90i
CP_{2N}_s	-2521.754647	0.576549	-2522.404824	-2521.828275	
CP_{2N}_t	-2521.765945	0.573546	-2522.420335	-2521.846789	
CP_{2N'}_s	-2521.728584	0.582295	-2522.377852	-2521.795557	
CP_{2N'}_t	-2521.741499	0.569889	-2522.389666	-2521.819777	
CP_{2N''}_s	-2521.736153	0.578959	-2522.387884	-2521.808925	
CP_{2N''}_t	-2521.752859	0.572674	-2522.405904	-2521.83323	
CP_{2A}_s	-2951.623882	0.756358	-2952.405879	-2951.649521	
CP_{2A}_t	-2951.640917	0.752725	-2952.418438	-2951.665713	
CP_{AN}_s	-2736.700464	0.664800	-2737.415769	-2736.750969	
CP_{AN}_t	-2736.702039	0.659581	-2737.420913	-2736.761332	
CP_N_s	-2197.243854	0.483209	-2197.805154	-2197.321945	
CP_N_t	-2197.277665	0.481274	-2197.841203	-2197.359929	
CP_A_s	-2412.202503	0.568600	-2412.822847	-2412.254247	
CP_A_t	-2412.211724	0.568225	-2412.841928	-2412.273703	
TS1_s	-2951.60584	0.755281	-2952.383956	-2951.628675	-180.62i
TS1_t	-2951.594479	0.74965	-2952.37592	-2951.62627	-335.09i
INT1_s	-2951.636281	0.757746	-2952.410866	-2951.65312	
INT1_t	-2951.620875	0.752181	-2952.397906	-2951.645725	
INT2_s	-2951.629894	0.755675	-2952.42366	-2951.667985	
INT2_t	-2951.643128	0.755368	-2952.424749	-2951.669381	

INT3_s	-3276.138532	0.850317	-3277.025928	-3276.175611	
INT3_t	-3276.120309	0.847929	-3276.996004	-3276.148075	
TS2_s	-3276.116733	0.853997	-3276.992856	-3276.138859	-447.80i
TS2_t	-3276.089787	0.848547	-3276.964866	-3276.116319	-499.00i
INT4_s	-3276.1373	0.854796	-3277.01109	-3276.156294	
INT4_t	-3276.133645	0.851758	-3277.011317	-3276.159559	
TS3_s	-3276.128253	0.856726	-3277.00287	-3276.146144	-257.47i
TS3_t	-3276.128584	0.84895	-3277.007639	-3276.158689	-249.15i
INT5_s	-3276.166596	0.858349	-3277.041196	-3276.182847	
INT5_t	-3276.236652	0.851547	-3277.10646	-3276.254913	
TS4_s	-2736.646879	0.663717	-2737.366707	-2736.70299	-396.90i
TS4_t	-2736.651304	0.661339	-2737.36347	-2736.702131	-300.76i
INT6_s	-2736.678398	0.668519	-2737.395099	-2736.72658	
INT6_t	-2736.658096	0.663669	-2737.369775	-2736.706106	
MECP1	-2951.617258				
MECP2	-2951.629053				
MECP3	-3276.120220				

Cartesian Coordinates

1a

C	-0.091838000	-1.214911000	0.000004000
C	0.609630000	0.000052000	0.000015000
C	-0.091902000	1.214941000	-0.000002000
C	-1.480706000	1.208014000	0.000000000
C	-2.175596000	-0.000037000	0.000003000
C	-1.480621000	-1.208068000	-0.000008000
H	0.460712000	-2.151348000	-0.000001000
H	0.460543000	2.151440000	-0.000012000
H	-2.023739000	2.150578000	-0.000006000
H	-3.263742000	-0.000095000	-0.000004000
H	-2.023640000	-2.150640000	-0.000009000
C	2.036593000	0.000044000	0.000000000
N	3.205215000	-0.000022000	-0.000005000

2a

C	-0.609164000	-0.000243000	0.000473000
C	0.609164000	-0.000166000	0.000436000
C	-2.030053000	-0.000080000	0.000216000
C	-2.746584000	-0.855833000	0.855441000
C	-2.746072000	0.855807000	-0.855299000
C	-4.135487000	-0.852331000	0.851802000
H	-2.196780000	-1.519885000	1.519181000
C	-4.134976000	0.852584000	-0.852218000
H	-2.195872000	1.519730000	-1.518840000
C	-4.834876000	0.000200000	-0.000346000
H	-4.676431000	-1.520493000	1.519550000
H	-4.675518000	1.520843000	-1.520195000
H	-5.923238000	0.000307000	-0.000567000
C	2.030053000	-0.000096000	0.000209000
C	2.746426000	0.855710000	0.855513000
C	2.746230000	-0.855807000	-0.855350000
C	4.135330000	0.852432000	0.851906000
H	2.196500000	1.519625000	1.519288000
C	4.135133000	-0.852360000	-0.852237000
H	2.196152000	-1.519772000	-1.518950000
C	4.834876000	0.000076000	-0.000287000
H	4.676151000	1.520634000	1.519714000
H	4.675799000	-1.520485000	-1.520248000
H	5.923238000	0.000144000	-0.000484000

CP_A

C	-0.809940000	1.931263000	0.397433000
Co	0.027248000	0.394726000	-0.314851000
P	1.708015000	-0.891652000	-0.887089000
P	-1.505398000	-1.084823000	-0.839547000
C	-1.147939000	-2.160815000	-2.309066000
H	-1.987725000	-2.849183000	-2.480137000
H	-1.123964000	-1.491355000	-3.181433000
C	1.435316000	-2.100073000	-2.270619000
H	1.425911000	-1.489467000	-3.185551000
H	2.317010000	-2.752022000	-2.360348000
C	0.161009000	-2.941210000	-2.197502000
H	0.194562000	-3.678247000	-3.012925000
H	0.152166000	-3.529018000	-1.266858000
C	0.492705000	2.085689000	0.415862000
C	1.529104000	2.998089000	0.849338000
C	1.227508000	4.334482000	1.176404000
C	2.865437000	2.580773000	0.966185000
C	2.222193000	5.211832000	1.587877000
H	0.192672000	4.669418000	1.109306000
C	3.861543000	3.458866000	1.375910000
H	3.109705000	1.547292000	0.721071000
C	3.545679000	4.780556000	1.685410000
H	1.965393000	6.241117000	1.835636000

H	4.890795000	3.109671000	1.450761000
H	4.324912000	5.471307000	2.003679000
C	-2.113269000	2.494471000	0.652627000
C	-2.430876000	3.804908000	0.249459000
C	-3.127303000	1.727938000	1.254275000
C	-3.708313000	4.320515000	0.437977000
H	-1.663437000	4.404796000	-0.239827000
C	-4.396303000	2.251756000	1.460374000
H	-2.900464000	0.701070000	1.545873000
C	-4.696545000	3.549900000	1.048316000
H	-3.933597000	5.334175000	0.108250000
H	-5.163810000	1.635206000	1.926793000
H	-5.695583000	3.956161000	1.197101000
C	-3.210342000	-0.529428000	-1.226768000
C	-4.361082000	-1.235471000	-0.862110000
C	-3.348556000	0.690602000	-1.900048000
C	-5.622946000	-0.731575000	-1.169013000
H	-4.273140000	-2.175678000	-0.317506000
C	-4.607715000	1.188480000	-2.215614000
H	-2.454420000	1.269970000	-2.138905000
C	-5.748343000	0.478274000	-1.847442000
H	-6.512329000	-1.285101000	-0.871259000
H	-4.698630000	2.147110000	-2.723620000
H	-6.735955000	0.874449000	-2.077802000
C	-1.688292000	-2.325030000	0.502214000
C	-2.137790000	-3.637014000	0.301391000
C	-1.267101000	-1.953212000	1.785858000
C	-2.166801000	-4.547990000	1.353686000
H	-2.461472000	-3.957116000	-0.689569000
C	-1.298360000	-2.860889000	2.840103000
H	-0.894378000	-0.938526000	1.948353000
C	-1.746287000	-4.161596000	2.624542000
H	-2.515036000	-5.564889000	1.179375000
H	-0.956109000	-2.554788000	3.827216000
H	-1.762218000	-4.877368000	3.444696000
C	2.144591000	-1.956844000	0.543381000
C	2.314970000	-3.344635000	0.478393000
C	2.233924000	-1.329444000	1.796079000
C	2.559677000	-4.085616000	1.633239000
H	2.256250000	-3.861216000	-0.479065000
C	2.497208000	-2.066181000	2.945053000
H	2.080130000	-0.249514000	1.861147000
C	2.653550000	-3.449325000	2.867373000
H	2.680638000	-5.165659000	1.564924000
H	2.569047000	-1.560074000	3.906494000
H	2.845078000	-4.030055000	3.768143000
C	3.328559000	-0.214214000	-1.427104000
C	3.370259000	1.087043000	-1.937419000
C	4.511568000	-0.959297000	-1.361590000
C	4.571401000	1.633545000	-2.381144000
H	2.453607000	1.680342000	-1.946327000
C	5.713562000	-0.411549000	-1.799735000
H	4.492369000	-1.969712000	-0.949571000
C	5.743738000	0.884847000	-2.311659000
H	4.594099000	2.652444000	-2.763863000
H	6.630754000	-0.995218000	-1.737125000
H	6.685831000	1.314691000	-2.648148000

CP_{2A}

C	-1.618225000	-1.325338000	0.721903000
C	-1.232939000	-1.841064000	-0.419990000
Co	-0.096119000	-0.380244000	0.107203000
P	1.722930000	-0.443457000	-1.249549000
P	-1.166368000	1.210465000	-1.208870000
C	-0.977342000	0.670630000	-2.976265000
H	-1.684473000	1.239963000	-3.595930000
H	-1.265048000	-0.389966000	-3.033116000
C	1.442742000	-0.230261000	-3.074820000
H	1.075919000	-1.205091000	-3.425455000

H	2.410101000	-0.069517000	-3.573266000
C	0.446854000	0.848106000	-3.505602000
H	0.408242000	0.839104000	-4.603907000
H	0.815163000	1.850193000	-3.237183000
C	0.631143000	0.935801000	1.621775000
C	0.925996000	-0.272679000	1.845485000
C	1.497677000	-1.317159000	2.649741000
C	2.647466000	-1.045322000	3.416624000
C	0.953835000	-2.611867000	2.694752000
C	3.229761000	-2.037237000	4.195220000
H	3.069691000	-0.040497000	3.390041000
C	1.535564000	-3.596162000	3.483278000
H	0.067730000	-2.827117000	2.097933000
C	2.678529000	-3.317438000	4.231238000
H	4.120070000	-1.809598000	4.779525000
H	1.095558000	-4.591982000	3.510895000
H	3.137922000	-4.093925000	4.840237000
C	0.581152000	2.340095000	1.884137000
C	1.771696000	3.075346000	2.039353000
C	-0.642131000	3.029123000	1.959533000
C	1.730669000	4.448598000	2.246799000
H	2.725231000	2.554446000	1.963350000
C	-0.676664000	4.399102000	2.179097000
H	-1.564565000	2.463509000	1.830290000
C	0.509873000	5.119102000	2.316335000
H	2.663756000	5.001487000	2.351189000
H	-1.636534000	4.912386000	2.228422000
H	0.482891000	6.196195000	2.471229000
C	-2.540663000	-1.374340000	1.828289000
C	-3.450842000	-2.437467000	1.987257000
C	-2.566709000	-0.332258000	2.770856000
C	-4.363619000	-2.440496000	3.033869000
H	-3.423283000	-3.266151000	1.280500000
C	-3.486225000	-0.332758000	3.811634000
H	-1.843104000	0.474957000	2.662485000
C	-4.391606000	-1.384179000	3.944670000
H	-5.060363000	-3.270857000	3.140864000
H	-3.494811000	0.488369000	4.526869000
H	-5.113098000	-1.385711000	4.760166000
C	-1.609583000	-2.780458000	-1.452050000
C	-0.687924000	-3.246110000	-2.406797000
C	-2.943560000	-3.227452000	-1.561985000
C	-1.072402000	-4.124026000	-3.413188000
H	0.348567000	-2.921873000	-2.328918000
C	-3.330653000	-4.090367000	-2.579019000
H	-3.677052000	-2.859241000	-0.845036000
C	-2.396898000	-4.547645000	-3.509167000
H	-0.333071000	-4.477706000	-4.130527000
H	-4.369176000	-4.412565000	-2.645922000
H	-2.700162000	-5.228181000	-4.302756000
C	3.098678000	0.715291000	-0.888544000
C	3.834074000	0.510046000	0.290073000
C	3.399528000	1.835843000	-1.672032000
C	4.835420000	1.397183000	0.669206000
H	3.627186000	-0.367453000	0.904643000
C	4.393640000	2.732681000	-1.284910000
H	2.849066000	2.022932000	-2.594059000
C	5.113336000	2.518317000	-0.112621000
H	5.400102000	1.212571000	1.582746000
H	4.610817000	3.597728000	-1.910240000
H	5.892935000	3.216506000	0.187209000
C	2.671009000	-2.021632000	-1.227224000
C	3.880355000	-2.163453000	-1.921173000
C	2.198448000	-3.094719000	-0.467696000
C	4.592261000	-3.356447000	-1.861615000
H	4.276290000	-1.324646000	-2.495705000
C	2.915894000	-4.286681000	-0.397204000
H	1.254743000	-2.982455000	0.067777000
C	4.111952000	-4.419203000	-1.096054000
H	5.530382000	-3.456021000	-2.405542000

H	2.539300000	-5.107921000	0.210635000
H	4.676426000	-5.348767000	-1.041940000
C	-2.973635000	1.141276000	-0.947802000
C	-3.727699000	0.095990000	-1.495497000
C	-3.602581000	2.016197000	-0.050423000
C	-5.063944000	-0.077851000	-1.145945000
H	-3.267083000	-0.605646000	-2.189408000
C	-4.938758000	1.844010000	0.296070000
H	-3.041075000	2.850314000	0.370563000
C	-5.672549000	0.789987000	-0.243445000
H	-5.628016000	-0.902062000	-1.581558000
H	-5.406990000	2.534919000	0.995275000
H	-6.714826000	0.648317000	0.036408000
C	-0.820973000	3.002137000	-1.391706000
C	-1.759102000	3.924657000	-1.872673000
C	0.472542000	3.448025000	-1.101826000
C	-1.409774000	5.262169000	-2.038178000
H	-2.770564000	3.595698000	-2.111139000
C	0.828066000	4.780818000	-1.281715000
H	1.200591000	2.740722000	-0.707874000
C	-0.117366000	5.693214000	-1.742606000
H	-2.150334000	5.971395000	-2.405061000
H	1.839437000	5.103533000	-1.036830000
H	0.149544000	6.741129000	-1.870627000

CP_{AN}

Co	0.432484000	-0.066328000	-0.335599000
P	-0.083934000	1.072557000	1.569932000
P	0.310224000	-2.089648000	0.568780000
C	0.578102000	-2.237547000	2.397689000
H	0.320325000	-3.253240000	2.728990000
H	1.659227000	-2.130804000	2.567519000
C	0.347400000	0.215962000	3.151758000
H	1.445433000	0.210349000	3.207122000
H	0.005404000	0.815744000	4.007040000
C	-0.181618000	-1.215295000	3.245437000
H	-0.130749000	-1.537267000	4.295810000
H	-1.250566000	-1.234091000	2.981742000
C	1.541881000	1.195133000	-1.224563000
C	2.286282000	0.261981000	-0.701292000
C	3.615719000	-0.275253000	-0.560499000
C	4.595198000	-0.072680000	-1.551521000
C	3.962063000	-1.056953000	0.555256000
C	5.856559000	-0.643202000	-1.432563000
H	4.339280000	0.524454000	-2.426680000
C	5.227276000	-1.614528000	0.681354000
H	3.199833000	-1.225315000	1.318329000
C	6.180078000	-1.416177000	-0.317072000
H	6.596173000	-0.483749000	-2.216374000
H	5.467838000	-2.220683000	1.553838000
H	7.168616000	-1.863492000	-0.228388000
C	1.469271000	2.510972000	-1.801312000
C	2.609933000	3.333561000	-1.873089000
C	0.241603000	3.037890000	-2.240838000
C	2.519454000	4.632268000	-2.356139000
H	3.561829000	2.941176000	-1.515243000
C	0.156923000	4.332676000	-2.736375000
H	-0.641154000	2.400192000	-2.178905000
C	1.294432000	5.137753000	-2.791911000
H	3.409865000	5.259185000	-2.389160000
H	-0.802364000	4.722801000	-3.074732000
H	1.226410000	6.156390000	-3.170537000
N	-1.309297000	0.008400000	-1.088868000
C	-2.435049000	-0.002221000	-1.425791000
C	-3.823257000	-0.038254000	-1.683463000
C	-4.368224000	0.447585000	-2.885905000
C	-4.677720000	-0.556623000	-0.689431000
C	-5.741673000	0.413118000	-3.083894000
H	-3.705681000	0.848242000	-3.650174000

C	-6.047241000	-0.582878000	-0.903588000
H	-4.244434000	-0.926727000	0.238514000
C	-6.584447000	-0.099926000	-2.097883000
H	-6.159066000	0.790206000	-4.015525000
H	-6.702235000	-0.983578000	-0.132095000
H	-7.660250000	-0.123079000	-2.260168000
C	0.911636000	2.603674000	1.708951000
C	0.373870000	3.893395000	1.652477000
C	2.307350000	2.459860000	1.751262000
C	1.208124000	5.009059000	1.640796000
H	-0.705814000	4.031320000	1.616919000
C	3.137757000	3.574138000	1.749538000
H	2.749758000	1.462355000	1.758168000
C	2.590170000	4.854394000	1.688945000
H	0.771037000	6.005228000	1.591999000
H	4.218132000	3.439616000	1.779711000
H	3.240116000	5.727757000	1.672850000
C	-1.813458000	1.606506000	1.817269000
C	-2.594766000	1.253144000	2.925604000
C	-2.433159000	2.303405000	0.765414000
C	-3.947562000	1.583046000	2.980336000
H	-2.149642000	0.718475000	3.763550000
C	-3.779092000	2.644163000	0.825992000
H	-1.841223000	2.572488000	-0.111397000
C	-4.544968000	2.276241000	1.931537000
H	-4.535341000	1.298823000	3.852068000
H	-4.238450000	3.180208000	-0.003653000
H	-5.603879000	2.525832000	1.971264000
C	1.497189000	-3.338431000	-0.082435000
C	1.865880000	-4.489566000	0.623508000
C	2.081386000	-3.101013000	-1.331434000
C	2.812547000	-5.367067000	0.102503000
H	1.413847000	-4.708708000	1.590823000
C	3.020345000	-3.982042000	-1.858579000
H	1.817087000	-2.190318000	-1.871852000
C	3.394013000	-5.113090000	-1.138064000
H	3.096685000	-6.253649000	0.667623000
H	3.477601000	-3.770425000	-2.823868000
H	4.140187000	-5.796515000	-1.540203000
C	-1.299285000	-2.956228000	0.340881000
C	-2.125211000	-3.392648000	1.383579000
C	-1.756919000	-3.115841000	-0.976492000
C	-3.368127000	-3.967516000	1.118607000
H	-1.805339000	-3.295675000	2.419887000
C	-2.991507000	-3.694783000	-1.242449000
H	-1.131683000	-2.768704000	-1.800555000
C	-3.806583000	-4.118382000	-0.192996000
H	-3.992783000	-4.301761000	1.945952000
H	-3.326219000	-3.804095000	-2.272998000
H	-4.779586000	-4.561200000	-0.399315000

CP_{AN}'

C	-0.390500000	-2.324285000	-0.797662000
Co	0.094737000	-0.477074000	-0.155819000
P	-1.631902000	0.493220000	-1.187160000
P	1.652546000	0.599095000	-1.419619000
C	1.197042000	0.832711000	-3.190296000
H	1.985710000	1.390753000	-3.714190000
H	1.190537000	-0.177032000	-3.622036000
C	-1.369213000	0.622290000	-3.022038000
H	-1.225249000	-0.400919000	-3.397273000
H	-2.283578000	1.013538000	-3.489793000
C	-0.168894000	1.485815000	-3.412593000
H	-0.255488000	1.727528000	-4.481225000
H	-0.223015000	2.452702000	-2.886607000
C	0.053346000	-0.139503000	1.717583000
C	-0.710287000	0.580232000	2.702400000
C	-2.113726000	0.628103000	2.621561000
C	-0.082094000	1.335368000	3.711127000

C	-2.859461000	1.385486000	3.513666000
H	-2.604334000	0.063694000	1.826944000
C	-0.829894000	2.112079000	4.588592000
H	1.006121000	1.323903000	3.780084000
C	-2.221093000	2.139763000	4.498251000
H	-3.945897000	1.401600000	3.430637000
H	-0.322858000	2.698738000	5.353726000
H	-2.803062000	2.747628000	5.188585000
C	-1.288708000	-3.291213000	-0.192474000
C	-1.991246000	-2.992984000	0.979382000
C	-1.497624000	-4.521567000	-0.835153000
C	-2.898530000	-3.908053000	1.499423000
H	-1.814502000	-2.031946000	1.461952000
C	-2.403713000	-5.432511000	-0.308579000
H	-0.947311000	-4.740997000	-1.748496000
C	-3.108401000	-5.125938000	0.856069000
H	-3.448027000	-3.666584000	2.407284000
H	-2.564772000	-6.385748000	-0.809271000
H	-3.822045000	-5.840739000	1.262529000
C	1.100215000	-0.853160000	1.398727000
C	2.319186000	-1.506411000	1.799097000
C	2.994711000	-1.151267000	2.981428000
C	2.889354000	-2.489850000	0.970774000
C	4.200740000	-1.754237000	3.315863000
H	2.558254000	-0.393428000	3.632136000
C	4.084867000	-3.103772000	1.318454000
H	2.379045000	-2.742688000	0.041362000
C	4.748477000	-2.734138000	2.487986000
H	4.715954000	-1.463161000	4.230322000
H	4.514065000	-3.859326000	0.661933000
H	5.693351000	-3.205804000	2.753534000
N	0.344149000	-2.080166000	-1.731257000
C	2.020246000	2.287768000	-0.813596000
C	2.158843000	2.472366000	0.571592000
C	2.100056000	3.410830000	-1.644979000
C	2.373253000	3.738213000	1.105861000
H	2.073233000	1.609195000	1.233623000
C	2.300345000	4.681039000	-1.108860000
H	2.002121000	3.302376000	-2.724151000
C	2.437746000	4.848882000	0.265969000
H	2.475952000	3.858533000	2.183576000
H	2.350831000	5.543290000	-1.771793000
H	2.591783000	5.842798000	0.682756000
C	3.298755000	-0.193823000	-1.530268000
C	3.459249000	-1.329749000	-2.338484000
C	4.375506000	0.224557000	-0.738096000
C	4.671728000	-2.011184000	-2.365225000
H	2.620204000	-1.700250000	-2.924090000
C	5.583430000	-0.465523000	-0.761417000
H	4.270565000	1.096390000	-0.093618000
C	5.738073000	-1.582649000	-1.577449000
H	4.780259000	-2.888273000	-3.001830000
H	6.406699000	-0.128068000	-0.133579000
H	6.684013000	-2.121745000	-1.595178000
C	-2.052779000	2.224948000	-0.763743000
C	-3.092063000	2.911769000	-1.407233000
C	-1.299780000	2.892734000	0.205348000
C	-3.367947000	4.235926000	-1.085104000
H	-3.699260000	2.398228000	-2.154457000
C	-1.576665000	4.218397000	0.531839000
H	-0.493533000	2.359332000	0.706303000
C	-2.609768000	4.890873000	-0.113717000
H	-4.178388000	4.759700000	-1.589811000
H	-0.981839000	4.718710000	1.294768000
H	-2.830173000	5.926834000	0.139478000
C	-3.258736000	-0.352446000	-1.130529000
C	-3.447584000	-1.529449000	-1.869680000
C	-4.275604000	0.054327000	-0.255245000
C	-4.612428000	-2.277487000	-1.734954000
H	-2.663198000	-1.880403000	-2.541212000

C	-5.440046000	-0.696508000	-0.119285000
H	-4.154561000	0.972040000	0.321011000
C	-5.611723000	-1.865753000	-0.856249000
H	-4.734291000	-3.192352000	-2.313008000
H	-6.218982000	-0.362390000	0.564696000
H	-6.520905000	-2.454310000	-0.746535000

CP_{2N}

C	3.362177000	0.702737000	1.130970000
Co	0.380783000	0.390842000	0.540981000
P	0.690810000	-1.228428000	-0.995370000
P	-0.642084000	1.828796000	-0.782643000
C	-0.264669000	1.676572000	-2.593765000
H	-0.928538000	2.353249000	-3.152297000
H	0.751187000	2.077773000	-2.719322000
C	0.798089000	-0.670672000	-2.752696000
H	1.762500000	-0.151883000	-2.854757000
H	0.837727000	-1.535474000	-3.430688000
C	-0.339292000	0.263079000	-3.171383000
H	-0.332728000	0.340909000	-4.268495000
H	-1.305406000	-0.195385000	-2.912365000
C	-2.139774000	-0.721883000	1.851618000
N	-1.066955000	-0.370465000	1.506720000
C	-3.472647000	-1.098196000	2.095046000
C	-4.187921000	-1.772659000	1.079616000
C	-4.127625000	-0.772351000	3.301745000
C	-5.517768000	-2.106147000	1.277902000
H	-3.684070000	-2.004697000	0.142770000
C	-5.461390000	-1.108317000	3.476670000
H	-3.579160000	-0.249708000	4.082751000
C	-6.164091000	-1.776775000	2.471894000
H	-6.061329000	-2.620835000	0.487135000
H	-5.960020000	-0.849260000	4.409146000
H	-7.209889000	-2.038955000	2.618531000
C	4.756485000	0.649699000	1.263462000
C	5.443275000	1.391225000	2.252911000
C	5.499757000	-0.179522000	0.387773000
C	6.821335000	1.294902000	2.357858000
H	4.878933000	2.030348000	2.928545000
C	6.875642000	-0.262495000	0.513947000
H	4.972899000	-0.753605000	-0.372540000
C	7.548660000	0.470184000	1.495859000
H	7.338088000	1.869504000	3.124832000
H	7.432052000	-0.910201000	-0.162379000
H	8.630291000	0.399326000	1.588636000
N	2.191024000	0.674085000	0.965007000
C	2.247866000	-2.190408000	-0.788943000
C	3.051113000	-2.622406000	-1.850870000
C	2.652380000	-2.489648000	0.520041000
C	4.221494000	-3.340774000	-1.610560000
H	2.766352000	-2.404487000	-2.879372000
C	3.811185000	-3.220560000	0.760036000
H	2.055394000	-2.115564000	1.354104000
C	4.601031000	-3.646606000	-0.306115000
H	4.835506000	-3.666687000	-2.448992000
H	4.111571000	-3.437556000	1.783745000
H	5.517217000	-4.204600000	-0.119473000
C	-0.316412000	3.628661000	-0.568153000
C	-1.230199000	4.619317000	-0.948151000
C	0.920095000	4.014401000	-0.037016000
C	-0.912146000	5.966198000	-0.800253000
H	-2.200215000	4.331183000	-1.355003000
C	1.241223000	5.362224000	0.101737000
H	1.625579000	3.240717000	0.272087000
C	0.324455000	6.339927000	-0.277026000
H	-1.632548000	6.728164000	-1.094574000
H	2.206556000	5.649557000	0.515789000
H	0.570648000	7.394178000	-0.160275000
C	-2.475329000	1.768812000	-0.732926000

C	-3.291879000	1.455165000	-1.827537000
C	-3.090321000	1.967047000	0.514125000
C	-4.672124000	1.330943000	-1.677801000
H	-2.857193000	1.313637000	-2.815900000
C	-4.467448000	1.856704000	0.661545000
H	-2.469764000	2.201419000	1.380711000
C	-5.263974000	1.525631000	-0.433361000
H	-5.286489000	1.083918000	-2.542620000
H	-4.920270000	2.003571000	1.641175000
H	-6.340353000	1.415055000	-0.313143000
C	-0.560607000	-2.574265000	-1.054793000
C	-1.308101000	-2.911326000	-2.189492000
C	-0.818584000	-3.264359000	0.139984000
C	-2.281533000	-3.908153000	-2.131920000
H	-1.133128000	-2.403721000	-3.136914000
C	-1.779342000	-4.266753000	0.194652000
H	-0.260016000	-2.999281000	1.038156000
C	-2.519337000	-4.589872000	-0.942454000
H	-2.851098000	-4.154946000	-3.026813000
H	-1.963024000	-4.787724000	1.133030000
H	-3.280288000	-5.367217000	-0.898627000

CP_{2N}'

C	-1.396758000	1.723722000	-0.859053000
Co	0.036066000	0.706192000	0.042546000
P	2.253784000	0.874191000	-0.468374000
P	-0.086196000	-1.351660000	-0.997604000
C	0.668240000	-1.225580000	-2.687720000
H	0.464186000	-2.148778000	-3.247750000
H	0.141137000	-0.410770000	-3.203523000
C	2.567803000	0.465695000	-2.242275000
H	1.981991000	1.206404000	-2.803995000
H	3.623908000	0.657284000	-2.478761000
C	2.169508000	-0.944073000	-2.679175000
H	2.548398000	-1.097496000	-3.699699000
H	2.678715000	-1.698277000	-2.058704000
C	-0.929715000	0.365006000	1.704205000
N	0.237329000	0.463380000	2.064487000
C	-2.276605000	0.130869000	2.195970000
C	-2.582032000	0.393067000	3.540692000
C	-3.286035000	-0.320671000	1.337225000
C	-3.878244000	0.213440000	4.007269000
H	-1.793101000	0.746195000	4.202431000
C	-4.576097000	-0.516950000	1.813687000
H	-3.048748000	-0.495851000	0.289507000
C	-4.877003000	-0.242860000	3.146340000
H	-4.111963000	0.427212000	5.049023000
H	-5.351605000	-0.865130000	1.133109000
H	-5.891623000	-0.381293000	3.516567000
C	-2.754351000	2.187469000	-0.636757000
C	-3.105043000	2.784775000	0.581779000
C	-3.739554000	2.001924000	-1.616860000
C	-4.412768000	3.188787000	0.814531000
H	-2.340803000	2.913689000	1.346822000
C	-5.053101000	2.383033000	-1.367265000
H	-3.464761000	1.551457000	-2.568696000
C	-5.393769000	2.976248000	-0.152973000
H	-4.672383000	3.649228000	1.766143000
H	-5.814015000	2.223217000	-2.129774000
H	-6.423387000	3.272715000	0.039123000
N	-0.461561000	1.742861000	-1.651455000
C	-1.746083000	-1.999766000	-1.403289000
C	-2.315770000	-3.084818000	-0.724302000
C	-2.547808000	-1.271541000	-2.296214000
C	-3.646779000	-3.433510000	-0.936526000
H	-1.714152000	-3.653532000	-0.015862000
C	-3.877843000	-1.621059000	-2.505900000
H	-2.127166000	-0.408443000	-2.814497000
C	-4.432961000	-2.703598000	-1.825266000

H	-4.073417000	-4.278853000	-0.398712000
H	-4.485941000	-1.041556000	-3.199865000
H	-5.474797000	-2.975314000	-1.986022000
C	0.782608000	-2.799210000	-0.294565000
C	0.956299000	-3.993867000	-1.008038000
C	1.328781000	-2.687628000	0.988604000
C	1.671948000	-5.048898000	-0.453417000
H	0.520321000	-4.100445000	-2.002466000
C	2.045746000	-3.746307000	1.543754000
H	1.194127000	-1.759060000	1.545138000
C	2.221274000	-4.923421000	0.823000000
H	1.803400000	-5.971863000	-1.016236000
H	2.474250000	-3.643527000	2.539361000
H	2.785626000	-5.748736000	1.254491000
C	2.936536000	2.578108000	-0.397515000
C	4.122732000	2.905261000	0.268989000
C	2.219002000	3.594470000	-1.046052000
C	4.582979000	4.220031000	0.283385000
H	4.692528000	2.130224000	0.779448000
C	2.688469000	4.903698000	-1.036768000
H	1.284976000	3.350666000	-1.553392000
C	3.870421000	5.221150000	-0.370203000
H	5.507051000	4.459984000	0.807284000
H	2.122904000	5.681706000	-1.547269000
H	4.233408000	6.247595000	-0.358314000
C	3.493084000	-0.099878000	0.455130000
C	3.408198000	-0.103891000	1.856386000
C	4.516803000	-0.831199000	-0.159066000
C	4.328671000	-0.817365000	2.616787000
H	2.597533000	0.438954000	2.340011000
C	5.426633000	-1.558595000	0.605020000
H	4.616140000	-0.835326000	-1.243381000
C	5.336646000	-1.551810000	1.993867000
H	4.251956000	-0.807149000	3.703092000
H	6.212240000	-2.127664000	0.110469000
H	6.050726000	-2.117823000	2.590059000

CP_{2N}''

C	0.201467000	-0.515943000	2.340548000
Co	-0.228195000	0.353209000	0.693451000
C	2.181463000	1.946677000	-0.298395000
N	1.199895000	1.441439000	0.114156000
C	3.393516000	2.423431000	-0.842660000
C	4.069571000	1.636210000	-1.799296000
C	3.948039000	3.655312000	-0.443383000
C	5.271804000	2.077058000	-2.330740000
H	3.642611000	0.680870000	-2.101660000
C	5.150861000	4.080733000	-0.988352000
H	3.426159000	4.262125000	0.293138000
C	5.818142000	3.297350000	-1.930553000
H	5.789073000	1.457976000	-3.061963000
H	5.573635000	5.033101000	-0.674175000
H	6.762389000	3.636976000	-2.351286000
C	1.259501000	-0.914546000	3.256339000
C	2.510775000	-0.283652000	3.217188000
C	1.051238000	-1.962345000	4.167180000
C	3.528446000	-0.683081000	4.075879000
H	2.664775000	0.523651000	2.500144000
C	2.075515000	-2.367625000	5.013981000
H	0.076234000	-2.446523000	4.193648000
C	3.314968000	-1.729147000	4.972475000
H	4.494074000	-0.180741000	4.043397000
H	1.907422000	-3.184096000	5.714740000
H	4.115043000	-2.048775000	5.638100000
N	-1.030587000	-0.598607000	2.236456000
P	-2.054834000	1.191677000	-0.291193000
C	-1.886815000	1.502882000	-2.108952000
H	-1.074264000	2.230257000	-2.254947000
H	-2.810046000	1.965453000	-2.488096000

C	-1.593541000	0.228354000	-2.900883000
C	-0.180372000	-0.334575000	-2.734884000
H	-1.746215000	0.445398000	-3.967467000
H	-2.340864000	-0.539975000	-2.645583000
P	0.199454000	-1.066163000	-1.076327000
H	0.017274000	-1.063913000	-3.533055000
H	0.558277000	0.470263000	-2.872488000
C	-2.684956000	2.785590000	0.348505000
C	-3.106084000	2.814436000	1.687225000
C	-2.716248000	3.971630000	-0.392766000
C	-3.562910000	3.994789000	2.259961000
H	-3.070774000	1.897165000	2.277140000
C	-3.166669000	5.156854000	0.186973000
H	-2.389930000	3.978746000	-1.432029000
C	-3.593638000	5.171195000	1.511068000
H	-3.892315000	3.999245000	3.297730000
H	-3.186658000	6.071949000	-0.403280000
H	-3.947017000	6.097258000	1.961351000
C	1.976355000	-1.508678000	-1.302794000
C	2.823505000	-1.377192000	-0.196970000
C	2.523151000	-1.938280000	-2.519010000
C	4.182946000	-1.659110000	-0.298983000
H	2.399203000	-1.032734000	0.746195000
C	3.885230000	-2.208851000	-2.627121000
H	1.884118000	-2.070788000	-3.392168000
C	4.718648000	-2.067113000	-1.518028000
H	4.823285000	-1.547909000	0.575368000
H	4.296833000	-2.538235000	-3.580226000
H	5.783424000	-2.277416000	-1.606145000
C	-3.575452000	0.161784000	-0.290662000
C	-3.499477000	-1.171454000	0.122103000
C	-4.794445000	0.660821000	-0.768941000
C	-4.617435000	-1.999438000	0.035683000
H	-2.561563000	-1.545794000	0.528659000
C	-5.911361000	-0.163766000	-0.846665000
H	-4.868236000	1.706614000	-1.073310000
C	-5.821341000	-1.498542000	-0.450335000
H	-4.540667000	-3.038606000	0.352646000
H	-6.855338000	0.233643000	-1.217007000
H	-6.695905000	-2.144355000	-0.515655000
C	-0.624444000	-2.700705000	-1.107051000
C	-1.337184000	-3.210207000	-2.197974000
C	-0.597794000	-3.441907000	0.084705000
C	-2.006924000	-4.428311000	-2.101255000
H	-1.381708000	-2.655092000	-3.134395000
C	-1.256334000	-4.662305000	0.176266000
H	-0.071278000	-3.040719000	0.952437000
C	-1.967443000	-5.157433000	-0.916530000
H	-2.562693000	-4.807040000	-2.957700000
H	-1.224266000	-5.224575000	1.108011000
H	-2.492945000	-6.107994000	-0.842105000

CP_N

Co	-0.072657000	0.755857000	-0.182146000
P	-2.159893000	0.805745000	0.394468000
P	0.450966000	-1.140344000	0.826610000
C	-0.481946000	-1.498704000	2.387611000
H	-0.233369000	-2.508407000	2.745831000
H	-0.076355000	-0.806112000	3.139443000
C	-2.455440000	0.132068000	2.105704000
H	-1.929276000	0.776378000	2.824258000
H	-3.529738000	0.213063000	2.327544000
C	-1.995007000	-1.314912000	2.280322000
H	-2.452909000	-1.712055000	3.197518000
H	-2.396719000	-1.928875000	1.458261000
N	1.573603000	1.459177000	-0.590631000
C	2.689557000	1.750183000	-0.857397000
C	4.027709000	2.061607000	-1.138125000
C	4.364828000	3.150229000	-1.976761000

C	5.066512000	1.277283000	-0.580661000
C	5.694050000	3.437443000	-2.239057000
H	3.570292000	3.754994000	-2.408222000
C	6.388719000	1.586522000	-0.852305000
H	4.809775000	0.433200000	0.056634000
C	6.714757000	2.664117000	-1.680018000
H	5.940653000	4.277759000	-2.885840000
H	7.178080000	0.976097000	-0.416360000
H	7.756246000	2.898633000	-1.889662000
C	-3.166024000	2.343494000	0.426920000
C	-3.630062000	2.874174000	-0.785862000
C	-3.417111000	3.057086000	1.604881000
C	-4.332370000	4.072678000	-0.817799000
H	-3.442525000	2.331782000	-1.713591000
C	-4.117342000	4.261188000	1.572584000
H	-3.063574000	2.675409000	2.561835000
C	-4.578411000	4.772426000	0.363211000
H	-4.690489000	4.463707000	-1.768944000
H	-4.305222000	4.799781000	2.500336000
H	-5.126353000	5.712708000	0.339148000
C	2.176197000	-1.277175000	1.441249000
C	3.000052000	-2.389950000	1.239428000
C	2.691136000	-0.175347000	2.141219000
C	4.302146000	-2.404797000	1.735941000
H	2.620755000	-3.252756000	0.692514000
C	3.984868000	-0.197857000	2.651372000
H	2.068193000	0.712893000	2.266782000
C	4.795508000	-1.314433000	2.448398000
H	4.931781000	-3.277873000	1.570411000
H	4.368394000	0.665657000	3.192798000
H	5.811741000	-1.330616000	2.838956000
C	-3.268631000	-0.311745000	-0.565780000
C	-4.653962000	-0.347189000	-0.360900000
C	-2.698958000	-1.204601000	-1.479491000
C	-5.446568000	-1.260532000	-1.048706000
H	-5.114112000	0.354927000	0.336257000
C	-3.489708000	-2.124087000	-2.165226000
H	-1.620112000	-1.175608000	-1.645858000
C	-4.864751000	-2.153040000	-1.949002000
H	-6.522804000	-1.277904000	-0.882639000
H	-3.026535000	-2.816557000	-2.866605000
H	-5.487140000	-2.868514000	-2.484300000
C	0.235949000	-2.651295000	-0.182632000
C	-0.541013000	-3.753366000	0.191653000
C	0.799449000	-2.636060000	-1.469798000
C	-0.749434000	-4.810025000	-0.692985000
H	-0.995750000	-3.794624000	1.180461000
C	0.601276000	-3.695294000	-2.347787000
H	1.395543000	-1.774525000	-1.778427000
C	-0.179919000	-4.785099000	-1.962741000
H	-1.360804000	-5.657056000	-0.385572000
H	1.051354000	-3.668002000	-3.338841000
H	-0.344939000	-5.610842000	-2.652703000

CP_N'

C	1.181248000	-2.084662000	0.809216000
Co	0.014321000	-0.921905000	-0.095630000
P	-2.063953000	-0.389543000	-0.641974000
P	0.893857000	0.863156000	-0.962476000
C	0.111087000	1.422336000	-2.552957000
H	0.653844000	2.292213000	-2.949456000
H	0.274441000	0.610150000	-3.276678000
C	-2.311499000	0.550951000	-2.218791000
H	-2.167246000	-0.185997000	-3.022278000
H	-3.357513000	0.880364000	-2.303440000
C	-1.378857000	1.744460000	-2.436484000
H	-1.692852000	2.250258000	-3.360979000
H	-1.523070000	2.481934000	-1.632648000
C	2.536700000	-2.406368000	1.238303000

C	2.860380000	-3.701387000	1.673083000
C	3.539574000	-1.429606000	1.205725000
C	4.160011000	-4.007256000	2.056107000
H	2.075536000	-4.455438000	1.699518000
C	4.838913000	-1.736992000	1.592897000
H	3.282659000	-0.425871000	0.866857000
C	5.152767000	-3.027250000	2.015509000
H	4.403702000	-5.015072000	2.389477000
H	5.609583000	-0.968223000	1.556896000
H	6.171244000	-3.271467000	2.313776000
N	0.045970000	-2.602048000	0.865799000
C	-3.400869000	-1.641254000	-0.755001000
C	-4.727698000	-1.299957000	-1.046072000
C	-3.071459000	-2.980815000	-0.523095000
C	-5.706268000	-2.284456000	-1.124958000
H	-5.001538000	-0.254382000	-1.197441000
C	-4.055391000	-3.965182000	-0.600605000
H	-2.043554000	-3.234535000	-0.260858000
C	-5.368709000	-3.620070000	-0.906111000
H	-6.735686000	-2.011219000	-1.352159000
H	-3.793315000	-5.005825000	-0.416714000
H	-6.135918000	-4.390518000	-0.966335000
C	2.668583000	0.873307000	-1.439434000
C	3.547399000	1.923316000	-1.153838000
C	3.170920000	-0.277249000	-2.062279000
C	4.898581000	1.820561000	-1.480183000
H	3.179191000	2.819904000	-0.655683000
C	4.514840000	-0.372359000	-2.403785000
H	2.501617000	-1.120765000	-2.244270000
C	5.384245000	0.676169000	-2.106782000
H	5.574701000	2.639895000	-1.240281000
H	4.890007000	-1.276104000	-2.880846000
H	6.441008000	0.596356000	-2.355863000
C	0.697856000	2.336522000	0.112508000
C	0.608441000	3.648702000	-0.370467000
C	0.566182000	2.120028000	1.490061000
C	0.385042000	4.712226000	0.499627000
H	0.708981000	3.844949000	-1.438431000
C	0.351346000	3.182480000	2.362443000
H	0.620530000	1.098244000	1.873287000
C	0.255041000	4.480511000	1.867276000
H	0.311345000	5.725562000	0.107884000
H	0.240426000	2.992500000	3.428697000
H	0.074306000	5.312301000	2.546035000
C	-2.683241000	0.745542000	0.660205000
C	-3.299295000	1.978423000	0.421241000
C	-2.453682000	0.353557000	1.988416000
C	-3.664627000	2.805488000	1.481851000
H	-3.498991000	2.305153000	-0.598991000
C	-2.833414000	1.171833000	3.046072000
H	-1.967933000	-0.605834000	2.182956000
C	-3.432313000	2.405418000	2.794531000
H	-4.133521000	3.767192000	1.278963000
H	-2.652561000	0.850013000	4.070572000
H	-3.717413000	3.054032000	3.621242000

TS1

C	1.411446000	0.287231000	1.348243000
C	1.984000000	0.342039000	0.151216000
Co	0.158219000	-0.102200000	-0.101339000
P	0.169381000	-2.020360000	-1.204117000
P	-0.612691000	1.190079000	-1.805041000
C	-0.428099000	0.487636000	-3.507161000
H	-0.977394000	1.116892000	-4.221132000
H	0.634847000	0.587765000	-3.770231000
C	0.161719000	-1.964641000	-3.050665000
H	1.175459000	-1.673092000	-3.362399000
H	-0.006130000	-2.971093000	-3.458927000
C	-0.851407000	-0.977632000	-3.630689000

H	-0.996495000	-1.210573000	-4.695369000
H	-1.834893000	-1.130297000	-3.156469000
C	-0.524277000	0.824139000	1.505902000
C	-1.366718000	-0.107747000	1.113825000
C	-2.695748000	-0.600835000	1.329826000
C	-3.233090000	-0.725412000	2.626883000
C	-3.488015000	-1.018347000	0.243482000
C	-4.511388000	-1.234710000	2.821813000
H	-2.618916000	-0.443595000	3.482393000
C	-4.774942000	-1.493673000	0.439241000
H	-3.067750000	-0.948114000	-0.759847000
C	-5.292388000	-1.612111000	1.730252000
H	-4.903685000	-1.333212000	3.833170000
H	-5.372493000	-1.794179000	-0.420851000
H	-6.296210000	-2.004074000	1.885291000
C	-0.536931000	2.162740000	2.064868000
C	-1.541542000	2.525725000	2.981857000
C	0.358428000	3.155739000	1.629050000
C	-1.648052000	3.833983000	3.437052000
H	-2.254702000	1.769800000	3.310747000
C	0.240125000	4.463669000	2.082050000
H	1.129598000	2.892123000	0.904841000
C	-0.757946000	4.810675000	2.991574000
H	-2.434529000	4.093519000	4.144428000
H	0.933201000	5.219565000	1.715192000
H	-0.842899000	5.834809000	3.350308000
C	1.822244000	-0.097902000	2.693895000
C	0.987977000	-0.145377000	3.825319000
C	3.160501000	-0.519291000	2.858015000
C	1.467534000	-0.595330000	5.051371000
H	-0.046135000	0.175156000	3.748644000
C	3.633512000	-0.962122000	4.084399000
H	3.823467000	-0.514017000	1.994139000
C	2.789985000	-1.003189000	5.194486000
H	0.794350000	-0.619695000	5.907097000
H	4.670945000	-1.282952000	4.171911000
H	3.161022000	-1.347762000	6.157974000
C	3.296977000	0.503604000	-0.414893000
C	4.230692000	1.385701000	0.165410000
C	3.663739000	-0.163501000	-1.598346000
C	5.474231000	1.589385000	-0.418483000
H	3.953040000	1.917796000	1.075521000
C	4.919210000	0.019079000	-2.162186000
H	2.937725000	-0.834090000	-2.060095000
C	5.828454000	0.903261000	-1.580521000
H	6.176367000	2.285330000	0.038504000
H	5.187749000	-0.520842000	-3.069102000
H	6.806342000	1.059215000	-2.032472000
C	0.231885000	2.808650000	-1.993363000
C	-0.394167000	4.047722000	-1.816048000
C	1.614459000	2.785421000	-2.230223000
C	0.346114000	5.226940000	-1.859880000
H	-1.466671000	4.096208000	-1.637058000
C	2.351893000	3.962706000	-2.277900000
H	2.124501000	1.831638000	-2.361847000
C	1.719755000	5.190009000	-2.083470000
H	-0.158116000	6.181182000	-1.713915000
H	3.425329000	3.915939000	-2.457376000
H	2.295835000	6.113549000	-2.109473000
C	-2.387163000	1.624081000	-1.716976000
C	-3.331886000	1.228563000	-2.673332000
C	-2.849180000	2.262050000	-0.553454000
C	-4.692203000	1.445527000	-2.464356000
H	-3.014600000	0.740665000	-3.593729000
C	-4.205309000	2.484903000	-0.349081000
H	-2.135145000	2.588844000	0.201201000
C	-5.134429000	2.066399000	-1.299451000
H	-5.409309000	1.126620000	-3.219468000
H	-4.534250000	2.973556000	0.567173000
H	-6.198615000	2.224271000	-1.133377000

C	1.670372000	-3.021951000	-0.851219000
C	2.341968000	-3.770114000	-1.825919000
C	2.201580000	-2.980875000	0.445014000
C	3.523225000	-4.439844000	-1.516996000
H	1.950268000	-3.831442000	-2.840327000
C	3.374790000	-3.660087000	0.756583000
H	1.701880000	-2.390028000	1.212853000
C	4.044690000	-4.383716000	-0.227081000
H	4.037059000	-5.009926000	-2.289646000
H	3.771469000	-3.607287000	1.769535000
H	4.971481000	-4.903250000	0.010232000
C	-1.181606000	-3.201877000	-0.812150000
C	-2.075362000	-3.722101000	-1.753940000
C	-1.371126000	-3.524601000	0.539318000
C	-3.129387000	-4.542703000	-1.354053000
H	-1.964431000	-3.486961000	-2.811919000
C	-2.410050000	-4.355613000	0.936266000
H	-0.706770000	-3.090536000	1.289721000
C	-3.298069000	-4.863421000	-0.011054000
H	-3.820374000	-4.932524000	-2.100295000
H	-2.544306000	-4.585616000	1.991980000
H	-4.125505000	-5.498804000	0.300080000

INT1

C	-0.420018000	1.685894000	1.057987000
C	-0.994537000	1.747977000	-0.215992000
Co	0.014156000	0.062081000	-0.096353000
P	1.631519000	-0.043080000	-1.524418000
P	-1.379531000	-1.104087000	-1.307299000
C	-1.272241000	-0.849712000	-3.134419000
H	-1.998713000	-1.499329000	-3.640829000
H	-1.609022000	0.179437000	-3.319966000
C	1.156949000	-0.003816000	-3.317969000
H	0.749254000	0.994730000	-3.526486000
H	2.063698000	-0.113889000	-3.929459000
C	0.124719000	-1.058168000	-3.720516000
H	0.040171000	-1.048501000	-4.816206000
H	0.491831000	-2.065274000	-3.468349000
C	-0.607293000	0.362751000	1.739802000
C	0.572355000	-0.421679000	1.571057000
C	1.427445000	-1.130576000	2.474883000
C	1.273788000	-1.020771000	3.876324000
C	2.446792000	-1.976357000	1.985701000
C	2.100765000	-1.723170000	4.740466000
H	0.477498000	-0.386565000	4.266401000
C	3.273642000	-2.673685000	2.852673000
H	2.564280000	-2.071595000	0.907954000
C	3.105746000	-2.549358000	4.233593000
H	1.965850000	-1.628421000	5.816817000
H	4.054454000	-3.318740000	2.451679000
H	3.755805000	-3.096405000	4.914478000
C	-1.894029000	-0.072903000	2.297484000
C	-2.047391000	-1.356799000	2.849632000
C	-3.002645000	0.788784000	2.319318000
C	-3.254612000	-1.756631000	3.410044000
H	-1.199418000	-2.042750000	2.844634000
C	-4.213313000	0.381548000	2.865233000
H	-2.903904000	1.784898000	1.888656000
C	-4.346018000	-0.889725000	3.421414000
H	-3.344417000	-2.754178000	3.838920000
H	-5.062478000	1.063876000	2.855276000
H	-5.293319000	-1.203256000	3.857555000
C	0.501315000	2.696983000	1.625920000
C	0.943624000	2.587014000	2.953202000
C	0.916492000	3.815217000	0.885118000
C	1.777991000	3.546458000	3.515588000
H	0.614711000	1.735477000	3.547682000
C	1.732515000	4.784659000	1.453713000
H	0.610807000	3.909568000	-0.155340000

C	2.172428000	4.655868000	2.770261000
H	2.108921000	3.434718000	4.547361000
H	2.044793000	5.639244000	0.854381000
H	2.815453000	5.415165000	3.212933000
C	-1.536302000	2.800597000	-0.994904000
C	-2.327224000	3.812653000	-0.386120000
C	-1.401463000	2.856385000	-2.404843000
C	-2.957302000	4.785442000	-1.143539000
H	-2.433347000	3.805072000	0.698935000
C	-2.025378000	3.840858000	-3.155541000
H	-0.776893000	2.106173000	-2.888586000
C	-2.818838000	4.808931000	-2.535312000
H	-3.563682000	5.541979000	-0.646501000
H	-1.894067000	3.857478000	-4.237185000
H	-3.317045000	5.574880000	-3.126339000
C	-1.186463000	-2.926633000	-1.125934000
C	-1.554984000	-3.838120000	-2.123218000
C	-0.617007000	-3.419899000	0.054399000
C	-1.338282000	-5.203228000	-1.950753000
H	-2.015029000	-3.487432000	-3.046551000
C	-0.416887000	-4.784582000	0.236525000
H	-0.292066000	-2.706288000	0.812506000
C	-0.768948000	-5.679636000	-0.771625000
H	-1.618932000	-5.897808000	-2.740960000
H	0.033661000	-5.144304000	1.160594000
H	-0.598450000	-6.747099000	-0.641327000
C	-3.160777000	-0.856652000	-0.977938000
C	-3.792412000	0.309731000	-1.432753000
C	-3.889228000	-1.757267000	-0.192082000
C	-5.124179000	0.559638000	-1.120766000
H	-3.241577000	1.036518000	-2.027912000
C	-5.221852000	-1.502929000	0.119099000
H	-3.410490000	-2.658447000	0.189120000
C	-5.843332000	-0.346897000	-0.344576000
H	-5.595330000	1.472678000	-1.482196000
H	-5.770854000	-2.209226000	0.740042000
H	-6.884545000	-0.148295000	-0.094825000
C	2.854866000	-1.428399000	-1.557057000
C	4.240597000	-1.229452000	-1.514383000
C	2.373450000	-2.745223000	-1.591072000
C	5.112980000	-2.315765000	-1.486661000
H	4.645060000	-0.219164000	-1.489069000
C	3.244499000	-3.829432000	-1.578074000
H	1.300566000	-2.926770000	-1.589241000
C	4.620279000	-3.617577000	-1.516671000
H	6.186666000	-2.139659000	-1.440649000
H	2.842156000	-4.841404000	-1.599884000
H	5.305381000	-4.463343000	-1.490013000
C	2.710451000	1.416514000	-1.314898000
C	2.948456000	2.365714000	-2.313886000
C	3.301392000	1.598204000	-0.054635000
C	3.761509000	3.469622000	-2.058984000
H	2.505903000	2.250561000	-3.302072000
C	4.129320000	2.685684000	0.189993000
H	3.093953000	0.879583000	0.741146000
C	4.357915000	3.627977000	-0.812106000
H	3.932226000	4.204533000	-2.844122000
H	4.571083000	2.815059000	1.176452000
H	4.991402000	4.491457000	-0.615351000

TS2

C	-1.384026000	1.018688000	1.330312000
C	-1.494900000	1.021772000	-0.028125000
Co	0.167306000	0.058637000	-0.147159000
P	1.630749000	0.966857000	-1.493690000
P	-0.608162000	-1.352430000	-1.555774000
C	-0.435014000	-0.974604000	-3.362217000
H	-0.838132000	-1.836238000	-3.927131000
H	-1.114229000	-0.123333000	-3.586438000

C	1.469935000	0.720680000	-3.335825000
H	0.768992000	1.488756000	-3.694867000
H	2.438771000	0.937440000	-3.806041000
C	0.972929000	-0.650700000	-3.789130000
H	1.025744000	-0.683752000	-4.886482000
H	1.648881000	-1.446992000	-3.441101000
C	-0.544808000	-0.176049000	1.729865000
C	0.856466000	-0.011829000	1.620841000
C	1.928591000	-0.359685000	2.494259000
C	1.730336000	-0.388191000	3.898426000
C	3.214700000	-0.703974000	2.013208000
C	2.758791000	-0.727297000	4.762369000
H	0.744653000	-0.132847000	4.286868000
C	4.236626000	-1.052030000	2.882580000
H	3.386891000	-0.707669000	0.938711000
C	4.019908000	-1.061887000	4.262424000
H	2.579643000	-0.737369000	5.836800000
H	5.214089000	-1.318098000	2.480873000
H	4.825657000	-1.331357000	4.943208000
C	-1.212449000	-1.403781000	2.198959000
C	-0.500143000	-2.606693000	2.364538000
C	-2.584393000	-1.407956000	2.499207000
C	-1.136436000	-3.760356000	2.802393000
H	0.563748000	-2.629532000	2.129935000
C	-3.220348000	-2.565789000	2.936346000
H	-3.154637000	-0.486508000	2.378528000
C	-2.503084000	-3.749492000	3.089836000
H	-0.562315000	-4.679218000	2.916099000
H	-4.287996000	-2.542304000	3.152807000
H	-3.000588000	-4.655491000	3.432610000
C	-1.713338000	2.080490000	2.283184000
C	-1.644459000	1.823852000	3.663756000
C	-2.086401000	3.372633000	1.868190000
C	-1.948531000	2.812365000	4.592306000
H	-1.367492000	0.823493000	3.997863000
C	-2.391080000	4.357268000	2.797936000
H	-2.118866000	3.600155000	0.802992000
C	-2.324900000	4.083976000	4.165255000
H	-1.893296000	2.588262000	5.656643000
H	-2.674541000	5.351690000	2.454774000
H	-2.560542000	4.859688000	4.891782000
C	-2.403549000	1.640518000	-0.953798000
C	-3.788220000	1.671361000	-0.676024000
C	-1.974572000	2.135259000	-2.202213000
C	-4.692079000	2.163708000	-1.606298000
H	-4.136115000	1.273400000	0.277275000
C	-2.881645000	2.633449000	-3.128425000
H	-0.906151000	2.131887000	-2.419005000
C	-4.247297000	2.643584000	-2.839781000
H	-5.756164000	2.165840000	-1.373301000
H	-2.523178000	3.018804000	-4.082332000
H	-4.959263000	3.024720000	-3.569652000
C	0.367314000	-2.907516000	-1.438253000
C	0.017436000	-4.067488000	-2.140948000
C	1.528842000	-2.910865000	-0.659313000
C	0.819107000	-5.202372000	-2.066455000
H	-0.896392000	-4.085359000	-2.736694000
C	2.333681000	-4.045153000	-0.585992000
H	1.790227000	-2.006655000	-0.102753000
C	1.979439000	-5.191964000	-1.291533000
H	0.537391000	-6.100953000	-2.613128000
H	3.234764000	-4.026036000	0.026917000
H	2.603621000	-6.082541000	-1.236963000
C	-2.339029000	-1.927110000	-1.439505000
C	-3.354123000	-1.310420000	-2.183931000
C	-2.686237000	-2.935508000	-0.530562000
C	-4.680181000	-1.704985000	-2.034102000
H	-3.118332000	-0.500928000	-2.874464000
C	-4.012436000	-3.329657000	-0.386367000
H	-1.915412000	-3.410015000	0.077635000

C	-5.012558000	-2.718179000	-1.138600000
H	-5.454924000	-1.209514000	-2.617665000
H	-4.260855000	-4.112272000	0.328842000
H	-6.050437000	-3.026408000	-1.022722000
C	3.417151000	0.623208000	-1.241614000
C	4.223406000	1.475522000	-0.476914000
C	3.959980000	-0.589436000	-1.690554000
C	5.535353000	1.124105000	-0.171806000
H	3.815086000	2.414178000	-0.104002000
C	5.270556000	-0.940697000	-1.383148000
H	3.345070000	-1.282122000	-2.265354000
C	6.062903000	-0.084385000	-0.620230000
H	6.145558000	1.796653000	0.428818000
H	5.671206000	-1.889423000	-1.737783000
H	7.086731000	-0.360412000	-0.373667000
C	1.569791000	2.797859000	-1.359176000
C	2.071278000	3.629531000	-2.369026000
C	1.004295000	3.382222000	-0.219512000
C	1.993903000	5.013785000	-2.247915000
H	2.533612000	3.194663000	-3.255189000
C	0.932816000	4.767647000	-0.096742000
H	0.614475000	2.739290000	0.570971000
C	1.421983000	5.584873000	-1.112557000
H	2.384423000	5.648774000	-3.041638000
H	0.486652000	5.204205000	0.795575000
H	1.360253000	6.668001000	-1.020484000

INT2

C	-2.099996000	1.122394000	-0.478187000
C	-0.846318000	1.555588000	-0.132783000
Co	0.548510000	0.171219000	-0.343464000
P	2.542902000	1.136536000	0.145821000
P	0.548650000	-1.120914000	1.512058000
C	1.399360000	-0.343649000	2.971037000
H	1.285756000	-1.024299000	3.826098000
H	0.865517000	0.578895000	3.237520000
C	3.188495000	1.173720000	1.876959000
H	2.748877000	2.069118000	2.339045000
H	4.274545000	1.343681000	1.861526000
C	2.880031000	-0.061500000	2.725612000
H	3.374732000	0.073049000	3.697612000
H	3.345955000	-0.954711000	2.280782000
C	-2.144004000	-0.235541000	-1.056095000
C	-3.393374000	-0.920147000	-1.445351000
C	-3.507699000	-1.579070000	-2.678701000
C	-4.485055000	-0.980090000	-0.563764000
C	-4.660586000	-2.281452000	-3.013397000
H	-2.671749000	-1.536480000	-3.376418000
C	-5.635095000	-1.687244000	-0.895188000
H	-4.415721000	-0.473992000	0.398648000
C	-5.730112000	-2.341636000	-2.122199000
H	-4.725184000	-2.782909000	-3.978286000
H	-6.463987000	-1.726767000	-0.188938000
H	-6.633115000	-2.891191000	-2.383755000
C	-3.322354000	1.939705000	-0.307884000
C	-4.255817000	2.079189000	-1.347570000
C	-3.584364000	2.605294000	0.899381000
C	-5.396909000	2.857872000	-1.187672000
H	-4.077509000	1.568706000	-2.293249000
C	-4.727708000	3.378702000	1.063714000
H	-2.867846000	2.511588000	1.715467000
C	-5.641200000	3.509207000	0.019494000
H	-6.102090000	2.953903000	-2.012187000
H	-4.906942000	3.882708000	2.012739000
H	-6.537913000	4.113829000	0.146061000
C	-0.538672000	2.897122000	0.353788000
C	-0.913960000	4.047000000	-0.370478000
C	0.213077000	3.100240000	1.525170000
C	-0.534379000	5.316925000	0.045201000

H	-1.504322000	3.921956000	-1.278288000
C	0.594103000	4.369837000	1.944032000
H	0.499386000	2.223316000	2.107998000
C	0.231025000	5.489924000	1.198667000
H	-0.831360000	6.184387000	-0.543839000
H	1.179840000	4.486214000	2.856490000
H	0.539011000	6.485435000	1.512990000
C	-0.914651000	-0.818641000	-1.127534000
C	-0.570083000	-2.161002000	-1.584671000
C	0.543722000	-2.334358000	-2.429657000
C	-1.228342000	-3.324732000	-1.135948000
C	0.991061000	-3.598570000	-2.798460000
H	1.057836000	-1.444230000	-2.797578000
C	-0.775091000	-4.587675000	-1.496063000
H	-2.106547000	-3.217039000	-0.500643000
C	0.338562000	-4.734650000	-2.324797000
H	1.858654000	-3.696605000	-3.451485000
H	-1.297681000	-5.470444000	-1.128649000
H	0.690851000	-5.727373000	-2.600447000
C	3.711470000	0.023197000	-0.731716000
C	3.444020000	-0.223837000	-2.087363000
C	4.765422000	-0.668103000	-0.123867000
C	4.193296000	-1.146731000	-2.808752000
H	2.632974000	0.319658000	-2.578238000
C	5.514691000	-1.595185000	-0.845065000
H	5.007863000	-0.494451000	0.923245000
C	5.226356000	-1.843533000	-2.184521000
H	3.965120000	-1.326024000	-3.858419000
H	6.325672000	-2.129992000	-0.353315000
H	5.809458000	-2.573531000	-2.742970000
C	2.974052000	2.794111000	-0.500113000
C	4.062075000	3.543641000	-0.038291000
C	2.165451000	3.321410000	-1.512398000
C	4.328928000	4.799118000	-0.574821000
H	4.709055000	3.149694000	0.745251000
C	2.438533000	4.573394000	-2.054792000
H	1.297617000	2.750722000	-1.850411000
C	3.517971000	5.315274000	-1.583800000
H	5.174352000	5.376730000	-0.204431000
H	1.791378000	4.977869000	-2.831302000
H	3.726265000	6.299933000	-1.998826000
C	-1.136395000	-1.371913000	2.167783000
C	-1.789399000	-2.610233000	2.161447000
C	-1.843198000	-0.239001000	2.598086000
C	-3.110601000	-2.714642000	2.590193000
H	-1.264413000	-3.497580000	1.810867000
C	-3.159560000	-0.347069000	3.033921000
H	-1.365110000	0.741853000	2.566579000
C	-3.796215000	-1.586867000	3.032513000
H	-3.605978000	-3.684094000	2.573463000
H	-3.694976000	0.543875000	3.358439000
H	-4.830246000	-1.670087000	3.363048000
C	1.346725000	-2.769467000	1.544491000
C	1.237572000	-3.634675000	2.643130000
C	2.162659000	-3.140697000	0.471506000
C	1.912448000	-4.850216000	2.653931000
H	0.606696000	-3.358185000	3.489113000
C	2.842301000	-4.356640000	0.483693000
H	2.255516000	-2.478214000	-0.389441000
C	2.714556000	-5.213878000	1.571780000
H	1.813301000	-5.517494000	3.508632000
H	3.463274000	-4.632025000	-0.367865000
H	3.239181000	-6.167950000	1.580922000

INT3

C	2.055521000	0.761406000	-0.608880000
C	0.764098000	1.217289000	-0.737626000
Co	-0.550956000	0.157984000	0.337019000
P	-2.593956000	1.174970000	-0.202581000

P	-0.954605000	-1.384088000	-1.375133000
C	-1.635285000	-0.573030000	-2.895097000
H	-1.655538000	-1.325875000	-3.695068000
H	-0.880402000	0.167553000	-3.191084000
C	-2.978009000	1.425083000	-1.988086000
H	-2.219286000	2.111868000	-2.390982000
H	-3.949304000	1.929027000	-2.087036000
C	-2.988223000	0.127081000	-2.786851000
H	-3.323550000	0.358447000	-3.807706000
H	-3.746689000	-0.550632000	-2.368907000
C	2.215125000	-0.378082000	0.300037000
C	3.547689000	-0.934150000	0.629870000
C	3.934674000	-1.080932000	1.969790000
C	4.453901000	-1.323159000	-0.367241000
C	5.176692000	-1.610378000	2.302696000
H	3.242761000	-0.765712000	2.751992000
C	5.693625000	-1.858532000	-0.035259000
H	4.173871000	-1.202380000	-1.413219000
C	6.061230000	-2.005480000	1.301041000
H	5.457564000	-1.711143000	3.350372000
H	6.379486000	-2.159853000	-0.826243000
H	7.034552000	-2.419596000	1.560056000
C	3.257016000	1.420162000	-1.191190000
C	4.274263000	1.897089000	-0.347750000
C	3.449727000	1.565393000	-2.571668000
C	5.408460000	2.518137000	-0.856209000
H	4.173287000	1.755076000	0.726876000
C	4.585954000	2.184142000	-3.087366000
H	2.708795000	1.162595000	-3.257819000
C	5.569364000	2.670613000	-2.232033000
H	6.176696000	2.877778000	-0.172431000
H	4.704077000	2.278480000	-4.166214000
H	6.458763000	3.153845000	-2.633269000
C	0.389426000	2.420760000	-1.488269000
C	-0.071093000	3.557766000	-0.794899000
C	0.406043000	2.508305000	-2.895297000
C	-0.424294000	4.727515000	-1.458143000
H	-0.159267000	3.506743000	0.292313000
C	0.018871000	3.665641000	-3.564613000
H	0.723014000	1.644424000	-3.478340000
C	-0.386337000	4.790710000	-2.850247000
H	-0.757474000	5.588623000	-0.879579000
H	0.045678000	3.690173000	-4.653532000
H	-0.674183000	5.702085000	-3.371098000
C	-0.024939000	1.112169000	2.129789000
C	1.162472000	1.636755000	2.759662000
C	1.447823000	1.182473000	4.059631000
C	2.014889000	2.559031000	2.142929000
C	2.571872000	1.648961000	4.726743000
H	0.782425000	0.458541000	4.526405000
C	3.131458000	3.028195000	2.827568000
H	1.804577000	2.893937000	1.129903000
C	3.415914000	2.574296000	4.112776000
H	2.789693000	1.290008000	5.730834000
H	3.789697000	3.746317000	2.341281000
H	4.296268000	2.940554000	4.637586000
N	-1.161347000	0.724394000	2.263650000
C	1.055187000	-0.849240000	0.851543000
C	0.901553000	-2.077297000	1.634961000
C	-0.031248000	-2.195434000	2.688570000
C	1.602427000	-3.251698000	1.275566000
C	-0.251541000	-3.408250000	3.335254000
H	-0.608309000	-1.325083000	2.991600000
C	1.369210000	-4.463183000	1.912698000
H	2.326273000	-3.200756000	0.465326000
C	0.437944000	-4.554915000	2.947831000
H	-0.980916000	-3.456474000	4.143732000
H	1.919816000	-5.347772000	1.592976000
H	0.254860000	-5.506378000	3.444690000
C	-3.152982000	2.749737000	0.548407000

C	-3.307346000	3.920664000	-0.203176000
C	-3.440601000	2.787260000	1.921303000
C	-3.725986000	5.102319000	0.403641000
H	-3.088362000	3.923122000	-1.268881000
C	-3.858173000	3.969164000	2.523187000
H	-3.338440000	1.881517000	2.514879000
C	-3.999039000	5.131668000	1.767895000
H	-3.839315000	6.003044000	-0.198319000
H	-4.078996000	3.979800000	3.589210000
H	-4.326648000	6.055987000	2.240765000
C	-3.954111000	0.053437000	0.323987000
C	-5.271316000	0.261728000	-0.108152000
C	-3.685036000	-1.037933000	1.155243000
C	-6.286087000	-0.613780000	0.260716000
H	-5.506844000	1.121885000	-0.736246000
C	-4.702955000	-1.910082000	1.534182000
H	-2.667134000	-1.208291000	1.507120000
C	-6.001975000	-1.704758000	1.081754000
H	-7.302937000	-0.442793000	-0.089146000
H	-4.470761000	-2.760125000	2.173945000
H	-6.796245000	-2.391859000	1.369143000
C	-2.078495000	-2.812455000	-1.108558000
C	-3.106984000	-3.157178000	-1.994253000
C	-1.903762000	-3.590519000	0.045377000
C	-3.945802000	-4.235982000	-1.723201000
H	-3.260043000	-2.593732000	-2.912257000
C	-2.725991000	-4.681521000	0.302693000
H	-1.113213000	-3.340108000	0.750533000
C	-3.759276000	-5.001144000	-0.575548000
H	-4.744882000	-4.482245000	-2.420536000
H	-2.558702000	-5.273495000	1.201755000
H	-4.414747000	-5.845557000	-0.369098000
C	0.530523000	-2.187579000	-2.095730000
C	1.396532000	-1.430020000	-2.896404000
C	0.843978000	-3.531444000	-1.862857000
C	2.538004000	-1.997880000	-3.451201000
H	1.186411000	-0.376714000	-3.069870000
C	1.992597000	-4.097090000	-2.411188000
H	0.190942000	-4.145892000	-1.246129000
C	2.842451000	-3.335187000	-3.207017000
H	3.198715000	-1.385411000	-4.063893000
H	2.219919000	-5.143301000	-2.212053000
H	3.739953000	-3.779595000	-3.633696000

INT3'

C	2.196927000	-0.112800000	-0.438688000
C	1.131689000	0.591198000	-0.937338000
Co	-0.599094000	0.092101000	0.014388000
P	-2.378815000	1.333181000	-0.739487000
P	-1.064434000	-1.579010000	-1.350872000
C	-1.776609000	-1.090859000	-2.996816000
H	-1.892882000	-2.013641000	-3.581191000
H	-1.029166000	-0.484043000	-3.524574000
C	-3.020436000	1.095712000	-2.454107000
H	-2.336651000	1.662911000	-3.101727000
H	-3.997727000	1.592392000	-2.541528000
C	-3.109408000	-0.355003000	-2.925351000
H	-3.562950000	-0.358336000	-3.926602000
H	-3.799497000	-0.926001000	-2.285379000
C	1.873824000	-1.108828000	0.595015000
C	2.908357000	-1.990445000	1.183764000
C	3.067998000	-2.106491000	2.571618000
C	3.744061000	-2.754059000	0.355814000
C	4.016987000	-2.967097000	3.113864000
H	2.426359000	-1.515741000	3.226198000
C	4.687745000	-3.620491000	0.896173000
H	3.639768000	-2.661430000	-0.724912000
C	4.829124000	-3.731735000	2.278369000
H	4.123616000	-3.041229000	4.195465000

H	5.319374000	-4.210390000	0.232513000
H	5.571302000	-4.406572000	2.702251000
C	3.596982000	0.147909000	-0.852130000
C	4.631952000	0.295735000	0.086439000
C	3.927645000	0.296787000	-2.207945000
C	5.931992000	0.585229000	-0.312747000
H	4.409620000	0.176769000	1.146309000
C	5.226959000	0.583468000	-2.610936000
H	3.137501000	0.192524000	-2.951566000
C	6.238629000	0.728898000	-1.664241000
H	6.712610000	0.698228000	0.438721000
H	5.451318000	0.692631000	-3.671462000
H	7.257761000	0.951006000	-1.976952000
C	1.265216000	1.818049000	-1.706507000
C	2.056725000	2.885202000	-1.221848000
C	0.519899000	2.063641000	-2.876793000
C	2.068406000	4.123913000	-1.852879000
H	2.657823000	2.722907000	-0.326850000
C	0.547774000	3.294078000	-3.520833000
H	-0.097890000	1.256717000	-3.273459000
C	1.312654000	4.341424000	-3.005257000
H	2.676555000	4.928944000	-1.439428000
H	-0.040709000	3.443433000	-4.426269000
H	1.319097000	5.312946000	-3.496354000
C	0.444625000	2.239156000	1.863721000
C	1.278224000	3.223508000	2.431882000
C	2.541737000	2.841455000	2.927900000
C	0.887041000	4.575825000	2.471886000
C	3.392025000	3.803560000	3.450790000
H	2.834570000	1.793945000	2.880669000
C	1.752048000	5.522475000	2.999824000
H	-0.086692000	4.861820000	2.078700000
C	3.002761000	5.143439000	3.490113000
H	4.368981000	3.507534000	3.827192000
H	1.449878000	6.567564000	3.028292000
H	3.675847000	5.893103000	3.900917000
N	-0.158996000	1.383168000	1.334051000
C	0.560552000	-1.171302000	0.957830000
C	-0.051920000	-2.059886000	1.944931000
C	-1.007565000	-1.558200000	2.850730000
C	0.209702000	-3.444907000	1.987911000
C	-1.674888000	-2.391151000	3.741338000
H	-1.224057000	-0.489460000	2.835637000
C	-0.467227000	-4.278773000	2.869924000
H	0.960814000	-3.858272000	1.316066000
C	-1.417161000	-3.760846000	3.749802000
H	-2.408121000	-1.968856000	4.428836000
H	-0.249623000	-5.346368000	2.871508000
H	-1.947878000	-4.418138000	4.436710000
C	-3.790019000	0.813988000	0.320036000
C	-5.021535000	0.358973000	-0.163310000
C	-3.581723000	0.827369000	1.708137000
C	-6.006352000	-0.094812000	0.713407000
H	-5.225807000	0.350355000	-1.232697000
C	-4.565418000	0.382038000	2.582900000
H	-2.627739000	1.184925000	2.097931000
C	-5.780007000	-0.090944000	2.085880000
H	-6.954178000	-0.455247000	0.316909000
H	-4.381367000	0.399424000	3.656100000
H	-6.547668000	-0.451996000	2.768094000
C	-2.474670000	3.161004000	-0.579160000
C	-3.712764000	3.811652000	-0.482835000
C	-1.304125000	3.925428000	-0.577961000
C	-3.776869000	5.197962000	-0.393920000
H	-4.632991000	3.226071000	-0.466073000
C	-1.371046000	5.315057000	-0.492457000
H	-0.336231000	3.433191000	-0.650874000
C	-2.604534000	5.953145000	-0.398910000
H	-4.744743000	5.691137000	-0.318423000
H	-0.447145000	5.892961000	-0.502315000

H	-2.656048000	7.038650000	-0.329637000
C	-2.327891000	-2.809332000	-0.833491000
C	-2.642543000	-3.919292000	-1.631850000
C	-3.044108000	-2.605868000	0.348331000
C	-3.642436000	-4.805322000	-1.248042000
H	-2.084438000	-4.101420000	-2.551346000
C	-4.043894000	-3.495323000	0.736297000
H	-2.807782000	-1.749496000	0.977833000
C	-4.344161000	-4.594951000	-0.060479000
H	-3.873214000	-5.665905000	-1.874042000
H	-4.579256000	-3.322944000	1.669006000
H	-5.123025000	-5.293520000	0.241397000
C	0.336610000	-2.610998000	-1.918722000
C	1.244030000	-2.077097000	-2.843474000
C	0.550516000	-3.908155000	-1.438830000
C	2.328052000	-2.828428000	-3.289215000
H	1.112839000	-1.056028000	-3.202824000
C	1.637418000	-4.657557000	-1.881989000
H	-0.140199000	-4.336484000	-0.714333000
C	2.524719000	-4.122460000	-2.812352000
H	3.026439000	-2.394341000	-4.002974000
H	1.791963000	-5.662548000	-1.492599000
H	3.375098000	-4.708353000	-3.157585000

TS3

C	1.982207000	0.851675000	-0.546931000
C	0.661995000	1.255095000	-0.663454000
Co	-0.612041000	0.049851000	0.235604000
P	-2.627160000	1.119521000	-0.224176000
P	-0.987111000	-1.417445000	-1.461945000
C	-1.779654000	-0.717786000	-2.986556000
H	-1.871432000	-1.533163000	-3.717082000
H	-1.068116000	0.001859000	-3.414230000
C	-3.089354000	1.257676000	-2.000579000
H	-2.345176000	1.922771000	-2.458276000
H	-4.054732000	1.774884000	-2.082592000
C	-3.135657000	-0.064307000	-2.764340000
H	-3.589959000	0.127766000	-3.746675000
H	-3.802763000	-0.782379000	-2.263903000
C	2.194599000	-0.360813000	0.213622000
C	3.546653000	-0.911413000	0.447189000
C	3.945600000	-1.261121000	1.746310000
C	4.467471000	-1.085927000	-0.596916000
C	5.216739000	-1.766096000	1.992586000
H	3.241848000	-1.125340000	2.567894000
C	5.734939000	-1.602017000	-0.352558000
H	4.177031000	-0.812035000	-1.610181000
C	6.117242000	-1.942428000	0.943587000
H	5.506421000	-2.021744000	3.010933000
H	6.430962000	-1.734442000	-1.179843000
H	7.112806000	-2.339643000	1.135423000
C	3.123869000	1.647928000	-1.071570000
C	4.179206000	2.049987000	-0.237878000
C	3.186066000	2.018696000	-2.422311000
C	5.239438000	2.803133000	-0.729809000
H	4.173197000	1.742917000	0.807881000
C	4.245987000	2.771139000	-2.918654000
H	2.387267000	1.704844000	-3.093790000
C	5.277738000	3.170514000	-2.073114000
H	6.044672000	3.100762000	-0.059249000
H	4.267081000	3.042890000	-3.973261000
H	6.108540000	3.758905000	-2.459225000
C	0.328683000	2.558567000	-1.255223000
C	0.378545000	3.720446000	-0.463038000
C	-0.035233000	2.719379000	-2.603117000
C	0.101832000	4.973676000	-0.995041000
H	0.631697000	3.625200000	0.593573000
C	-0.324222000	3.972388000	-3.137256000
H	-0.054790000	1.839537000	-3.250466000

C	-0.254790000	5.109525000	-2.335650000
H	0.152153000	5.851490000	-0.351734000
H	-0.588612000	4.060926000	-4.190800000
H	-0.475867000	6.091168000	-2.751415000
C	0.152620000	0.359832000	2.133231000
C	1.241889000	0.825620000	2.980400000
C	1.405981000	0.202395000	4.226797000
C	2.124443000	1.841214000	2.594291000
C	2.447632000	0.583899000	5.064826000
H	0.720302000	-0.591315000	4.518728000
C	3.159050000	2.218915000	3.443157000
H	1.995787000	2.325293000	1.629528000
C	3.329011000	1.590418000	4.675183000
H	2.570521000	0.090697000	6.027416000
H	3.838316000	3.011911000	3.133591000
H	4.144426000	1.887243000	5.332062000
N	-1.059037000	0.182432000	2.194912000
C	1.048674000	-0.918025000	0.764093000
C	0.950033000	-2.289934000	1.295669000
C	0.079079000	-2.687731000	2.331585000
C	1.709779000	-3.316643000	0.690349000
C	-0.015631000	-4.014717000	2.737750000
H	-0.551791000	-1.951007000	2.820785000
C	1.612420000	-4.640369000	1.096516000
H	2.381018000	-3.062005000	-0.125882000
C	0.748060000	-5.004634000	2.126643000
H	-0.703676000	-4.274819000	3.541838000
H	2.214770000	-5.394939000	0.590569000
H	0.667488000	-6.043090000	2.443363000
C	-2.764910000	2.847204000	0.373025000
C	-3.110542000	3.915225000	-0.460620000
C	-2.471043000	3.106459000	1.719874000
C	-3.168267000	5.212679000	0.042271000
H	-3.312286000	3.753489000	-1.517495000
C	-2.533171000	4.402719000	2.218273000
H	-2.178486000	2.285197000	2.373676000
C	-2.882696000	5.460712000	1.380647000
H	-3.426367000	6.034095000	-0.624834000
H	-2.302188000	4.587572000	3.266103000
H	-2.926683000	6.476316000	1.770663000
C	-4.139019000	0.348193000	0.511733000
C	-5.303689000	0.114284000	-0.232477000
C	-4.139876000	-0.012016000	1.868340000
C	-6.421221000	-0.478149000	0.350486000
H	-5.360598000	0.395686000	-1.281013000
C	-5.262215000	-0.592091000	2.450934000
H	-3.245476000	0.147162000	2.463902000
C	-6.405377000	-0.836106000	1.694244000
H	-7.310162000	-0.653463000	-0.253368000
H	-5.237985000	-0.859375000	3.506499000
H	-7.280022000	-1.297398000	2.149816000
C	-2.172468000	-2.740211000	-1.023734000
C	-2.649211000	-3.668138000	-1.960968000
C	-2.682376000	-2.769675000	0.278079000
C	-3.611937000	-4.603745000	-1.599420000
H	-2.255871000	-3.664371000	-2.978538000
C	-3.648927000	-3.705068000	0.640000000
H	-2.320998000	-2.044209000	1.009529000
C	-4.114518000	-4.620798000	-0.298071000
H	-3.974017000	-5.320947000	-2.334259000
H	-4.041052000	-3.708807000	1.655603000
H	-4.871998000	-5.351231000	-0.018565000
C	0.428539000	-2.255348000	-2.251639000
C	1.371785000	-1.452553000	-2.909850000
C	0.624788000	-3.639999000	-2.219850000
C	2.479393000	-2.021820000	-3.527898000
H	1.244336000	-0.369227000	-2.915996000
C	1.735124000	-4.207972000	-2.840499000
H	-0.079581000	-4.276948000	-1.687323000
C	2.664531000	-3.403066000	-3.493419000

H	3.204608000	-1.380276000	-4.027487000
H	1.877692000	-5.286955000	-2.801443000
H	3.534638000	-3.849549000	-3.971456000

INT4

C	-1.892193000	-1.067873000	-0.126671000
C	-0.576031000	-1.255347000	-0.596307000
Co	0.648000000	0.085562000	0.082261000
P	2.769954000	-0.388368000	-0.659591000
P	0.261039000	1.566864000	-1.532716000
C	1.162608000	1.312924000	-3.142213000
H	0.869543000	2.145666000	-3.796584000
H	0.775488000	0.401933000	-3.617329000
C	3.268400000	0.004794000	-2.404895000
H	2.978220000	-0.870249000	-3.003482000
H	4.365101000	0.058624000	-2.448581000
C	2.680283000	1.270105000	-3.028678000
H	3.103071000	1.369838000	-4.038613000
H	3.013957000	2.166336000	-2.485603000
C	-2.083332000	0.015263000	0.774163000
C	-3.408259000	0.578703000	1.068981000
C	-3.741735000	1.044192000	2.353916000
C	-4.368017000	0.721547000	0.051435000
C	-4.985274000	1.605864000	2.613645000
H	-3.004048000	0.973255000	3.153560000
C	-5.603876000	1.299763000	0.307290000
H	-4.117866000	0.393322000	-0.956473000
C	-5.923988000	1.738731000	1.591597000
H	-5.220042000	1.950944000	3.619345000
H	-6.320792000	1.412608000	-0.505487000
H	-6.894873000	2.188104000	1.793472000
C	-3.016646000	-1.965879000	-0.503013000
C	-3.927346000	-2.425957000	0.460399000
C	-3.199322000	-2.395493000	-1.825772000
C	-4.978184000	-3.268652000	0.116697000
H	-3.804364000	-2.111052000	1.495869000
C	-4.251587000	-3.234127000	-2.174968000
H	-2.493104000	-2.072978000	-2.589431000
C	-5.149017000	-3.674733000	-1.204874000
H	-5.667600000	-3.611276000	0.887044000
H	-4.369071000	-3.548288000	-3.211333000
H	-5.972612000	-4.333248000	-1.475997000
C	-0.174113000	-2.458702000	-1.308360000
C	-0.471211000	-3.735901000	-0.780398000
C	0.601627000	-2.414869000	-2.480255000
C	0.006871000	-4.889480000	-1.385101000
H	-1.061345000	-3.801407000	0.134906000
C	1.067916000	-3.570872000	-3.094035000
H	0.837913000	-1.438854000	-2.903038000
C	0.781193000	-4.819027000	-2.544741000
H	-0.221807000	-5.858830000	-0.943045000
H	1.668620000	-3.496594000	-4.000630000
H	1.160506000	-5.726618000	-3.010611000
C	0.129240000	-0.379418000	2.040827000
C	-0.280379000	-1.574605000	2.826593000
C	0.707746000	-2.488982000	3.223428000
C	-1.603015000	-1.819003000	3.211370000
C	0.377334000	-3.628059000	3.945826000
H	1.740790000	-2.279094000	2.951553000
C	-1.936141000	-2.961917000	3.931793000
H	-2.382190000	-1.107033000	2.949684000
C	-0.950059000	-3.876203000	4.293445000
H	1.159180000	-4.327963000	4.238151000
H	-2.973698000	-3.135675000	4.213758000
H	-1.212844000	-4.773090000	4.852052000
N	1.374660000	-0.084789000	1.815756000
C	-0.874539000	0.560293000	1.363421000
C	-0.805507000	1.973559000	1.836544000
C	-0.004649000	2.370157000	2.921807000

C	-1.547906000	2.978256000	1.192774000
C	0.067433000	3.701726000	3.317638000
H	0.589218000	1.628358000	3.450226000
C	-1.476736000	4.308226000	1.586235000
H	-2.197495000	2.701841000	0.366639000
C	-0.662729000	4.683859000	2.652068000
H	0.702035000	3.971606000	4.161136000
H	-2.059310000	5.056935000	1.049134000
H	-0.599168000	5.726095000	2.960507000
C	3.326386000	-2.125510000	-0.491518000
C	4.489122000	-2.602811000	-1.108959000
C	2.574431000	-2.993092000	0.302548000
C	4.879278000	-3.927597000	-0.941863000
H	5.100225000	-1.936738000	-1.718082000
C	2.970490000	-4.315695000	0.479201000
H	1.660919000	-2.624387000	0.766553000
C	4.120665000	-4.786252000	-0.147201000
H	5.782444000	-4.290753000	-1.429965000
H	2.363107000	-4.980582000	1.092662000
H	4.428190000	-5.822991000	-0.019773000
C	4.042582000	0.487647000	0.327967000
C	4.632587000	1.681195000	-0.103207000
C	4.398692000	-0.018551000	1.586470000
C	5.550506000	2.354652000	0.699173000
H	4.376532000	2.104381000	-1.072656000
C	5.316621000	0.653263000	2.385237000
H	3.946449000	-0.943385000	1.937655000
C	5.893760000	1.843594000	1.946916000
H	5.995945000	3.282471000	0.343018000
H	5.582614000	0.243337000	3.358126000
H	6.612116000	2.368003000	2.574922000
C	0.891424000	3.235381000	-1.110129000
C	0.743968000	4.339937000	-1.961030000
C	1.641901000	3.376011000	0.062504000
C	1.312667000	5.565152000	-1.628957000
H	0.173174000	4.243018000	-2.885624000
C	2.219667000	4.600546000	0.388022000
H	1.763963000	2.517330000	0.727434000
C	2.049856000	5.696763000	-0.452109000
H	1.184639000	6.419186000	-2.292260000
H	2.796492000	4.692143000	1.306981000
H	2.494364000	6.656961000	-0.194895000
C	-1.424406000	1.793848000	-2.220859000
C	-1.967792000	0.710493000	-2.926232000
C	-2.187137000	2.961336000	-2.100010000
C	-3.230566000	0.792298000	-3.503016000
H	-1.393185000	-0.213937000	-3.012766000
C	-3.457104000	3.040001000	-2.668110000
H	-1.788819000	3.815559000	-1.554873000
C	-3.980633000	1.959895000	-3.372717000
H	-3.635461000	-0.065619000	-4.037799000
H	-4.039292000	3.953000000	-2.555509000
H	-4.974279000	2.023496000	-3.813087000

TS4

C	-2.210282000	-0.401773000	-0.270888000
C	-1.038098000	-1.025346000	-0.744636000
Co	0.622175000	-0.269948000	0.054282000
P	2.555126000	-1.194724000	-0.602400000
P	0.829988000	1.441554000	-1.441801000
C	1.567649000	0.903372000	-3.066589000
H	1.567670000	1.777836000	-3.731427000
H	0.882720000	0.172872000	-3.518830000
C	3.057852000	-1.075082000	-2.375176000
H	2.393583000	-1.761784000	-2.917664000
H	4.069490000	-1.489447000	-2.491468000
C	2.976154000	0.326374000	-2.975785000
H	3.398797000	0.290071000	-3.989999000
H	3.616495000	1.022676000	-2.412008000

C	-2.006350000	0.596631000	0.731092000
C	-3.002817000	1.638463000	1.028294000
C	-3.186238000	2.143106000	2.328771000
C	-3.780147000	2.192298000	-0.002581000
C	-4.116183000	3.140862000	2.587947000
H	-2.575914000	1.754713000	3.143487000
C	-4.697960000	3.202757000	0.252777000
H	-3.640700000	1.828988000	-1.018652000
C	-4.877266000	3.678139000	1.550290000
H	-4.242807000	3.507269000	3.605312000
H	-5.275762000	3.622048000	-0.570107000
H	-5.601594000	4.465442000	1.752589000
C	-3.573130000	-0.773923000	-0.727151000
C	-4.634139000	-0.898816000	0.183488000
C	-3.842482000	-1.034326000	-2.079283000
C	-5.907815000	-1.261288000	-0.238952000
H	-4.446500000	-0.710970000	1.240404000
C	-5.116149000	-1.392336000	-2.506267000
H	-3.031929000	-0.960047000	-2.803541000
C	-6.157355000	-1.506128000	-1.587692000
H	-6.710647000	-1.355897000	0.490905000
H	-5.296139000	-1.585434000	-3.563073000
H	-7.155180000	-1.787898000	-1.919972000
C	-1.099558000	-2.297679000	-1.447263000
C	-1.822460000	-3.384916000	-0.906137000
C	-0.329264000	-2.544436000	-2.599038000
C	-1.732711000	-4.652796000	-1.466009000
H	-2.430818000	-3.220021000	-0.015983000
C	-0.274058000	-3.802887000	-3.183688000
H	0.227660000	-1.711822000	-3.030744000
C	-0.963271000	-4.871139000	-2.609750000
H	-2.279337000	-5.479120000	-1.012408000
H	0.323735000	-3.957926000	-4.081483000
H	-0.901152000	-5.864801000	-3.049786000
C	-0.346864000	-0.908815000	1.943448000
C	-1.312428000	-1.803695000	2.631524000
C	-0.982778000	-3.161734000	2.766308000
C	-2.537375000	-1.356595000	3.136930000
C	-1.858770000	-4.043661000	3.384390000
H	-0.028559000	-3.500268000	2.364584000
C	-3.417331000	-2.242295000	3.751440000
H	-2.808107000	-0.306850000	3.044907000
C	-3.083042000	-3.588551000	3.874906000
H	-1.592320000	-5.095757000	3.475233000
H	-4.368388000	-1.876935000	4.136286000
H	-3.774777000	-4.282016000	4.350426000
N	0.852370000	-1.279050000	1.682371000
C	-0.759179000	0.487902000	1.432710000
C	-0.086237000	1.633086000	2.090692000
C	0.788746000	1.469474000	3.181348000
C	-0.265390000	2.943839000	1.605698000
C	1.449372000	2.556863000	3.746071000
H	0.962267000	0.473230000	3.582553000
C	0.379180000	4.028456000	2.180849000
H	-0.922976000	3.102951000	0.752868000
C	1.248018000	3.844872000	3.256205000
H	2.121632000	2.392436000	4.587731000
H	0.223001000	5.024470000	1.766511000
H	1.766808000	4.693433000	3.699046000
C	2.794270000	-2.980706000	-0.281092000
C	4.070155000	-3.554264000	-0.334599000
C	1.690154000	-3.793182000	-0.013395000
C	4.235208000	-4.921158000	-0.134626000
H	4.942032000	-2.924239000	-0.519150000
C	1.856268000	-5.161236000	0.184391000
H	0.701326000	-3.344096000	0.044536000
C	3.127082000	-5.726766000	0.123867000
H	5.231666000	-5.358287000	-0.175639000
H	0.983947000	-5.781763000	0.387144000
H	3.257962000	-6.796173000	0.282318000

C	3.979865000	-0.436743000	0.283391000
C	5.152673000	-0.014893000	-0.354555000
C	3.861882000	-0.238679000	1.668465000
C	6.175523000	0.598292000	0.367291000
H	5.282784000	-0.155948000	-1.426281000
C	4.884912000	0.370097000	2.386017000
H	2.948476000	-0.558907000	2.168987000
C	6.044485000	0.794787000	1.738023000
H	7.076992000	0.924361000	-0.149135000
H	4.773075000	0.517000000	3.459600000
H	6.842512000	1.277345000	2.300178000
C	1.999022000	2.793341000	-1.023904000
C	2.302229000	3.832262000	-1.916377000
C	2.688316000	2.724878000	0.190036000
C	3.272853000	4.775754000	-1.597748000
H	1.766516000	3.908884000	-2.863868000
C	3.664976000	3.665222000	0.508083000
H	2.445577000	1.932012000	0.898785000
C	3.959125000	4.689841000	-0.385718000
H	3.497689000	5.579614000	-2.297111000
H	4.185880000	3.593247000	1.461659000
H	4.721474000	5.427798000	-0.140543000
C	-0.653378000	2.299199000	-2.094927000
C	-1.529326000	1.567477000	-2.910441000
C	-0.952612000	3.640809000	-1.828269000
C	-2.654460000	2.165698000	-3.467784000
H	-1.327365000	0.512318000	-3.103238000
C	-2.086553000	4.236747000	-2.376179000
H	-0.284810000	4.228134000	-1.198264000
C	-2.934748000	3.505539000	-3.203127000
H	-3.321572000	1.578342000	-4.097169000
H	-2.304834000	5.280294000	-2.155226000
H	-3.818197000	3.974583000	-3.633184000

INT5

C	2.102951000	1.082318000	-0.138639000
C	0.897482000	1.375524000	-0.743686000
Co	-0.608945000	0.231560000	-0.236333000
P	-2.774323000	0.655614000	-0.792987000
P	-0.382585000	-1.352616000	-1.788217000
C	-1.318870000	-1.048148000	-3.370760000
H	-1.098283000	-1.882011000	-4.051311000
H	-0.908562000	-0.146122000	-3.846086000
C	-3.293337000	0.388643000	-2.546070000
H	-2.883544000	1.246593000	-3.099912000
H	-4.386954000	0.484540000	-2.616077000
C	-2.828316000	-0.917841000	-3.185421000
H	-3.303538000	-1.001199000	-4.173158000
H	-3.197004000	-1.778835000	-2.605983000
C	2.128813000	-0.073187000	0.752891000
C	3.361255000	-0.887709000	0.832057000
C	3.794398000	-1.452776000	2.044017000
C	4.164732000	-1.078091000	-0.301837000
C	4.976091000	-2.177369000	2.117936000
H	3.181661000	-1.329126000	2.936471000
C	5.344362000	-1.809807000	-0.232115000
H	3.844733000	-0.651098000	-1.250814000
C	5.758869000	-2.360347000	0.978062000
H	5.291232000	-2.599119000	3.071057000
H	5.942709000	-1.949113000	-1.131901000
H	6.687185000	-2.926502000	1.035714000
C	3.343362000	1.862902000	-0.359494000
C	4.197019000	2.166179000	0.712287000
C	3.702544000	2.325719000	-1.634343000
C	5.356361000	2.909325000	0.519838000
H	3.934390000	1.815021000	1.711191000
C	4.860438000	3.069021000	-1.829469000
H	3.056625000	2.089110000	-2.480240000
C	5.694325000	3.365308000	-0.752556000

H	5.999080000	3.135733000	1.369472000
H	5.117761000	3.414889000	-2.829899000
H	6.602987000	3.945455000	-0.904890000
C	0.597663000	2.635995000	-1.415780000
C	0.933367000	3.880159000	-0.844513000
C	-0.174978000	2.650638000	-2.591253000
C	0.503551000	5.070138000	-1.418966000
H	1.516138000	3.892677000	0.075686000
C	-0.582316000	3.840554000	-3.183236000
H	-0.465971000	1.691615000	-3.024012000
C	-0.250370000	5.058792000	-2.593451000
H	0.758998000	6.018228000	-0.947002000
H	-1.177156000	3.818508000	-4.095941000
H	-0.584819000	5.993649000	-3.040107000
C	0.139825000	0.820181000	2.012249000
C	0.372627000	1.295875000	3.403683000
C	-0.593105000	2.099763000	4.028204000
C	1.543503000	0.984800000	4.105346000
C	-0.390002000	2.575472000	5.316306000
H	-1.495748000	2.344632000	3.469945000
C	1.749230000	1.468606000	5.393992000
H	2.307059000	0.373880000	3.625328000
C	0.782143000	2.261328000	6.005996000
H	-1.149886000	3.196033000	5.789484000
H	2.669816000	1.224345000	5.921936000
H	0.939738000	2.634668000	7.016596000
N	-0.731923000	1.384204000	1.264890000
C	0.983812000	-0.352797000	1.512361000
C	0.637671000	-1.687616000	2.034327000
C	-0.272908000	-1.858006000	3.096012000
C	1.099514000	-2.859154000	1.396431000
C	-0.665987000	-3.125597000	3.516259000
H	-0.680068000	-0.984804000	3.603252000
C	0.718481000	-4.120086000	1.825368000
H	1.752821000	-2.764936000	0.530386000
C	-0.164892000	-4.266459000	2.895654000
H	-1.370220000	-3.217791000	4.342537000
H	1.085054000	-4.998587000	1.294148000
H	-0.475111000	-5.256975000	3.224412000
C	1.273719000	-1.713541000	-2.482028000
C	1.950233000	-2.923810000	-2.294368000
C	1.895741000	-0.703645000	-3.231874000
C	3.201970000	-3.131523000	-2.870765000
H	1.492520000	-3.714216000	-1.699726000
C	3.139769000	-0.916416000	-3.816661000
H	1.399930000	0.262200000	-3.350624000
C	3.793490000	-2.135728000	-3.642335000
H	3.717309000	-4.077106000	-2.710283000
H	3.605450000	-0.122809000	-4.399005000
H	4.769631000	-2.301619000	-4.095226000
C	-1.090697000	-2.990162000	-1.358853000
C	-1.087355000	-4.068023000	-2.256813000
C	-1.755769000	-3.134761000	-0.137775000
C	-1.730346000	-5.258227000	-1.935430000
H	-0.568041000	-3.976823000	-3.211988000
C	-2.412572000	-4.321310000	0.180291000
H	-1.744614000	-2.316385000	0.583543000
C	-2.399770000	-5.383558000	-0.717365000
H	-1.714736000	-6.089528000	-2.638549000
H	-2.921829000	-4.409601000	1.138504000
H	-2.908337000	-6.314314000	-0.470808000
C	-3.864684000	-0.447262000	0.183170000
C	-4.864266000	-1.260516000	-0.361110000
C	-3.616457000	-0.514335000	1.564247000
C	-5.594864000	-2.125255000	0.452413000
H	-5.080443000	-1.228640000	-1.428588000
C	-4.347810000	-1.375321000	2.373507000
H	-2.832470000	0.112684000	1.995468000
C	-5.337919000	-2.186800000	1.818688000
H	-6.366670000	-2.754989000	0.012569000

H	-4.140875000	-1.416123000	3.442053000
H	-5.906592000	-2.866321000	2.451305000
C	-3.502308000	2.303984000	-0.469161000
C	-4.892902000	2.476193000	-0.489077000
C	-2.676778000	3.410401000	-0.252614000
C	-5.448237000	3.738196000	-0.309191000
H	-5.544994000	1.612975000	-0.634352000
C	-3.236829000	4.673690000	-0.075731000
H	-1.599581000	3.274000000	-0.205540000
C	-4.618336000	4.840038000	-0.104895000
H	-6.529969000	3.862236000	-0.324768000
H	-2.583130000	5.528786000	0.089410000
H	-5.053098000	5.828355000	0.037386000

TS5

C	2.069009000	1.241372000	0.238452000
C	0.840259000	1.622653000	-0.327039000
Co	-0.524501000	0.245058000	-0.261539000
P	-2.631083000	0.696761000	-0.952594000
P	-0.088196000	-1.111720000	-1.913998000
C	-0.857148000	-0.596805000	-3.531522000
H	-0.510456000	-1.296382000	-4.304531000
H	-0.454672000	0.389457000	-3.803489000
C	-2.996691000	0.618240000	-2.763063000
H	-2.611556000	1.562989000	-3.175751000
H	-4.085517000	0.648846000	-2.918350000
C	-2.383452000	-0.565424000	-3.508560000
H	-2.744701000	-0.536243000	-4.546444000
H	-2.758190000	-1.513648000	-3.091787000
C	2.078125000	0.009771000	0.950277000
C	3.355701000	-0.686175000	1.210092000
C	3.640040000	-1.268358000	2.455060000
C	4.329319000	-0.779983000	0.204068000
C	4.845433000	-1.918993000	2.685636000
H	2.895718000	-1.209493000	3.248855000
C	5.532304000	-1.437031000	0.429177000
H	4.120307000	-0.337463000	-0.768460000
C	5.798414000	-2.008890000	1.671971000
H	5.044066000	-2.357151000	3.662536000
H	6.264864000	-1.504700000	-0.374615000
H	6.742596000	-2.520596000	1.851392000
C	3.284591000	2.084217000	0.133692000
C	4.095508000	2.317525000	1.255255000
C	3.653009000	2.691211000	-1.075917000
C	5.228041000	3.119048000	1.170235000
H	3.824221000	1.858868000	2.205924000
C	4.786398000	3.491724000	-1.164742000
H	3.034496000	2.528268000	-1.958066000
C	5.581525000	3.708833000	-0.041716000
H	5.837320000	3.286126000	2.057336000
H	5.050750000	3.947962000	-2.117970000
H	6.469525000	4.335149000	-0.109944000
C	0.565185000	2.957587000	-0.877515000
C	0.833701000	4.137963000	-0.163701000
C	-0.068425000	3.074639000	-2.123275000
C	0.467337000	5.377614000	-0.674047000
H	1.314956000	4.063023000	0.810477000
C	-0.415277000	4.315609000	-2.649095000
H	-0.301102000	2.156094000	-2.665474000
C	-0.155059000	5.472922000	-1.919757000
H	0.668283000	6.279431000	-0.097140000
H	-0.906440000	4.377996000	-3.619588000
H	-0.440958000	6.445997000	-2.315914000
C	-0.097103000	0.536785000	1.990060000
C	-0.504228000	0.585340000	3.420068000
C	-1.683370000	1.253190000	3.779472000
C	0.297917000	0.043569000	4.432653000
C	-2.052781000	1.366571000	5.115301000
H	-2.293212000	1.690104000	2.988939000

C	-0.069768000	0.159292000	5.767440000
H	1.218791000	-0.471480000	4.160848000
C	-1.249368000	0.817795000	6.113005000
H	-2.973014000	1.885277000	5.379266000
H	0.568198000	-0.261742000	6.542769000
H	-1.539514000	0.904780000	7.158792000
N	-0.501882000	1.502384000	1.210173000
C	0.840406000	-0.501143000	1.474117000
C	0.611884000	-1.942887000	1.744364000
C	-0.459293000	-2.410620000	2.531769000
C	1.363036000	-2.926035000	1.065438000
C	-0.721813000	-3.769033000	2.676576000
H	-1.115078000	-1.704926000	3.034134000
C	1.101535000	-4.280781000	1.211104000
H	2.154564000	-2.615428000	0.387691000
C	0.063541000	-4.719312000	2.030608000
H	-1.561475000	-4.082045000	3.297021000
H	1.703256000	-5.000638000	0.656435000
H	-0.147424000	-5.781845000	2.139239000
C	1.664207000	-1.256988000	-2.442745000
C	2.413654000	-2.435767000	-2.354295000
C	2.285018000	-0.104400000	-2.945828000
C	3.737040000	-2.468646000	-2.790425000
H	1.957288000	-3.338230000	-1.948934000
C	3.602113000	-0.139988000	-3.392256000
H	1.725346000	0.833394000	-2.979235000
C	4.330253000	-1.327107000	-3.321640000
H	4.306475000	-3.393335000	-2.710328000
H	4.065585000	0.765410000	-3.781542000
H	5.363265000	-1.355663000	-3.664559000
C	-0.690041000	-2.847164000	-1.858930000
C	-0.472966000	-3.749743000	-2.910867000
C	-1.475878000	-3.252332000	-0.777102000
C	-1.022623000	-5.026264000	-2.873038000
H	0.143707000	-3.453594000	-3.760838000
C	-2.033992000	-4.528275000	-0.740968000
H	-1.640150000	-2.566408000	0.054472000
C	-1.807610000	-5.416331000	-1.787306000
H	-0.841549000	-5.719234000	-3.693357000
H	-2.638202000	-4.823310000	0.115788000
H	-2.239859000	-6.415496000	-1.760647000
C	-3.688590000	-0.613062000	-0.222747000
C	-4.591101000	-1.409124000	-0.936000000
C	-3.504086000	-0.870263000	1.145325000
C	-5.282074000	-2.440231000	-0.301123000
H	-4.758749000	-1.234002000	-1.998423000
C	-4.197415000	-1.893389000	1.780144000
H	-2.794970000	-0.261645000	1.711986000
C	-5.086602000	-2.686796000	1.054865000
H	-5.974882000	-3.055775000	-0.872927000
H	-4.036939000	-2.074364000	2.842461000
H	-5.624548000	-3.495931000	1.545985000
C	-3.549341000	2.217119000	-0.490963000
C	-4.941347000	2.279622000	-0.643594000
C	-2.862210000	3.338351000	-0.014805000
C	-5.632621000	3.447086000	-0.340592000
H	-5.488375000	1.401044000	-0.990891000
C	-3.558630000	4.507690000	0.286206000
H	-1.787126000	3.283072000	0.138120000
C	-4.939263000	4.565425000	0.122106000
H	-6.714164000	3.484969000	-0.462090000
H	-3.012283000	5.375162000	0.653660000
H	-5.480581000	5.479928000	0.360207000

INT6

C	2.463986000	0.759893000	0.134735000
C	1.322426000	1.564888000	-0.307210000
Co	-0.504609000	0.140175000	0.010116000
P	-2.424800000	0.928054000	-0.853758000

P	-0.161651000	-1.294438000	-1.635285000
C	-0.584177000	-0.615430000	-3.300357000
H	-0.396727000	-1.387151000	-4.060220000
H	0.138031000	0.191392000	-3.493053000
C	-2.283948000	1.216773000	-2.678551000
H	-1.468455000	1.938841000	-2.837349000
H	-3.206184000	1.688949000	-3.046212000
C	-2.000262000	-0.063674000	-3.459414000
H	-2.154771000	0.147131000	-4.526738000
H	-2.745822000	-0.829927000	-3.195978000
C	2.231051000	-0.085447000	1.193591000
C	3.291122000	-0.600628000	2.087576000
C	3.188178000	-0.316855000	3.461285000
C	4.380198000	-1.374188000	1.662174000
C	4.136204000	-0.775043000	4.366395000
H	2.350482000	0.288130000	3.809825000
C	5.327501000	-1.838472000	2.570768000
H	4.469779000	-1.636956000	0.612536000
C	5.212825000	-1.543338000	3.926054000
H	4.034299000	-0.530007000	5.422568000
H	6.160853000	-2.441585000	2.212360000
H	5.954133000	-1.909488000	4.634230000
C	3.804502000	1.110665000	-0.393016000
C	4.310723000	2.408070000	-0.239521000
C	4.556871000	0.190154000	-1.131286000
C	5.539763000	2.762959000	-0.786021000
H	3.726010000	3.142772000	0.314309000
C	5.782326000	0.543698000	-1.686047000
H	4.145851000	-0.803395000	-1.299882000
C	6.281057000	1.832322000	-1.511721000
H	5.919523000	3.774243000	-0.648499000
H	6.342495000	-0.190804000	-2.264616000
H	7.239403000	2.113889000	-1.945140000
C	1.318267000	2.316741000	-1.578820000
C	0.634075000	3.538483000	-1.687455000
C	1.945674000	1.811255000	-2.729211000
C	0.563272000	4.214099000	-2.900813000
H	0.155583000	3.942244000	-0.797195000
C	1.874382000	2.488147000	-3.941845000
H	2.481521000	0.864092000	-2.668552000
C	1.178398000	3.692235000	-4.038778000
H	0.029765000	5.163388000	-2.956105000
H	2.365490000	2.068455000	-4.819349000
H	1.124132000	4.222601000	-4.987854000
C	0.157433000	1.127226000	1.672129000
C	-0.537458000	1.733271000	2.826619000
C	-1.280574000	2.913818000	2.668194000
C	-0.404777000	1.204937000	4.120676000
C	-1.888712000	3.523907000	3.758224000
H	-1.367028000	3.348714000	1.674830000
C	-1.012620000	1.818724000	5.209940000
H	0.186397000	0.303913000	4.274238000
C	-1.762834000	2.979200000	5.035042000
H	-2.464106000	4.436291000	3.605347000
H	-0.890296000	1.390137000	6.203458000
H	-2.236954000	3.460940000	5.888666000
N	0.388673000	1.954608000	0.601844000
C	0.816078000	-0.188879000	1.612564000
C	0.232958000	-1.360440000	2.296547000
C	-1.153343000	-1.383616000	2.587081000
C	0.943186000	-2.551009000	2.560942000
C	-1.782567000	-2.512317000	3.094152000
H	-1.751525000	-0.492804000	2.391408000
C	0.308597000	-3.680337000	3.072330000
H	2.008783000	-2.603835000	2.354560000
C	-1.056313000	-3.676187000	3.347987000
H	-2.855115000	-2.479635000	3.287258000
H	0.898847000	-4.577031000	3.257696000
H	-1.545707000	-4.561036000	3.751208000
C	1.511811000	-2.003138000	-1.929966000

C	2.085734000	-2.744124000	-0.887860000
C	2.216580000	-1.884957000	-3.134005000
C	3.304636000	-3.390966000	-1.060176000
H	1.559124000	-2.824098000	0.064610000
C	3.447186000	-2.519417000	-3.300765000
H	1.810408000	-1.299359000	-3.957316000
C	3.988736000	-3.283685000	-2.270919000
H	3.725746000	-3.970436000	-0.239424000
H	3.980823000	-2.416714000	-4.244357000
H	4.945014000	-3.785932000	-2.406499000
C	-1.147687000	-2.848185000	-1.548866000
C	-1.833292000	-3.395687000	-2.639055000
C	-1.211648000	-3.511739000	-0.316184000
C	-2.570322000	-4.569373000	-2.496605000
H	-1.798678000	-2.911763000	-3.613785000
C	-1.934648000	-4.691345000	-0.177430000
H	-0.702454000	-3.091079000	0.551343000
C	-2.622109000	-5.221090000	-1.267521000
H	-3.103489000	-4.976593000	-3.354224000
H	-1.965677000	-5.186228000	0.792527000
H	-3.198330000	-6.138624000	-1.159825000
C	-3.867250000	-0.201486000	-0.762690000
C	-5.063454000	0.066821000	-1.442295000
C	-3.772930000	-1.367532000	0.001284000
C	-6.129891000	-0.822255000	-1.370440000
H	-5.163511000	0.984747000	-2.023121000
C	-4.841284000	-2.258401000	0.077739000
H	-2.847537000	-1.582143000	0.536867000
C	-6.018693000	-1.988794000	-0.612705000
H	-7.053641000	-0.605230000	-1.904503000
H	-4.742995000	-3.165877000	0.672247000
H	-6.854909000	-2.684078000	-0.559935000
C	-3.156096000	2.502770000	-0.277797000
C	-4.037244000	2.505234000	0.811732000
C	-2.771693000	3.728545000	-0.835328000
C	-4.527537000	3.701366000	1.323915000
H	-4.337683000	1.559823000	1.265117000
C	-3.256444000	4.925904000	-0.315581000
H	-2.080282000	3.751332000	-1.676943000
C	-4.135768000	4.916260000	0.764814000
H	-5.209839000	3.684253000	2.172347000
H	-2.946904000	5.870549000	-0.760684000
H	-4.514553000	5.852950000	1.170282000

3aa

C	-1.220758000	0.105952000	-0.023245000
C	-1.162084000	-1.304602000	0.044237000
C	-0.000011000	0.812226000	-0.000092000
C	0.000182000	2.299712000	-0.000083000
C	-0.550866000	3.012917000	-1.070407000
C	0.551509000	3.012698000	1.070242000
C	-0.545752000	4.403628000	-1.073285000
H	-0.990932000	2.466781000	-1.904331000
C	0.546739000	4.403420000	1.073213000
H	0.991467000	2.466418000	1.904129000
C	0.000568000	5.103538000	-0.000001000
H	-0.974462000	4.942515000	-1.916390000
H	0.975618000	4.942130000	1.916347000
H	0.000693000	6.192082000	0.000033000
C	-2.516417000	0.820665000	-0.130042000
C	-3.389288000	0.530352000	-1.185897000
C	-2.902093000	1.784823000	0.809870000
C	-4.609920000	1.186509000	-1.301578000
H	-3.103367000	-0.224964000	-1.917616000
C	-4.125732000	2.435919000	0.699140000
H	-2.231390000	2.023817000	1.634378000
C	-4.983756000	2.140580000	-0.357984000
H	-5.273083000	0.949117000	-2.131656000
H	-4.409576000	3.178962000	1.442437000

H	-5.940371000	2.652475000	-0.446166000
C	-2.353554000	-2.181527000	0.170427000
C	-2.341821000	-3.427684000	-0.471396000
C	-3.464262000	-1.847073000	0.957481000
C	-3.418170000	-4.299181000	-0.356492000
H	-1.466261000	-3.698630000	-1.057360000
C	-4.534166000	-2.726063000	1.083774000
H	-3.487249000	-0.897095000	1.487356000
C	-4.520757000	-3.950928000	0.420635000
H	-3.394691000	-5.257137000	-0.873561000
H	-5.382616000	-2.451760000	1.708323000
H	-5.363673000	-4.633662000	0.514587000
C	1.161747000	-1.304737000	-0.044299000
C	2.353169000	-2.181725000	-0.170538000
C	2.341487000	-3.427776000	0.471455000
C	3.463797000	-1.847316000	-0.957715000
C	3.417861000	-4.299257000	0.356593000
H	1.465976000	-3.698686000	1.057520000
C	4.533722000	-2.726277000	-1.083959000
H	3.486715000	-0.897350000	-1.487629000
C	4.520379000	-3.951063000	-0.420652000
H	3.394456000	-5.257137000	0.873807000
H	5.382141000	-2.452038000	-1.708576000
H	5.363315000	-4.633777000	-0.514563000
N	-0.000186000	-1.965678000	-0.000076000
C	1.220626000	0.105798000	0.023174000
C	2.516378000	0.820308000	0.130093000
C	3.389035000	0.529915000	1.186120000
C	2.902354000	1.784296000	-0.809851000
C	4.609792000	1.185801000	1.301883000
H	3.102818000	-0.225282000	1.917846000
C	4.126139000	2.435120000	-0.699042000
H	2.231789000	2.023339000	-1.634461000
C	4.983959000	2.139679000	0.358212000
H	5.272825000	0.948375000	2.132053000
H	4.410256000	3.178013000	-1.442381000
H	5.940679000	2.651369000	0.446470000

TS6

C	-1.501314000	1.213466000	-1.211874000
Co	0.086181000	0.112236000	-0.329555000
P	-0.836220000	-1.946033000	-0.520550000
P	1.992422000	-0.584719000	-1.073947000
C	1.882774000	-1.679129000	-2.559055000
H	2.890116000	-1.837774000	-2.968495000
H	1.326606000	-1.098834000	-3.308982000
C	-0.296593000	-2.918951000	-2.005310000
H	-0.791759000	-2.417653000	-2.848680000
H	-0.743347000	-3.921749000	-1.946953000
C	1.198370000	-3.014938000	-2.289141000
H	1.331131000	-3.660091000	-3.169524000
H	1.711575000	-3.530927000	-1.463506000
C	-0.727312000	1.807475000	0.449643000
C	-1.638594000	2.522242000	1.349391000
C	-1.805551000	2.096443000	2.675299000
C	-2.340921000	3.659727000	0.923984000
C	-2.659526000	2.772384000	3.539730000
H	-1.256193000	1.218062000	3.016211000
C	-3.192284000	4.336372000	1.789917000
H	-2.225168000	3.997070000	-0.106107000
C	-3.362077000	3.892560000	3.099780000
H	-2.776368000	2.422934000	4.564891000
H	-3.732087000	5.213797000	1.436590000
H	-4.034681000	4.418620000	3.774938000
C	-2.963534000	1.340420000	-1.093807000
C	-3.663193000	0.836721000	0.007226000
C	-3.674508000	1.933794000	-2.142755000
C	-5.047167000	0.927625000	0.063178000
H	-3.107512000	0.354945000	0.811292000

C	-5.060390000	2.036658000	-2.078484000
H	-3.123758000	2.311343000	-3.003035000
C	-5.750275000	1.536911000	-0.975285000
H	-5.579637000	0.517713000	0.920014000
H	-5.604904000	2.509264000	-2.894844000
H	-6.835058000	1.618610000	-0.926428000
C	0.599523000	1.777735000	0.414550000
C	1.670377000	2.637184000	0.846424000
C	2.932745000	2.142896000	1.219027000
C	1.479941000	4.034111000	0.855399000
C	3.959015000	3.002674000	1.585961000
H	3.103802000	1.066759000	1.205931000
C	2.511563000	4.892109000	1.210348000
H	0.506799000	4.430525000	0.567828000
C	3.757046000	4.381975000	1.576687000
H	4.929747000	2.594137000	1.864029000
H	2.344159000	5.968317000	1.202423000
H	4.566811000	5.056344000	1.850368000
N	-0.743416000	0.896820000	-2.135508000
C	2.966676000	-1.613309000	0.093849000
C	3.945621000	-2.528186000	-0.317801000
C	2.659367000	-1.534161000	1.458056000
C	4.599437000	-3.335506000	0.608656000
H	4.195735000	-2.618890000	-1.375418000
C	3.317216000	-2.334362000	2.387485000
H	1.877904000	-0.844072000	1.783683000
C	4.286594000	-3.239053000	1.963101000
H	5.354455000	-4.043774000	0.271276000
H	3.057723000	-2.262157000	3.442264000
H	4.794878000	-3.874820000	2.686147000
C	3.132789000	0.717708000	-1.667978000
C	2.557529000	1.854116000	-2.249611000
C	4.522877000	0.638042000	-1.541703000
C	3.366030000	2.894991000	-2.694237000
H	1.469079000	1.915940000	-2.322289000
C	5.327558000	1.685028000	-1.984075000
H	4.980836000	-0.231145000	-1.069346000
C	4.750459000	2.815199000	-2.557156000
H	2.910399000	3.781208000	-3.132775000
H	6.408524000	1.621744000	-1.868029000
H	5.380266000	3.638629000	-2.890149000
C	-0.399380000	-2.988822000	0.915879000
C	0.143880000	-4.274148000	0.821006000
C	-0.569448000	-2.423448000	2.188742000
C	0.519467000	-4.970695000	1.968071000
H	0.280797000	-4.741153000	-0.153328000
C	-0.219730000	-3.127937000	3.334834000
H	-0.974329000	-1.411099000	2.267774000
C	0.335587000	-4.402428000	3.225207000
H	0.954197000	-5.964757000	1.876832000
H	-0.367357000	-2.677220000	4.314996000
H	0.627403000	-4.949985000	4.119809000
C	-2.643702000	-2.202805000	-0.718586000
C	-3.248194000	-1.709401000	-1.884284000
C	-3.441634000	-2.825884000	0.245877000
C	-4.615957000	-1.849120000	-2.084176000
H	-2.647590000	-1.169833000	-2.618904000
C	-4.814797000	-2.955147000	0.046736000
H	-2.989907000	-3.217079000	1.156910000
C	-5.403925000	-2.471147000	-1.117673000
H	-5.071651000	-1.445906000	-2.987047000
H	-5.424544000	-3.442657000	0.806099000
H	-6.477724000	-2.569136000	-1.268782000

INT7

C	-1.667484000	1.321129000	-0.934145000
Co	0.051792000	0.081360000	-0.431889000
P	-0.776129000	-2.041586000	-0.452565000
P	1.985459000	-0.577042000	-1.064192000

C	1.863581000	-1.701284000	-2.533194000
H	2.864754000	-1.824184000	-2.969317000
H	1.263919000	-1.152620000	-3.273603000
C	-0.246386000	-3.035144000	-1.920169000
H	-0.789279000	-2.575387000	-2.758205000
H	-0.643525000	-4.055712000	-1.823611000
C	1.245093000	-3.063454000	-2.237292000
H	1.388103000	-3.708898000	-3.115757000
H	1.800659000	-3.548045000	-1.420077000
C	-0.951967000	1.957595000	0.198987000
C	-1.635965000	2.780898000	1.223678000
C	-1.267553000	2.674143000	2.572398000
C	-2.607247000	3.731505000	0.874984000
C	-1.851298000	3.483168000	3.540788000
H	-0.508152000	1.941491000	2.848592000
C	-3.189099000	4.542443000	1.842810000
H	-2.901053000	3.835884000	-0.168824000
C	-2.816731000	4.420762000	3.180306000
H	-1.551165000	3.381290000	4.582803000
H	-3.937901000	5.276787000	1.549488000
H	-3.276078000	5.054375000	3.937198000
C	-3.156860000	1.265313000	-0.951150000
C	-3.900483000	0.900889000	0.178168000
C	-3.833855000	1.528898000	-2.147596000
C	-5.286012000	0.807320000	0.113131000
H	-3.380786000	0.674758000	1.110282000
C	-5.221635000	1.456438000	-2.206851000
H	-3.248195000	1.789154000	-3.028461000
C	-5.953168000	1.094737000	-1.076280000
H	-5.848263000	0.503514000	0.995184000
H	-5.736229000	1.680323000	-3.140842000
H	-7.039450000	1.030790000	-1.123520000
C	0.424699000	1.733080000	0.223768000
C	1.472049000	2.621007000	0.664693000
C	2.713481000	2.151900000	1.132587000
C	1.298401000	4.019291000	0.570058000
C	3.731705000	3.028242000	1.480914000
H	2.873736000	1.077054000	1.210824000
C	2.316530000	4.894232000	0.920251000
H	0.347498000	4.404662000	0.204286000
C	3.541020000	4.405180000	1.375715000
H	4.685436000	2.633304000	1.829123000
H	2.156966000	5.968067000	0.832245000
H	4.341620000	5.092508000	1.644001000
N	-0.985580000	0.731757000	-1.900424000
C	3.014337000	-1.572055000	0.087864000
C	4.029878000	-2.436489000	-0.344583000
C	2.718844000	-1.520147000	1.455290000
C	4.730289000	-3.221627000	0.566621000
H	4.274837000	-2.501512000	-1.405380000
C	3.424591000	-2.296402000	2.369936000
H	1.905109000	-0.874267000	1.792241000
C	4.429337000	-3.151478000	1.925638000
H	5.513752000	-3.890763000	0.214481000
H	3.174931000	-2.245506000	3.428320000
H	4.975490000	-3.769175000	2.636664000
C	3.085474000	0.731420000	-1.715072000
C	2.476421000	1.779778000	-2.417200000
C	4.469621000	0.746994000	-1.520849000
C	3.245668000	2.827262000	-2.912065000
H	1.390133000	1.779215000	-2.534109000
C	5.234889000	1.799560000	-2.016517000
H	4.951466000	-0.050096000	-0.954877000
C	4.624407000	2.841669000	-2.708765000
H	2.763392000	3.645118000	-3.444786000
H	6.310670000	1.811012000	-1.847810000
H	5.222502000	3.670337000	-3.084328000
C	-0.274423000	-3.011854000	1.009775000
C	0.311379000	-4.280157000	0.949048000
C	-0.450661000	-2.409844000	2.265189000

C	0.720018000	-4.927290000	2.113638000
H	0.453461000	-4.773276000	-0.011687000
C	-0.066101000	-3.065609000	3.428702000
H	-0.889813000	-1.409771000	2.318791000
C	0.528831000	-4.325025000	3.353639000
H	1.186317000	-5.909046000	2.049621000
H	-0.219438000	-2.589083000	4.395612000
H	0.845610000	-4.834118000	4.262358000
C	-2.582865000	-2.314798000	-0.565644000
C	-3.243482000	-1.811987000	-1.696390000
C	-3.319725000	-2.995267000	0.408971000
C	-4.610102000	-2.007493000	-1.854497000
H	-2.685797000	-1.225874000	-2.428906000
C	-4.692042000	-3.177408000	0.250717000
H	-2.821839000	-3.392769000	1.292424000
C	-5.337666000	-2.690016000	-0.881621000
H	-5.112778000	-1.599217000	-2.729297000
H	-5.255519000	-3.709150000	1.015955000
H	-6.410761000	-2.830934000	-1.002068000

CPA_t

C	-0.716860000	1.858486000	0.548578000
Co	0.257479000	0.596385000	-0.694468000
P	1.716786000	-1.220883000	-0.701260000
P	-1.459414000	-0.879146000	-1.124207000
C	-1.108414000	-2.021316000	-2.546910000
H	-2.010721000	-2.606369000	-2.777096000
H	-0.925148000	-1.384759000	-3.424035000
C	1.447230000	-2.324343000	-2.169326000
H	1.652550000	-1.690707000	-3.044050000
H	2.226815000	-3.099299000	-2.172886000
C	0.069252000	-2.970225000	-2.314461000
H	0.116045000	-3.662150000	-3.168058000
H	-0.144649000	-3.596391000	-1.436591000
C	0.476597000	2.261104000	0.193823000
C	1.503933000	3.225709000	0.538639000
C	1.281800000	4.179231000	1.549209000
C	2.751696000	3.211717000	-0.103539000
C	2.274728000	5.086159000	1.896962000
H	0.319337000	4.188985000	2.060686000
C	3.744513000	4.118262000	0.247474000
H	2.925841000	2.469581000	-0.882668000
C	3.509975000	5.059678000	1.248256000
H	2.087096000	5.818815000	2.680880000
H	4.707602000	4.084841000	-0.260901000
H	4.287254000	5.770186000	1.525380000
C	-1.999995000	2.234299000	1.060293000
C	-2.428178000	3.574998000	0.905040000
C	-2.921817000	1.314811000	1.602187000
C	-3.709029000	3.963864000	1.268914000
H	-1.734723000	4.296897000	0.473363000
C	-4.195142000	1.715090000	1.979342000
H	-2.628724000	0.271327000	1.708044000
C	-4.603339000	3.039574000	1.812166000
H	-4.013451000	5.001172000	1.131710000
H	-4.885386000	0.980679000	2.393055000
H	-5.608326000	3.346448000	2.095931000
C	-3.115221000	-0.194543000	-1.488223000
C	-4.307033000	-0.915327000	-1.353973000
C	-3.172653000	1.151302000	-1.868970000
C	-5.530863000	-0.302328000	-1.604609000
H	-4.283795000	-1.955007000	-1.028388000
C	-4.396612000	1.763667000	-2.118563000
H	-2.245609000	1.725094000	-1.932726000
C	-5.576890000	1.037302000	-1.985740000
H	-6.453127000	-0.870043000	-1.491768000
H	-4.427936000	2.816504000	-2.393197000
H	-6.536585000	1.518197000	-2.167642000
C	-1.701345000	-2.091686000	0.234743000

C	-2.315316000	-3.338537000	0.042195000
C	-1.174555000	-1.797646000	1.499187000
C	-2.410968000	-4.254623000	1.085709000
H	-2.708736000	-3.609363000	-0.938269000
C	-1.278754000	-2.708290000	2.546221000
H	-0.657537000	-0.847388000	1.646827000
C	-1.894948000	-3.939696000	2.340953000
H	-2.886203000	-5.219417000	0.915590000
H	-0.854145000	-2.462069000	3.517576000
H	-1.961499000	-4.660104000	3.154597000
C	2.011079000	-2.333401000	0.705303000
C	1.846444000	-3.726345000	0.647139000
C	2.232043000	-1.740368000	1.964080000
C	1.913832000	-4.498132000	1.802988000
H	1.670305000	-4.218702000	-0.308428000
C	2.325679000	-2.516801000	3.110808000
H	2.324983000	-0.654123000	2.033471000
C	2.160309000	-3.901773000	3.037976000
H	1.780604000	-5.577078000	1.735479000
H	2.515995000	-2.038731000	4.070727000
H	2.216371000	-4.509275000	3.939330000
C	3.363575000	-0.519460000	-1.104329000
C	3.460522000	0.265686000	-2.263573000
C	4.485590000	-0.649385000	-0.282072000
C	4.655150000	0.896778000	-2.596569000
H	2.577001000	0.410886000	-2.890768000
C	5.675096000	0.002470000	-0.604813000
H	4.430919000	-1.260854000	0.617290000
C	5.763454000	0.774164000	-1.760606000
H	4.715101000	1.498070000	-3.502326000
H	6.537574000	-0.097689000	0.051992000
H	6.694985000	1.279094000	-2.010924000

CP_{2A_q}

C	-0.278883000	-2.265253000	0.469158000
C	0.480084000	-2.250446000	-0.567070000
Co	0.280262000	-0.411596000	0.269075000
P	1.691963000	0.775416000	-1.182755000
P	-1.648558000	0.242327000	-1.159204000
C	-1.093946000	-0.126865000	-2.897943000
H	-1.984817000	-0.115228000	-3.541214000
H	-0.695759000	-1.152126000	-2.919552000
C	1.389183000	0.596779000	-2.994432000
H	1.672564000	-0.434987000	-3.244059000
H	2.079029000	1.246839000	-3.551906000
C	-0.051534000	0.847701000	-3.447125000
H	-0.065223000	0.777536000	-4.543541000
H	-0.358911000	1.878417000	-3.214053000
C	-0.157467000	0.912335000	1.776134000
C	0.905279000	0.199729000	2.034558000
C	1.887158000	-0.290748000	2.941406000
C	2.633245000	0.623326000	3.727377000
C	2.255529000	-1.657489000	2.998519000
C	3.694254000	0.190341000	4.507580000
H	2.361759000	1.679180000	3.704950000
C	3.306720000	-2.078512000	3.796899000
H	1.696748000	-2.376901000	2.398857000
C	4.044192000	-1.161507000	4.552811000
H	4.251080000	0.916007000	5.099790000
H	3.558712000	-3.138131000	3.831251000
H	4.874079000	-1.496506000	5.171717000
C	-1.207444000	1.767850000	2.193765000
C	-0.921735000	3.056270000	2.716624000
C	-2.569099000	1.435337000	1.983830000
C	-1.938785000	3.962953000	2.964299000
H	0.116994000	3.329460000	2.900765000
C	-3.578104000	2.346230000	2.254154000
H	-2.810762000	0.438758000	1.614328000
C	-3.276913000	3.624579000	2.729897000

H	-1.690189000	4.948445000	3.358034000
H	-4.617032000	2.056948000	2.090217000
H	-4.070283000	4.342509000	2.927253000
C	-1.139953000	-2.930392000	1.408131000
C	-1.391504000	-4.307915000	1.254091000
C	-1.774857000	-2.240612000	2.453269000
C	-2.264786000	-4.963817000	2.109991000
H	-0.888809000	-4.851520000	0.454627000
C	-2.651160000	-2.902614000	3.303546000
H	-1.565377000	-1.180324000	2.586606000
C	-2.903684000	-4.262591000	3.133140000
H	-2.450789000	-6.028598000	1.978346000
H	-3.139363000	-2.351762000	4.105328000
H	-3.592931000	-4.778249000	3.799477000
C	0.964654000	-2.996504000	-1.702879000
C	2.212678000	-2.749913000	-2.299797000
C	0.166555000	-4.026923000	-2.242990000
C	2.640847000	-3.494124000	-3.392720000
H	2.855858000	-1.979488000	-1.878655000
C	0.591234000	-4.756213000	-3.346199000
H	-0.794396000	-4.246870000	-1.778142000
C	1.830157000	-4.493194000	-3.928857000
H	3.617479000	-3.290832000	-3.828847000
H	-0.046196000	-5.541987000	-3.748508000
H	2.164498000	-5.068852000	-4.789735000
C	1.712599000	2.588430000	-0.921597000
C	1.943771000	3.057301000	0.380357000
C	1.502763000	3.522460000	-1.943258000
C	1.942111000	4.419917000	0.653904000
H	2.122745000	2.340673000	1.181568000
C	1.501865000	4.888588000	-1.666338000
H	1.333661000	3.195541000	-2.967372000
C	1.713898000	5.341108000	-0.368471000
H	2.120972000	4.764465000	1.671387000
H	1.328869000	5.599230000	-2.472932000
H	1.707152000	6.408086000	-0.152683000
C	3.470357000	0.382166000	-0.986796000
C	4.457185000	1.004666000	-1.761723000
C	3.854664000	-0.511618000	0.018380000
C	5.801702000	0.725155000	-1.539814000
H	4.173539000	1.726821000	-2.528785000
C	5.201017000	-0.779639000	0.250250000
H	3.088814000	-0.994744000	0.625911000
C	6.174995000	-0.163324000	-0.531289000
H	6.563049000	1.211582000	-2.147505000
H	5.480173000	-1.464548000	1.049222000
H	7.229154000	-0.368419000	-0.352226000
C	-3.100636000	-0.853375000	-1.009777000
C	-2.996673000	-2.188428000	-1.427110000
C	-4.270756000	-0.452522000	-0.346638000
C	-4.018715000	-3.097210000	-1.177030000
H	-2.096939000	-2.523791000	-1.942277000
C	-5.294915000	-1.361692000	-0.103589000
H	-4.378343000	0.583599000	-0.026261000
C	-5.171030000	-2.689524000	-0.508768000
H	-3.910085000	-4.131759000	-1.501614000
H	-6.196267000	-1.029274000	0.409060000
H	-5.968513000	-3.401685000	-0.305603000
C	-2.362732000	1.910072000	-1.381667000
C	-3.503807000	2.119766000	-2.170259000
C	-1.732334000	3.011833000	-0.793698000
C	-4.010024000	3.402534000	-2.349042000
H	-4.007515000	1.268560000	-2.630277000
C	-2.239415000	4.295783000	-0.975429000
H	-0.854563000	2.857159000	-0.168354000
C	-3.378785000	4.492720000	-1.750256000
H	-4.900935000	3.552810000	-2.956963000
H	-1.744651000	5.137594000	-0.493425000
H	-3.780562000	5.495564000	-1.886899000

INT2_q

C	-2.307541000	0.950075000	-0.523517000
C	-1.227617000	1.582695000	0.030888000
Co	0.386113000	0.427403000	-0.243537000
P	2.538658000	1.285078000	0.001413000
P	0.546521000	-0.926478000	1.635905000
C	1.331337000	-0.015072000	3.049768000
H	1.328689000	-0.666614000	3.934569000
H	0.690991000	0.843416000	3.296065000
C	2.902654000	1.624880000	1.788199000
H	2.224051000	2.442571000	2.072355000
H	3.916413000	2.045693000	1.855801000
C	2.758790000	0.447774000	2.755938000
H	3.217381000	0.747359000	3.708770000
H	3.352978000	-0.409388000	2.401209000
C	-2.052622000	-0.353121000	-1.193335000
C	-3.180510000	-1.276510000	-1.465801000
C	-3.318206000	-1.936601000	-2.694428000
C	-4.113541000	-1.556340000	-0.456264000
C	-4.347046000	-2.848723000	-2.904224000
H	-2.601304000	-1.727797000	-3.488293000
C	-5.133268000	-2.478675000	-0.659111000
H	-4.018567000	-1.048501000	0.503621000
C	-5.256972000	-3.128157000	-1.886187000
H	-4.438172000	-3.346473000	-3.868786000
H	-5.836703000	-2.689457000	0.146448000
H	-6.059733000	-3.845586000	-2.049876000
C	-3.673730000	1.522946000	-0.513618000
C	-4.484049000	1.507084000	-1.659686000
C	-4.193910000	2.114346000	0.647602000
C	-5.754479000	2.072149000	-1.648037000
H	-4.104493000	1.046190000	-2.571041000
C	-5.466005000	2.674280000	0.663650000
H	-3.577945000	2.129395000	1.547041000
C	-6.253394000	2.657222000	-0.486020000
H	-6.360788000	2.052376000	-2.552666000
H	-5.846772000	3.124526000	1.579653000
H	-7.251024000	3.093405000	-0.475253000
C	-1.179740000	2.961109000	0.492768000
C	-1.697775000	4.033002000	-0.267944000
C	-0.476966000	3.298276000	1.667666000
C	-1.503282000	5.352703000	0.119821000
H	-2.244817000	3.807004000	-1.182590000
C	-0.296815000	4.617462000	2.066353000
H	-0.063162000	2.484520000	2.267506000
C	-0.801692000	5.657591000	1.287808000
H	-1.905171000	6.156623000	-0.496517000
H	0.249219000	4.836452000	2.983891000
H	-0.649431000	6.693400000	1.585586000
C	-0.750062000	-0.708638000	-1.429016000
C	-0.286919000	-2.003516000	-1.919747000
C	0.673099000	-2.081320000	-2.946991000
C	-0.679443000	-3.213967000	-1.310839000
C	1.218882000	-3.298851000	-3.340619000
H	0.979525000	-1.157442000	-3.440396000
C	-0.122890000	-4.427734000	-1.694119000
H	-1.431244000	-3.181248000	-0.521553000
C	0.832523000	-4.480772000	-2.709100000
H	1.950944000	-3.325952000	-4.148026000
H	-0.435681000	-5.343767000	-1.193273000
H	1.267733000	-5.433231000	-3.007462000
C	3.875054000	0.144222000	-0.505459000
C	3.687524000	-0.579162000	-1.690959000
C	5.044718000	-0.070638000	0.233813000
C	4.641592000	-1.490783000	-2.128428000
H	2.764258000	-0.443781000	-2.256664000
C	5.997638000	-0.989511000	-0.199768000
H	5.219246000	0.477630000	1.159203000
C	5.798820000	-1.700203000	-1.380396000

H	4.471792000	-2.049633000	-3.047342000
H	6.898605000	-1.150642000	0.389647000
H	6.542453000	-2.421771000	-1.714119000
C	2.996032000	2.885852000	-0.756343000
C	4.324805000	3.237590000	-1.023409000
C	1.974625000	3.802307000	-1.032070000
C	4.624572000	4.488722000	-1.553071000
H	5.126459000	2.525019000	-0.825664000
C	2.279650000	5.057350000	-1.551343000
H	0.936861000	3.533345000	-0.833783000
C	3.603137000	5.400759000	-1.814350000
H	5.659622000	4.752575000	-1.764178000
H	1.475026000	5.762424000	-1.752826000
H	3.841333000	6.379269000	-2.228065000
C	-1.082463000	-1.401450000	2.304765000
C	-1.543329000	-2.723324000	2.296258000
C	-1.945081000	-0.385381000	2.742830000
C	-2.830797000	-3.024225000	2.734683000
H	-0.892320000	-3.521349000	1.939927000
C	-3.224108000	-0.691435000	3.195812000
H	-1.618941000	0.655790000	2.706946000
C	-3.669744000	-2.012422000	3.193067000
H	-3.178989000	-4.055471000	2.713230000
H	-3.881609000	0.107559000	3.534573000
H	-4.676082000	-2.249319000	3.534406000
C	1.539062000	-2.461997000	1.629949000
C	1.727980000	-3.222465000	2.793554000
C	2.171245000	-2.862083000	0.448901000
C	2.537185000	-4.352604000	2.773375000
H	1.224771000	-2.935723000	3.718122000
C	2.986696000	-3.991531000	0.430091000
H	2.012348000	-2.294136000	-0.467595000
C	3.171860000	-4.735201000	1.590923000
H	2.673874000	-4.938107000	3.681099000
H	3.465974000	-4.288233000	-0.501582000
H	3.806789000	-5.619676000	1.577903000

INT5_q

C	1.879746000	1.458602000	-0.086264000
C	0.596269000	1.596384000	-0.555906000
Co	-0.810493000	0.227119000	-0.171473000
P	-3.133807000	0.451008000	-0.583543000
P	-0.540190000	-1.453016000	-1.750450000
C	-1.687908000	-1.267763000	-3.208902000
H	-1.484144000	-2.103785000	-3.892715000
H	-1.372719000	-0.358550000	-3.742486000
C	-3.670087000	0.123098000	-2.319636000
H	-3.289449000	0.963028000	-2.919736000
H	-4.766128000	0.186973000	-2.380815000
C	-3.179249000	-1.205237000	-2.897548000
H	-3.725787000	-1.388772000	-3.833411000
H	-3.451193000	-2.037326000	-2.230066000
C	2.327281000	0.207807000	0.572352000
C	3.676235000	-0.289890000	0.190520000
C	4.561124000	-0.786805000	1.160412000
C	4.126595000	-0.226659000	-1.134028000
C	5.832507000	-1.227267000	0.816424000
H	4.236711000	-0.828340000	2.200451000
C	5.395967000	-0.673236000	-1.483503000
H	3.459814000	0.170368000	-1.896561000
C	6.255794000	-1.177127000	-0.510924000
H	6.500465000	-1.604394000	1.589404000
H	5.714057000	-0.623346000	-2.524506000
H	7.253423000	-1.519273000	-0.781871000
C	2.931250000	2.493176000	-0.287640000
C	3.776669000	2.846278000	0.773887000
C	3.119641000	3.136521000	-1.518937000
C	4.757377000	3.820247000	0.619357000
H	3.647868000	2.348201000	1.736294000

C	4.10202000	4.106695000	-1.678589000
H	2.484669000	2.858497000	-2.360996000
C	4.923993000	4.456580000	-0.608556000
H	5.396345000	4.082524000	1.461574000
H	4.232345000	4.588876000	-2.646638000
H	5.694272000	5.215915000	-0.733646000
C	0.066908000	2.825144000	-1.149002000
C	0.214032000	4.090433000	-0.543179000
C	-0.755222000	2.755237000	-2.292965000
C	-0.432964000	5.210759000	-1.051888000
H	0.836273000	4.175016000	0.346944000
C	-1.383017000	3.878818000	-2.816320000
H	-0.906632000	1.776034000	-2.758119000
C	-1.231288000	5.116598000	-2.192366000
H	-0.311114000	6.172087000	-0.553241000
H	-2.008944000	3.786794000	-3.703871000
H	-1.737593000	5.996579000	-2.585074000
C	0.448616000	0.188537000	2.241203000
C	0.728481000	0.767618000	3.582335000
C	-0.326695000	1.276376000	4.354352000
C	2.030736000	0.842905000	4.096415000
C	-0.086217000	1.839874000	5.598960000
H	-1.333103000	1.220714000	3.941966000
C	2.272310000	1.410909000	5.343798000
H	2.859939000	0.454981000	3.504015000
C	1.215208000	1.910139000	6.099904000
H	-0.916265000	2.230258000	6.186338000
H	3.290723000	1.464628000	5.725521000
H	1.402673000	2.354524000	7.076114000
N	-0.716009000	0.245316000	1.716838000
C	1.590050000	-0.473038000	1.515615000
C	1.762790000	-1.906007000	1.831899000
C	1.439537000	-2.433128000	3.095221000
C	2.117893000	-2.820984000	0.821802000
C	1.494854000	-3.801983000	3.339573000
H	1.144258000	-1.761508000	3.899553000
C	2.166512000	-4.185791000	1.064513000
H	2.340508000	-2.440630000	-0.173950000
C	1.858314000	-4.687916000	2.328557000
H	1.246910000	-4.177906000	4.331401000
H	2.427237000	-4.866397000	0.253738000
H	1.888747000	-5.759574000	2.518706000
C	1.020065000	-1.572338000	-2.702523000
C	1.835954000	-2.707661000	-2.747880000
C	1.388500000	-0.446536000	-3.454833000
C	2.980168000	-2.723006000	-3.542974000
H	1.574427000	-3.586676000	-2.159628000
C	2.517227000	-0.472189000	-4.266583000
H	0.791887000	0.465741000	-3.390467000
C	3.315137000	-1.613968000	-4.314557000
H	3.610462000	-3.610450000	-3.560215000
H	2.784288000	0.409504000	-4.847229000
H	4.204697000	-1.633552000	-4.941935000
C	-0.926882000	-3.133131000	-1.152309000
C	-0.981858000	-4.256790000	-1.988421000
C	-1.226667000	-3.279801000	0.207753000
C	-1.317898000	-5.502808000	-1.469749000
H	-0.747557000	-4.158101000	-3.049501000
C	-1.573644000	-4.525561000	0.723512000
H	-1.171810000	-2.407970000	0.864704000
C	-1.615326000	-5.636744000	-0.113327000
H	-1.351993000	-6.371933000	-2.124745000
H	-1.797874000	-4.624224000	1.784182000
H	-1.880194000	-6.613199000	0.289165000
C	-4.048884000	-0.814144000	0.380067000
C	-5.091924000	-1.589003000	-0.143531000
C	-3.664606000	-1.012661000	1.715087000
C	-5.727322000	-2.547546000	0.642338000
H	-5.419405000	-1.452782000	-1.173768000
C	-4.308581000	-1.964523000	2.498958000

H	-2.838778000	-0.427432000	2.123695000
C	-5.336195000	-2.738848000	1.964453000
H	-6.532216000	-3.145134000	0.217386000
H	-3.998004000	-2.107302000	3.532890000
H	-5.832143000	-3.490406000	2.576541000
C	-4.021672000	2.000186000	-0.191832000
C	-5.420359000	2.068003000	-0.232445000
C	-3.288315000	3.141302000	0.144964000
C	-6.073151000	3.263044000	0.046306000
H	-6.000608000	1.173816000	-0.467750000
C	-3.944807000	4.338829000	0.420831000
H	-2.199959000	3.091406000	0.185647000
C	-5.334078000	4.400985000	0.370645000
H	-7.160657000	3.307786000	0.015873000
H	-3.362326000	5.222960000	0.674302000
H	-5.846706000	5.336494000	0.588978000

TS1_q

C	1.484532000	-0.532710000	1.324905000
C	2.069560000	-0.424212000	0.143535000
Co	0.113157000	-0.086092000	-0.011960000
P	-0.765618000	-1.743117000	-1.390893000
P	0.137120000	1.540216000	-1.695837000
C	0.139539000	0.934084000	-3.439608000
H	0.027473000	1.789371000	-4.120125000
H	1.143463000	0.526115000	-3.626471000
C	-0.559059000	-1.531011000	-3.214347000
H	0.496833000	-1.740848000	-3.437115000
H	-1.143404000	-2.296598000	-3.743829000
C	-0.915094000	-0.137018000	-3.734065000
H	-1.044222000	-0.198828000	-4.823808000
H	-1.894109000	0.176260000	-3.337716000
C	-0.209459000	0.699883000	1.711643000
C	-1.357747000	0.165142000	1.309051000
C	-2.770216000	0.272303000	1.482944000
C	-3.367004000	0.115833000	2.756377000
C	-3.630872000	0.475371000	0.379689000
C	-4.745766000	0.166099000	2.910616000
H	-2.726067000	-0.063823000	3.620654000
C	-5.003723000	0.551219000	0.547225000
H	-3.189877000	0.583559000	-0.612317000
C	-5.576605000	0.391530000	1.811715000
H	-5.177992000	0.037911000	3.902685000
H	-5.637233000	0.724299000	-0.322771000
H	-6.656612000	0.439158000	1.938539000
C	0.286899000	1.839519000	2.450144000
C	-0.466524000	2.343618000	3.528071000
C	1.474217000	2.505541000	2.090180000
C	-0.043646000	3.471761000	4.219581000
H	-1.392908000	1.840557000	3.803097000
C	1.882871000	3.639488000	2.778781000
H	2.058391000	2.129364000	1.249281000
C	1.130820000	4.126029000	3.849141000
H	-0.637146000	3.846216000	5.052450000
H	2.795223000	4.150604000	2.474245000
H	1.457901000	5.011973000	4.390596000
C	1.711063000	-1.274889000	2.552527000
C	0.680898000	-1.661856000	3.428430000
C	3.027348000	-1.673267000	2.856654000
C	0.957760000	-2.420529000	4.558463000
H	-0.343857000	-1.375191000	3.196952000
C	3.299428000	-2.421050000	3.995200000
H	3.830714000	-1.395711000	2.175863000
C	2.267466000	-2.800174000	4.852156000
H	0.143524000	-2.718440000	5.217388000
H	4.325412000	-2.714513000	4.212662000
H	2.481530000	-3.388469000	5.742726000
C	3.267008000	-0.698172000	-0.576528000
C	4.512999000	-0.187013000	-0.140004000

C	3.242147000	-1.391701000	-1.809248000
C	5.659319000	-0.353334000	-0.903392000
H	4.550023000	0.377173000	0.792621000
C	4.398058000	-1.571374000	-2.554123000
H	2.292013000	-1.802647000	-2.153117000
C	5.616351000	-1.045974000	-2.115824000
H	6.602015000	0.061940000	-0.547930000
H	4.350983000	-2.124955000	-3.491576000
H	6.519040000	-1.177266000	-2.708952000
C	1.539398000	2.715847000	-1.675678000
C	1.413771000	4.033978000	-1.220199000
C	2.813961000	2.239223000	-2.016463000
C	2.534731000	4.851749000	-1.106269000
H	0.435986000	4.426161000	-0.946265000
C	3.931333000	3.059863000	-1.903062000
H	2.945047000	1.212796000	-2.357059000
C	3.796173000	4.367666000	-1.442322000
H	2.417648000	5.873486000	-0.748368000
H	4.910945000	2.664977000	-2.167243000
H	4.671669000	5.007693000	-1.346442000
C	-1.348976000	2.599803000	-1.596571000
C	-2.209789000	2.840118000	-2.675026000
C	-1.682831000	3.136013000	-0.342498000
C	-3.376108000	3.582332000	-2.500399000
H	-1.978279000	2.449841000	-3.664847000
C	-2.837328000	3.890550000	-0.173959000
H	-1.033483000	2.951301000	0.513224000
C	-3.693873000	4.107585000	-1.251208000
H	-4.036635000	3.752275000	-3.349153000
H	-3.077841000	4.287597000	0.810652000
H	-4.609474000	4.680412000	-1.115946000
C	0.133858000	-3.305057000	-1.058519000
C	0.525625000	-4.199177000	-2.061913000
C	0.490857000	-3.582871000	0.266987000
C	1.272878000	-5.330705000	-1.744741000
H	0.253831000	-4.016701000	-3.100844000
C	1.233158000	-4.714492000	0.584714000
H	0.203562000	-2.888774000	1.056149000
C	1.632681000	-5.588252000	-0.424060000
H	1.577225000	-6.013677000	-2.536273000
H	1.512726000	-4.897187000	1.621649000
H	2.226821000	-6.467886000	-0.182863000
C	-2.515657000	-2.239666000	-1.201201000
C	-3.471134000	-2.111900000	-2.214856000
C	-2.927728000	-2.690882000	0.060861000
C	-4.805802000	-2.430602000	-1.972123000
H	-3.184801000	-1.757418000	-3.204576000
C	-4.255823000	-3.017974000	0.298074000
H	-2.199960000	-2.760687000	0.870729000
C	-5.200814000	-2.884276000	-0.717510000
H	-5.538205000	-2.322600000	-2.770746000
H	-4.559374000	-3.353962000	1.288021000
H	-6.245265000	-3.124587000	-0.526938000

TS3_q

C	2.259343000	0.463771000	-0.202986000
C	1.149723000	1.153341000	-0.630834000
Co	-0.583651000	0.449302000	0.122622000
P	-2.811580000	1.257300000	-0.379002000
P	-0.910104000	-1.219340000	-1.632651000
C	-1.802669000	-0.590430000	-3.144596000
H	-1.844910000	-1.418988000	-3.865163000
H	-1.184684000	0.188324000	-3.612200000
C	-3.311188000	1.269178000	-2.160338000
H	-2.656609000	2.010605000	-2.641250000
H	-4.328383000	1.678915000	-2.242761000
C	-3.216312000	-0.071320000	-2.889151000
H	-3.712815000	0.040034000	-3.863577000
H	-3.793487000	-0.839466000	-2.351119000

C	2.017264000	-0.688680000	0.669889000
C	3.065287000	-1.719506000	0.844317000
C	3.337955000	-2.296803000	2.093233000
C	3.790151000	-2.181746000	-0.264865000
C	4.296245000	-3.294103000	2.229546000
H	2.777693000	-1.960971000	2.964559000
C	4.738235000	-3.189400000	-0.133485000
H	3.586901000	-1.749620000	-1.244149000
C	5.000558000	-3.748171000	1.115680000
H	4.492928000	-3.722267000	3.211498000
H	5.276031000	-3.538939000	-1.014711000
H	5.748750000	-4.532188000	1.221790000
C	3.643832000	0.869485000	-0.542817000
C	4.616016000	0.971368000	0.463273000
C	4.011908000	1.206641000	-1.852455000
C	5.903537000	1.407963000	0.172390000
H	4.343120000	0.713129000	1.487188000
C	5.301434000	1.634920000	-2.147470000
H	3.263617000	1.137406000	-2.642384000
C	6.253703000	1.739837000	-1.135199000
H	6.638394000	1.488948000	0.972638000
H	5.565326000	1.889743000	-3.173248000
H	7.263313000	2.077150000	-1.364681000
C	1.151330000	2.421996000	-1.351584000
C	1.948703000	3.523840000	-0.968483000
C	0.234792000	2.636637000	-2.400720000
C	1.808058000	4.761642000	-1.583800000
H	2.680966000	3.390774000	-0.172959000
C	0.109903000	3.867605000	-3.032865000
H	-0.398499000	1.799972000	-2.699177000
C	0.889914000	4.945741000	-2.618967000
H	2.429986000	5.594653000	-1.256976000
H	-0.610385000	3.990853000	-3.841551000
H	0.784441000	5.918391000	-3.095923000
C	0.151739000	1.066796000	2.185905000
C	1.412708000	1.565134000	2.734506000
C	2.194196000	0.783869000	3.589880000
C	1.814830000	2.866538000	2.421126000
C	3.367925000	1.299366000	4.126847000
H	1.863200000	-0.224919000	3.832569000
C	3.006953000	3.367711000	2.936006000
H	1.191429000	3.469806000	1.762172000
C	3.783799000	2.587590000	3.789152000
H	3.967822000	0.687999000	4.798749000
H	3.329128000	4.372619000	2.667486000
H	4.715321000	2.982179000	4.191206000
N	-1.026217000	1.348651000	2.139109000
C	0.771768000	-0.770700000	1.258756000
C	0.179341000	-1.939211000	1.900624000
C	-0.696353000	-1.834296000	3.003383000
C	0.356834000	-3.230291000	1.348414000
C	-1.350477000	-2.950140000	3.517591000
H	-0.873678000	-0.858286000	3.450937000
C	-0.295372000	-4.339030000	1.864563000
H	1.023335000	-3.342372000	0.493744000
C	-1.158742000	-4.209613000	2.954049000
H	-2.019911000	-2.830096000	4.369512000
H	-0.140902000	-5.314703000	1.403479000
H	-1.679217000	-5.079132000	3.352338000
C	-3.036867000	3.014924000	0.062543000
C	-1.901218000	3.823311000	0.180110000
C	-4.303689000	3.581945000	0.239190000
C	-2.029690000	5.181996000	0.450506000
H	-0.911071000	3.382369000	0.059806000
C	-4.430001000	4.938627000	0.521611000
H	-5.193437000	2.954605000	0.167545000
C	-3.293879000	5.740066000	0.623481000
H	-1.136270000	5.799700000	0.530615000
H	-5.418527000	5.372143000	0.664360000
H	-3.396111000	6.801407000	0.843875000

C	-4.182556000	0.385431000	0.460952000
C	-5.336501000	-0.015758000	-0.188658000
C	-4.010043000	0.049701000	1.814002000
C	-6.333581000	-0.737335000	0.494029000
H	-5.520945000	0.230796000	-1.236637000
C	-4.988091000	-0.669886000	2.490980000
H	-3.095423000	0.354833000	2.322062000
C	-6.151231000	-1.068521000	1.833339000
H	-7.239391000	-1.042862000	-0.027060000
H	-4.836409000	-0.925733000	3.538730000
H	-6.913482000	-1.637116000	2.363546000
C	-2.014094000	-2.622555000	-1.222150000
C	-2.339071000	-3.618115000	-2.156066000
C	-2.632058000	-2.647273000	0.031290000
C	-3.256724000	-4.612552000	-1.836692000
H	-1.859932000	-3.620366000	-3.136304000
C	-3.559861000	-3.636279000	0.348657000
H	-2.374066000	-1.894641000	0.776683000
C	-3.872611000	-4.619099000	-0.584472000
H	-3.495836000	-5.383762000	-2.567282000
H	-4.024841000	-3.635818000	1.333066000
H	-4.594170000	-5.396698000	-0.338844000
C	0.562139000	-1.968414000	-2.410570000
C	1.405133000	-1.131906000	-3.158167000
C	0.910975000	-3.316105000	-2.262508000
C	2.542680000	-1.640618000	-3.776282000
H	1.169976000	-0.069082000	-3.248090000
C	2.058177000	-3.820346000	-2.871298000
H	0.277791000	-3.977426000	-1.671914000
C	2.869763000	-2.988850000	-3.637667000
H	3.183765000	-0.977881000	-4.355487000
H	2.318503000	-4.869434000	-2.740935000
H	3.765170000	-3.385181000	-4.113601000

TS5_q

C	2.008199000	1.399981000	0.181175000
C	0.704019000	1.759476000	-0.198393000
Co	-0.889548000	0.572140000	-0.505365000
P	-3.086309000	0.452147000	-1.020650000
P	-0.269589000	-1.114701000	-1.952709000
C	-1.247206000	-0.853753000	-3.525483000
H	-0.847982000	-1.538013000	-4.286686000
H	-1.023735000	0.163947000	-3.880402000
C	-3.523893000	0.119288000	-2.779547000
H	-3.294979000	1.047059000	-3.323839000
H	-4.607411000	-0.034499000	-2.888055000
C	-2.758165000	-1.052603000	-3.395344000
H	-3.167719000	-1.228518000	-4.399888000
H	-2.962035000	-1.975077000	-2.828563000
C	2.298634000	0.128265000	0.762467000
C	3.698988000	-0.360303000	0.729676000
C	4.312269000	-0.904461000	1.867928000
C	4.450934000	-0.289314000	-0.451034000
C	5.622108000	-1.365529000	1.826312000
H	3.742454000	-0.963760000	2.795599000
C	5.758857000	-0.756528000	-0.498160000
H	3.986856000	0.132984000	-1.340800000
C	6.352583000	-1.296939000	0.640623000
H	6.078334000	-1.777973000	2.725173000
H	6.316092000	-0.698938000	-1.432987000
H	7.378812000	-1.659494000	0.606960000
C	3.098402000	2.392546000	-0.006250000
C	4.021061000	2.658004000	1.017086000
C	3.227343000	3.108631000	-1.205175000
C	5.030836000	3.597713000	0.847735000
H	3.935966000	2.112794000	1.956895000
C	4.237497000	4.048186000	-1.378814000
H	2.521796000	2.911115000	-2.012446000
C	5.146001000	4.296617000	-0.352580000

H	5.731819000	3.787778000	1.659341000
H	4.317888000	4.587083000	-2.322100000
H	5.938952000	5.030643000	-0.486794000
C	0.274894000	3.165690000	-0.347491000
C	0.364806000	4.078736000	0.717367000
C	-0.331488000	3.604898000	-1.536869000
C	-0.140486000	5.368414000	0.598470000
H	0.823606000	3.747921000	1.648501000
C	-0.811668000	4.903311000	-1.668898000
H	-0.425476000	2.896140000	-2.365074000
C	-0.726122000	5.788911000	-0.595737000
H	-0.072370000	6.054587000	1.441873000
H	-1.270017000	5.220520000	-2.604568000
H	-1.118638000	6.800463000	-0.687898000
C	0.208973000	0.184384000	2.035936000
C	-0.098821000	0.181281000	3.493245000
C	-1.350501000	0.615623000	3.953500000
C	0.876255000	-0.165917000	4.439901000
C	-1.624577000	0.679558000	5.314783000
H	-2.097488000	0.923017000	3.222713000
C	0.604342000	-0.096307000	5.801012000
H	1.855466000	-0.493086000	4.091258000
C	-0.649370000	0.321577000	6.244139000
H	-2.603758000	1.014978000	5.653176000
H	1.376654000	-0.364675000	6.519982000
H	-0.863302000	0.373885000	7.310396000
N	-0.458725000	1.034710000	1.308847000
C	1.331093000	-0.596756000	1.505340000
C	1.359213000	-2.055562000	1.682338000
C	0.549641000	-2.749491000	2.611926000
C	2.084179000	-2.865706000	0.774698000
C	0.530842000	-4.137539000	2.675052000
H	-0.089094000	-2.201374000	3.297766000
C	2.056349000	-4.250966000	0.835581000
H	2.666428000	-2.390778000	-0.010555000
C	1.293620000	-4.907208000	1.799677000
H	-0.101663000	-4.622124000	3.419004000
H	2.628931000	-4.824424000	0.106271000
H	1.269693000	-5.994615000	1.847055000
C	1.416462000	-1.054280000	-2.670169000
C	2.292178000	-2.144329000	-2.724908000
C	1.833307000	0.170120000	-3.214897000
C	3.537168000	-2.020954000	-3.339279000
H	1.999572000	-3.097117000	-2.285384000
C	3.070747000	0.288706000	-3.838891000
H	1.179885000	1.041715000	-3.133471000
C	3.923367000	-0.812106000	-3.911238000
H	4.209245000	-2.877242000	-3.366814000
H	3.375896000	1.247302000	-4.256081000
H	4.894777000	-0.720458000	-4.394356000
C	-0.619806000	-2.885215000	-1.651276000
C	-0.479237000	-3.871159000	-2.638732000
C	-1.130871000	-3.248067000	-0.402244000
C	-0.833360000	-5.189572000	-2.372976000
H	-0.079152000	-3.607316000	-3.618798000
C	-1.499301000	-4.564753000	-0.139687000
H	-1.228809000	-2.489989000	0.374965000
C	-1.348251000	-5.536448000	-1.123583000
H	-0.712430000	-5.949220000	-3.143817000
H	-1.889888000	-4.826408000	0.842223000
H	-1.628882000	-6.568736000	-0.919980000
C	-3.841908000	-0.933341000	-0.088203000
C	-4.777531000	-1.830436000	-0.613141000
C	-3.394132000	-1.119030000	1.228390000
C	-5.251599000	-2.888343000	0.160517000
H	-5.139259000	-1.715567000	-1.635044000
C	-3.873221000	-2.168327000	2.003568000
H	-2.639142000	-0.441973000	1.634040000
C	-4.802685000	-3.059078000	1.467552000
H	-5.973485000	-3.584591000	-0.263201000

H	-3.507269000	-2.294959000	3.022086000
H	-5.172536000	-3.889877000	2.066074000
C	-4.118223000	1.895429000	-0.579910000
C	-5.488457000	1.952533000	-0.864511000
C	-3.507232000	2.972090000	0.073080000
C	-6.230933000	3.075613000	-0.517656000
H	-5.980778000	1.108689000	-1.350616000
C	-4.253712000	4.096250000	0.420018000
H	-2.441613000	2.927077000	0.307947000
C	-5.612293000	4.149880000	0.122256000
H	-7.295453000	3.113717000	-0.743300000
H	-3.764667000	4.930670000	0.919654000
H	-6.195442000	5.029146000	0.391286000

CP_{2N}_s

C	-2.203071000	2.194655000	0.287397000
Co	0.031964000	0.263374000	-0.390430000
P	1.603116000	-1.219524000	-0.828771000
P	-1.509015000	-1.255819000	-0.819194000
C	-1.225358000	-2.482175000	-2.169786000
H	-2.064305000	-3.191860000	-2.158972000
H	-1.335126000	-1.905133000	-3.099251000
C	1.328236000	-2.319568000	-2.287676000
H	1.247457000	-1.659988000	-3.163444000
H	2.235159000	-2.918602000	-2.442551000
C	0.107133000	-3.222248000	-2.173294000
H	0.106884000	-3.919177000	-3.021986000
H	0.200886000	-3.845534000	-1.272838000
C	2.197048000	2.239100000	0.378352000
N	1.339021000	1.497768000	0.089177000
C	3.287487000	3.081665000	0.691583000
C	4.588110000	2.547016000	0.640610000
C	3.087965000	4.430744000	1.034068000
C	5.672453000	3.363120000	0.925798000
H	4.726592000	1.500768000	0.374688000
C	4.184726000	5.231005000	1.318518000
H	2.079177000	4.834865000	1.070754000
C	5.474358000	4.701750000	1.264156000
H	6.678579000	2.951593000	0.883839000
H	4.034520000	6.274824000	1.583508000
H	6.328951000	5.336484000	1.487535000
C	-3.348256000	2.973584000	0.567672000
C	-4.607827000	2.346817000	0.520964000
C	-3.247547000	4.341717000	0.874960000
C	-5.750003000	3.091466000	0.773560000
H	-4.669322000	1.285938000	0.283915000
C	-4.401152000	5.069391000	1.128467000
H	-2.270318000	4.817306000	0.908487000
C	-5.649863000	4.449273000	1.076886000
H	-6.724144000	2.608831000	0.733238000
H	-4.327709000	6.127854000	1.366267000
H	-6.549285000	5.028035000	1.274897000
N	-1.311520000	1.481035000	0.029096000
C	-3.166333000	-0.648680000	-1.310972000
C	-4.343460000	-1.244042000	-0.842711000
C	-3.251014000	0.394047000	-2.243237000
C	-5.583363000	-0.803905000	-1.303922000
H	-4.292479000	-2.055133000	-0.116748000
C	-4.489777000	0.830231000	-2.702458000
H	-2.336477000	0.871397000	-2.599699000
C	-5.658018000	0.231188000	-2.232947000
H	-6.492695000	-1.275786000	-0.936667000
H	-4.544058000	1.642464000	-3.424497000
H	-6.626937000	0.573743000	-2.590767000
C	3.275935000	-0.581080000	-1.212115000
C	4.437896000	-1.115741000	-0.645462000
C	3.387698000	0.444605000	-2.161486000
C	5.690471000	-0.643500000	-1.037159000
H	4.367576000	-1.905166000	0.101678000

C	4.638440000	0.911893000	-2.551428000
H	2.483995000	0.883518000	-2.588304000
C	5.792871000	0.365059000	-1.991838000
H	6.588224000	-1.069844000	-0.593650000
H	4.712669000	1.707017000	-3.290515000
H	6.771485000	0.730357000	-2.296961000
C	-1.816035000	-2.231725000	0.690682000
C	-1.791280000	-3.629643000	0.728370000
C	-2.045705000	-1.523027000	1.880362000
C	-1.977441000	-4.305033000	1.933191000
H	-1.632879000	-4.205364000	-0.181818000
C	-2.248347000	-2.199403000	3.077140000
H	-2.060784000	-0.431852000	1.860593000
C	-2.205083000	-3.593152000	3.106833000
H	-1.949122000	-5.392663000	1.950077000
H	-2.434261000	-1.638607000	3.991152000
H	-2.352832000	-4.123351000	4.045491000
C	1.812964000	-2.380641000	0.561511000
C	2.341068000	-3.669653000	0.404227000
C	1.393858000	-1.968127000	1.833115000
C	2.440693000	-4.527191000	1.495765000
H	2.678291000	-4.009859000	-0.575224000
C	1.498621000	-2.824950000	2.924222000
H	0.963903000	-0.971309000	1.953070000
C	2.018374000	-4.105961000	2.755374000
H	2.849484000	-5.526700000	1.362216000
H	1.163409000	-2.494930000	3.905525000
H	2.093613000	-4.779991000	3.606370000

CP_{2N}_t

C	3.478361000	0.681832000	-0.859244000
Co	0.401622000	0.366097000	-0.826771000
P	-0.448225000	1.957578000	0.597763000
P	0.656519000	-1.281394000	0.770891000
C	1.133897000	-0.602454000	2.418171000
H	1.214872000	-1.422142000	3.145438000
H	2.151248000	-0.201258000	2.295161000
C	0.272762000	1.845050000	2.296222000
H	1.320305000	2.162639000	2.191217000
H	-0.207814000	2.604091000	2.930212000
C	0.206039000	0.477988000	2.978032000
H	0.464789000	0.621155000	4.036046000
H	-0.828818000	0.109909000	2.976132000
C	-2.330091000	-0.633509000	-1.865676000
N	-1.245686000	-0.241455000	-1.665594000
C	-3.657998000	-1.107095000	-1.987804000
C	-4.378864000	-1.359956000	-0.805531000
C	-4.251655000	-1.314132000	-3.243712000
C	-5.684561000	-1.819217000	-0.891489000
H	-3.902630000	-1.190469000	0.158781000
C	-5.559698000	-1.773674000	-3.309448000
H	-3.685513000	-1.113463000	-4.150072000
C	-6.274656000	-2.026188000	-2.138697000
H	-6.245136000	-2.016215000	0.019710000
H	-6.024645000	-1.935827000	-4.278762000
H	-7.299346000	-2.386311000	-2.199235000
C	4.879721000	0.502077000	-0.785069000
C	5.765198000	1.394249000	-1.413365000
C	5.371047000	-0.608203000	-0.072693000
C	7.131487000	1.169167000	-1.326702000
H	5.374857000	2.248238000	-1.961483000
C	6.739935000	-0.818076000	-0.000296000
H	4.672569000	-1.292032000	0.407364000
C	7.619103000	0.066724000	-0.624560000
H	7.821129000	1.855973000	-1.811080000
H	7.121844000	-1.678195000	0.545363000
H	8.691754000	-0.103266000	-0.564140000
N	2.308735000	0.752555000	-0.875580000
C	-0.131607000	3.710180000	0.184628000

C	-0.803787000	4.750627000	0.839412000
C	0.816360000	4.019809000	-0.796596000
C	-0.523784000	6.075023000	0.522421000
H	-1.559819000	4.520337000	1.591177000
C	1.095197000	5.347162000	-1.113180000
H	1.335382000	3.211762000	-1.314247000
C	0.426448000	6.374282000	-0.453323000
H	-1.051455000	6.877455000	1.034048000
H	1.830571000	5.579449000	-1.881047000
H	0.640189000	7.411536000	-0.702996000
C	2.041479000	-2.419563000	0.383431000
C	2.737008000	-3.139398000	1.363702000
C	2.421366000	-2.566561000	-0.957390000
C	3.794592000	-3.973772000	1.010078000
H	2.450566000	-3.058018000	2.411798000
C	3.470940000	-3.409346000	-1.313198000
H	1.890158000	-2.004109000	-1.728886000
C	4.163177000	-4.109254000	-0.327676000
H	4.326419000	-4.527200000	1.781622000
H	3.753256000	-3.513204000	-2.358894000
H	4.988226000	-4.763744000	-0.601670000
C	-2.257603000	1.925233000	0.853262000
C	-2.878260000	1.733835000	2.093461000
C	-3.066339000	2.088231000	-0.282877000
C	-4.268503000	1.689809000	2.192036000
H	-2.284233000	1.638569000	3.000601000
C	-4.451852000	2.052261000	-0.182562000
H	-2.598181000	2.255422000	-1.253692000
C	-5.057363000	1.843245000	1.056163000
H	-4.733656000	1.545548000	3.165312000
H	-5.062163000	2.182221000	-1.074762000
H	-6.142189000	1.809055000	1.135054000
C	-0.743180000	-2.408133000	1.102089000
C	-1.354591000	-2.556000000	2.352539000
C	-1.251859000	-3.133763000	0.013626000
C	-2.453570000	-3.399624000	2.506835000
H	-0.971059000	-2.026495000	3.223046000
C	-2.340415000	-3.983042000	0.171603000
H	-0.779978000	-3.035837000	-0.965243000
C	-2.950406000	-4.111317000	1.418943000
H	-2.915268000	-3.506243000	3.486543000
H	-2.719261000	-4.541012000	-0.682912000
H	-3.807375000	-4.770461000	1.542354000

CP_{2N'}_s

C	-1.679840000	1.266916000	-1.061926000
Co	-0.069925000	0.546447000	-0.133621000
P	2.064412000	1.130153000	-0.577428000
P	0.383672000	-1.343762000	-1.039079000
C	0.974041000	-1.132143000	-2.765092000
H	0.939544000	-2.108908000	-3.264446000
H	0.242810000	-0.488109000	-3.267616000
C	2.489427000	0.905849000	-2.350118000
H	1.787645000	1.553619000	-2.892016000
H	3.494075000	1.306568000	-2.536857000
C	2.372309000	-0.527367000	-2.869898000
H	2.664013000	-0.530068000	-3.927828000
H	3.091420000	-1.182436000	-2.358166000
C	-1.032186000	0.139940000	1.547992000
N	0.151882000	0.307958000	1.811984000
C	-2.343460000	-0.154371000	2.078592000
C	-2.636651000	0.195206000	3.407393000
C	-3.322487000	-0.769351000	1.286962000
C	-3.899189000	-0.062966000	3.924413000
H	-1.871102000	0.671828000	4.016264000
C	-4.574729000	-1.043462000	1.819693000
H	-3.095104000	-1.016664000	0.251568000
C	-4.867502000	-0.683118000	3.133932000

H	-4.128289000	0.214499000	4.950915000
H	-5.330251000	-1.522339000	1.199396000
H	-5.854076000	-0.885017000	3.546010000
C	-3.076135000	1.576435000	-0.855626000
C	-3.487912000	2.254915000	0.299728000
C	-4.026209000	1.178030000	-1.808097000
C	-4.832473000	2.538637000	0.495193000
H	-2.745422000	2.554477000	1.037680000
C	-5.372705000	1.442363000	-1.590373000
H	-3.699394000	0.667581000	-2.711952000
C	-5.777019000	2.121237000	-0.441563000
H	-5.146582000	3.072938000	1.389031000
H	-6.109221000	1.129889000	-2.327512000
H	-6.832149000	2.330191000	-0.278845000
N	-0.737990000	1.285254000	-1.843651000
C	2.084743000	2.936700000	-0.330478000
C	2.898356000	3.549790000	0.631828000
C	1.238335000	3.730701000	-1.121422000
C	2.871727000	4.931994000	0.788699000
H	3.569147000	2.952522000	1.245286000
C	1.223733000	5.111785000	-0.961971000
H	0.588970000	3.266043000	-1.861999000
C	2.036700000	5.714734000	-0.004548000
H	3.515195000	5.398771000	1.531409000
H	0.571878000	5.717969000	-1.587420000
H	2.021041000	6.795174000	0.121562000
C	-1.164433000	-2.280783000	-1.164037000
C	-1.452234000	-3.304221000	-0.251645000
C	-2.127896000	-1.907646000	-2.112925000
C	-2.682806000	-3.952312000	-0.298582000
H	-0.711422000	-3.595050000	0.492309000
C	-3.354325000	-2.561705000	-2.155943000
H	-1.918588000	-1.100054000	-2.814826000
C	-3.633541000	-3.582702000	-1.247527000
H	-2.898800000	-4.749114000	0.409710000
H	-4.094589000	-2.274807000	-2.900430000
H	-4.594376000	-4.092030000	-1.281562000
C	1.584635000	-2.449683000	-0.245605000
C	2.247099000	-3.423349000	-1.009781000
C	1.839177000	-2.364541000	1.128456000
C	3.153491000	-4.288204000	-0.407400000
H	2.053491000	-3.517292000	-2.077396000
C	2.745166000	-3.236898000	1.724947000
H	1.342650000	-1.600687000	1.724487000
C	3.405303000	-4.194244000	0.960046000
H	3.662061000	-5.038785000	-1.008508000
H	2.942372000	-3.157245000	2.792043000
H	4.117521000	-4.870336000	1.428490000
C	3.435379000	0.453624000	0.395747000
C	4.560468000	-0.126587000	-0.203971000
C	3.347528000	0.482555000	1.797536000
C	5.573401000	-0.671792000	0.579991000
H	4.663096000	-0.148056000	-1.287090000
C	4.371725000	-0.046602000	2.574434000
H	2.466487000	0.907831000	2.273187000
C	5.482227000	-0.631506000	1.968467000
H	6.441059000	-1.120379000	0.100905000
H	4.298001000	-0.007957000	3.659525000
H	6.278936000	-1.052141000	2.578615000

CP_{2N'}_t

C	-1.190000000	-1.895056000	-1.004845000
Co	-0.098769000	-0.419172000	0.003256000
P	-1.454222000	1.420080000	-0.533487000
P	1.759566000	0.485630000	-1.052011000
C	1.314834000	1.183270000	-2.698601000
H	2.234381000	1.546269000	-3.176698000
H	0.936003000	0.356697000	-3.314153000
C	-1.143858000	1.861487000	-2.296633000

H	-1.381827000	0.965518000	-2.885360000
H	-1.870502000	2.626368000	-2.601282000
C	0.282713000	2.308650000	-2.628284000
H	0.256316000	2.797423000	-3.610660000
H	0.622220000	3.082824000	-1.923102000
C	0.361111000	-1.167362000	1.856325000
N	-0.430782000	-0.285906000	2.082221000
C	1.264938000	-2.252248000	2.118708000
C	1.544186000	-2.594519000	3.453691000
C	1.863990000	-2.959285000	1.064735000
C	2.420699000	-3.636722000	3.718646000
H	1.072378000	-2.040074000	4.261405000
C	2.738759000	-3.998990000	1.345669000
H	1.647770000	-2.684804000	0.031830000
C	3.017062000	-4.337060000	2.669141000
H	2.640653000	-3.905186000	4.749111000
H	3.207123000	-4.543529000	0.528638000
H	3.704012000	-5.152022000	2.886755000
C	-2.313207000	-2.644264000	-0.515335000
C	-2.943938000	-2.304843000	0.690069000
C	-2.810475000	-3.692351000	-1.309548000
C	-4.070918000	-3.007365000	1.093499000
H	-2.559758000	-1.477271000	1.284745000
C	-3.935233000	-4.388292000	-0.890368000
H	-2.313624000	-3.941887000	-2.244274000
C	-4.565826000	-4.045933000	0.306223000
H	-4.569757000	-2.737901000	2.021471000
H	-4.324218000	-5.199709000	-1.500954000
H	-5.450144000	-4.593222000	0.625615000
N	-0.363181000	-1.528761000	-1.800244000
C	-3.223682000	0.966977000	-0.505392000
C	-4.016704000	1.248977000	0.614729000
C	-3.769174000	0.199010000	-1.544722000
C	-5.324707000	0.779799000	0.687814000
H	-3.614401000	1.850406000	1.429020000
C	-5.077687000	-0.267348000	-1.467597000
H	-3.170618000	-0.051602000	-2.420329000
C	-5.858024000	0.019336000	-0.350580000
H	-5.932021000	1.017258000	1.559067000
H	-5.485957000	-0.860484000	-2.283862000
H	-6.881163000	-0.345982000	-0.290971000
C	3.098293000	-0.696777000	-1.395673000
C	4.223763000	-0.757385000	-0.562653000
C	2.949114000	-1.649503000	-2.414746000
C	5.189407000	-1.740301000	-0.757016000
H	4.347945000	-0.028218000	0.237323000
C	3.919513000	-2.628964000	-2.604633000
H	2.067952000	-1.632520000	-3.054188000
C	5.040855000	-2.676117000	-1.777986000
H	6.063392000	-1.771460000	-0.109503000
H	3.800702000	-3.355422000	-3.406093000
H	5.799916000	-3.440249000	-1.932811000
C	-1.327728000	2.982516000	0.391627000
C	-1.283378000	4.229999000	-0.243511000
C	-1.255512000	2.929855000	1.792552000
C	-1.165110000	5.397771000	0.504968000
H	-1.343453000	4.302091000	-1.328009000
C	-1.156556000	4.101005000	2.536808000
H	-1.264236000	1.963751000	2.295720000
C	-1.104147000	5.336299000	1.894500000
H	-1.127555000	6.359687000	-0.001901000
H	-1.111712000	4.047002000	3.622959000
H	-1.017202000	6.251375000	2.476616000
C	2.547030000	1.885380000	-0.203012000
C	3.626480000	2.568411000	-0.783022000
C	2.042177000	2.320449000	1.026652000
C	4.181789000	3.670033000	-0.143676000
H	4.041367000	2.227430000	-1.732189000
C	2.596603000	3.429219000	1.662772000
H	1.203925000	1.792419000	1.483333000

C	3.663842000	4.103373000	1.077526000
H	5.020293000	4.194064000	-0.597575000
H	2.190180000	3.765245000	2.614671000
H	4.098202000	4.969024000	1.573404000

CP_{2N}'_s

C	-2.121996000	-1.380356000	0.844977000
Co	-0.401077000	-0.750562000	0.394330000
P	-0.383583000	-0.614199000	-1.742401000
P	1.636329000	-1.633561000	0.307564000
C	1.570312000	-3.174154000	-0.689049000
H	2.480447000	-3.768981000	-0.541550000
H	0.735320000	-3.756348000	-0.276477000
C	0.007701000	-2.238261000	-2.513347000
H	-0.809077000	-2.894458000	-2.183520000
H	-0.103279000	-2.128262000	-3.600923000
C	1.346993000	-2.893891000	-2.172391000
H	1.391997000	-3.844846000	-2.718712000
H	2.181108000	-2.290165000	-2.556216000
C	-0.171189000	2.132662000	1.425441000
N	-0.247298000	1.067503000	0.943368000
C	-0.059633000	3.432658000	1.973501000
C	0.948756000	4.297251000	1.509749000
C	-0.954764000	3.858657000	2.970609000
C	1.051952000	5.574380000	2.041220000
H	1.639468000	3.953864000	0.741216000
C	-0.833667000	5.137509000	3.494795000
H	-1.729596000	3.181623000	3.323037000
C	0.164546000	5.994467000	3.032053000
H	1.830293000	6.245243000	1.685655000
H	-1.521908000	5.468894000	4.268416000
H	0.252801000	6.995883000	3.447064000
C	-3.494397000	-1.056105000	1.162745000
C	-3.911115000	0.282256000	1.155436000
C	-4.431500000	-2.076247000	1.397203000
C	-5.245970000	0.598043000	1.374079000
H	-3.174454000	1.059002000	0.949298000
C	-5.762587000	-1.753476000	1.622196000
H	-4.099497000	-3.112866000	1.393340000
C	-6.170797000	-0.418865000	1.608148000
H	-5.570653000	1.636311000	1.358684000
H	-6.488574000	-2.542848000	1.805430000
H	-7.216497000	-0.171371000	1.779598000
N	-1.396302000	-2.357924000	0.565313000
C	-2.073583000	-0.260966000	-2.331521000
C	-3.071615000	-1.227909000	-2.130169000
C	-2.420596000	0.962923000	-2.918082000
C	-4.383304000	-0.975843000	-2.510785000
H	-2.829324000	-2.174848000	-1.648563000
C	-3.738780000	1.212179000	-3.290491000
H	-1.660572000	1.718235000	-3.105729000
C	-4.721525000	0.248100000	-3.085359000
H	-5.146049000	-1.733980000	-2.344467000
H	-3.994484000	2.164350000	-3.750524000
H	-5.750909000	0.448503000	-3.374624000
C	2.027293000	-2.185991000	1.997004000
C	1.157355000	-3.092549000	2.622396000
C	3.139593000	-1.700281000	2.696154000
C	1.416620000	-3.524417000	3.918422000
H	0.274488000	-3.451897000	2.093289000
C	3.386483000	-2.132817000	3.995748000
H	3.820423000	-0.996258000	2.219898000
C	2.529248000	-3.044697000	4.607053000
H	0.743849000	-4.235105000	4.393888000
H	4.257378000	-1.758929000	4.530209000
H	2.727651000	-3.381213000	5.622454000
C	0.702279000	0.631218000	-2.496003000
C	1.640050000	0.293398000	-3.479926000
C	0.627527000	1.964338000	-2.061180000

C	2.493247000	1.260828000	-4.003461000
H	1.705925000	-0.725131000	-3.855224000
C	1.467553000	2.931119000	-2.600894000
H	-0.101840000	2.242991000	-1.302510000
C	2.410861000	2.578868000	-3.564983000
H	3.220447000	0.981000000	-4.762573000
H	1.383989000	3.964913000	-2.269770000
H	3.075780000	3.333730000	-3.979504000
C	3.106498000	-0.740585000	-0.283877000
C	4.200081000	-1.391465000	-0.869772000
C	3.139379000	0.652703000	-0.145321000
C	5.297636000	-0.660518000	-1.314949000
H	4.201892000	-2.475805000	-0.976285000
C	4.241484000	1.380662000	-0.580965000
H	2.283050000	1.161537000	0.297873000
C	5.319772000	0.725168000	-1.171191000
H	6.141039000	-1.175870000	-1.769793000
H	4.255385000	2.463837000	-0.469988000
H	6.179866000	1.293824000	-1.518795000

CP_{2N}’_t

C	2.132005000	1.744982000	0.911622000
Co	0.455573000	0.678356000	0.387981000
P	1.249530000	-0.490369000	-1.452482000
P	-1.214641000	1.796340000	-0.768004000
C	-0.593742000	2.339706000	-2.417917000
H	-1.379845000	2.932203000	-2.905394000
H	0.260713000	3.008032000	-2.245963000
C	1.177258000	0.546257000	-2.978808000
H	1.921450000	1.341139000	-2.832122000
H	1.547181000	-0.054250000	-3.820946000
C	-0.175113000	1.176343000	-3.318419000
H	-0.111590000	1.552806000	-4.347546000
H	-0.966669000	0.410729000	-3.335221000
C	-1.285804000	-1.291545000	2.076629000
N	-0.573244000	-0.583677000	1.477623000
C	-2.158147000	-2.175235000	2.755439000
C	-2.935068000	-3.077875000	2.006516000
C	-2.246762000	-2.149161000	4.157987000
C	-3.794088000	-3.944208000	2.666520000
H	-2.855096000	-3.083753000	0.921325000
C	-3.109040000	-3.025820000	4.800175000
H	-1.642906000	-1.444978000	4.724953000
C	-3.880970000	-3.919819000	4.058491000
H	-4.400218000	-4.641997000	2.093982000
H	-3.181801000	-3.010765000	5.884708000
H	-4.556415000	-4.602325000	4.569274000
C	3.274408000	1.273907000	1.650042000
C	3.389115000	-0.075564000	2.011954000
C	4.305405000	2.177683000	1.954797000
C	4.531724000	-0.521042000	2.661360000
H	2.589183000	-0.771001000	1.754188000
C	5.440297000	1.721518000	2.611461000
H	4.204826000	3.222312000	1.669447000
C	5.556259000	0.376012000	2.960402000
H	4.627865000	-1.570760000	2.928836000
H	6.240409000	2.418517000	2.849771000
H	6.451407000	0.025004000	3.469337000
N	1.490059000	2.538279000	0.268646000
C	3.024845000	-0.928272000	-1.370257000
C	3.469087000	-2.244211000	-1.196440000
C	3.968432000	0.110371000	-1.366641000
C	4.824865000	-2.512743000	-1.024768000
H	2.756113000	-3.067275000	-1.207778000
C	5.321484000	-0.162135000	-1.200108000
H	3.645098000	1.146180000	-1.479003000
C	5.753156000	-1.475114000	-1.024420000
H	5.156113000	-3.541824000	-0.899777000
H	6.039848000	0.655554000	-1.201833000

H	6.811608000	-1.688472000	-0.890872000
C	-1.821764000	3.313003000	0.028053000
C	-2.846088000	3.221216000	0.981990000
C	-1.223633000	4.556447000	-0.209355000
C	-3.276090000	4.352770000	1.665736000
H	-3.320145000	2.258275000	1.176134000
C	-1.658048000	5.686902000	0.477187000
H	-0.410787000	4.646892000	-0.927131000
C	-2.684008000	5.588794000	1.412989000
H	-4.078765000	4.270027000	2.395794000
H	-1.191339000	6.649270000	0.277406000
H	-3.022594000	6.474753000	1.945945000
C	-2.732913000	0.882383000	-1.210482000
C	-3.885530000	1.549241000	-1.650364000
C	-2.723585000	-0.517387000	-1.196846000
C	-5.000677000	0.828720000	-2.063799000
H	-3.910643000	2.638996000	-1.660279000
C	-3.837521000	-1.237709000	-1.623304000
H	-1.831777000	-1.045869000	-0.859464000
C	-4.977601000	-0.565596000	-2.053948000
H	-5.890601000	1.356840000	-2.400094000
H	-3.809298000	-2.326661000	-1.623514000
H	-5.850140000	-1.125754000	-2.384124000
C	0.391832000	-2.042660000	-1.869866000
C	-0.105129000	-2.330563000	-3.145897000
C	0.149892000	-2.954948000	-0.829970000
C	-0.829452000	-3.498261000	-3.375605000
H	0.066265000	-1.643811000	-3.972875000
C	-0.558642000	-4.128771000	-1.064304000
H	0.526870000	-2.738726000	0.171282000
C	-1.057792000	-4.398299000	-2.338444000
H	-1.212262000	-3.706052000	-4.372580000
H	-0.721598000	-4.834606000	-0.251244000
H	-1.619099000	-5.311947000	-2.523042000

CP_{2A}_s

C	-1.682254000	1.404320000	0.603979000
C	-0.901711000	2.062534000	-0.184808000
Co	-0.168884000	0.258780000	0.135395000
P	1.927653000	0.839158000	-0.529604000
P	-0.638848000	-0.615507000	-1.775696000
C	-0.149197000	0.487420000	-3.165927000
H	-0.559622000	0.061242000	-4.091037000
H	-0.688899000	1.429266000	-3.002974000
C	1.980459000	1.600170000	-2.213187000
H	1.468748000	2.569229000	-2.127094000
H	3.025809000	1.807269000	-2.474721000
C	1.343241000	0.771503000	-3.326415000
H	1.473133000	1.323291000	-4.266763000
H	1.897738000	-0.166848000	-3.463470000
C	0.499065000	-1.076991000	1.451284000
C	-0.781782000	-1.142274000	1.346255000
C	-2.858930000	1.432386000	1.431424000
C	-2.798509000	1.040030000	2.779738000
C	-4.085534000	1.876522000	0.907789000
C	-3.932836000	1.082471000	3.577512000
H	-1.847971000	0.697156000	3.187431000
C	-5.223278000	1.895113000	1.704574000
H	-4.131084000	2.213310000	-0.126896000
C	-5.151042000	1.494669000	3.038153000
H	-3.871526000	0.779790000	4.620809000
H	-6.168931000	2.236184000	1.287906000
H	-6.043519000	1.512603000	3.660126000
C	-1.967148000	-1.807615000	1.825681000
C	-1.866250000	-2.615236000	2.975703000
C	-3.215739000	-1.676276000	1.198612000
C	-2.987043000	-3.257536000	3.482298000
H	-0.899330000	-2.720895000	3.466617000
C	-4.331514000	-2.331051000	1.703060000

H	-3.306609000	-1.031846000	0.328347000
C	-4.222656000	-3.117405000	2.848118000
H	-2.898970000	-3.872625000	4.375567000
H	-5.293875000	-2.210774000	1.208374000
H	-5.099580000	-3.621182000	3.249769000
C	1.724221000	-1.553833000	2.050293000
C	2.202488000	-0.940940000	3.222198000
C	2.430872000	-2.650387000	1.528637000
C	3.345711000	-1.417100000	3.854212000
H	1.651560000	-0.104738000	3.650170000
C	3.576254000	-3.114330000	2.161711000
H	2.084627000	-3.125497000	0.613463000
C	4.039715000	-2.502086000	3.324936000
H	3.692117000	-0.938372000	4.767987000
H	4.114383000	-3.960347000	1.737742000
H	4.936521000	-2.871391000	3.818006000
C	-0.693171000	3.342294000	-0.839517000
C	0.164643000	4.309344000	-0.287517000
C	-1.367444000	3.660559000	-2.032930000
C	0.361910000	5.528935000	-0.924956000
H	0.658052000	4.108929000	0.658934000
C	-1.158124000	4.877919000	-2.670832000
H	-2.074729000	2.950380000	-2.460180000
C	-0.282948000	5.814567000	-2.125861000
H	1.026509000	6.262392000	-0.471567000
H	-1.692014000	5.098605000	-3.592946000
H	-0.119110000	6.766717000	-2.625417000
C	0.106989000	-2.232869000	-2.171040000
C	0.537741000	-2.526834000	-3.473896000
C	0.202305000	-3.226698000	-1.189144000
C	1.084718000	-3.771443000	-3.772833000
H	0.449430000	-1.788810000	-4.268335000
C	0.739438000	-4.473953000	-1.494379000
H	-0.145729000	-3.023642000	-0.178091000
C	1.193661000	-4.744980000	-2.782743000
H	1.420340000	-3.980593000	-4.786320000
H	0.804487000	-5.234349000	-0.718441000
H	1.622133000	-5.716805000	-3.018347000
C	3.363866000	-0.299134000	-0.532516000
C	4.431424000	-0.118681000	0.357127000
C	3.408265000	-1.381903000	-1.422485000
C	5.519895000	-0.985561000	0.338777000
H	4.413566000	0.697137000	1.076761000
C	4.500502000	-2.243040000	-1.441594000
H	2.579699000	-1.574423000	-2.099503000
C	5.562390000	-2.045227000	-0.562765000
H	6.336827000	-0.831438000	1.041249000
H	4.515264000	-3.072934000	-2.146274000
H	6.416859000	-2.719010000	-0.575824000
C	-2.417413000	-0.894116000	-2.073760000
C	-3.291210000	0.201143000	-2.074685000
C	-2.941255000	-2.181505000	-2.249417000
C	-4.657137000	0.017367000	-2.253709000
H	-2.898683000	1.202649000	-1.904597000
C	-4.310813000	-2.362201000	-2.423342000
H	-2.283441000	-3.047912000	-2.247148000
C	-5.170514000	-1.267506000	-2.424118000
H	-5.323452000	0.878009000	-2.252441000
H	-4.705552000	-3.367273000	-2.555505000
H	-6.240423000	-1.413460000	-2.556485000
C	2.470123000	2.186009000	0.571415000
C	3.394340000	3.152994000	0.157600000
C	1.940691000	2.260200000	1.865008000
C	3.766120000	4.182013000	1.017542000
H	3.826415000	3.108732000	-0.841232000
C	2.323153000	3.281427000	2.729811000
H	1.198693000	1.526568000	2.182741000
C	3.231980000	4.247744000	2.303522000
H	4.477644000	4.934049000	0.682743000
H	1.900974000	3.330846000	3.731533000

H	3.524916000	5.053307000	2.973590000
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CP_{2A}_t

C	1.113403000	-1.842955000	0.897419000
C	0.993432000	-2.018646000	-0.362617000
Co	0.004255000	-0.359292000	0.243398000
P	-1.517193000	-0.206035000	-1.618280000
P	1.571315000	1.048494000	-0.931331000
C	1.552749000	0.756062000	-2.762170000
H	2.369636000	1.351218000	-3.190633000
H	1.791642000	-0.301849000	-2.942965000
C	-0.892845000	0.137930000	-3.322968000
H	-0.562310000	-0.833488000	-3.714969000
H	-1.742995000	0.449824000	-3.945906000
C	0.250563000	1.142788000	-3.459908000
H	0.460945000	1.247108000	-4.532354000
H	-0.058128000	2.145419000	-3.130796000
C	-0.688656000	0.997466000	1.541819000
C	-1.237176000	-0.144729000	1.715955000
C	1.639898000	-2.224454000	2.181401000
C	1.458294000	-1.452323000	3.339489000
C	2.414883000	-3.397645000	2.256112000
C	2.040488000	-1.840575000	4.539484000
H	0.863521000	-0.541176000	3.283633000
C	2.990568000	-3.780333000	3.459857000
H	2.557347000	-3.997884000	1.358812000
C	2.806842000	-3.003397000	4.603369000
H	1.894638000	-1.233894000	5.430614000
H	3.586453000	-4.689415000	3.506663000
H	3.260361000	-3.305402000	5.545002000
C	1.521116000	-2.579918000	-1.579640000
C	2.919050000	-2.721331000	-1.676527000
C	0.724125000	-2.951068000	-2.673358000
C	3.497693000	-3.186604000	-2.850647000
H	3.539314000	-2.439454000	-0.826425000
C	1.309887000	-3.438031000	-3.836017000
H	-0.359186000	-2.875835000	-2.595141000
C	2.696833000	-3.544147000	-3.934467000
H	4.580716000	-3.275217000	-2.915930000
H	0.679618000	-3.736590000	-4.671379000
H	3.151654000	-3.914108000	-4.850783000
C	-2.140885000	-1.018750000	2.416280000
C	-3.235504000	-0.444543000	3.091010000
C	-1.977718000	-2.412115000	2.444109000
C	-4.140718000	-1.250674000	3.767601000
H	-3.359433000	0.637673000	3.073942000
C	-2.881780000	-3.210803000	3.132422000
H	-1.125856000	-2.857789000	1.931825000
C	-3.967055000	-2.634371000	3.790121000
H	-4.983292000	-0.797608000	4.285758000
H	-2.739604000	-4.289248000	3.156318000
H	-4.676810000	-3.262854000	4.323639000
C	-0.525073000	2.390492000	1.848777000
C	-1.645091000	3.239192000	1.803661000
C	0.725432000	2.925318000	2.195116000
C	-1.508588000	4.589163000	2.100330000
H	-2.611396000	2.829085000	1.512032000
C	0.849290000	4.271770000	2.508676000
H	1.599705000	2.273875000	2.208964000
C	-0.264778000	5.108434000	2.457242000
H	-2.380767000	5.239046000	2.054612000
H	1.823564000	4.674499000	2.777943000
H	-0.161981000	6.166041000	2.691496000
C	3.255492000	0.551462000	-0.438267000
C	3.483264000	0.294373000	0.920105000
C	4.312665000	0.383202000	-1.341627000
C	4.728567000	-0.130471000	1.369498000
H	2.661020000	0.399603000	1.629763000
C	5.562203000	-0.037405000	-0.892094000

H	4.166806000	0.565578000	-2.404917000
C	5.771584000	-0.298417000	0.460349000
H	4.878142000	-0.341321000	2.427228000
H	6.374404000	-0.166461000	-1.604916000
H	6.746910000	-0.635502000	0.805182000
C	1.584118000	2.873007000	-0.882016000
C	0.358008000	3.545094000	-0.959124000
C	2.766243000	3.617833000	-0.805774000
C	0.309952000	4.933597000	-0.979864000
H	-0.570150000	2.973195000	-0.962529000
C	2.715276000	5.009732000	-0.815927000
H	3.728312000	3.111480000	-0.734301000
C	1.491478000	5.668993000	-0.906622000
H	-0.654512000	5.437367000	-1.029606000
H	3.639001000	5.581742000	-0.753829000
H	1.458388000	6.756707000	-0.911394000
C	-2.598428000	-1.660488000	-1.846507000
C	-2.444739000	-2.773340000	-1.013980000
C	-3.617072000	-1.661786000	-2.809788000
C	-3.290278000	-3.872876000	-1.139635000
H	-1.650900000	-2.773464000	-0.266486000
C	-4.452680000	-2.764774000	-2.942252000
H	-3.767940000	-0.790158000	-3.447258000
C	-4.291448000	-3.870054000	-2.106262000
H	-3.165281000	-4.730079000	-0.480618000
H	-5.238704000	-2.760214000	-3.694557000
H	-4.952664000	-4.728061000	-2.208273000
C	-2.757273000	1.100882000	-1.299412000
C	-3.706259000	0.867296000	-0.292175000
C	-2.790860000	2.320641000	-1.985044000
C	-4.656864000	1.831056000	0.023435000
H	-3.712524000	-0.088069000	0.234177000
C	-3.735122000	3.292538000	-1.656107000
H	-2.083640000	2.523091000	-2.788314000
C	-4.667889000	3.051898000	-0.651796000
H	-5.394416000	1.625301000	0.797652000
H	-3.747750000	4.234530000	-2.201189000
H	-5.410285000	3.807565000	-0.403651000

CP_{AN_s}

C	-1.678468000	-0.608799000	-1.456492000
C	-2.115828000	0.496199000	-0.875464000
Co	-0.372934000	0.166322000	-0.386747000
P	-0.838222000	-0.379567000	1.645651000
P	0.685779000	2.013607000	0.289695000
C	0.005953000	2.939475000	1.741847000
H	0.722517000	3.717351000	2.035707000
H	-0.881734000	3.459217000	1.354697000
C	-1.422279000	1.019466000	2.681723000
H	-2.288670000	1.444915000	2.152429000
H	-1.804710000	0.617346000	3.629403000
C	-0.391313000	2.111177000	2.958753000
H	-0.816625000	2.794994000	3.705149000
H	0.498248000	1.680891000	3.436501000
C	2.295370000	-1.177943000	-1.209988000
C	-2.026587000	-1.718657000	-2.300311000
C	-1.126401000	-2.782632000	-2.490033000
C	-3.295381000	-1.792332000	-2.906862000
C	-1.487064000	-3.890499000	-3.244551000
H	-0.146714000	-2.723894000	-2.015208000
C	-3.648600000	-2.896514000	-3.670230000
H	-3.995150000	-0.968342000	-2.772353000
C	-2.749118000	-3.950021000	-3.836124000
H	-0.785823000	-4.712379000	-3.375934000
H	-4.631151000	-2.941302000	-4.135579000
H	-3.031773000	-4.817626000	-4.428863000
C	3.547970000	-1.739643000	-1.555298000
C	3.748424000	-2.324657000	-2.817258000
C	4.588435000	-1.709622000	-0.609751000

C	4.986680000	-2.870478000	-3.124716000
H	2.935468000	-2.341538000	-3.539838000
C	5.819801000	-2.259657000	-0.935413000
H	4.415464000	-1.246684000	0.360127000
C	6.020292000	-2.838405000	-2.188589000
H	5.147911000	-3.322711000	-4.100233000
H	6.628842000	-2.235443000	-0.208731000
H	6.988357000	-3.267117000	-2.438055000
C	-3.273678000	1.273586000	-0.518392000
C	-3.183367000	2.658640000	-0.292812000
C	-4.508820000	0.630390000	-0.312547000
C	-4.296307000	3.380623000	0.116970000
H	-2.230144000	3.157808000	-0.474204000
C	-5.611502000	1.352200000	0.127789000
H	-4.575889000	-0.446145000	-0.470678000
C	-5.509668000	2.726888000	0.338397000
H	-4.221623000	4.455665000	0.268058000
H	-6.557366000	0.842148000	0.300527000
H	-6.377989000	3.291788000	0.671125000
N	1.267892000	-0.731593000	-0.875008000
C	-2.237792000	-1.554372000	1.648005000
C	-3.455692000	-1.285441000	2.281056000
C	-2.094783000	-2.743443000	0.919815000
C	-4.508560000	-2.194746000	2.186893000
H	-3.605114000	-0.362263000	2.837151000
C	-3.148413000	-3.641974000	0.819144000
H	-1.157886000	-2.949918000	0.400706000
C	-4.359537000	-3.368473000	1.455332000
H	-5.452128000	-1.974292000	2.682424000
H	-3.026779000	-4.550945000	0.232719000
H	-5.187063000	-4.070350000	1.376576000
C	0.462949000	-1.198852000	2.635427000
C	0.636955000	-0.932296000	4.000971000
C	1.315390000	-2.121537000	2.014582000
C	1.660433000	-1.549168000	4.715409000
H	-0.027429000	-0.245133000	4.521482000
C	2.330668000	-2.743921000	2.733063000
H	1.181091000	-2.350167000	0.959637000
C	2.514326000	-2.448658000	4.082083000
H	1.784188000	-1.329768000	5.773887000
H	2.981080000	-3.461251000	2.235651000
H	3.313635000	-2.928228000	4.643171000
C	0.648046000	3.305098000	-1.003201000
C	1.226551000	4.561589000	-0.770105000
C	0.037765000	3.053722000	-2.236424000
C	1.181936000	5.547375000	-1.749286000
H	1.727720000	4.765501000	0.176434000
C	-0.003155000	4.042533000	-3.217302000
H	-0.416186000	2.079311000	-2.423000000
C	0.565867000	5.288845000	-2.973532000
H	1.631337000	6.519671000	-1.558147000
H	-0.481850000	3.836759000	-4.172361000
H	0.532930000	6.061850000	-3.738510000
C	2.471055000	1.811073000	0.641937000
C	2.901345000	1.246792000	1.851479000
C	3.431287000	2.115530000	-0.333397000
C	4.255581000	1.039859000	2.098745000
H	2.179883000	0.953797000	2.611997000
C	4.784640000	1.898551000	-0.088142000
H	3.120416000	2.537096000	-1.288310000
C	5.202388000	1.371502000	1.131569000
H	4.567162000	0.617857000	3.052780000
H	5.515604000	2.148390000	-0.854674000
H	6.261795000	1.212753000	1.324752000

CP_{AN_t}

C	-1.384404000	1.818578000	1.166662000
C	-2.283711000	1.044549000	0.715748000
Co	-0.371673000	0.342319000	0.371743000

P	0.590094000	1.138221000	-1.589433000
P	-1.101650000	-1.626067000	-0.672845000
C	-1.749976000	-1.367168000	-2.376613000
H	-1.965441000	-2.345122000	-2.829087000
H	-2.722315000	-0.869959000	-2.247860000
C	-0.641541000	0.910836000	-2.953352000
H	-1.583981000	1.379275000	-2.636554000
H	-0.289150000	1.471052000	-3.829989000
C	-0.873225000	-0.550887000	-3.331486000
H	-1.361271000	-0.572447000	-4.314731000
H	0.100739000	-1.040762000	-3.478228000
C	2.132804000	-0.727156000	1.992324000
C	-0.917499000	3.058738000	1.734326000
C	0.451186000	3.323889000	1.890277000
C	-1.851783000	4.043436000	2.099912000
C	0.877831000	4.547996000	2.388530000
H	1.177693000	2.566128000	1.594515000
C	-1.418557000	5.262499000	2.604436000
H	-2.914121000	3.838975000	1.978304000
C	-0.055172000	5.519270000	2.746724000
H	1.942566000	4.748535000	2.491089000
H	-2.148661000	6.018524000	2.886057000
H	0.279490000	6.477933000	3.137692000
C	3.285776000	-1.172246000	2.684012000
C	3.533159000	-0.740935000	3.998603000
C	4.178150000	-2.047824000	2.039735000
C	4.669718000	-1.186856000	4.657562000
H	2.835661000	-0.063540000	4.485211000
C	5.307001000	-2.486621000	2.716269000
H	3.970868000	-2.374162000	1.022427000
C	5.553542000	-2.057378000	4.020304000
H	4.867115000	-0.855592000	5.673976000
H	6.000691000	-3.163945000	2.224189000
H	6.441874000	-2.403691000	4.543703000
C	-3.612915000	0.575528000	0.435953000
C	-4.182266000	0.755288000	-0.836168000
C	-4.374084000	-0.051183000	1.436930000
C	-5.474801000	0.316639000	-1.099542000
H	-3.607163000	1.266717000	-1.608303000
C	-5.661911000	-0.493098000	1.164066000
H	-3.939295000	-0.192473000	2.424096000
C	-6.215475000	-0.315715000	-0.102986000
H	-5.907550000	0.475510000	-2.085290000
H	-6.236946000	-0.982516000	1.947766000
H	-7.225069000	-0.663179000	-0.311450000
N	1.188497000	-0.384685000	1.394327000
C	-2.428951000	-2.532461000	0.196210000
C	-3.519137000	-3.120145000	-0.452122000
C	-2.328259000	-2.638821000	1.590182000
C	-4.484185000	-3.806784000	0.280714000
H	-3.629990000	-3.041243000	-1.532368000
C	-3.281266000	-3.342658000	2.317754000
H	-1.504210000	-2.144325000	2.110112000
C	-4.363132000	-3.927203000	1.662363000
H	-5.332888000	-4.252931000	-0.234151000
H	-3.187701000	-3.423085000	3.399140000
H	-5.115465000	-4.471043000	2.230036000
C	0.183210000	-2.922346000	-0.864002000
C	0.575591000	-3.437565000	-2.104757000
C	0.822094000	-3.399828000	0.290173000
C	1.591401000	-4.387343000	-2.191035000
H	0.089977000	-3.109272000	-3.020995000
C	1.830141000	-4.353902000	0.204353000
H	0.513859000	-3.032935000	1.268623000
C	2.226136000	-4.843298000	-1.040019000
H	1.881778000	-4.774387000	-3.165735000
H	2.301507000	-4.723184000	1.114031000
H	3.015209000	-5.589350000	-1.109349000
C	0.833172000	2.942698000	-1.532195000
C	2.107538000	3.501802000	-1.368668000

C	-0.286927000	3.785467000	-1.492783000
C	2.256226000	4.873752000	-1.187539000
H	2.988718000	2.861284000	-1.389770000
C	-0.134242000	5.155649000	-1.311620000
H	-1.290914000	3.367155000	-1.578614000
C	1.137573000	5.702849000	-1.158393000
H	3.252408000	5.296044000	-1.069661000
H	-1.013307000	5.796398000	-1.279890000
H	1.255553000	6.774503000	-1.011746000
C	2.115375000	0.474676000	-2.337345000
C	2.682064000	1.054971000	-3.482300000
C	2.697142000	-0.678718000	-1.799509000
C	3.808129000	0.491818000	-4.071299000
H	2.245098000	1.960374000	-3.905047000
C	3.821903000	-1.245501000	-2.396079000
H	2.253790000	-1.142375000	-0.917911000
C	4.378267000	-0.660396000	-3.529110000
H	4.242577000	0.950696000	-4.957081000
H	4.259252000	-2.150394000	-1.976987000
H	5.257814000	-1.100672000	-3.994529000

CP_Ns

Co	-0.091172000	0.911244000	0.012556000
P	-2.188699000	0.779918000	0.523125000
P	0.319292000	-0.937726000	0.941683000
C	-0.513708000	-1.240785000	2.562589000
H	-0.230740000	-2.250683000	2.891586000
H	-0.023623000	-0.550803000	3.264182000
C	-2.519984000	0.340809000	2.281195000
H	-2.015412000	1.097241000	2.897946000
H	-3.593028000	0.438736000	2.489562000
C	-2.028309000	-1.060815000	2.628097000
H	-2.351196000	-1.302742000	3.649087000
H	-2.528610000	-1.789629000	1.974656000
N	1.629540000	1.291949000	-0.506031000
C	2.744943000	1.480766000	-0.816667000
C	4.107914000	1.635674000	-1.143945000
C	4.589291000	2.831368000	-1.707556000
C	4.985861000	0.564883000	-0.884688000
C	5.939170000	2.947016000	-2.003981000
H	3.903286000	3.651419000	-1.904581000
C	6.332089000	0.702468000	-1.186355000
H	4.598350000	-0.354189000	-0.448609000
C	6.809963000	1.888557000	-1.744248000
H	6.315768000	3.869004000	-2.439987000
H	7.013393000	-0.121289000	-0.986338000
H	7.867165000	1.988589000	-1.979177000
C	-2.945602000	2.422006000	0.303474000
C	-4.046780000	2.639178000	-0.532934000
C	-2.359516000	3.508848000	0.971170000
C	-4.563681000	3.923218000	-0.680918000
H	-4.502441000	1.804002000	-1.062970000
C	-2.883486000	4.788118000	0.822083000
H	-1.490649000	3.347639000	1.612857000
C	-3.986043000	4.995580000	-0.004977000
H	-5.423620000	4.085524000	-1.327239000
H	-2.429267000	5.624512000	1.349001000
H	-4.394200000	5.996804000	-0.124836000
C	2.071113000	-1.207326000	1.389870000
C	2.763416000	-2.375816000	1.054151000
C	2.725357000	-0.209740000	2.127191000
C	4.086395000	-2.545619000	1.461041000
H	2.269192000	-3.158897000	0.481028000
C	4.042952000	-0.384463000	2.534813000
H	2.197504000	0.714330000	2.370426000
C	4.725256000	-1.555030000	2.202346000
H	4.615155000	-3.460458000	1.201210000
H	4.540443000	0.394669000	3.108681000
H	5.756461000	-1.692717000	2.521410000

C	-3.188701000	-0.396578000	-0.438745000
C	-4.382268000	-0.947414000	0.045997000
C	-2.729894000	-0.772135000	-1.707755000
C	-5.094651000	-1.863292000	-0.722192000
H	-4.763852000	-0.662007000	1.026143000
C	-3.447625000	-1.681268000	-2.477801000
H	-1.791247000	-0.355991000	-2.079503000
C	-4.627815000	-2.231154000	-1.982670000
H	-6.019006000	-2.288245000	-0.336658000
H	-3.078936000	-1.968129000	-3.460635000
H	-5.187089000	-2.948111000	-2.580249000
C	-0.123114000	-2.326454000	-0.145641000
C	-0.945327000	-3.386373000	0.251993000
C	0.353794000	-2.288716000	-1.465522000
C	-1.294387000	-4.382601000	-0.657198000
H	-1.312983000	-3.448804000	1.274608000
C	0.017417000	-3.292788000	-2.364982000
H	0.991082000	-1.460657000	-1.782231000
C	-0.815671000	-4.337092000	-1.963279000
H	-1.937732000	-5.200237000	-0.339009000
H	0.399966000	-3.258918000	-3.383131000
H	-1.088385000	-5.118263000	-2.669867000

CP_{N_t}

Co	0.275183000	-0.960300000	-0.167276000
P	2.442363000	-0.669199000	0.364609000
P	-0.537256000	0.812554000	1.057201000
C	0.427524000	1.206576000	2.579218000
H	0.046697000	2.140599000	3.015385000
H	0.180256000	0.417884000	3.304303000
C	2.644344000	-0.047485000	2.099946000
H	2.276477000	-0.821248000	2.788351000
H	3.721776000	0.051214000	2.290751000
C	1.943863000	1.282150000	2.385933000
H	2.374019000	1.692296000	3.308928000
H	2.195665000	2.006724000	1.596699000
N	-1.399576000	-1.560202000	-0.882899000
C	-2.521316000	-1.765597000	-1.148793000
C	-3.905132000	-1.910528000	-1.398125000
C	-4.404444000	-2.971133000	-2.172916000
C	-4.777384000	-0.958698000	-0.836433000
C	-5.772655000	-3.073063000	-2.378431000
H	-3.719774000	-3.698893000	-2.601204000
C	-6.141872000	-1.079898000	-1.051246000
H	-4.372441000	-0.144602000	-0.236505000
C	-6.638896000	-2.132884000	-1.819589000
H	-6.167191000	-3.890381000	-2.976756000
H	-6.820285000	-0.349441000	-0.615999000
H	-7.710264000	-2.222119000	-1.985011000
C	3.678360000	-2.004366000	0.248714000
C	4.328512000	-2.243820000	-0.969809000
C	3.936012000	-2.848912000	1.336021000
C	5.226996000	-3.298171000	-1.091182000
H	4.141193000	-1.591980000	-1.822928000
C	4.836438000	-3.902826000	1.209750000
H	3.439050000	-2.686651000	2.291857000
C	5.482966000	-4.129116000	-0.002448000
H	5.732387000	-3.468675000	-2.039451000
H	5.035067000	-4.546633000	2.063983000
H	6.187534000	-4.952293000	-0.098554000
C	-2.249156000	0.625010000	1.670771000
C	-3.177079000	1.674012000	1.677845000
C	-2.643090000	-0.635116000	2.143964000
C	-4.468898000	1.464756000	2.157128000
H	-2.889110000	2.657337000	1.307346000
C	-3.930168000	-0.839543000	2.631043000
H	-1.933637000	-1.465267000	2.123933000
C	-4.846048000	0.211494000	2.635632000
H	-5.180750000	2.287912000	2.162456000

H	-4.221772000	-1.821416000	2.998201000
H	-5.855135000	0.052180000	3.010457000
C	3.139484000	0.690495000	-0.628303000
C	4.459704000	1.127639000	-0.453650000
C	2.320053000	1.346389000	-1.552678000
C	4.940365000	2.206917000	-1.186362000
H	5.115795000	0.611794000	0.248279000
C	2.799537000	2.430298000	-2.283406000
H	1.289989000	1.009986000	-1.698122000
C	4.109836000	2.861095000	-2.097075000
H	5.966980000	2.539772000	-1.048717000
H	2.147903000	2.935596000	-2.993396000
H	4.490391000	3.706640000	-2.666304000
C	-0.572475000	2.349409000	0.081770000
C	0.053226000	3.537496000	0.473304000
C	-1.221788000	2.302255000	-1.162689000
C	0.032974000	4.652693000	-0.362394000
H	0.559390000	3.605518000	1.434797000
C	-1.249489000	3.418562000	-1.989961000
H	-1.717009000	1.380933000	-1.478022000
C	-0.615593000	4.595915000	-1.592324000
H	0.524001000	5.570437000	-0.045703000
H	-1.764068000	3.370964000	-2.947542000
H	-0.630912000	5.468963000	-2.241241000

CP_{A_s}

C	1.543643000	0.530592000	0.996945000
Co	0.007507000	0.050988000	0.146753000
P	0.151030000	-1.163974000	-1.629724000
P	-1.342483000	1.502911000	-0.767990000
C	-1.490575000	1.652535000	-2.595942000
H	-2.342341000	2.305127000	-2.831108000
H	-0.587075000	2.151653000	-2.975699000
C	-0.397873000	-0.559205000	-3.278833000
H	0.442886000	0.021371000	-3.683859000
H	-0.506698000	-1.427384000	-3.943276000
C	-1.666616000	0.293580000	-3.271315000
H	-1.977054000	0.456390000	-4.310940000
H	-2.496945000	-0.249221000	-2.793421000
C	0.867742000	-0.308644000	1.742150000
C	1.842090000	-1.760934000	-1.914185000
C	2.163841000	-3.121901000	-1.959496000
C	2.852570000	-0.803127000	-2.083305000
C	3.481933000	-3.515425000	-2.176111000
H	1.386509000	-3.873357000	-1.829077000
C	4.165700000	-1.202870000	-2.299737000
H	2.611000000	0.259871000	-2.031153000
C	4.481278000	-2.560131000	-2.344462000
H	3.727108000	-4.574618000	-2.214629000
H	4.943508000	-0.452147000	-2.425494000
H	5.509676000	-2.873892000	-2.510406000
C	-0.891269000	-2.591846000	-1.215972000
C	-1.993614000	-2.988750000	-1.982805000
C	-0.652775000	-3.221822000	0.018583000
C	-2.840078000	-3.994566000	-1.523470000
H	-2.198973000	-2.518863000	-2.943152000
C	-1.500952000	-4.226200000	0.471577000
H	0.203726000	-2.918333000	0.622674000
C	-2.599785000	-4.609276000	-0.296525000
H	-3.690785000	-4.299280000	-2.129159000
H	-1.302239000	-4.708081000	1.427281000
H	-3.266561000	-5.392253000	0.058341000
C	-3.009676000	1.004834000	-0.229783000
C	-4.122538000	1.845238000	-0.352149000
C	-3.168582000	-0.272026000	0.324789000
C	-5.374888000	1.403323000	0.061389000
H	-4.005870000	2.849748000	-0.760668000
C	-4.422329000	-0.713413000	0.736637000
H	-2.298786000	-0.928675000	0.434456000

C	-5.525576000	0.125889000	0.601716000
H	-6.237949000	2.058662000	-0.034437000
H	-4.533672000	-1.708489000	1.163487000
H	-6.507979000	-0.212440000	0.924225000
C	-1.085641000	3.196744000	-0.163949000
C	-1.011073000	4.305264000	-1.015943000
C	-0.904158000	3.377160000	1.215486000
C	-0.758197000	5.571996000	-0.494031000
H	-1.150274000	4.191467000	-2.089614000
C	-0.658511000	4.643246000	1.731286000
H	-0.948355000	2.514800000	1.882624000
C	-0.580391000	5.742009000	0.875948000
H	-0.702701000	6.428187000	-1.162976000
H	-0.521921000	4.773427000	2.802543000
H	-0.380717000	6.732303000	1.279394000
C	0.720519000	-1.011021000	2.989670000
C	1.731209000	-0.956085000	3.967279000
C	-0.434866000	-1.768555000	3.251863000
C	1.589577000	-1.647071000	5.163154000
H	2.621928000	-0.359142000	3.777331000
C	-0.571597000	-2.458852000	4.448046000
H	-1.224231000	-1.800031000	2.499188000
C	0.441732000	-2.401431000	5.404966000
H	2.376641000	-1.597585000	5.912571000
H	-1.471499000	-3.039549000	4.641163000
H	0.334695000	-2.941785000	6.343116000
C	2.710769000	1.290370000	0.649780000
C	3.978806000	0.861369000	1.082469000
C	2.615039000	2.425088000	-0.175183000
C	5.119809000	1.549280000	0.690740000
H	4.055266000	-0.028856000	1.704893000
C	3.758739000	3.116802000	-0.549138000
H	1.629622000	2.756041000	-0.505467000
C	5.012720000	2.677267000	-0.122415000
H	6.097563000	1.207140000	1.023236000
H	3.676389000	4.002400000	-1.175762000
H	5.908275000	3.218025000	-0.421212000

CPA_t

C	0.884709000	2.131208000	-0.314697000
Co	0.030801000	0.493576000	0.194345000
P	-1.793090000	-0.822502000	0.915158000
P	1.687651000	-1.090728000	0.696818000
C	1.292831000	-1.916878000	2.302377000
H	2.096577000	-2.633344000	2.521468000
H	1.336703000	-1.155781000	3.094342000
C	-1.303777000	-1.762238000	2.431052000
H	-1.184031000	-1.008221000	3.222412000
H	-2.168953000	-2.367641000	2.735207000
C	-0.054678000	-2.641126000	2.339266000
H	-0.050860000	-3.287665000	3.226464000
H	-0.128185000	-3.322259000	1.479083000
C	-0.382832000	2.202410000	-0.555697000
C	-3.293828000	0.061671000	1.440903000
C	-4.579076000	-0.408586000	1.150320000
C	-3.138250000	1.275097000	2.124119000
C	-5.692946000	0.328486000	1.544542000
H	-4.710473000	-1.344489000	0.608278000
C	-4.253705000	2.000092000	2.526548000
H	-2.137090000	1.665745000	2.318088000
C	-5.532110000	1.528892000	2.232259000
H	-6.690529000	-0.038927000	1.313204000
H	-4.125115000	2.942943000	3.053472000
H	-6.405278000	2.102913000	2.534846000
C	-2.332937000	-2.057657000	-0.301213000
C	-2.515910000	-3.410738000	0.005322000
C	-2.572739000	-1.615455000	-1.611236000
C	-2.924976000	-4.304541000	-0.981799000
H	-2.349970000	-3.777131000	1.017201000

C	-2.999088000	-2.506186000	-2.588977000
H	-2.421865000	-0.563375000	-1.863442000
C	-3.168400000	-3.854563000	-2.276431000
H	-3.061284000	-5.354859000	-0.733506000
H	-3.193101000	-2.149384000	-3.598458000
H	-3.493567000	-4.554405000	-3.043296000
C	1.525094000	-2.423775000	-0.531994000
C	2.069911000	-3.697021000	-0.315850000
C	0.816190000	-2.174706000	-1.712728000
C	1.891745000	-4.702183000	-1.259035000
H	2.640770000	-3.901278000	0.590442000
C	0.643650000	-3.180782000	-2.659820000
H	0.396962000	-1.181303000	-1.895177000
C	1.176791000	-4.445181000	-2.429420000
H	2.316144000	-5.688625000	-1.084925000
H	0.088189000	-2.976331000	-3.572718000
H	1.041233000	-5.234562000	-3.165766000
C	3.463148000	-0.723544000	0.772777000
C	4.160941000	-0.641008000	1.982553000
C	4.128903000	-0.439719000	-0.427886000
C	5.509741000	-0.292721000	1.987554000
H	3.660832000	-0.850299000	2.927328000
C	5.473767000	-0.093624000	-0.416953000
H	3.588480000	-0.487257000	-1.374197000
C	6.166306000	-0.019569000	0.790832000
H	6.048121000	-0.239644000	2.931605000
H	5.981632000	0.125969000	-1.353763000
H	7.219912000	0.251819000	0.798402000
C	-1.508626000	3.013198000	-0.951766000
C	-2.799090000	2.477471000	-1.071679000
C	-1.312692000	4.380698000	-1.218871000
C	-3.869584000	3.282769000	-1.436894000
H	-2.955740000	1.420289000	-0.860869000
C	-2.384746000	5.181953000	-1.587484000
H	-0.312597000	4.801913000	-1.127499000
C	-3.664558000	4.637023000	-1.694738000
H	-4.866426000	2.853269000	-1.516310000
H	-2.223286000	6.238498000	-1.790593000
H	-4.502132000	5.269880000	-1.980596000
C	2.236110000	2.623883000	-0.380304000
C	3.072101000	2.584826000	0.746929000
C	2.732040000	3.159868000	-1.581623000
C	4.364435000	3.087559000	0.680936000
H	2.689388000	2.164382000	1.676532000
C	4.034852000	3.638524000	-1.646250000
H	2.085403000	3.193613000	-2.457162000
C	4.851705000	3.608355000	-0.516753000
H	4.998366000	3.062404000	1.564967000
H	4.411163000	4.048573000	-2.581226000
H	5.868010000	3.993362000	-0.569967000

TS1_s

C	-1.777612000	0.691544000	0.743699000
C	-1.708786000	1.052409000	-0.509491000
Co	-0.041831000	0.168036000	-0.059299000
P	1.530186000	1.495970000	-0.889688000
P	-0.075167000	-1.042566000	-1.822507000
C	-0.080254000	-0.091349000	-3.393857000
H	-0.278076000	-0.781554000	-4.224642000
H	-0.939986000	0.593087000	-3.345951000
C	1.427228000	1.877541000	-2.701517000
H	0.592710000	2.583204000	-2.809179000
H	2.339765000	2.411545000	-2.996094000
C	1.199456000	0.702456000	-3.649408000
H	1.148874000	1.105755000	-4.669253000
H	2.067818000	0.030320000	-3.646862000
C	0.683782000	-0.598845000	1.525911000
C	-0.607738000	-0.912823000	1.405852000
C	-2.461159000	1.077179000	1.965558000

C	-1.805427000	1.210675000	3.199800000
C	-3.822949000	1.412309000	1.883313000
C	-2.487336000	1.687437000	4.311048000
H	-0.751049000	0.947233000	3.277153000
C	-4.501198000	1.882621000	3.001426000
H	-4.339883000	1.308730000	0.930043000
C	-3.838287000	2.020936000	4.218458000
H	-1.963147000	1.793505000	5.258784000
H	-5.555497000	2.138914000	2.920874000
H	-4.372968000	2.381911000	5.094215000
C	-1.551475000	-1.929191000	1.828829000
C	-1.072550000	-2.962315000	2.659806000
C	-2.879683000	-2.004272000	1.373566000
C	-1.893972000	-4.020943000	3.021528000
H	-0.039782000	-2.933279000	3.003521000
C	-3.699360000	-3.059949000	1.747779000
H	-3.262045000	-1.238579000	0.701289000
C	-3.214420000	-4.069966000	2.575975000
H	-1.502550000	-4.809808000	3.660596000
H	-4.723621000	-3.097786000	1.381637000
H	-3.861554000	-4.892514000	2.873435000
C	1.756883000	-0.849894000	2.455048000
C	1.465626000	-0.951898000	3.833659000
C	3.097085000	-0.975563000	2.045151000
C	2.476983000	-1.159000000	4.759961000
H	0.430246000	-0.860101000	4.163170000
C	4.100946000	-1.213555000	2.975521000
H	3.337513000	-0.909276000	0.986281000
C	3.798618000	-1.297339000	4.333574000
H	2.234897000	-1.223819000	5.818809000
H	5.129675000	-1.323531000	2.636887000
H	4.589743000	-1.471299000	5.059912000
C	-2.460814000	1.831974000	-1.463877000
C	-1.944233000	3.027300000	-1.993995000
C	-3.741450000	1.412493000	-1.870501000
C	-2.683108000	3.772571000	-2.904599000
H	-0.980372000	3.390463000	-1.638719000
C	-4.463958000	2.150130000	-2.801217000
H	-4.153856000	0.493121000	-1.454508000
C	-3.937241000	3.330077000	-3.323595000
H	-2.279890000	4.708399000	-3.286412000
H	-5.450083000	1.809104000	-3.110218000
H	-4.508164000	3.910282000	-4.045009000
C	1.355116000	-2.171986000	-1.963121000
C	1.843293000	-2.567802000	-3.217201000
C	1.973592000	-2.667359000	-0.810040000
C	2.943401000	-3.415469000	-3.308080000
H	1.366923000	-2.218607000	-4.132074000
C	3.067399000	-3.522781000	-0.902846000
H	1.598722000	-2.371522000	0.168214000
C	3.561131000	-3.889375000	-2.152072000
H	3.315395000	-3.709904000	-4.287181000
H	3.538541000	-3.892585000	0.006224000
H	4.423132000	-4.549002000	-2.227537000
C	3.301337000	1.151533000	-0.617836000
C	4.010924000	1.815425000	0.391004000
C	3.952013000	0.155979000	-1.361895000
C	5.341983000	1.495427000	0.643703000
H	3.521177000	2.585487000	0.984824000
C	5.281775000	-0.161536000	-1.104951000
H	3.418397000	-0.395180000	-2.135001000
C	5.980021000	0.507060000	-0.100653000
H	5.879925000	2.020893000	1.430192000
H	5.771278000	-0.936058000	-1.692690000
H	7.020292000	0.257966000	0.099192000
C	-1.514367000	-2.146176000	-1.931352000
C	-2.682426000	-1.743565000	-2.592107000
C	-1.479702000	-3.395071000	-1.296790000
C	-3.793526000	-2.580845000	-2.619888000
H	-2.726270000	-0.778112000	-3.094214000

C	-2.591024000	-4.229792000	-1.332730000
H	-0.579110000	-3.717552000	-0.774462000
C	-3.749313000	-3.824078000	-1.991347000
H	-4.692754000	-2.264323000	-3.145415000
H	-2.552712000	-5.196925000	-0.835577000
H	-4.618015000	-4.478737000	-2.019337000
C	1.263060000	3.127461000	-0.114271000
C	1.591252000	4.323790000	-0.766190000
C	0.684444000	3.183992000	1.160284000
C	1.324494000	5.548105000	-0.160045000
H	2.058412000	4.305688000	-1.749943000
C	0.420104000	4.408670000	1.764737000
H	0.435377000	2.256719000	1.678430000
C	0.733767000	5.592590000	1.101420000
H	1.581204000	6.471377000	-0.675349000
H	-0.039313000	4.434657000	2.751075000
H	0.520755000	6.551991000	1.568061000

TS1_t

C	-0.776624000	-0.435962000	1.780672000
C	-1.024531000	-1.254088000	0.822459000
Co	-0.065657000	0.302160000	-0.109675000
P	-1.769999000	0.957133000	-1.547764000
P	1.229535000	-0.960202000	-1.644671000
C	0.695312000	-0.781612000	-3.417276000
H	1.582215000	-0.889055000	-4.054568000
H	0.039832000	-1.635126000	-3.644266000
C	-1.513874000	0.508879000	-3.314312000
H	-1.928506000	-0.499633000	-3.451481000
H	-2.119799000	1.168619000	-3.949688000
C	-0.045152000	0.514056000	-3.754667000
H	-0.013243000	0.649315000	-4.843404000
H	0.485126000	1.386316000	-3.337828000
C	1.124172000	1.491146000	0.914499000
C	1.151094000	0.380206000	1.579778000
C	-1.374846000	0.171307000	2.955124000
C	-0.838561000	1.245325000	3.681783000
C	-2.595109000	-0.390425000	3.387638000
C	-1.505220000	1.742642000	4.796538000
H	0.100303000	1.695515000	3.371148000
C	-3.247712000	0.106135000	4.506635000
H	-3.023826000	-1.217948000	2.822197000
C	-2.706340000	1.177553000	5.216634000
H	-1.074951000	2.577427000	5.345757000
H	-4.186454000	-0.343908000	4.824263000
H	-3.218524000	1.567962000	6.093170000
C	2.039430000	-0.573433000	2.210805000
C	3.390464000	-0.527391000	1.811547000
C	1.643941000	-1.536700000	3.153250000
C	4.306322000	-1.437382000	2.321343000
H	3.700780000	0.219139000	1.080456000
C	2.570508000	-2.439715000	3.662042000
H	0.611095000	-1.572430000	3.491250000
C	3.899127000	-2.401084000	3.242786000
H	5.342343000	-1.395900000	1.990164000
H	2.252205000	-3.177302000	4.395975000
H	4.617426000	-3.115471000	3.639410000
C	1.710868000	2.797956000	0.807162000
C	2.637037000	3.211950000	1.786464000
C	1.408322000	3.674412000	-0.249317000
C	3.245060000	4.455706000	1.697340000
H	2.874787000	2.538682000	2.609473000
C	2.024020000	4.915932000	-0.335415000
H	0.682586000	3.367155000	-1.002505000
C	2.943703000	5.310296000	0.635909000
H	3.959998000	4.761942000	2.458195000
H	1.777853000	5.582382000	-1.160007000
H	3.422071000	6.285238000	0.569787000
C	-1.633651000	-2.463719000	0.372638000

C	-1.883623000	-2.717604000	-0.986742000
C	-1.972090000	-3.454824000	1.317084000
C	-2.475747000	-3.904601000	-1.390304000
H	-1.593118000	-1.965272000	-1.721656000
C	-2.545509000	-4.649502000	0.906700000
H	-1.759588000	-3.275082000	2.370851000
C	-2.804061000	-4.876745000	-0.445457000
H	-2.666003000	-4.083966000	-2.446699000
H	-2.793942000	-5.409625000	1.644430000
H	-3.253846000	-5.814760000	-0.763453000
C	2.941837000	-0.324457000	-1.649833000
C	4.063793000	-1.152888000	-1.527448000
C	3.125269000	1.063781000	-1.703633000
C	5.338791000	-0.596693000	-1.458155000
H	3.940781000	-2.233472000	-1.470041000
C	4.398311000	1.618292000	-1.628233000
H	2.259317000	1.721988000	-1.782308000
C	5.509096000	0.785609000	-1.501290000
H	6.204475000	-1.249655000	-1.363199000
H	4.517382000	2.700325000	-1.655630000
H	6.506939000	1.214306000	-1.434885000
C	1.424319000	-2.757284000	-1.430858000
C	1.525077000	-3.645050000	-2.509559000
C	1.491310000	-3.263241000	-0.126499000
C	1.670088000	-5.011304000	-2.283794000
H	1.502329000	-3.277565000	-3.534257000
C	1.644572000	-4.626795000	0.096365000
H	1.407254000	-2.583122000	0.721206000
C	1.725767000	-5.504636000	-0.982509000
H	1.744737000	-5.691606000	-3.129745000
H	1.688673000	-5.002432000	1.117348000
H	1.835876000	-6.573336000	-0.810283000
C	-1.837456000	2.782789000	-1.530178000
C	-2.061824000	3.408483000	-0.294009000
C	-1.570442000	3.574915000	-2.652412000
C	-2.049326000	4.793532000	-0.190455000
H	-2.235143000	2.802984000	0.598054000
C	-1.541980000	4.964377000	-2.541281000
H	-1.378969000	3.120047000	-3.622979000
C	-1.784870000	5.575087000	-1.314636000
H	-2.232705000	5.264590000	0.772818000
H	-1.335115000	5.569112000	-3.422044000
H	-1.763882000	6.659655000	-1.231820000
C	-3.454332000	0.384912000	-1.155448000
C	-4.346583000	-0.065896000	-2.136013000
C	-3.845517000	0.345230000	0.189759000
C	-5.596529000	-0.559640000	-1.773938000
H	-4.076499000	-0.032105000	-3.190029000
C	-5.099280000	-0.138753000	0.546522000
H	-3.161671000	0.683420000	0.968099000
C	-5.973629000	-0.601045000	-0.434039000
H	-6.280471000	-0.908686000	-2.544795000
H	-5.389041000	-0.159030000	1.595888000
H	-6.950547000	-0.990148000	-0.155224000

INT1_s

C	-1.173835000	1.367431000	0.939769000
C	-1.583692000	1.120018000	-0.373468000
Co	-0.050632000	0.109002000	-0.165098000
P	1.575706000	0.664110000	-1.536171000
P	-0.627885000	-1.620335000	-1.344321000
C	-0.619223000	-1.356303000	-3.165191000
H	-0.989719000	-2.265079000	-3.656986000
H	-1.368985000	-0.580351000	-3.370592000
C	1.206015000	0.451217000	-3.335796000
H	0.426303000	1.182318000	-3.590271000
H	2.099998000	0.727545000	-3.910651000
C	0.733343000	-0.943769000	-3.744888000
H	0.654121000	-0.963763000	-4.839643000

H	1.496459000	-1.695714000	-3.497793000
C	0.646303000	-0.101245000	1.543768000
C	-0.740316000	0.113172000	1.679243000
C	-0.940293000	2.700103000	1.520409000
C	-0.652095000	2.829806000	2.887087000
C	-1.049394000	3.866000000	0.745087000
C	-0.462669000	4.082977000	3.458686000
H	-0.601612000	1.933834000	3.504837000
C	-0.880277000	5.116899000	1.321872000
H	-1.237709000	3.785711000	-0.325287000
C	-0.581228000	5.231807000	2.679364000
H	-0.241209000	4.163901000	4.521073000
H	-0.961949000	6.008858000	0.703094000
H	-0.445504000	6.213439000	3.128716000
C	-1.717556000	-0.784514000	2.310876000
C	-1.311964000	-1.991911000	2.905842000
C	-3.075978000	-0.442160000	2.363913000
C	-2.233675000	-2.820283000	3.532131000
H	-0.260352000	-2.278807000	2.878872000
C	-4.000599000	-1.281849000	2.973509000
H	-3.400090000	0.502982000	1.930455000
C	-3.583572000	-2.471265000	3.566372000
H	-1.897680000	-3.747270000	3.993507000
H	-5.051238000	-0.998488000	2.997815000
H	-4.304956000	-3.120771000	4.058166000
C	1.701246000	-0.366722000	2.468225000
C	1.511001000	-0.194812000	3.859757000
C	2.962327000	-0.808561000	2.010419000
C	2.541771000	-0.449610000	4.749313000
H	0.535386000	0.128043000	4.221469000
C	3.988980000	-1.065959000	2.904739000
H	3.106183000	-0.955126000	0.942237000
C	3.782393000	-0.882654000	4.273690000
H	2.385901000	-0.313844000	5.817279000
H	4.954773000	-1.407203000	2.537154000
H	4.590534000	-1.079791000	4.975441000
C	-2.628135000	1.649364000	-1.195026000
C	-2.454344000	1.797618000	-2.586475000
C	-3.874177000	2.002621000	-0.634717000
C	-3.484980000	2.263382000	-3.387637000
H	-1.480947000	1.559963000	-3.013217000
C	-4.913940000	2.439507000	-1.442080000
H	-4.010850000	1.915461000	0.441861000
C	-4.723841000	2.567786000	-2.818610000
H	-3.332044000	2.387795000	-4.457515000
H	-5.875095000	2.691939000	-0.999670000
H	-5.539007000	2.916411000	-3.449165000
C	0.419436000	-3.098882000	-1.092514000
C	0.609113000	-4.058158000	-2.096275000
C	1.072518000	-3.266596000	0.134116000
C	1.448623000	-5.147492000	-1.877657000
H	0.105685000	-3.963233000	-3.057114000
C	1.899985000	-4.362022000	0.357083000
H	0.947976000	-2.508045000	0.905766000
C	2.095955000	-5.301016000	-0.653273000
H	1.593736000	-5.881365000	-2.667714000
H	2.402846000	-4.471946000	1.316507000
H	2.752499000	-6.152939000	-0.488580000
C	3.275656000	-0.018715000	-1.406889000
C	4.384581000	0.790924000	-1.127657000
C	3.473988000	-1.400687000	-1.551472000
C	5.651388000	0.229691000	-0.984082000
H	4.263789000	1.866221000	-1.016980000
C	4.741783000	-1.956741000	-1.416403000
H	2.629185000	-2.059182000	-1.739544000
C	5.834635000	-1.142959000	-1.124754000
H	6.499690000	0.874459000	-0.763205000
H	4.871046000	-3.031377000	-1.532674000
H	6.825782000	-1.577347000	-1.010864000
C	-2.317751000	-2.204980000	-0.988045000

C	-3.426384000	-1.587114000	-1.584769000
C	-2.529247000	-3.217196000	-0.043625000
C	-4.716635000	-1.979502000	-1.245598000
H	-3.290066000	-0.794789000	-2.319372000
C	-3.822437000	-3.605238000	0.292174000
H	-1.680062000	-3.705452000	0.432375000
C	-4.917633000	-2.988059000	-0.305531000
H	-5.566768000	-1.495301000	-1.723069000
H	-3.971045000	-4.391612000	1.029524000
H	-5.927993000	-3.293944000	-0.041422000
C	1.807490000	2.456924000	-1.310773000
C	1.688932000	3.389308000	-2.347765000
C	2.107259000	2.912769000	-0.017092000
C	1.869084000	4.748019000	-2.094116000
H	1.471871000	3.065721000	-3.364109000
C	2.305913000	4.265567000	0.227564000
H	2.183338000	2.195665000	0.802677000
C	2.181715000	5.187109000	-0.810892000
H	1.775340000	5.463223000	-2.908841000
H	2.533719000	4.602810000	1.236880000
H	2.325075000	6.248465000	-0.618023000

INT1_t

C	-0.627989000	-0.402363000	1.834951000
C	-0.894148000	-1.235711000	0.790556000
Co	-0.024501000	0.226298000	-0.197302000
P	-1.582355000	1.049064000	-1.654656000
P	1.226446000	-1.029230000	-1.792503000
C	0.733618000	-0.857466000	-3.569594000
H	1.613716000	-1.035859000	-4.200629000
H	0.014921000	-1.659278000	-3.789814000
C	-1.363791000	0.596143000	-3.428506000
H	-1.864186000	-0.372337000	-3.570279000
H	-1.921888000	1.315132000	-4.043382000
C	0.087594000	0.486224000	-3.907654000
H	0.098855000	0.606097000	-4.998634000
H	0.696412000	1.317354000	-3.516738000
C	0.816994000	1.382199000	1.028083000
C	0.783782000	0.184861000	1.715051000
C	-1.503207000	0.072181000	2.918171000
C	-1.044580000	1.030796000	3.835796000
C	-2.800309000	-0.445028000	3.084748000
C	-1.856481000	1.466003000	4.876808000
H	-0.037535000	1.433260000	3.732420000
C	-3.605735000	-0.013474000	4.130009000
H	-3.175274000	-1.185740000	2.379360000
C	-3.139413000	0.945606000	5.029247000
H	-1.481901000	2.208715000	5.578181000
H	-4.605105000	-0.429446000	4.246157000
H	-3.772362000	1.281120000	5.847861000
C	1.915276000	-0.602249000	2.226228000
C	3.226299000	-0.369440000	1.777079000
C	1.691553000	-1.633669000	3.152759000
C	4.276094000	-1.155421000	2.232563000
H	3.411368000	0.415503000	1.043100000
C	2.747425000	-2.415406000	3.608980000
H	0.681109000	-1.814405000	3.518732000
C	4.041141000	-2.183181000	3.146583000
H	5.283182000	-0.971768000	1.862824000
H	2.559541000	-3.207201000	4.331565000
H	4.865620000	-2.799279000	3.499091000
C	1.558894000	2.596553000	1.127082000
C	2.290125000	2.895579000	2.301113000
C	1.554450000	3.541844000	0.078399000
C	3.004547000	4.077557000	2.404558000
H	2.298127000	2.171870000	3.115744000
C	2.270642000	4.723454000	0.187896000
H	0.967439000	3.332835000	-0.815524000
C	2.998435000	4.992595000	1.348449000

H	3.569254000	4.293428000	3.308870000
H	2.255789000	5.444167000	-0.627373000
H	3.557103000	5.922389000	1.435260000
C	-1.653118000	-2.393124000	0.473349000
C	-2.054650000	-2.660788000	-0.854355000
C	-1.923304000	-3.371267000	1.460390000
C	-2.730041000	-3.826495000	-1.174025000
H	-1.814981000	-1.927181000	-1.626933000
C	-2.578382000	-4.546665000	1.129488000
H	-1.599153000	-3.188497000	2.484839000
C	-2.990483000	-4.777483000	-0.184801000
H	-3.041594000	-4.009854000	-2.200564000
H	-2.774116000	-5.290561000	1.899181000
H	-3.506457000	-5.700698000	-0.439471000
C	2.939503000	-0.400641000	-1.741510000
C	4.057931000	-1.237921000	-1.661431000
C	3.124827000	0.989182000	-1.706834000
C	5.333695000	-0.690446000	-1.549838000
H	3.930042000	-2.319480000	-1.671862000
C	4.399613000	1.533722000	-1.596700000
H	2.257374000	1.651011000	-1.740522000
C	5.507561000	0.691431000	-1.513773000
H	6.197123000	-1.349978000	-1.485957000
H	4.525094000	2.614567000	-1.560984000
H	6.506133000	1.112814000	-1.418106000
C	1.354038000	-2.818087000	-1.510399000
C	1.216174000	-3.772802000	-2.525340000
C	1.563196000	-3.251274000	-0.193288000
C	1.264383000	-5.131195000	-2.222162000
H	1.077484000	-3.468706000	-3.561121000
C	1.619090000	-4.607305000	0.104090000
H	1.672394000	-2.517775000	0.605211000
C	1.458763000	-5.550838000	-0.908990000
H	1.152838000	-5.863627000	-3.019030000
H	1.776305000	-4.925673000	1.133280000
H	1.489722000	-6.613214000	-0.676176000
C	-1.511193000	2.876301000	-1.644584000
C	-1.825596000	3.536497000	-0.447542000
C	-1.066320000	3.629522000	-2.737045000
C	-1.725326000	4.918815000	-0.355632000
H	-2.141710000	2.959319000	0.423109000
C	-0.949043000	5.015609000	-2.635607000
H	-0.809177000	3.147221000	-3.678808000
C	-1.282100000	5.662049000	-1.449451000
H	-1.983507000	5.417531000	0.576182000
H	-0.604784000	5.589314000	-3.493867000
H	-1.195449000	6.744022000	-1.374750000
C	-3.320947000	0.630734000	-1.306061000
C	-4.249865000	0.338651000	-2.312568000
C	-3.723660000	0.559670000	0.032795000
C	-5.550269000	-0.029402000	-1.979543000
H	-3.970107000	0.399874000	-3.362683000
C	-5.026621000	0.203170000	0.361758000
H	-3.006024000	0.772550000	0.824914000
C	-5.940415000	-0.100435000	-0.644379000
H	-6.263243000	-0.256755000	-2.769398000
H	-5.322724000	0.156135000	1.408559000
H	-6.957436000	-0.390687000	-0.389511000

INT2_s

C	-2.225039000	0.932829000	-0.264481000
C	-0.991669000	1.335381000	0.157065000
Co	0.452944000	0.134134000	-0.341245000
P	2.524904000	1.005288000	0.275478000
P	0.154169000	-0.961825000	1.481277000
C	0.818523000	-0.111438000	2.982032000
H	0.591629000	-0.786907000	3.818545000
H	0.235409000	0.800245000	3.154166000
C	2.710620000	1.373019000	2.062523000

H	2.077146000	2.247053000	2.267333000
H	3.744709000	1.678696000	2.270636000
C	2.310220000	0.204910000	2.964824000
H	2.610965000	0.451598000	3.991254000
H	2.874884000	-0.702045000	2.699699000
C	-2.224351000	-0.355984000	-1.000734000
C	-3.429723000	-1.039222000	-1.486458000
C	-3.450418000	-1.698422000	-2.725977000
C	-4.578135000	-1.096755000	-0.678751000
C	-4.576573000	-2.399640000	-3.138529000
H	-2.576692000	-1.642734000	-3.374098000
C	-5.697121000	-1.812526000	-1.086748000
H	-4.577327000	-0.589079000	0.284709000
C	-5.702982000	-2.463181000	-2.318846000
H	-4.579000000	-2.894450000	-4.107797000
H	-6.572611000	-1.856000000	-0.441103000
H	-6.584403000	-3.012447000	-2.643458000
C	-3.413265000	1.798476000	-0.154203000
C	-4.271424000	1.989886000	-1.249880000
C	-3.697112000	2.480461000	1.038650000
C	-5.369642000	2.835919000	-1.151919000
H	-4.067473000	1.476301000	-2.187991000
C	-4.800560000	3.319342000	1.138209000
H	-3.042620000	2.337224000	1.898182000
C	-5.641517000	3.500509000	0.042180000
H	-6.017793000	2.976447000	-2.014641000
H	-5.006898000	3.832195000	2.075767000
H	-6.505760000	4.157054000	0.118535000
C	-0.568314000	2.700181000	0.461757000
C	-0.401264000	3.601122000	-0.610136000
C	-0.300677000	3.173285000	1.758673000
C	0.027198000	4.904243000	-0.394679000
H	-0.625310000	3.257319000	-1.620272000
C	0.121636000	4.480130000	1.976377000
H	-0.480659000	2.519334000	2.612068000
C	0.298449000	5.347044000	0.898681000
H	0.146264000	5.579626000	-1.239818000
H	0.297113000	4.829761000	2.992322000
H	0.631882000	6.368804000	1.068731000
C	-0.955539000	-0.803203000	-1.170383000
C	-0.304447000	-1.889504000	-1.870482000
C	0.800798000	-1.543939000	-2.681567000
C	-0.580205000	-3.256756000	-1.673548000
C	1.613296000	-2.522635000	-3.249973000
H	0.981277000	-0.485962000	-2.900502000
C	0.221885000	-4.226832000	-2.256884000
H	-1.443262000	-3.538112000	-1.071981000
C	1.328576000	-3.867336000	-3.032611000
H	2.451257000	-2.234214000	-3.882691000
H	-0.011532000	-5.279233000	-2.105890000
H	1.951572000	-4.637531000	-3.482206000
C	3.961378000	-0.059904000	-0.125037000
C	4.066235000	-0.548167000	-1.434765000
C	4.931202000	-0.433359000	0.811150000
C	5.112127000	-1.386306000	-1.801292000
H	3.315168000	-0.269702000	-2.175797000
C	5.976704000	-1.278589000	0.444960000
H	4.885700000	-0.069518000	1.835755000
C	6.069482000	-1.757395000	-0.858175000
H	5.181715000	-1.750424000	-2.824656000
H	6.723241000	-1.559449000	1.184821000
H	6.888043000	-2.415808000	-1.140892000
C	2.876540000	2.564129000	-0.598295000
C	3.455220000	3.676326000	0.019618000
C	2.536093000	2.637655000	-1.956094000
C	3.694509000	4.836485000	-0.713143000
H	3.719164000	3.647351000	1.075644000
C	2.785532000	3.791489000	-2.689001000
H	2.061631000	1.780322000	-2.443196000
C	3.366254000	4.894370000	-2.064957000

H	4.143874000	5.698112000	-0.223487000
H	2.520871000	3.834023000	-3.743458000
C	3.560069000	5.801360000	-2.633695000
H	-1.523686000	-1.431315000	1.999321000
C	-2.033896000	-2.704105000	1.715035000
C	-2.335443000	-0.503438000	2.663925000
C	-3.328597000	-3.042632000	2.096409000
H	-1.407794000	-3.436705000	1.207291000
C	-3.628245000	-0.845656000	3.047794000
H	-1.960996000	0.498373000	2.873771000
C	-4.125696000	-2.116023000	2.764672000
H	-3.715501000	-4.033589000	1.868897000
H	-4.248435000	-0.114321000	3.562428000
H	-5.138203000	-2.382399000	3.061234000
C	1.121735000	-2.507481000	1.488058000
C	1.043189000	-3.381795000	2.583742000
C	2.023747000	-2.785002000	0.456930000
C	1.855771000	-4.508012000	2.637778000
H	0.334677000	-3.186971000	3.389510000
C	2.840019000	-3.911561000	0.515941000
H	2.088212000	-2.124260000	-0.407151000
C	2.757582000	-4.771850000	1.606015000
H	1.785529000	-5.182897000	3.488220000
H	3.537604000	-4.109738000	-0.296004000
H	3.393184000	-5.653635000	1.654913000

INT2_t

C	-2.152622000	0.932117000	-0.652303000
C	-0.907799000	1.389386000	-0.200474000
Co	0.511769000	0.121409000	-0.242936000
P	2.675832000	0.930106000	0.234629000
P	0.196611000	-0.900265000	1.810796000
C	1.198225000	-0.169366000	3.189062000
H	0.986852000	-0.759842000	4.091014000
H	0.843653000	0.849468000	3.393331000
C	3.199869000	0.978099000	2.008208000
H	2.852004000	1.947276000	2.395063000
H	4.297718000	1.011859000	2.039990000
C	2.701627000	-0.147475000	2.919244000
H	3.214031000	-0.032704000	3.883193000
H	3.018196000	-1.130263000	2.541084000
C	-2.067186000	-0.367017000	-1.267192000
C	-3.177478000	-1.131113000	-1.853502000
C	-2.993414000	-1.847073000	-3.048069000
C	-4.430537000	-1.198459000	-1.220037000
C	-4.024090000	-2.605934000	-3.588946000
H	-2.033169000	-1.792390000	-3.558972000
C	-5.454104000	-1.970532000	-1.755163000
H	-4.593411000	-0.643823000	-0.298020000
C	-5.256450000	-2.675257000	-2.941740000
H	-3.865842000	-3.143468000	-4.521596000
H	-6.415059000	-2.017579000	-1.246187000
H	-6.062381000	-3.272068000	-3.363686000
C	-3.388673000	1.722588000	-0.532779000
C	-4.245562000	1.895555000	-1.631697000
C	-3.720330000	2.338284000	0.683195000
C	-5.395175000	2.667345000	-1.515245000
H	-3.998916000	1.427806000	-2.583872000
C	-4.881363000	3.092875000	0.802059000
H	-3.062981000	2.202370000	1.541659000
C	-5.720310000	3.263115000	-0.297445000
H	-6.042316000	2.803082000	-2.379408000
H	-5.131143000	3.552962000	1.756239000
H	-6.625852000	3.859433000	-0.206570000
C	-0.603566000	2.758262000	0.173807000
C	-1.023647000	3.845310000	-0.622979000
C	0.197406000	3.039516000	1.297116000
C	-0.632992000	5.140657000	-0.316697000
H	-1.647931000	3.652838000	-1.494252000

C	0.579469000	4.337059000	1.608263000
H	0.508755000	2.207180000	1.928532000
C	0.174438000	5.393305000	0.793981000
H	-0.957271000	5.963884000	-0.950536000
H	1.197699000	4.528016000	2.484312000
H	0.481160000	6.410914000	1.026345000
C	-0.759750000	-0.835219000	-1.189349000
C	-0.119880000	-2.069165000	-1.596123000
C	1.184202000	-1.978052000	-2.130128000
C	-0.647589000	-3.352107000	-1.338135000
C	1.935257000	-3.119538000	-2.394776000
H	1.587190000	-0.991358000	-2.373792000
C	0.101009000	-4.485358000	-1.615164000
H	-1.652834000	-3.443323000	-0.928086000
C	1.392846000	-4.375531000	-2.139589000
H	2.938349000	-3.020453000	-2.807068000
H	-0.320366000	-5.468959000	-1.415846000
H	1.970050000	-5.273410000	-2.351532000
C	3.926351000	-0.127682000	-0.589106000
C	4.104513000	0.010491000	-1.973693000
C	4.657017000	-1.110050000	0.089658000
C	4.991302000	-0.811745000	-2.659439000
H	3.558087000	0.784557000	-2.514910000
C	5.539512000	-1.938581000	-0.600973000
H	4.552015000	-1.233668000	1.166502000
C	5.708219000	-1.792832000	-1.974778000
H	5.129664000	-0.680261000	-3.730775000
H	6.105900000	-2.691722000	-0.056518000
H	6.403997000	-2.434847000	-2.510785000
C	3.063827000	2.596478000	-0.392924000
C	4.099700000	3.376186000	0.134718000
C	2.296138000	3.101345000	-1.448727000
C	4.351381000	4.644049000	-0.380365000
H	4.716922000	2.996871000	0.948374000
C	2.557138000	4.364662000	-1.969596000
H	1.473087000	2.504541000	-1.849402000
C	3.581807000	5.138936000	-1.431535000
H	5.155915000	5.245730000	0.037479000
H	1.948652000	4.749496000	-2.785667000
H	3.782292000	6.130798000	-1.831272000
C	0.698450000	-2.649998000	1.874362000
C	0.066150000	-3.602282000	2.684048000
C	1.810053000	-3.031525000	1.112464000
C	0.541894000	-4.909665000	2.722611000
H	-0.800580000	-3.322314000	3.281747000
C	2.296670000	-4.332960000	1.170414000
H	2.288870000	-2.307503000	0.450594000
C	1.658546000	-5.275799000	1.972235000
H	0.042108000	-5.645383000	3.349477000
H	3.162171000	-4.609565000	0.569712000
H	2.027360000	-6.298766000	2.011532000
C	-1.514351000	-0.839258000	2.413265000
C	-1.934535000	0.089939000	3.373930000
C	-2.468996000	-1.679760000	1.822064000
C	-3.274677000	0.163494000	3.745631000
H	-1.219773000	0.762961000	3.844497000
C	-3.804546000	-1.610450000	2.203311000
H	-2.157403000	-2.403961000	1.067826000
C	-4.211479000	-0.685554000	3.163177000
H	-3.584909000	0.886275000	4.497656000
H	-4.529353000	-2.280023000	1.743720000
H	-5.257092000	-0.628612000	3.457833000

INT3_s

C	-1.643135000	-1.418706000	-0.414218000
C	-0.428726000	-1.097108000	-0.940932000
Co	0.442629000	0.370345000	-0.019824000
P	2.558337000	0.681558000	-1.002865000
P	-0.554020000	1.841910000	-1.368394000

C	0.221380000	2.141413000	-3.025192000
H	-0.353266000	2.963465000	-3.472402000
H	0.053915000	1.268887000	-3.668921000
C	2.627019000	1.314561000	-2.724371000
H	2.337221000	0.479494000	-3.375957000
H	3.667357000	1.555721000	-2.980615000
C	1.703073000	2.502150000	-2.989360000
H	1.972817000	2.931775000	-3.962643000
H	1.874771000	3.303640000	-2.253798000
C	-2.103421000	-0.548220000	0.674744000
C	-3.439246000	-0.677145000	1.294435000
C	-3.604186000	-0.694169000	2.685809000
C	-4.580867000	-0.750474000	0.483911000
C	-4.873460000	-0.769205000	3.249749000
H	-2.722960000	-0.644374000	3.325720000
C	-5.849985000	-0.815893000	1.047564000
H	-4.461670000	-0.749035000	-0.599369000
C	-6.001268000	-0.826105000	2.432845000
H	-4.983222000	-0.784956000	4.332639000
H	-6.724999000	-0.863018000	0.400920000
H	-6.994056000	-0.883560000	2.874872000
C	-2.390516000	-2.619608000	-0.854706000
C	-2.957336000	-3.491934000	0.088397000
C	-2.522727000	-2.940680000	-2.212741000
C	-3.623929000	-4.643414000	-0.315094000
H	-2.882942000	-3.255255000	1.149263000
C	-3.193002000	-4.089941000	-2.616856000
H	-2.095030000	-2.272414000	-2.959420000
C	-3.746265000	-4.947406000	-1.669094000
H	-4.055629000	-5.304870000	0.433909000
H	-3.286879000	-4.314779000	-3.677808000
H	-4.273637000	-5.845590000	-1.983881000
C	0.412262000	-1.922028000	-1.802585000
C	0.967224000	-3.117865000	-1.305659000
C	0.659220000	-1.600331000	-3.148724000
C	1.706002000	-3.960645000	-2.125013000
H	0.776168000	-3.392822000	-0.268624000
C	1.390713000	-2.447772000	-3.974050000
H	0.217760000	-0.693867000	-3.562294000
C	1.917557000	-3.632488000	-3.463789000
H	2.113555000	-4.885232000	-1.720222000
H	1.536803000	-2.190375000	-5.022106000
H	2.487910000	-4.299653000	-4.107229000
C	-1.195572000	0.401240000	1.025286000
C	-1.276552000	1.428684000	2.057957000
C	-0.193513000	1.648601000	2.930547000
C	-2.386575000	2.289942000	2.164468000
C	-0.204991000	2.693902000	3.848335000
H	0.661342000	0.973575000	2.888327000
C	-2.394482000	3.334812000	3.078593000
H	-3.250633000	2.112758000	1.526109000
C	-1.301116000	3.549913000	3.918934000
H	0.643690000	2.837065000	4.516127000
H	-3.264255000	3.986470000	3.141827000
H	-1.311696000	4.371144000	4.632589000
N	1.115597000	-0.882647000	1.230550000
C	1.373922000	-1.775894000	1.935794000
C	1.613808000	-2.898990000	2.761766000
C	2.810804000	-3.021042000	3.486360000
C	0.625669000	-3.897395000	2.837498000
C	3.012084000	-4.139398000	4.282085000
H	3.563572000	-2.238160000	3.423980000
C	0.847429000	-5.011660000	3.633893000
H	-0.296981000	-3.783535000	2.270375000
C	2.035375000	-5.132670000	4.354559000
H	3.934241000	-4.238354000	4.849372000
H	0.088888000	-5.787968000	3.695443000
H	2.200811000	-6.007374000	4.979444000
C	3.373263000	1.977581000	0.000867000
C	4.110263000	3.032406000	-0.549307000

C	3.199503000	1.934284000	1.392679000
C	4.655355000	4.016268000	0.271623000
H	4.264198000	3.097267000	-1.625075000
C	3.748438000	2.913860000	2.213554000
H	2.610830000	1.128729000	1.835288000
C	4.476997000	3.960033000	1.651843000
H	5.224462000	4.830759000	-0.171574000
H	3.600736000	2.863255000	3.290958000
H	4.903650000	4.732321000	2.288353000
C	3.740995000	-0.709862000	-0.987515000
C	4.134482000	-1.360986000	-2.161107000
C	4.225389000	-1.182927000	0.241040000
C	4.986213000	-2.461320000	-2.106653000
H	3.774518000	-1.023925000	-3.130131000
C	5.072110000	-2.283585000	0.292129000
H	3.954889000	-0.667282000	1.162426000
C	5.452443000	-2.929356000	-0.883132000
H	5.283224000	-2.953533000	-3.030936000
H	5.448643000	-2.633011000	1.252037000
H	6.118502000	-3.788603000	-0.843243000
C	-2.298920000	1.587488000	-1.831208000
C	-3.336300000	2.316900000	-1.238002000
C	-2.616034000	0.629310000	-2.802866000
C	-4.657704000	2.101417000	-1.619491000
H	-3.108551000	3.065995000	-0.482435000
C	-3.937315000	0.414805000	-3.183075000
H	-1.825416000	0.034599000	-3.260859000
C	-4.960641000	1.154794000	-2.594789000
H	-5.452854000	2.675823000	-1.148526000
H	-4.165285000	-0.336199000	-3.937030000
H	-5.994152000	0.988178000	-2.891811000
C	-0.455435000	3.532210000	-0.685909000
C	-1.108556000	4.605016000	-1.311102000
C	0.364184000	3.788372000	0.415979000
C	-0.957589000	5.897638000	-0.822422000
H	-1.751070000	4.426573000	-2.173758000
C	0.520092000	5.083322000	0.902041000
H	0.875306000	2.967172000	0.914609000
C	-0.144684000	6.138411000	0.9525278000
H	-1.476566000	6.721379000	-1.308186000
H	1.153572000	5.258413000	1.769807000
H	-0.031858000	7.151812000	0.665165000

INT3_t

C	2.027184000	0.715768000	-0.652656000
C	0.743210000	1.276777000	-0.782998000
Co	-0.672378000	0.198827000	0.018544000
P	-2.780293000	1.248312000	-0.213411000
P	-1.172729000	-1.304850000	-1.656371000
C	-2.162325000	-0.554438000	-3.032002000
H	-2.223738000	-1.314669000	-3.822411000
H	-1.593903000	0.283820000	-3.457042000
C	-3.636584000	1.202457000	-1.849316000
H	-3.195714000	2.017686000	-2.438946000
H	-4.685642000	1.491385000	-1.695438000
C	-3.563933000	-0.109957000	-2.629088000
H	-4.160277000	0.013542000	-3.542804000
H	-4.049660000	-0.922204000	-2.068537000
C	2.047537000	-0.507385000	0.101289000
C	3.285347000	-1.252700000	0.415380000
C	3.618157000	-1.563246000	1.740854000
C	4.144728000	-1.669927000	-0.610579000
C	4.783676000	-2.262693000	2.034428000
H	2.955573000	-1.244638000	2.546328000
C	5.299008000	-2.387190000	-0.317258000
H	3.894637000	-1.428662000	-1.643437000
C	5.625583000	-2.681146000	1.005905000
H	5.032909000	-2.484269000	3.071029000
H	5.951262000	-2.713001000	-1.125512000

H	6.534635000	-3.233981000	1.234195000
C	3.244759000	1.338374000	-1.213286000
C	4.425372000	1.457340000	-0.459470000
C	3.238235000	1.867566000	-2.513998000
C	5.544733000	2.094061000	-0.982238000
H	4.463083000	1.043457000	0.547317000
C	4.363974000	2.485626000	-3.043986000
H	2.331603000	1.789283000	-3.112931000
C	5.521314000	2.606802000	-2.277784000
H	6.444477000	2.183900000	-0.376126000
H	4.336115000	2.879957000	-4.057880000
H	6.401594000	3.096740000	-2.688702000
C	0.533485000	2.629040000	-1.276499000
C	1.259173000	3.724796000	-0.761488000
C	-0.467571000	2.905250000	-2.226453000
C	0.966390000	5.024658000	-1.152096000
H	2.052596000	3.540830000	-0.037244000
C	-0.736729000	4.200980000	-2.645064000
H	-1.022046000	2.065637000	-2.645224000
C	-0.030798000	5.271261000	-2.096426000
H	1.527779000	5.854013000	-0.725276000
H	-1.506708000	4.381133000	-3.393707000
H	-0.252953000	6.290244000	-2.405544000
C	0.782590000	-0.924024000	0.506153000
C	0.475991000	-2.130875000	1.268231000
C	-0.514590000	-2.100226000	2.271090000
C	1.080644000	-3.374532000	0.984632000
C	-0.878604000	-3.248622000	2.963086000
H	-1.006767000	-1.155390000	2.502080000
C	0.697560000	-4.523944000	1.663100000
H	1.848118000	-3.428178000	0.214953000
C	-0.278517000	-4.468370000	2.658021000
H	-1.644893000	-3.193474000	3.735332000
H	1.171158000	-5.472930000	1.418476000
H	-0.569079000	-5.371555000	3.190601000
N	-0.327692000	1.174737000	1.955276000
C	0.605861000	1.241227000	2.659369000
C	1.814230000	1.235168000	3.396403000
C	2.946347000	1.854169000	2.838431000
C	1.909369000	0.531509000	4.608770000
C	4.165691000	1.761222000	3.493303000
H	2.858784000	2.380421000	1.889465000
C	3.137169000	0.450133000	5.251140000
H	1.027844000	0.047874000	5.023414000
C	4.262071000	1.060698000	4.695665000
H	5.045486000	2.232542000	3.060428000
H	3.218703000	-0.094474000	6.188566000
H	5.221231000	0.989110000	5.203656000
C	-3.878076000	0.253830000	0.871156000
C	-5.059451000	-0.360780000	0.438878000
C	-3.478281000	0.072339000	2.204639000
C	-5.805301000	-1.154967000	1.307305000
H	-5.416171000	-0.224579000	-0.579888000
C	-4.223485000	-0.721287000	3.070238000
H	-2.580104000	0.572773000	2.565709000
C	-5.385268000	-1.346393000	2.620429000
H	-6.720067000	-1.625408000	0.952048000
H	-3.900425000	-0.844698000	4.102711000
H	-5.968639000	-1.969357000	3.295435000
C	-3.115312000	2.955152000	0.343676000
C	-2.063151000	3.810823000	0.679417000
C	-4.435288000	3.417830000	0.438837000
C	-2.324760000	5.117232000	1.085063000
H	-1.037436000	3.453210000	0.616635000
C	-4.693326000	4.721545000	0.845106000
H	-5.266783000	2.749790000	0.209260000
C	-3.636797000	5.574039000	1.165071000
H	-1.497278000	5.778307000	1.336768000
H	-5.720605000	5.073055000	0.917001000
H	-3.840722000	6.594738000	1.482631000

C	0.318999000	-1.857700000	-2.546373000
C	0.838249000	-3.150209000	-2.401405000
C	1.006601000	-0.938497000	-3.351409000
C	2.007441000	-3.518270000	-3.062752000
H	0.319325000	-3.875637000	-1.776625000
C	2.171662000	-1.309768000	-4.014937000
H	0.632822000	0.081832000	-3.453695000
C	2.671943000	-2.603298000	-3.875266000
H	2.396631000	-4.527815000	-2.944717000
H	2.691183000	-0.585514000	-4.639842000
H	3.581489000	-2.895229000	-4.396571000
C	-2.130934000	-2.820416000	-1.319904000
C	-2.318717000	-3.792362000	-2.315176000
C	-2.757116000	-2.985385000	-0.080980000
C	-3.106293000	-4.909553000	-2.064911000
H	-1.833730000	-3.679540000	-3.285467000
C	-3.544850000	-4.107020000	0.168335000
H	-2.627079000	-2.234025000	0.696790000
C	-3.718346000	-5.069153000	-0.821039000
H	-3.243187000	-5.659536000	-2.841289000
H	-4.019623000	-4.223020000	1.141280000
H	-4.331707000	-5.946958000	-0.627528000

TS2_s

C	1.754129000	1.181120000	-0.399667000
C	0.404401000	1.398583000	-0.552125000
Co	-0.711470000	0.057666000	0.140944000
P	-2.931396000	0.759317000	-0.196333000
P	-0.637511000	-1.097265000	-1.776397000
C	-1.736824000	-0.505487000	-3.143924000
H	-1.598570000	-1.218686000	-3.967491000
H	-1.373313000	0.463661000	-3.507948000
C	-3.562628000	0.805450000	-1.920805000
H	-3.126032000	1.703084000	-2.380169000
H	-4.648491000	0.969281000	-1.901003000
C	-3.212446000	-0.412159000	-2.772474000
H	-3.794149000	-0.354221000	-3.701459000
H	-3.532825000	-1.343409000	-2.280493000
C	2.101205000	-0.086144000	0.220445000
C	3.493882000	-0.555559000	0.314749000
C	3.991667000	-1.108930000	1.504085000
C	4.351638000	-0.458472000	-0.791142000
C	5.309701000	-1.539880000	1.587509000
H	3.335446000	-1.198809000	2.368531000
C	5.660603000	-0.918090000	-0.715514000
H	3.976283000	-0.024414000	-1.716512000
C	6.147578000	-1.451997000	0.476449000
H	5.683107000	-1.950967000	2.523764000
H	6.307071000	-0.848699000	-1.588829000
H	7.177416000	-1.797799000	0.540003000
C	2.760013000	2.213537000	-0.757370000
C	3.824067000	2.524447000	0.104410000
C	2.669902000	2.914136000	-1.967941000
C	4.751226000	3.504769000	-0.229589000
H	3.934984000	1.977319000	1.039857000
C	3.597634000	3.893972000	-2.304137000
H	1.860753000	2.679822000	-2.657970000
C	4.641952000	4.195658000	-1.434272000
H	5.566777000	3.728142000	0.455677000
H	3.505384000	4.421472000	-3.251680000
H	5.369336000	4.961632000	-1.694906000
C	-0.251554000	2.667129000	-0.862635000
C	-0.360891000	3.629812000	0.158774000
C	-0.762128000	2.987331000	-2.131326000
C	-0.919937000	4.875293000	-0.095393000
H	0.005463000	3.383613000	1.154890000
C	-1.324843000	4.233580000	-2.383931000
H	-0.666724000	2.263989000	-2.941959000
C	-1.400320000	5.183605000	-1.366834000

H	-0.987089000	5.608622000	0.705888000
H	-1.689654000	4.470367000	-3.382026000
H	-1.837844000	6.160357000	-1.563520000
C	1.003277000	-0.774712000	0.724443000
C	0.917047000	-2.163428000	1.189726000
C	-0.100863000	-2.553729000	2.084481000
C	1.747825000	-3.185027000	0.683734000
C	-0.276228000	-3.880262000	2.462570000
H	-0.787067000	-1.801401000	2.474820000
C	1.563149000	-4.511462000	1.051524000
H	2.548047000	-2.926523000	-0.005549000
C	0.553988000	-4.869974000	1.945701000
H	-1.077027000	-4.140482000	3.153921000
H	2.220487000	-5.275256000	0.639488000
H	0.417452000	-5.910450000	2.232420000
N	-0.740144000	0.795494000	1.983435000
C	0.354616000	0.405534000	2.322219000
C	1.422582000	0.438953000	3.293013000
C	1.578460000	-0.572912000	4.250453000
C	2.336304000	1.501877000	3.232397000
C	2.646615000	-0.513062000	5.138796000
H	0.872069000	-1.398608000	4.289848000
C	3.402895000	1.543068000	4.120771000
H	2.203050000	2.282002000	2.484580000
C	3.561913000	0.535860000	5.071892000
H	2.764697000	-1.293959000	5.886548000
H	4.110428000	2.368111000	4.071241000
H	4.398470000	0.571766000	5.766117000
C	-3.954510000	-0.514115000	0.635285000
C	-5.061601000	-1.123456000	0.033106000
C	-3.561951000	-0.944965000	1.912739000
C	-5.750628000	-2.141985000	0.686799000
H	-5.399409000	-0.808772000	-0.952513000
C	-4.252687000	-1.961497000	2.564966000
H	-2.705210000	-0.478281000	2.398642000
C	-5.346886000	-2.566471000	1.950189000
H	-6.609556000	-2.604125000	0.204564000
H	-3.936073000	-2.278946000	3.557189000
H	-5.887819000	-3.363360000	2.456377000
C	-3.504318000	2.339416000	0.516089000
C	-4.056336000	3.353233000	-0.275495000
C	-3.376300000	2.551925000	1.897228000
C	-4.471185000	4.550966000	0.301271000
H	-4.165177000	3.226616000	-1.350018000
C	-3.790719000	3.749859000	2.467005000
H	-2.945185000	1.779202000	2.528245000
C	-4.338751000	4.753768000	1.670796000
H	-4.901040000	5.327413000	-0.329050000
H	-3.689172000	3.897041000	3.540356000
H	-4.667183000	5.689232000	2.119238000
C	0.960005000	-1.251441000	-2.646062000
C	1.730529000	-2.418885000	-2.587551000
C	1.430195000	-0.171323000	-3.405674000
C	2.931236000	-2.507962000	-3.287873000
H	1.380563000	-3.269736000	-2.006737000
C	2.624881000	-0.263793000	-4.111587000
H	0.858277000	0.756494000	-3.443670000
C	3.376363000	-1.436581000	-4.056977000
H	3.517900000	-3.422851000	-3.233183000
H	2.971175000	0.584993000	-4.698265000
H	4.311697000	-1.510833000	-4.608223000
C	-1.266065000	-2.803897000	-1.606503000
C	-1.150447000	-3.720698000	-2.663494000
C	-1.981270000	-3.174221000	-0.465409000
C	-1.713924000	-4.986586000	-2.558544000
H	-0.607457000	-3.446855000	-3.568110000
C	-2.550774000	-4.441168000	-0.363563000
H	-2.094928000	-2.470903000	0.357201000
C	-2.412037000	-5.350129000	-1.406697000
H	-1.610109000	-5.692131000	-3.380270000

H	-3.098243000	-4.711911000	0.537678000
H	-2.851252000	-6.342604000	-1.328755000

TS2_t

C	2.103861000	0.988041000	-0.362645000
C	0.859679000	1.485818000	-0.663521000
Co	-0.684783000	0.376247000	-0.015106000
P	-2.949566000	0.982146000	-0.236026000
P	-0.780230000	-0.970777000	-1.862151000
C	-1.813188000	-0.266344000	-3.232132000
H	-1.712434000	-0.963267000	-4.074899000
H	-1.376445000	0.683187000	-3.567327000
C	-3.606204000	1.076729000	-1.954727000
H	-3.198926000	2.011152000	-2.367256000
H	-4.692401000	1.232911000	-1.890550000
C	-3.288055000	-0.093420000	-2.883521000
H	-3.841316000	0.063481000	-3.818758000
H	-3.673513000	-1.036112000	-2.467040000
C	2.099684000	-0.308700000	0.293155000
C	3.344497000	-1.075508000	0.494554000
C	3.651664000	-1.661182000	1.730984000
C	4.243772000	-1.233936000	-0.570369000
C	4.831442000	-2.376070000	1.899307000
H	2.959671000	-1.548819000	2.565164000
C	5.408584000	-1.973643000	-0.407671000
H	4.014305000	-0.775203000	-1.531171000
C	5.710356000	-2.540565000	0.829622000
H	5.063668000	-2.811032000	2.869673000
H	6.089041000	-2.098603000	-1.248305000
H	6.629670000	-3.107817000	0.960887000
C	3.349376000	1.742289000	-0.650996000
C	4.409408000	1.815092000	0.267106000
C	3.480895000	2.437256000	-1.862516000
C	5.547621000	2.562980000	-0.013589000
H	4.345049000	1.267522000	1.206890000
C	4.619809000	3.181896000	-2.145834000
H	2.670266000	2.388405000	-2.589278000
C	5.658515000	3.250083000	-1.220249000
H	6.354998000	2.606487000	0.715125000
H	4.697551000	3.709911000	-3.094448000
H	6.551253000	3.832106000	-1.439512000
C	0.501100000	2.847803000	-1.000051000
C	0.985752000	3.932362000	-0.234409000
C	-0.442407000	3.130938000	-2.008109000
C	0.542252000	5.225185000	-0.473405000
H	1.716085000	3.737937000	0.550037000
C	-0.873360000	4.428058000	-2.256038000
H	-0.828162000	2.302663000	-2.602881000
C	-0.387981000	5.481514000	-1.483621000
H	0.928193000	6.045258000	0.129652000
H	-1.595567000	4.618711000	-3.048201000
H	-0.732456000	6.497243000	-1.665244000
C	0.868842000	-0.764267000	0.752535000
C	0.504467000	-2.104395000	1.215808000
C	-0.534725000	-2.298523000	2.147178000
C	1.112411000	-3.260945000	0.681185000
C	-0.930552000	-3.570196000	2.545202000
H	-1.067547000	-1.431880000	2.539609000
C	0.708145000	-4.530324000	1.071232000
H	1.918114000	-3.150301000	-0.040896000
C	-0.310371000	-4.695840000	2.010061000
H	-1.741054000	-3.679614000	3.264763000
H	1.197394000	-5.401754000	0.639633000
H	-0.621861000	-5.693283000	2.312886000
N	-0.622389000	1.189947000	1.813574000
C	0.329847000	0.594930000	2.265334000
C	1.313216000	0.466990000	3.314895000
C	2.437674000	1.304949000	3.254007000
C	1.196668000	-0.479606000	4.341618000

C	3.436599000	1.189295000	4.211675000
H	2.516327000	2.037121000	2.452055000
C	2.202869000	-0.581309000	5.295858000
H	0.327634000	-1.130459000	4.388318000
C	3.323853000	0.244159000	5.230437000
H	4.305456000	1.842313000	4.161335000
H	2.108982000	-1.311897000	6.096028000
H	4.108762000	0.154757000	5.978074000
C	-3.999771000	-0.229753000	0.629024000
C	-5.046621000	-0.929187000	0.020285000
C	-3.697955000	-0.486549000	1.975248000
C	-5.768221000	-1.879345000	0.740236000
H	-5.310691000	-0.739827000	-1.018815000
C	-4.418556000	-1.436726000	2.689523000
H	-2.899204000	0.076170000	2.461128000
C	-5.451430000	-2.140537000	2.070308000
H	-6.580973000	-2.417126000	0.256320000
H	-4.179964000	-1.622445000	3.735370000
H	-6.016052000	-2.884392000	2.628628000
C	-3.475273000	2.575657000	0.474144000
C	-2.547618000	3.580464000	0.762465000
C	-4.840881000	2.810063000	0.692296000
C	-2.983327000	4.809015000	1.252542000
H	-1.485136000	3.400590000	0.614816000
C	-5.269214000	4.038170000	1.181551000
H	-5.569953000	2.024442000	0.489894000
C	-4.339791000	5.039337000	1.461305000
H	-2.253831000	5.585154000	1.476285000
H	-6.329856000	4.212784000	1.349816000
H	-4.676471000	5.998865000	1.848665000
C	0.809348000	-1.262348000	-2.706475000
C	1.454933000	-2.504752000	-2.680721000
C	1.409938000	-0.201313000	-3.399303000
C	2.661848000	-2.686153000	-3.352144000
H	1.003439000	-3.339957000	-2.148963000
C	2.612770000	-0.385938000	-4.072439000
H	0.937413000	0.782617000	-3.404858000
C	3.238700000	-1.631774000	-4.054237000
H	3.151028000	-3.657846000	-3.324294000
H	3.063798000	0.446294000	-4.609321000
H	4.179114000	-1.776565000	-4.582252000
C	-1.563361000	-2.614464000	-1.711946000
C	-1.551990000	-3.512487000	-2.791823000
C	-2.277768000	-2.949609000	-0.559734000
C	-2.221627000	-4.726667000	-2.701585000
H	-1.005505000	-3.266007000	-3.702409000
C	-2.948876000	-4.167135000	-0.471188000
H	-2.304993000	-2.260714000	0.281458000
C	-2.918232000	-5.057613000	-1.538777000
H	-2.200342000	-5.417865000	-3.541631000
H	-3.489703000	-4.414771000	0.440706000
H	-3.438298000	-6.011044000	-1.470825000

INT4_s

C	1.884739000	1.002870000	-0.335102000
C	0.579348000	1.235739000	-0.722886000
Co	-0.646897000	0.065214000	0.016272000
P	-2.728986000	0.763399000	-0.636741000
P	-0.472033000	-1.533337000	-1.624055000
C	-1.455093000	-1.186967000	-3.160589000
H	-1.335439000	-2.065924000	-3.807944000
H	-0.990583000	-0.347660000	-3.695067000
C	-3.233750000	0.484981000	-2.380470000
H	-2.692593000	1.228434000	-2.981105000
H	-4.299772000	0.728418000	-2.485151000
C	-2.935641000	-0.911800000	-2.921532000
H	-3.461269000	-1.021700000	-3.878917000
H	-3.356729000	-1.686746000	-2.262609000
C	2.074368000	-0.127265000	0.546335000

C	3.360146000	-0.828552000	0.596185000
C	3.821257000	-1.441480000	1.776456000
C	4.181530000	-0.891577000	-0.543905000
C	5.053182000	-2.075425000	1.818310000
H	3.204695000	-1.411035000	2.670469000
C	5.404355000	-1.546014000	-0.508398000
H	3.839043000	-0.434879000	-1.469022000
C	5.849251000	-2.134328000	0.673852000
H	5.396165000	-2.527655000	2.746279000
H	6.014896000	-1.593359000	-1.408157000
H	6.813706000	-2.637214000	0.705900000
C	3.000272000	1.910632000	-0.696209000
C	3.888491000	2.339111000	0.300595000
C	3.184375000	2.376727000	-2.003863000
C	4.932081000	3.205302000	-0.004312000
H	3.750381000	1.989329000	1.324962000
C	4.229411000	3.241810000	-2.309058000
H	2.502701000	2.049260000	-2.789122000
C	5.106930000	3.658293000	-1.310395000
H	5.609583000	3.531499000	0.782308000
H	4.360900000	3.590905000	-3.331493000
H	5.923860000	4.336126000	-1.548973000
C	0.101413000	2.443676000	-1.387768000
C	0.070809000	3.641175000	-0.649927000
C	-0.306545000	2.471058000	-2.729597000
C	-0.330593000	4.826537000	-1.250970000
H	0.376057000	3.622682000	0.395876000
C	-0.692536000	3.663748000	-3.332904000
H	-0.276565000	1.551590000	-3.315504000
C	-0.703422000	4.845044000	-2.594601000
H	-0.350138000	5.744887000	-0.667373000
H	-0.976929000	3.671784000	-4.383778000
H	-1.006537000	5.778904000	-3.063824000
C	0.932475000	-0.470765000	1.333416000
C	0.652611000	-1.805257000	1.899399000
C	-0.224154000	-1.960982000	2.990703000
C	1.157432000	-2.976639000	1.301050000
C	-0.566936000	-3.223873000	3.464258000
H	-0.640137000	-1.079799000	3.478857000
C	0.819109000	-4.233623000	1.777483000
H	1.820187000	-2.888091000	0.442615000
C	-0.045828000	-4.367160000	2.864357000
H	-1.243207000	-3.311835000	4.312976000
H	1.217910000	-5.119685000	1.284892000
H	-0.316480000	-5.354377000	3.233150000
N	-0.820657000	1.149438000	1.554328000
C	0.263119000	0.720430000	2.072157000
C	0.879938000	1.324048000	3.270316000
C	1.794915000	0.632126000	4.072329000
C	0.535045000	2.642499000	3.608397000
C	2.362006000	1.244862000	5.183856000
H	2.029018000	-0.406161000	3.846184000
C	1.107821000	3.254049000	4.715033000
H	-0.182422000	3.170001000	2.980674000
C	2.025225000	2.558704000	5.503053000
H	3.064653000	0.694425000	5.805947000
H	0.843380000	4.279684000	4.964419000
H	2.475289000	3.040713000	6.368465000
C	-3.863730000	-0.283702000	0.349003000
C	-4.994382000	-0.896083000	-0.207469000
C	-3.565314000	-0.520769000	1.700532000
C	-5.800731000	-1.726653000	0.565516000
H	-5.261073000	-0.726777000	-1.248892000
C	-4.374198000	-1.351196000	2.469972000
H	-2.690100000	-0.051304000	2.148715000
C	-5.491771000	-1.959537000	1.903460000
H	-6.676680000	-2.191779000	0.118156000
H	-4.128089000	-1.521425000	3.516930000
H	-6.124317000	-2.610607000	2.503431000
C	-3.223087000	2.478307000	-0.285961000

C	-3.524847000	3.379061000	-1.314616000
C	-3.278670000	2.921199000	1.045238000
C	-3.871655000	4.694297000	-1.019749000
H	-3.487306000	3.068782000	-2.356275000
C	-3.618386000	4.238016000	1.331466000
H	-3.048139000	2.234653000	1.854606000
C	-3.914967000	5.128459000	0.301285000
H	-4.107392000	5.380499000	-1.831242000
H	-3.661721000	4.567113000	2.367915000
H	-4.188024000	6.156829000	0.529473000
C	1.152130000	-1.914447000	-2.370505000
C	1.822635000	-3.129255000	-2.180266000
C	1.738695000	-0.945192000	-3.198376000
C	3.037905000	-3.371998000	-2.816171000
H	1.383298000	-3.898832000	-1.547004000
C	2.944476000	-1.194671000	-3.844886000
H	1.247296000	0.018632000	-3.340602000
C	3.596373000	-2.411954000	-3.655528000
H	3.545108000	-4.321833000	-2.659573000
H	3.378946000	-0.432388000	-4.489264000
H	4.540121000	-2.609757000	-4.159896000
C	-1.219170000	-3.124518000	-1.137705000
C	-1.210673000	-4.236882000	-1.992354000
C	-1.914133000	-3.204028000	0.072666000
C	-1.867663000	-5.406423000	-1.626804000
H	-0.678530000	-4.192404000	-2.943188000
C	-2.586477000	-4.369017000	0.430468000
H	-1.913735000	-2.354844000	0.756838000
C	-2.558866000	-5.472610000	-0.416673000
H	-1.846519000	-6.267831000	-2.291217000
H	-3.118509000	-4.411346000	1.379316000
H	-3.076058000	-6.388385000	-0.137442000

INT4_t

C	2.156276000	1.070459000	-0.227125000
C	0.970253000	1.210014000	-0.869414000
Co	-0.788013000	0.425636000	-0.660279000
P	-3.075891000	0.222543000	-0.838762000
P	-0.456113000	-1.340271000	-2.081555000
C	-1.582279000	-1.344742000	-3.553938000
H	-1.310245000	-2.200821000	-4.185816000
H	-1.357268000	-0.449943000	-4.152583000
C	-3.675738000	-0.178727000	-2.536417000
H	-3.463193000	0.723547000	-3.129072000
H	-4.771348000	-0.265434000	-2.510944000
C	-3.072757000	-1.409437000	-3.216756000
H	-3.616321000	-1.564957000	-4.158159000
H	-3.264589000	-2.307323000	-2.612652000
C	2.318745000	0.025929000	0.804131000
C	3.597347000	-0.718419000	0.786117000
C	4.292862000	-1.004016000	1.970840000
C	4.170898000	-1.100498000	-0.434242000
C	5.509739000	-1.671000000	1.937335000
H	3.867623000	-0.693458000	2.925424000
C	5.383454000	-1.780117000	-0.467023000
H	3.651079000	-0.864079000	-1.363022000
C	6.057228000	-2.067959000	0.717275000
H	6.039386000	-1.875982000	2.865558000
H	5.807450000	-2.077897000	-1.424845000
H	7.012057000	-2.589185000	0.691510000
C	3.316733000	1.928935000	-0.559375000
C	4.178989000	2.365657000	0.457681000
C	3.568562000	2.351257000	-1.872231000
C	5.245791000	3.209478000	0.172623000
H	3.997940000	2.044747000	1.484043000
C	4.637196000	3.192581000	-2.158093000
H	2.920875000	1.997805000	-2.674753000
C	5.479308000	3.626454000	-1.136268000
H	5.898883000	3.543232000	0.976611000

H	4.819947000	3.504617000	-3.184787000
H	6.318578000	4.281601000	-1.360198000
C	0.424019000	2.366752000	-1.567526000
C	0.508293000	3.649511000	-0.971876000
C	-0.396148000	2.230020000	-2.711088000
C	-0.162077000	4.730708000	-1.516255000
H	1.115614000	3.765028000	-0.074976000
C	-1.081677000	3.322953000	-3.245519000
H	-0.451513000	1.266288000	-3.215599000
C	-0.965486000	4.572752000	-2.652983000
H	-0.067850000	5.710659000	-1.051754000
H	-1.694115000	3.192910000	-4.136101000
H	-1.494578000	5.426960000	-3.070059000
C	0.303188000	0.902307000	1.937867000
C	0.333429000	1.764604000	3.139025000
C	-0.739542000	2.628385000	3.408060000
C	1.450884000	1.777636000	3.984814000
C	-0.693075000	3.481874000	4.500768000
H	-1.604277000	2.616159000	2.744689000
C	1.496659000	2.640585000	5.074218000
H	2.286415000	1.108203000	3.780672000
C	0.425220000	3.491155000	5.336090000
H	-1.531221000	4.144703000	4.706142000
H	2.370680000	2.647261000	5.721907000
H	0.459813000	4.161956000	6.192037000
N	-0.562508000	1.101310000	1.024086000
C	1.343793000	-0.177824000	1.755536000
C	1.174764000	-1.395256000	2.571392000
C	0.433770000	-1.391112000	3.769313000
C	1.646282000	-2.643324000	2.111031000
C	0.234051000	-2.558786000	4.499898000
H	0.016703000	-0.462229000	4.149911000
C	1.453250000	-3.803260000	2.844934000
H	2.157777000	-2.700077000	1.152290000
C	0.756081000	-3.768863000	4.053257000
H	-0.328673000	-2.515541000	5.430643000
H	1.834569000	-4.747507000	2.460590000
H	0.608782000	-4.679663000	4.630186000
C	-3.807459000	-1.001027000	0.289352000
C	-3.452249000	-0.903367000	1.644331000
C	-4.645220000	-2.040735000	-0.125221000
C	-3.934586000	-1.825966000	2.563907000
H	-2.786008000	-0.101600000	1.971112000
C	-5.118500000	-2.969812000	0.799399000
H	-4.938835000	-2.131764000	-1.170335000
C	-4.764785000	-2.864463000	2.141385000
H	-3.655887000	-1.739798000	3.612567000
H	-5.768938000	-3.776508000	0.467334000
H	-5.137577000	-3.591037000	2.860552000
C	-3.938928000	1.778326000	-0.453625000
C	-5.331473000	1.806229000	-0.298472000
C	-3.206305000	2.963864000	-0.334655000
C	-5.979674000	3.008006000	-0.037981000
H	-5.906855000	0.882058000	-0.367115000
C	-3.860573000	4.165906000	-0.076554000
H	-2.119878000	2.943461000	-0.432586000
C	-5.244687000	4.188510000	0.070802000
H	-7.060565000	3.024425000	0.085037000
H	-3.282999000	5.084295000	0.013949000
H	-5.755163000	5.127155000	0.276818000
C	-0.964710000	-2.832062000	-1.175957000
C	-1.302727000	-4.026425000	-1.830924000
C	-1.058480000	-2.770254000	0.217397000
C	-1.732693000	-5.127246000	-1.099055000
H	-1.227573000	-4.097803000	-2.916470000
C	-1.482579000	-3.874778000	0.951084000
H	-0.804080000	-1.844578000	0.739152000
C	-1.824378000	-5.050739000	0.291597000
H	-1.996264000	-6.048690000	-1.614091000
H	-1.548549000	-3.805628000	2.035103000

H	-2.165179000	-5.913976000	0.860000000
C	1.187841000	-1.696103000	-2.780593000
C	1.825987000	-0.707111000	-3.543536000
C	1.841713000	-2.913989000	-2.560921000
C	3.077611000	-0.944180000	-4.101745000
H	1.345405000	0.260064000	-3.698936000
C	3.097366000	-3.145900000	-3.118066000
H	1.371674000	-3.683783000	-1.951016000
C	3.713096000	-2.167707000	-3.893620000
H	3.560873000	-0.168731000	-4.692901000
H	3.596768000	-4.095995000	-2.938993000
H	4.693224000	-2.352417000	-4.328844000

TS3_s

C	1.553424000	1.595039000	0.295252000
C	0.249963000	1.682222000	-0.195047000
Co	-0.562385000	0.001910000	-0.175068000
P	-2.565362000	0.376240000	-1.053361000
P	0.218615000	-1.204131000	-1.917272000
C	-0.559045000	-0.762267000	-3.543820000
H	-0.116422000	-1.426511000	-4.297804000
H	-0.249745000	0.257352000	-3.812570000
C	-2.792861000	0.280914000	-2.872573000
H	-2.413173000	1.229222000	-3.277903000
H	-3.870197000	0.268508000	-3.088203000
C	-2.077469000	-0.878411000	-3.562149000
H	-2.413288000	-0.905153000	-4.606839000
H	-2.380686000	-1.843210000	-3.128097000
C	1.878164000	0.359326000	0.930281000
C	3.288818000	0.004482000	1.161104000
C	3.696226000	-0.561033000	2.381300000
C	4.265118000	0.257892000	0.186036000
C	5.030917000	-0.852777000	2.621046000
H	2.953930000	-0.756622000	3.152583000
C	5.597219000	-0.058668000	0.415100000
H	3.964321000	0.696483000	-0.762038000
C	5.986437000	-0.609927000	1.634330000
H	5.328814000	-1.272556000	3.579365000
H	6.335938000	0.132399000	-0.361159000
H	7.032335000	-0.846635000	1.818837000
C	2.497047000	2.740326000	0.260317000
C	3.156265000	3.137362000	1.432309000
C	2.737838000	3.459901000	-0.916747000
C	4.031850000	4.216676000	1.425276000
H	2.974366000	2.590163000	2.357527000
C	3.615702000	4.538609000	-0.925243000
H	2.234535000	3.164417000	-1.836833000
C	4.266425000	4.919989000	0.245508000
H	4.530514000	4.512460000	2.346132000
H	3.792917000	5.083197000	-1.850807000
H	4.952311000	5.764573000	0.239654000
C	-0.355005000	2.881880000	-0.778483000
C	-0.770910000	3.947062000	0.032859000
C	-0.498307000	2.996850000	-2.168599000
C	-1.294550000	5.099691000	-0.540939000
H	-0.682804000	3.851689000	1.113123000
C	-1.000641000	4.160845000	-2.741653000
H	-0.187078000	2.164443000	-2.802712000
C	-1.400109000	5.216916000	-1.926091000
H	-1.620709000	5.916422000	0.100254000
H	-1.081979000	4.241726000	-3.824488000
H	-1.798790000	6.127760000	-2.368502000
C	-0.299284000	0.275260000	2.085585000
C	-0.625686000	0.149594000	3.526286000
C	0.288476000	-0.368857000	4.452889000
C	-1.861276000	0.624170000	3.990739000
C	-0.022071000	-0.411129000	5.805626000
H	1.245715000	-0.752811000	4.105531000
C	-2.172145000	0.581010000	5.344020000

H	-2.560627000	1.046908000	3.270922000
C	-1.254458000	0.061259000	6.255092000
H	0.700543000	-0.811483000	6.513459000
H	-3.133937000	0.953407000	5.690647000
H	-1.497850000	0.025376000	7.314881000
N	-0.971614000	1.109343000	1.343749000
C	0.811205000	-0.486251000	1.424568000
C	0.942242000	-1.956166000	1.619660000
C	-0.032527000	-2.688261000	2.324587000
C	1.937447000	-2.702359000	0.958537000
C	0.016163000	-4.074819000	2.409287000
H	-0.854895000	-2.170734000	2.811630000
C	1.980650000	-4.088484000	1.035630000
H	2.687063000	-2.190158000	0.361907000
C	1.029064000	-4.787592000	1.773710000
H	-0.754797000	-4.600381000	2.971201000
H	2.765443000	-4.626690000	0.505620000
H	1.064740000	-5.873296000	1.835116000
C	-3.553878000	1.816387000	-0.547064000
C	-3.889691000	2.834602000	-1.446802000
C	-3.958935000	1.931471000	0.789794000
C	-4.612199000	3.943101000	-1.015584000
H	-3.584796000	2.780561000	-2.489152000
C	-4.677802000	3.040173000	1.216804000
H	-3.717343000	1.140684000	1.496098000
C	-5.003982000	4.051437000	0.315015000
H	-4.865604000	4.726096000	-1.727820000
H	-4.988224000	3.112816000	2.257266000
H	-5.568241000	4.919644000	0.649166000
C	-3.430759000	-1.088047000	-0.379545000
C	-4.245994000	-1.915623000	-1.163407000
C	-3.210007000	-1.438943000	0.963462000
C	-4.813847000	-3.064879000	-0.622109000
H	-4.451954000	-1.665358000	-2.202178000
C	-3.782781000	-2.587086000	1.502986000
H	-2.590480000	-0.804072000	1.596093000
C	-4.579517000	-3.407036000	0.708408000
H	-5.446776000	-3.694562000	-1.243811000
H	-3.605013000	-2.835763000	2.548268000
H	-5.025432000	-4.307609000	1.125570000
C	1.977466000	-0.958611000	-2.363847000
C	2.948876000	-1.962590000	-2.267164000
C	2.355349000	0.294879000	-2.868988000
C	4.253706000	-1.725645000	-2.694697000
H	2.680505000	-2.941248000	-1.872162000
C	3.654173000	0.525326000	-3.310368000
H	1.624532000	1.103433000	-2.918687000
C	4.606083000	-0.489561000	-3.229846000
H	4.995542000	-2.517947000	-2.616319000
H	3.923924000	1.502315000	-3.707490000
H	5.622365000	-0.313771000	-3.576848000
C	-0.064928000	-3.005751000	-1.902405000
C	0.426898000	-3.844633000	-2.914054000
C	-0.879171000	-3.549421000	-0.905122000
C	0.125256000	-5.201443000	-2.907908000
H	1.058622000	-3.436154000	-3.703539000
C	-1.190209000	-4.906589000	-0.906450000
H	-1.260604000	-2.908831000	-0.109897000
C	-0.684272000	-5.733965000	-1.903794000
H	0.518266000	-5.846183000	-3.691407000
H	-1.819819000	-5.313520000	-0.116723000
H	-0.919968000	-6.796358000	-1.904179000

TS3_t

C	2.098681000	1.330915000	0.370889000
C	0.839101000	1.636160000	-0.054268000
Co	-0.825961000	0.642220000	-0.393875000
P	-3.080566000	0.445656000	-0.871514000
P	-0.208494000	-0.618322000	-2.208757000

C	-1.206748000	-0.227309000	-3.724970000
H	-0.826698000	-0.848477000	-4.547115000
H	-0.988064000	0.813125000	-4.009263000
C	-3.447295000	0.554630000	-2.675380000
H	-3.192129000	1.585769000	-2.961824000
H	-4.533158000	0.467507000	-2.822069000
C	-2.712530000	-0.440870000	-3.574822000
H	-3.157957000	-0.374549000	-4.576322000
H	-2.898895000	-1.470756000	-3.235798000
C	2.373344000	0.004348000	0.909906000
C	3.747066000	-0.527602000	0.752500000
C	4.390395000	-1.186202000	1.810506000
C	4.443324000	-0.360026000	-0.451646000
C	5.683380000	-1.671442000	1.665229000
H	3.864110000	-1.313465000	2.756484000
C	5.732887000	-0.855976000	-0.601593000
H	3.957292000	0.157565000	-1.277978000
C	6.358911000	-1.511722000	0.456033000
H	6.169631000	-2.171684000	2.500334000
H	6.253127000	-0.723763000	-1.549089000
H	7.372549000	-1.890831000	0.342732000
C	3.183145000	2.336620000	0.265013000
C	4.092609000	2.498505000	1.320893000
C	3.313746000	3.163214000	-0.858902000
C	5.092409000	3.461227000	1.256065000
H	4.006176000	1.861049000	2.200673000
C	4.317681000	4.122570000	-0.926619000
H	2.626206000	3.035830000	-1.694730000
C	5.210353000	4.275801000	0.131475000
H	5.784311000	3.575423000	2.088137000
H	4.407053000	4.749835000	-1.811680000
H	5.997953000	5.024584000	0.078992000
C	0.237495000	2.926979000	-0.393933000
C	0.173714000	3.966051000	0.556435000
C	-0.447536000	3.099253000	-1.615525000
C	-0.528015000	5.129837000	0.282591000
H	0.687038000	3.835091000	1.507259000
C	-1.165299000	4.266128000	-1.878506000
H	-0.381404000	2.322190000	-2.379153000
C	-1.206499000	5.281670000	-0.931156000
H	-0.553566000	5.928953000	1.021132000
H	-1.679649000	4.383011000	-2.830671000
H	-1.761258000	6.195134000	-1.134543000
C	0.242154000	0.040775000	2.122884000
C	-0.082594000	0.009015000	3.567722000
C	-1.368205000	0.344482000	4.015219000
C	0.919053000	-0.260426000	4.511309000
C	-1.650080000	0.384845000	5.374674000
H	-2.137112000	0.586196000	3.281860000
C	0.635838000	-0.212568000	5.871011000
H	1.924763000	-0.502182000	4.167204000
C	-0.650177000	0.103580000	6.305285000
H	-2.652801000	0.638807000	5.712249000
H	1.421809000	-0.418706000	6.594369000
H	-0.872196000	0.136310000	7.369879000
N	-0.426346000	0.872159000	1.390638000
C	1.399069000	-0.718966000	1.584972000
C	1.414742000	-2.196332000	1.694710000
C	0.749864000	-2.927617000	2.696360000
C	1.992886000	-2.938075000	0.641404000
C	0.719409000	-4.319608000	2.672740000
H	0.256318000	-2.416955000	3.516877000
C	1.958112000	-4.322990000	0.618055000
H	2.457373000	-2.407151000	-0.186960000
C	1.329248000	-5.028778000	1.642733000
H	0.212017000	-4.851383000	3.475832000
H	2.408996000	-4.854673000	-0.218845000
H	1.301608000	-6.116532000	1.628844000
C	-3.878406000	-1.079887000	-0.280462000
C	-3.633919000	-1.443388000	1.052453000

C	-4.688498000	-1.899660000	-1.071835000
C	-4.197507000	-2.595454000	1.585319000
H	-2.986833000	-0.816557000	1.670936000
C	-5.242410000	-3.062171000	-0.538890000
H	-4.898765000	-1.636758000	-2.107916000
C	-5.000160000	-3.410307000	0.786751000
H	-4.005333000	-2.861749000	2.623116000
H	-5.870656000	-3.694082000	-1.163239000
H	-5.438093000	-4.316674000	1.199712000
C	-4.083993000	1.787100000	-0.156553000
C	-5.478866000	1.793810000	-0.293193000
C	-3.452295000	2.827865000	0.532353000
C	-6.226883000	2.836586000	0.239993000
H	-5.981862000	0.972732000	-0.806039000
C	-4.206236000	3.871311000	1.064579000
H	-2.368117000	2.817551000	0.658283000
C	-5.590133000	3.877080000	0.917162000
H	-7.309568000	2.836932000	0.132486000
H	-3.707064000	4.678324000	1.597968000
H	-6.178831000	4.690969000	1.335559000
C	-0.645142000	-2.354225000	-1.886288000
C	-0.674593000	-3.317824000	-2.905885000
C	-1.018787000	-2.725848000	-0.590978000
C	-1.068956000	-4.621436000	-2.626257000
H	-0.383210000	-3.048906000	-3.921880000
C	-1.419872000	-4.028593000	-0.311528000
H	-0.992265000	-1.987639000	0.213491000
C	-1.444693000	-4.975758000	-1.329899000
H	-1.087582000	-5.363011000	-3.422261000
H	-1.705222000	-4.298270000	0.702924000
H	-1.756486000	-5.996357000	-1.116455000
C	1.492384000	-0.609695000	-2.866039000
C	2.024756000	0.616968000	-3.289066000
C	2.276514000	-1.763879000	-2.980628000
C	3.295422000	0.683538000	-3.850879000
H	1.438304000	1.531619000	-3.181867000
C	3.552300000	-1.693152000	-3.536270000
H	1.887558000	-2.723141000	-2.640977000
C	4.058673000	-0.475585000	-3.982755000
H	3.692588000	1.642736000	-4.177763000
H	4.152374000	-2.597155000	-3.619389000
H	5.052898000	-0.425850000	-4.422265000

INT5_s

C	1.786921000	1.452754000	0.322900000
C	0.352436000	1.758227000	0.284257000
Co	-0.592314000	0.030142000	-0.032729000
P	-2.514411000	0.680465000	-0.954989000
P	0.069799000	-1.161676000	-1.831633000
C	-0.566935000	-0.499130000	-3.443446000
H	-0.156568000	-1.144447000	-4.231152000
H	-0.149748000	0.503470000	-3.609353000
C	-2.686175000	0.741066000	-2.782305000
H	-2.178664000	1.661185000	-3.105438000
H	-3.748733000	0.875051000	-3.027291000
C	-2.086014000	-0.443402000	-3.532012000
H	-2.372510000	-0.356004000	-4.587839000
H	-2.519003000	-1.393323000	-3.183094000
C	2.096224000	0.240521000	0.892467000
C	3.475020000	-0.117797000	1.258123000
C	3.751976000	-0.537562000	2.569535000
C	4.531815000	-0.007993000	0.346588000
C	5.052394000	-0.833529000	2.956442000
H	2.935028000	-0.617824000	3.287756000
C	5.828392000	-0.330163000	0.728206000
H	4.321157000	0.319142000	-0.669109000
C	6.093933000	-0.739927000	2.033642000
H	5.255022000	-1.143109000	3.979613000
H	6.637012000	-0.255513000	0.003039000

H	7.110956000	-0.983702000	2.333755000
C	2.798126000	2.518960000	0.088524000
C	3.453909000	3.069741000	1.198800000
C	3.125366000	3.001723000	-1.182633000
C	4.410206000	4.066513000	1.040951000
H	3.213068000	2.699252000	2.195022000
C	4.085983000	3.995904000	-1.342752000
H	2.632980000	2.585310000	-2.058499000
C	4.731393000	4.531748000	-0.231877000
H	4.906983000	4.479928000	1.916387000
H	4.330547000	4.352792000	-2.341590000
H	5.481299000	5.309964000	-0.357512000
C	-0.116605000	2.986363000	-0.397188000
C	-0.613429000	4.063843000	0.344445000
C	-0.016819000	3.110298000	-1.788013000
C	-0.965470000	5.249537000	-0.292560000
H	-0.705989000	3.961618000	1.424070000
C	-0.386034000	4.288298000	-2.427779000
H	0.358875000	2.261329000	-2.364199000
C	-0.850814000	5.366979000	-1.676005000
H	-1.338547000	6.085782000	0.295719000
H	-0.300590000	4.370847000	-3.510137000
H	-1.126636000	6.296551000	-2.170285000
C	-0.067821000	0.192097000	1.984198000
C	-0.718382000	-0.112057000	3.274878000
C	-0.114447000	-0.969355000	4.208426000
C	-1.885489000	0.570173000	3.651803000
C	-0.681654000	-1.163991000	5.460769000
H	0.809089000	-1.484082000	3.952244000
C	-2.456990000	0.366939000	4.901800000
H	-2.317261000	1.284265000	2.954481000
C	-1.862161000	-0.508443000	5.807887000
H	-0.195053000	-1.826408000	6.173286000
H	-3.364484000	0.902280000	5.173957000
H	-2.307309000	-0.667612000	6.787802000
N	-0.425619000	1.374418000	1.401698000
C	0.954765000	-0.601008000	1.320374000
C	0.999470000	-2.084622000	1.464634000
C	-0.191949000	-2.776592000	1.765067000
C	2.134550000	-2.874219000	1.214070000
C	-0.243087000	-4.157421000	1.857843000
H	-1.112986000	-2.212175000	1.903494000
C	2.080005000	-4.265800000	1.289237000
H	3.077073000	-2.415435000	0.938217000
C	0.900538000	-4.919688000	1.622687000
H	-1.192008000	-4.641566000	2.086916000
H	2.983315000	-4.838511000	1.084992000
H	0.866017000	-6.005141000	1.684813000
C	-3.395253000	2.182872000	-0.408807000
C	-3.580945000	3.281148000	-1.255208000
C	-3.887454000	2.248023000	0.901448000
C	-4.243583000	4.416961000	-0.798053000
H	-3.199777000	3.272495000	-2.273598000
C	-4.541314000	3.385504000	1.357511000
H	-3.781104000	1.389771000	1.562450000
C	-4.719989000	4.475719000	0.507492000
H	-4.379229000	5.262512000	-1.469930000
H	-4.922184000	3.416564000	2.376415000
H	-5.235658000	5.365731000	0.861919000
C	-3.577922000	-0.700961000	-0.412965000
C	-4.477318000	-1.369653000	-1.251614000
C	-3.420498000	-1.153114000	0.906621000
C	-5.191531000	-2.468092000	-0.780463000
H	-4.630164000	-1.037410000	-2.276989000
C	-4.135323000	-2.250161000	1.377578000
H	-2.726920000	-0.638400000	1.573140000
C	-5.019388000	-2.913554000	0.529460000
H	-5.888868000	-2.978608000	-1.441406000
H	-3.997943000	-2.580262000	2.406629000
H	-5.580154000	-3.773970000	0.888964000

C	1.863578000	-1.210116000	-2.201566000
C	2.651900000	-2.329859000	-1.906775000
C	2.467136000	-0.113188000	-2.831871000
C	4.000317000	-2.356111000	-2.255236000
H	2.204894000	-3.195739000	-1.423350000
C	3.810444000	-0.146026000	-3.192685000
H	1.880104000	0.775706000	-3.062777000
C	4.580105000	-1.272566000	-2.909150000
H	4.596185000	-3.236450000	-2.021226000
H	4.255663000	0.713668000	-3.690592000
H	5.630528000	-1.301902000	-3.191933000
C	-0.468061000	-2.902463000	-1.993560000
C	0.029856000	-3.710561000	-3.028085000
C	-1.469903000	-3.408906000	-1.162419000
C	-0.454965000	-4.999807000	-3.209093000
H	0.809215000	-3.331442000	-3.689469000
C	-1.958936000	-4.700440000	-1.348313000
H	-1.865785000	-2.792591000	-0.357742000
C	-1.450488000	-5.497538000	-2.367805000
H	-0.056971000	-5.618529000	-4.010714000
H	-2.736088000	-5.080663000	-0.687164000
H	-1.828749000	-6.507575000	-2.512097000

INT5_t

C	2.839848000	-0.868196000	-0.698044000
C	1.440433000	-0.980567000	-0.713213000
Co	-1.311731000	-0.254667000	-0.269027000
P	-3.463606000	-0.670478000	-0.705395000
P	-1.342213000	-0.801238000	1.957736000
C	-2.483236000	-2.221327000	2.244898000
H	-2.510206000	-2.460475000	3.317103000
H	-2.021150000	-3.087978000	1.746888000
C	-4.095129000	-2.144887000	0.215620000
H	-3.563658000	-3.030162000	-0.164103000
H	-5.161307000	-2.277487000	-0.014474000
C	-3.914260000	-2.028210000	1.728341000
H	-4.542139000	-2.794711000	2.201299000
H	-4.322096000	-1.065074000	2.073141000
C	3.395198000	0.430964000	-0.659539000
C	4.860280000	0.615684000	-0.518664000
C	5.749486000	0.071660000	-1.452434000
C	5.373591000	1.337911000	0.565822000
C	7.120563000	0.253056000	-1.308173000
H	5.360484000	-0.496587000	-2.296594000
C	6.745558000	1.502827000	0.718898000
H	4.686795000	1.778386000	1.289009000
C	7.622256000	0.963819000	-0.220103000
H	7.800005000	-0.166727000	-2.046982000
H	7.130555000	2.059957000	1.570476000
H	8.695607000	1.099242000	-0.104972000
C	3.679682000	-2.091089000	-0.687620000
C	3.542632000	-3.043321000	-1.705109000
C	4.596957000	-2.334133000	0.342553000
C	4.300707000	-4.209424000	-1.692493000
H	2.834375000	-2.863294000	-2.513965000
C	5.344319000	-3.505941000	0.362172000
H	4.724171000	-1.595671000	1.132319000
C	5.199346000	-4.446855000	-0.655239000
H	4.188120000	-4.934660000	-2.495754000
H	6.047782000	-3.682333000	1.173540000
H	5.789548000	-5.360788000	-0.642448000
C	0.687051000	-2.255720000	-0.665340000
C	-0.395567000	-2.433291000	-1.547868000
C	0.980909000	-3.269834000	0.256321000
C	-1.168126000	-3.594483000	-1.500630000
H	-0.588083000	-1.687502000	-2.321393000
C	0.200222000	-4.418722000	0.307287000
H	1.812726000	-3.143244000	0.948159000
C	-0.875279000	-4.585751000	-0.567681000

H	-1.985612000	-3.722616000	-2.209545000
H	0.434304000	-5.190854000	1.038280000
H	-1.471918000	-5.495412000	-0.531055000
C	1.160158000	1.347593000	-0.858431000
C	0.166631000	2.406279000	-1.145661000
C	-1.081240000	2.418495000	-0.502471000
C	0.398235000	3.341910000	-2.163251000
C	-2.063477000	3.341335000	-0.856316000
H	-1.262816000	1.764633000	0.361764000
C	-0.587474000	4.251408000	-2.527966000
H	1.355274000	3.344067000	-2.681202000
C	-1.820187000	4.255474000	-1.876909000
H	-3.015941000	3.342602000	-0.329012000
H	-0.390910000	4.961426000	-3.328425000
H	-2.586746000	4.973424000	-2.160233000
N	0.639304000	0.104983000	-0.759851000
C	2.546563000	1.558428000	-0.753278000
C	3.084784000	2.939837000	-0.725415000
C	4.052160000	3.362566000	-1.645385000
C	2.615774000	3.851890000	0.227781000
C	4.530820000	4.667364000	-1.616380000
H	4.429412000	2.660086000	-2.387616000
C	3.103307000	5.153676000	0.264051000
H	1.863741000	3.529339000	0.949825000
C	4.059813000	5.565672000	-0.660929000
H	5.277389000	4.983485000	-2.341923000
H	2.735363000	5.848423000	1.016337000
H	4.439596000	6.584863000	-0.635846000
C	-4.724787000	0.592465000	-0.304546000
C	-4.505809000	1.436572000	0.791788000
C	-5.917832000	0.712042000	-1.027633000
C	-5.465664000	2.371904000	1.169126000
H	-3.570899000	1.366380000	1.350645000
C	-6.870710000	1.656342000	-0.656753000
H	-6.098662000	0.068839000	-1.889014000
C	-6.648683000	2.484014000	0.442472000
H	-5.282197000	3.017579000	2.026378000
H	-7.791964000	1.745765000	-1.228953000
H	-7.397429000	3.219548000	0.729362000
C	-3.750440000	-1.070607000	-2.462122000
C	-4.526371000	-2.150294000	-2.900333000
C	-3.117656000	-0.258495000	-3.415676000
C	-4.665257000	-2.411343000	-4.262207000
H	-5.028103000	-2.795873000	-2.180423000
C	-3.267114000	-0.513479000	-4.774363000
H	-2.502706000	0.582423000	-3.082400000
C	-4.038961000	-1.593990000	-5.199270000
H	-5.269306000	-3.254740000	-4.590854000
H	-2.776366000	0.127961000	-5.503527000
H	-4.150351000	-1.799584000	-6.261784000
C	-1.919597000	0.486075000	3.132667000
C	-2.966611000	0.288982000	4.040607000
C	-1.310075000	1.748663000	3.078191000
C	-3.403503000	1.330899000	4.855841000
H	-3.453802000	-0.680811000	4.121559000
C	-1.739891000	2.785904000	3.898200000
H	-0.482547000	1.920797000	2.387418000
C	-2.796380000	2.581211000	4.783994000
H	-4.221313000	1.160041000	5.553060000
H	-1.250363000	3.756264000	3.844316000
H	-3.140584000	3.393392000	5.420757000
C	0.235646000	-1.340524000	2.718448000
C	0.379727000	-2.523922000	3.451629000
C	1.369334000	-0.547610000	2.491314000
C	1.629057000	-2.912143000	3.929988000
H	-0.480296000	-3.163680000	3.641695000
C	2.613928000	-0.928170000	2.981135000
H	1.278952000	0.372840000	1.909679000
C	2.749201000	-2.119155000	3.692633000
H	1.726238000	-3.838899000	4.492266000

H	3.482944000	-0.296855000	2.797648000
H	3.725796000	-2.427519000	4.061126000

TS4_s

C	1.261991000	0.860782000	0.924106000
C	0.315108000	1.645990000	0.452147000
Co	-0.300717000	-0.124027000	0.153565000
P	0.544391000	-0.286635000	-1.894578000
P	-2.451394000	-0.318348000	-0.468254000
C	-2.890245000	-0.223150000	-2.266303000
H	-3.850093000	-0.737658000	-2.406428000
H	-3.078239000	0.840070000	-2.476381000
C	-0.567461000	0.025825000	-3.333708000
H	-0.763103000	1.106565000	-3.391447000
H	-0.006762000	-0.234381000	-4.241544000
C	-1.873515000	-0.756701000	-3.273964000
H	-2.341751000	-0.724259000	-4.266216000
H	-1.652426000	-1.818680000	-3.090853000
C	0.299141000	-0.435290000	2.134206000
C	1.298085000	-0.962577000	3.061284000
C	1.419420000	-2.352482000	3.184533000
C	2.095034000	-0.116448000	3.838963000
C	2.347653000	-2.886565000	4.070670000
H	0.783191000	-3.001705000	2.584373000
C	3.011273000	-0.658523000	4.730370000
H	1.996235000	0.962399000	3.731938000
C	3.146161000	-2.041905000	4.839333000
H	2.444484000	-3.965972000	4.164768000
H	3.626798000	0.000077000	5.338720000
H	3.872321000	-2.463323000	5.531096000
C	2.710731000	0.803571000	0.938509000
C	3.384106000	-0.426864000	0.867432000
C	3.466648000	1.985772000	0.995577000
C	4.771391000	-0.475292000	0.874236000
H	2.802793000	-1.347636000	0.804224000
C	4.854539000	1.932603000	0.997962000
H	2.953088000	2.946744000	1.025455000
C	5.512050000	0.703554000	0.946429000
H	5.277648000	-1.437487000	0.823599000
H	5.427891000	2.856744000	1.039945000
H	6.599374000	0.665903000	0.959551000
C	-0.265676000	2.929161000	0.271738000
C	-1.184122000	3.165249000	-0.772339000
C	0.026905000	3.979029000	1.168322000
C	-1.784007000	4.404315000	-0.921374000
H	-1.423003000	2.343207000	-1.450043000
C	-0.579812000	5.217070000	1.015171000
H	0.717237000	3.795159000	1.990453000
C	-1.485428000	5.432734000	-0.025115000
H	-2.495689000	4.571871000	-1.727080000
H	-0.352842000	6.019363000	1.713801000
H	-1.963269000	6.403751000	-0.135085000
N	-0.918920000	-0.485706000	1.962203000
C	2.024842000	0.670376000	-2.324382000
C	3.305995000	0.109271000	-2.352204000
C	1.875590000	2.047585000	-2.542603000
C	4.414966000	0.910068000	-2.608384000
H	3.440470000	-0.953863000	-2.158014000
C	2.986098000	2.843983000	-2.798591000
H	0.886630000	2.506652000	-2.503929000
C	4.257574000	2.275337000	-2.832066000
H	5.407223000	0.463718000	-2.623387000
H	2.857398000	3.910531000	-2.970761000
H	5.127501000	2.898503000	-3.028847000
C	0.924198000	-2.056961000	-2.061815000
C	1.542023000	-2.610466000	-3.190715000
C	0.497328000	-2.906178000	-1.031856000
C	1.736125000	-3.985440000	-3.275869000
H	1.880774000	-1.962382000	-3.999566000

C	0.680946000	-4.282873000	-1.121772000
H	-0.003738000	-2.488637000	-0.149683000
C	1.304836000	-4.820508000	-2.244841000
H	2.222347000	-4.409248000	-4.151940000
H	0.332921000	-4.931128000	-0.319934000
H	1.454043000	-5.895503000	-2.320404000
C	-3.129435000	-1.916992000	0.084328000
C	-3.578018000	-2.057199000	1.404989000
C	-3.131726000	-3.033972000	-0.761464000
C	-4.031109000	-3.290645000	1.860841000
H	-3.574965000	-1.196572000	2.070612000
C	-3.583809000	-4.266199000	-0.298777000
H	-2.784675000	-2.949138000	-1.790698000
C	-4.033650000	-4.396256000	1.012926000
H	-4.387993000	-3.386337000	2.884123000
H	-3.590377000	-5.123810000	-0.968651000
H	-4.391916000	-5.358478000	1.372807000
C	-3.539050000	0.952860000	0.269743000
C	-4.776863000	1.246937000	-0.320449000
C	-3.143114000	1.667788000	1.406097000
C	-5.587909000	2.247786000	0.204622000
H	-5.120317000	0.691106000	-1.191530000
C	-3.959514000	2.664938000	1.931111000
H	-2.188759000	1.443285000	1.875896000
C	-5.178102000	2.962751000	1.327850000
H	-6.545530000	2.465157000	-0.263931000
H	-3.634736000	3.216160000	2.811583000
H	-5.812507000	3.747537000	1.734790000

TS4_t

C	0.502768000	-2.235517000	-0.643481000
Co	0.084899000	-0.086129000	-0.233001000
P	-1.582465000	1.113948000	-1.311672000
P	1.864845000	1.075768000	-1.052737000
C	1.570094000	1.492313000	-2.823373000
H	2.460293000	2.002958000	-3.215871000
H	1.467717000	0.541326000	-3.364650000
C	-1.012347000	1.633941000	-2.987458000
H	-0.961802000	0.708550000	-3.578354000
H	-1.799464000	2.243664000	-3.452082000
C	0.331636000	2.366552000	-3.041810000
H	0.417457000	2.822382000	-4.036514000
H	0.338515000	3.211830000	-2.334599000
C	-0.674324000	-1.722528000	0.772827000
C	-1.920098000	-2.475600000	0.663461000
C	-2.020105000	-3.703978000	-0.005560000
C	-3.075072000	-1.930671000	1.256147000
C	-3.238561000	-4.371539000	-0.070408000
H	-1.139128000	-4.148672000	-0.463957000
C	-4.288405000	-2.597250000	1.180702000
H	-3.008646000	-0.965236000	1.758698000
C	-4.374546000	-3.821717000	0.517532000
H	-3.298345000	-5.328561000	-0.584586000
H	-5.174554000	-2.154996000	1.631657000
H	-5.327397000	-4.343701000	0.458294000
C	1.392128000	-3.311063000	-0.203122000
C	2.332261000	-3.771464000	-1.140909000
C	1.370052000	-3.861181000	1.083414000
C	3.235622000	-4.762130000	-0.786638000
H	2.347938000	-3.325173000	-2.132974000
C	2.286158000	-4.847410000	1.432254000
H	0.636521000	-3.516631000	1.809334000
C	3.218109000	-5.299506000	0.500704000
H	3.965314000	-5.109776000	-1.515234000
H	2.266583000	-5.269793000	2.434346000
H	3.930209000	-6.074401000	0.776884000
C	-0.219656000	-0.751164000	1.539392000
C	-0.157134000	-0.236077000	2.870597000
C	0.332255000	1.061967000	3.117131000

C	-0.600741000	-1.018620000	3.958191000
C	0.354268000	1.571693000	4.406735000
H	0.695493000	1.656291000	2.276899000
C	-0.568598000	-0.504485000	5.245409000
H	-0.979547000	-2.022489000	3.770203000
C	-0.095006000	0.789677000	5.471850000
H	0.731598000	2.576238000	4.586507000
H	-0.914756000	-1.111048000	6.079338000
H	-0.070575000	1.186942000	6.484425000
N	0.377678000	-1.555005000	-1.659944000
C	-1.995384000	2.643617000	-0.421720000
C	-2.091140000	3.900296000	-1.030558000
C	-2.131850000	2.552645000	0.972587000
C	-2.308553000	5.040248000	-0.259672000
H	-1.991554000	3.998030000	-2.110803000
C	-2.354310000	3.690104000	1.740497000
H	-2.046954000	1.577947000	1.458353000
C	-2.437202000	4.938088000	1.123708000
H	-2.378237000	6.012309000	-0.743411000
H	-2.454353000	3.602151000	2.820875000
H	-2.603702000	5.831803000	1.721609000
C	2.405675000	2.645543000	-0.303692000
C	3.740965000	3.064412000	-0.372830000
C	1.461338000	3.468119000	0.324718000
C	4.118588000	4.286286000	0.174492000
H	4.486597000	2.428095000	-0.849702000
C	1.842140000	4.692945000	0.866076000
H	0.420949000	3.147745000	0.392870000
C	3.171365000	5.101681000	0.792251000
H	5.157958000	4.603225000	0.119714000
H	1.096981000	5.323125000	1.348401000
H	3.472823000	6.055694000	1.219813000
C	-3.158220000	0.265032000	-1.626406000
C	-3.105095000	-1.026723000	-2.171323000
C	-4.399242000	0.832856000	-1.316415000
C	-4.279057000	-1.728220000	-2.418703000
H	-2.138090000	-1.485258000	-2.386010000
C	-5.570990000	0.120363000	-1.558994000
H	-4.450931000	1.833117000	-0.887889000
C	-5.512837000	-1.156555000	-2.111194000
H	-4.229746000	-2.730550000	-2.839778000
H	-6.533140000	0.568907000	-1.319561000
H	-6.430776000	-1.710100000	-2.299481000
C	3.321627000	-0.008713000	-1.022412000
C	4.065689000	-0.334609000	-2.161171000
C	3.665133000	-0.587836000	0.208995000
C	5.141300000	-1.216096000	-2.065714000
H	3.812911000	0.097468000	-3.128170000
C	4.740869000	-1.462232000	0.301429000
H	3.075058000	-0.354357000	1.098679000
C	5.480237000	-1.777799000	-0.837922000
H	5.716559000	-1.461252000	-2.956252000
H	4.993321000	-1.910759000	1.260326000
H	6.318364000	-2.468443000	-0.768234000

INT6_s

C	1.131313000	0.639548000	1.379498000
C	0.277184000	1.468169000	0.617450000
Co	-0.334889000	-0.087581000	0.036573000
P	0.641410000	-0.364839000	-1.984080000
P	-2.423946000	-0.090126000	-0.659069000
C	-2.719158000	0.118360000	-2.469539000
H	-3.753868000	-0.186460000	-2.676458000
H	-2.672664000	1.198463000	-2.670594000
C	-0.367567000	0.006045000	-3.481489000
H	-0.432946000	1.097313000	-3.597267000
H	0.179819000	-0.367387000	-4.357239000
C	-1.761868000	-0.607199000	-3.416339000
H	-2.199672000	-0.581016000	-4.422344000

H	-1.679389000	-1.673497000	-3.157844000
C	0.405552000	-0.443703000	2.085161000
C	1.004661000	-1.275272000	3.151396000
C	0.581456000	-2.602530000	3.295059000
C	1.923461000	-0.744071000	4.065212000
C	1.081666000	-3.389621000	4.325634000
H	-0.148774000	-2.999266000	2.590163000
C	2.414391000	-1.530960000	5.099891000
H	2.246671000	0.291535000	3.968137000
C	2.000209000	-2.855979000	5.227754000
H	0.753164000	-4.421870000	4.428326000
H	3.122332000	-1.109533000	5.810381000
H	2.391449000	-3.472014000	6.034808000
C	2.607362000	0.707118000	1.282165000
C	3.363344000	-0.477619000	1.259820000
C	3.284105000	1.929698000	1.168039000
C	4.749144000	-0.435636000	1.179018000
H	2.855354000	-1.440413000	1.308264000
C	4.671457000	1.968587000	1.080725000
H	2.720836000	2.861354000	1.149927000
C	5.410500000	0.788370000	1.098185000
H	5.315001000	-1.365434000	1.174940000
H	5.176836000	2.929090000	0.999917000
H	6.496643000	0.821750000	1.039797000
C	-0.005815000	2.850855000	0.459236000
C	-0.726843000	3.305755000	-0.666749000
C	0.298350000	3.770477000	1.488380000
C	-1.122291000	4.627610000	-0.765667000
H	-0.974195000	2.583746000	-1.447594000
C	-0.101597000	5.093948000	1.385023000
H	0.825475000	3.415250000	2.372865000
C	-0.810370000	5.523178000	0.261602000
H	-1.681892000	4.968486000	-1.633852000
H	0.129085000	5.794855000	2.183895000
H	-1.126597000	6.561506000	0.186683000
N	-0.834306000	-0.632541000	1.692355000
C	2.198198000	0.519474000	-2.295819000
C	3.443998000	-0.096363000	-2.133176000
C	2.147887000	1.882336000	-2.624371000
C	4.614948000	0.633030000	-2.317839000
H	3.500306000	-1.148811000	-1.859115000
C	3.320252000	2.605638000	-2.811126000
H	1.187637000	2.387301000	-2.734239000
C	4.556474000	1.980587000	-2.660711000
H	5.577576000	0.142806000	-2.186623000
H	3.267685000	3.659455000	-3.076681000
H	5.474255000	2.546538000	-2.806541000
C	0.981193000	-2.144442000	-2.143630000
C	1.667511000	-2.681751000	-3.241365000
C	0.491078000	-3.005392000	-1.152732000
C	1.861562000	-4.055153000	-3.338441000
H	2.063090000	-2.021188000	-4.013722000
C	0.682385000	-4.380838000	-1.254338000
H	-0.054459000	-2.595582000	-0.295844000
C	1.369124000	-4.903937000	-2.346590000
H	2.398558000	-4.466616000	-4.190458000
H	0.295182000	-5.040399000	-0.480573000
H	1.522769000	-5.977918000	-2.428009000
C	-3.324810000	-1.607420000	-0.208493000
C	-3.653046000	-1.825553000	1.137687000
C	-3.642712000	-2.587931000	-1.157459000
C	-4.293879000	-2.998603000	1.518473000
H	-3.401702000	-1.076259000	1.884316000
C	-4.281908000	-3.761795000	-0.768509000
H	-3.406740000	-2.441505000	-2.209987000
C	-4.607052000	-3.969553000	0.568953000
H	-4.553644000	-3.152660000	2.563671000
H	-4.531582000	-4.511316000	-1.516610000
H	-5.110407000	-4.885579000	0.871011000
C	-3.356534000	1.290441000	0.091646000

C	-4.366104000	1.958580000	-0.614947000
C	-3.045407000	1.708944000	1.392169000
C	-5.035886000	3.033065000	-0.036654000
H	-4.645747000	1.642416000	-1.618159000
C	-3.723113000	2.778296000	1.968047000
H	-2.261021000	1.193768000	1.946281000
C	-4.712745000	3.448210000	1.252514000
H	-5.817437000	3.542764000	-0.596413000
H	-3.470423000	3.093497000	2.978668000
H	-5.236744000	4.289812000	1.700901000

INT6_t

C	-0.529854000	-2.177531000	-0.593966000
Co	-0.024035000	-0.089601000	-0.262008000
P	1.625709000	1.099929000	-1.354133000
P	-1.722265000	1.195742000	-0.965120000
C	-1.486731000	1.682300000	-2.726402000
H	-2.375180000	2.241652000	-3.050415000
H	-1.446282000	0.755207000	-3.315859000
C	1.083717000	1.745138000	-2.987642000
H	0.992837000	0.862056000	-3.635587000
H	1.891244000	2.353904000	-3.416989000
C	-0.233135000	2.525283000	-2.971588000
H	-0.341062000	3.012515000	-3.948901000
H	-0.186039000	3.346755000	-2.238833000
C	0.467149000	-1.907497000	0.562222000
C	1.756531000	-2.608872000	0.545381000
C	1.891206000	-3.817057000	-0.154006000
C	2.871071000	-2.089470000	1.223566000
C	3.107126000	-4.491888000	-0.166517000
H	1.032123000	-4.231913000	-0.680976000
C	4.084272000	-2.761077000	1.201858000
H	2.780242000	-1.139607000	1.752385000
C	4.206240000	-3.966035000	0.507747000
H	3.195531000	-5.432718000	-0.706096000
H	4.944643000	-2.338986000	1.717495000
H	5.159301000	-4.490760000	0.491238000
C	-1.694260000	-3.049046000	-0.361686000
C	-2.626846000	-3.245438000	-1.390720000
C	-1.875221000	-3.697558000	0.866827000
C	-3.723843000	-4.068904000	-1.186438000
H	-2.473665000	-2.737885000	-2.341437000
C	-2.982015000	-4.513933000	1.070416000
H	-1.140523000	-3.565083000	1.660828000
C	-3.907016000	-4.700384000	0.044961000
H	-4.446481000	-4.215389000	-1.987096000
H	-3.117419000	-5.015594000	2.026235000
H	-4.768970000	-5.345900000	0.202121000
C	0.017059000	-0.914544000	1.409010000
C	0.105222000	-0.599549000	2.796924000
C	-0.197421000	0.703303000	3.248751000
C	0.482612000	-1.578637000	3.743904000
C	-0.098524000	1.022918000	4.593520000
H	-0.517412000	1.448205000	2.518214000
C	0.571185000	-1.254118000	5.088136000
H	0.718576000	-2.584907000	3.399378000
C	0.284687000	0.045121000	5.514340000
H	-0.331971000	2.029741000	4.933085000
H	0.864955000	-2.011465000	5.811456000
H	0.353006000	0.294070000	6.571352000
N	-0.293745000	-1.501200000	-1.669953000
C	2.139209000	2.532994000	-0.365135000
C	2.266024000	3.827511000	-0.880401000
C	2.338566000	2.324261000	1.009285000
C	2.578625000	4.891466000	-0.036923000
H	2.120331000	4.014660000	-1.943348000
C	2.655651000	3.386025000	1.848422000
H	2.230350000	1.318187000	1.421771000
C	2.770943000	4.674086000	1.325196000

H	2.673601000	5.894262000	-0.447997000
H	2.807140000	3.209162000	2.911746000
H	3.013067000	5.508464000	1.980161000
C	-2.125955000	2.766265000	-0.131016000
C	-3.393900000	3.345046000	-0.280895000
C	-1.157718000	3.428176000	0.632396000
C	-3.679828000	4.566493000	0.318840000
H	-4.161825000	2.831771000	-0.860281000
C	-1.446308000	4.653268000	1.228950000
H	-0.171484000	2.982798000	0.762084000
C	-2.706964000	5.222464000	1.072433000
H	-4.667397000	5.007427000	0.200560000
H	-0.682873000	5.158468000	1.817869000
H	-2.936153000	6.177073000	1.541486000
C	3.139132000	0.150739000	-1.684208000
C	3.014178000	-1.123852000	-2.256817000
C	4.409493000	0.639423000	-1.353835000
C	4.148148000	-1.887793000	-2.507093000
H	2.023877000	-1.519675000	-2.486670000
C	5.539009000	-0.134782000	-1.603091000
H	4.517223000	1.625683000	-0.904537000
C	5.410334000	-1.396169000	-2.179076000
H	4.043641000	-2.877722000	-2.946832000
H	6.523544000	0.252541000	-1.348644000
H	6.295589000	-1.999781000	-2.369788000
C	-3.271799000	0.247671000	-0.927985000
C	-4.067962000	0.037179000	-2.059225000
C	-3.673642000	-0.292303000	0.302944000
C	-5.253459000	-0.688107000	-1.955643000
H	-3.773403000	0.440058000	-3.026761000
C	-4.859764000	-1.008080000	0.403408000
H	-3.044212000	-0.151883000	1.184306000
C	-5.651599000	-1.206513000	-0.726937000
H	-5.867812000	-0.843817000	-2.840246000
H	-5.161518000	-1.423574000	1.362733000
H	-6.577394000	-1.773378000	-0.649662000

MECP1

C	-1.99272090	0.02114510	1.12148590
C	-2.37247390	-0.17076240	-0.05791830
Co	-0.11361170	-0.00169630	0.19073320
P	-0.06085370	2.05196530	-0.90107370
P	0.16132890	-1.19729810	-1.67077690
C	-0.23031310	-0.41456060	-3.28546910
H	0.11026690	-1.08798340	-4.08291910
H	-1.32647980	-0.36622740	-3.36344710
C	-0.35725960	2.07690090	-2.71688260
H	-1.43865190	1.96508610	-2.86860570
H	-0.08805180	3.06464840	-3.11318750
C	0.37597200	0.97739310	-3.47923030
H	0.34668440	1.21741770	-4.55029660
H	1.44303530	0.97340140	-3.20436640
C	1.57004000	-0.15774430	0.94993550
C	0.71738440	-0.95555140	1.57378850
C	-2.31387860	0.26325630	2.50860190
C	-1.36452140	0.66263540	3.46042740
C	-3.65663290	0.13018130	2.90660620
C	-1.74379190	0.92608630	4.77047680
H	-0.32270350	0.76881400	3.15852760
C	-4.02872640	0.38990830	4.21945390
H	-4.40061460	-0.17425650	2.17276190
C	-3.07568680	0.78835440	5.15549160
H	-0.99412830	1.23558170	5.49543470
H	-5.07061040	0.28150250	4.51324250
H	-3.37029820	0.98966570	6.18308250
C	0.67038710	-2.00521600	2.56257370
C	1.88054390	-2.56640330	3.02327350
C	-0.53972230	-2.54986120	3.03260350
C	1.87548170	-3.61607480	3.93128230

H	2.82393690	-2.17716440	2.64066870
C	-0.53881970	-3.59135150	3.95053700
H	-1.48156350	-2.14475420	2.66845230
C	0.66692740	-4.12361440	4.40669290
H	2.81741160	-4.04175330	4.27066520
H	-1.48276090	-3.99365980	4.31165300
H	0.66501530	-4.93991340	5.12617640
C	2.94891190	0.25405800	0.89516730
C	3.71217280	0.29480810	2.07862080
C	3.56086160	0.61806990	-0.31410050
C	5.04346910	0.68768450	2.04341360
H	3.23960200	0.03620490	3.02555460
C	4.90041560	0.97758570	-0.34960640
H	2.96919960	0.60022060	-1.22754640
C	5.64403950	1.02044300	0.82930360
H	5.62030460	0.72248000	2.96580860
H	5.36272860	1.23867280	-1.29992260
H	6.69175870	1.31330440	0.80244050
C	-3.18989840	-0.22961670	-1.23282250
C	-3.58004920	0.96670590	-1.86699780
C	-3.67350540	-1.44893070	-1.74104280
C	-4.38078010	0.93710310	-3.00155970
H	-3.26608260	1.91731640	-1.43941290
C	-4.47581770	-1.46723830	-2.87651040
H	-3.42732900	-2.37807550	-1.23353060
C	-4.81842790	-0.28088960	-3.52147760
H	-4.67772810	1.87236140	-3.47254210
H	-4.84062140	-2.42102210	-3.25357180
H	-5.44188320	-0.30255330	-4.41280480
C	1.86757820	-1.83268960	-1.87142000
C	2.38945010	-2.64511640	-0.85466680
C	2.66231890	-1.55827530	-2.99020310
C	3.67798150	-3.15420210	-0.94569600
H	1.77824590	-2.88491120	0.01645950
C	3.95702770	-2.06727250	-3.07716450
H	2.28491190	-0.94771120	-3.80807590
C	4.46955880	-2.85942790	-2.05511710
H	4.06487390	-3.78521870	-0.14762280
H	4.56278820	-1.84456550	-3.95323810
H	5.48037480	-3.25532390	-2.12592800
C	-0.80172330	-2.74602960	-1.64886520
C	-1.10470170	-3.32229170	-0.41093110
C	-1.22482580	-3.38018950	-2.82264480
C	-1.82837630	-4.50833750	-0.34233690
H	-0.78852830	-2.82206250	0.50250470
C	-1.95720310	-4.56156170	-2.75120530
H	-1.00064800	-2.95274580	-3.79861570
C	-2.26317780	-5.12549330	-1.51359010
H	-2.05932730	-4.94313640	0.62875100
H	-2.29179940	-5.04332800	-3.66764440
H	-2.83740350	-6.04834580	-1.46388210
C	-1.29852190	3.23646770	-0.25377150
C	-1.56128890	3.23259380	1.11988550
C	-1.97872470	4.15100140	-1.06879540
C	-2.49464230	4.10254330	1.67262730
H	-1.03591080	2.52988310	1.76441420
C	-2.91213980	5.02393060	-0.51535860
H	-1.79022080	4.18787850	-2.14078330
C	-3.17607790	4.99824490	0.85237450
H	-2.69384770	4.06847960	2.74265430
H	-3.43554780	5.72893830	-1.15822600
H	-3.91198960	5.67753460	1.27734820
C	1.49226900	2.99515980	-0.68790460
C	1.90811450	3.27232020	0.62162950
C	2.28794910	3.42742320	-1.75415270
C	3.08105630	3.97617610	0.86034290
H	1.30901670	2.92160930	1.46419950
C	3.46916730	4.12658240	-1.51332110
H	1.99905990	3.22467470	-2.78435400
C	3.86729170	4.40222300	-0.20888020

H	3.38924020	4.18079610	1.88374960
H	4.07740990	4.45869020	-2.35262430
H	4.79036750	4.94743940	-0.02343230

MECP2

C	-2.23605931	0.93960524	-0.28602112
C	-0.98997940	1.35155232	0.10703773
Co	0.44783264	0.14308689	-0.33979475
P	2.52463073	1.00791422	0.27306865
P	0.16309077	-0.98559965	1.51121789
C	0.82775287	-0.12244738	3.00552996
H	0.61197964	-0.78778592	3.85302507
H	0.24208008	0.78926702	3.17128583
C	2.70772725	1.37142634	2.06202228
H	2.06990211	2.24237958	2.26695598
H	3.74020294	1.68409131	2.26854417
C	2.31787890	0.20308582	2.97033029
H	2.62779837	0.45526658	3.99270108
H	2.88363106	-0.70255166	2.70324803
C	-2.23040292	-0.34265876	-1.01544869
C	-3.43045416	-1.04217624	-1.48726185
C	-3.45114157	-1.70406361	-2.72588965
C	-4.57818558	-1.10100973	-0.67777561
C	-4.57784563	-2.40395004	-3.13799836
H	-2.57815472	-1.64792973	-3.37481211
C	-5.69729962	-1.81641378	-1.08518260
H	-4.57723021	-0.59348204	0.28566147
C	-5.70435116	-2.46563449	-2.31845347
H	-4.58033231	-2.89985719	-4.10668949
H	-6.57188623	-1.86198616	-0.43851713
H	-6.58652916	-3.01352262	-2.64323762
C	-3.42581914	1.79865686	-0.15706384
C	-4.28735480	1.99162185	-1.24975263
C	-3.70235975	2.48038592	1.03725226
C	-5.38186640	2.84162868	-1.14862605
H	-4.08562157	1.47842942	-2.18843874
C	-4.80427981	3.32120957	1.14085332
H	-3.04420461	2.33683141	1.89417112
C	-5.64742441	3.50590852	0.04718103
H	-6.03078007	2.98531102	-2.00999002
H	-5.00761483	3.83355586	2.07946827
H	-6.50955569	4.16486708	0.12594496
C	-0.57195463	2.71486323	0.42332852
C	-0.40055000	3.62804670	0.63663769
C	-0.30748979	3.16901096	1.72767303
C	0.02889821	4.92734671	-0.40195323
H	-0.61610607	3.29644011	-1.65241329
C	0.11523123	4.47259424	1.96419345
H	-0.48867981	2.50090346	2.56993936
C	0.29602819	5.35307545	0.89838259
H	0.15369456	5.61311742	-1.23778242
H	0.28887898	4.80819289	2.98521712
H	0.63147352	6.37163069	1.08189436
C	-0.94908320	-0.77263106	-1.19636584
C	-0.29787894	-1.86507112	-1.88845015
C	0.81314236	-1.53395000	-2.69740390
C	-0.58516482	-3.22921480	-1.68243591
C	1.61849405	-2.52319476	-3.25677152
H	1.00442622	-0.47914843	-2.91937033
C	0.21255142	-4.20959059	-2.25392179
H	-1.45168379	-3.49897873	-1.08055366
C	1.32309658	-3.86419267	-3.03036657
H	2.46138899	-2.24592999	-3.88797015
H	-0.02649701	-5.25908055	-2.09167728
H	1.94205724	-4.64202235	-3.47213619
C	3.95941272	-0.05936417	-0.12778021
C	4.06499071	-0.54834729	-1.43723726
C	4.92880679	-0.43249340	0.80907164
C	5.11135772	-1.38661689	-1.80258180

H	3.31524660	-0.26931710	-2.17922319
C	5.97462008	-1.27774377	0.44405797
H	4.88273480	-0.06782435	1.83331319
C	6.06826247	-1.75712542	-0.85883107
H	5.18204843	-1.75087247	-2.82586980
H	6.72083575	-1.55782462	1.18454954
H	6.88740198	-2.41516100	-1.14079904
C	2.87844725	2.56884456	-0.59794343
C	3.45870900	3.68059613	0.01946573
C	2.53702781	2.64333879	-1.95554587
C	3.69708143	4.84128801	-0.71299245
H	3.72452696	3.65135875	1.07508625
C	2.78746838	3.79692070	-2.68852623
H	2.05869844	1.78758414	-2.44137679
C	3.36842828	4.89975534	-2.06472843
H	4.14634175	5.70297887	-0.22331549
H	2.52266514	3.83935928	-3.74300218
H	3.56185144	5.80699833	-2.63329143
C	-1.51756178	-1.44792330	2.02202930
C	-2.03441821	-2.71692035	1.73106917
C	-2.33292154	-0.51258733	2.67222791
C	-3.33498900	-3.04710821	2.09959466
H	-1.40838377	-3.45330548	1.22847889
C	-3.63108497	-0.84723903	3.04520633
H	-1.95562307	0.48848224	2.88203542
C	-4.13228836	-2.11596574	2.76163592
H	-3.72602179	-4.03562922	1.86844278
H	-4.25202268	-0.11171133	3.55313254
H	-5.14717122	-2.37819294	3.05389153
C	1.12776348	-2.53073821	1.51893698
C	1.05527517	-3.41355435	2.60793700
C	2.02310701	-2.80007255	0.47961730
C	1.87008251	-4.53875113	2.64887017
H	0.35050311	-3.22579963	3.41877910
C	2.84228936	-3.92502242	0.52594348
H	2.08000613	-2.13224168	-0.38010141
C	2.76771730	-4.79259884	1.61083736
H	1.80597341	-5.22056227	3.49434074
H	3.53566017	-4.11576536	-0.29127762
H	3.40661405	-5.67246164	1.65083666

MECP3

C	2.00521300	1.05379320	-0.26858060
C	0.76145890	1.31868980	-0.78488930
Co	-0.65726340	0.19558500	-0.17772250
P	-2.86093750	0.71537160	-0.72076770
P	-0.50061120	-1.48828360	-1.75749490
C	-1.53647770	-1.19300800	-3.26970660
H	-1.40898310	-2.07806510	-3.90770380
H	-1.10432150	-0.35110590	-3.82785090
C	-3.36361000	0.43143580	-2.46148780
H	-2.84898450	1.19692350	-3.05922240
H	-4.43842030	0.63423620	-2.56710250
C	-3.02067010	-0.95674650	-3.00156450
H	-3.55870770	-1.08947380	-3.94891580
H	-3.40775760	-1.73992320	-2.33084010
C	2.14790570	-0.11995840	0.59457040
C	3.41610680	-0.87223510	0.55916640
C	3.98537180	-1.37542820	1.74174070
C	4.11961520	-1.04529860	-0.64189660
C	5.20980370	-2.02650740	1.72317990
H	3.46305800	-1.23145040	2.68616510
C	5.33708720	-1.71396630	-0.66403280
H	3.69562360	-0.65562660	-1.56555090
C	5.89021070	-2.20190020	0.51780160
H	5.64162430	-2.39100400	2.65288210
H	5.85897300	-1.84762440	-1.61002580
H	6.85317110	-2.70858740	0.50379650
C	3.18464000	1.89726970	-0.56979910

C	4.08755880	2.21879040	0.45438460
C	3.41718080	2.41045810	-1.85276420
C	5.18278540	3.03687070	0.20379910
H	3.91565240	1.82687700	1.45793100
C	4.51577580	3.22392080	-2.10441180
H	2.73081360	2.15442410	-2.66023640
C	5.40116770	3.54180030	-1.07649130
H	5.86977390	3.28198390	1.01116970
H	4.68524780	3.60717930	-3.10869890
H	6.26113800	4.17878460	-1.27387790
C	0.28662140	2.53556520	-1.42072990
C	0.36936500	3.76804990	-0.74281090
C	-0.34962820	2.50751210	-2.67531910
C	-0.15840580	4.92053170	-1.30897830
H	0.84864710	3.79778680	0.23525900
C	-0.85691010	3.66690510	-3.24981870
H	-0.42125430	1.55540680	-3.20420290
C	-0.76788950	4.87651150	-2.56342690
H	-0.09183210	5.86447040	-0.77117390
H	-1.32719470	3.62742190	-4.23153470
H	-1.17602330	5.78457550	-3.00305220
C	1.10194330	-0.46012410	1.46806070
C	0.82463800	-1.80078450	2.00362850
C	-0.03805330	-1.96711380	3.10545160
C	1.28984670	-2.96758360	1.36138380
C	-0.39342760	-3.23322830	3.55804000
H	-0.43702270	-1.09151770	3.61660580
C	0.93830590	-4.22769300	1.81827170
H	1.92386750	-2.87599590	0.48181930
C	0.09826350	-4.37095430	2.92360660
H	-1.05887160	-3.32822960	4.41420810
H	1.30794190	-5.10904760	1.29583660
H	-0.17931970	-5.36174530	3.27752660
N	-0.69977070	1.14731400	1.40804860
C	0.30848640	0.69667380	2.06023240
C	0.76283990	1.32633840	3.31643910
C	1.71720410	0.72797400	4.15021300
C	0.26198500	2.59467740	3.65194100
C	2.16395790	1.38378940	5.29151620
H	2.09353520	-0.26668220	3.91410740
C	0.71526480	3.24964510	4.78779560
H	-0.46926600	3.05537490	2.98808240
C	1.66815370	2.64649610	5.61028210
H	2.90199270	0.90750380	5.93377940
H	0.33220300	4.23891140	5.03091860
H	2.02748060	3.16310290	6.49793770
C	-3.96130680	-0.33444010	0.28959680
C	-5.11690290	-0.93348310	-0.22504870
C	-3.60964780	-0.57377470	1.62733900
C	-5.90520880	-1.74980690	0.58138480
H	-5.41397950	-0.76647420	-1.25902000
C	-4.40286640	-1.38557560	2.43112050
H	-2.69917190	-0.12922220	2.03295730
C	-5.55154320	-1.97742580	1.90886520
H	-6.80350190	-2.20451110	0.16926610
H	-4.11982050	-1.55994350	3.46786480
H	-6.17011840	-2.61769740	2.53446620
C	-3.33844850	2.43181060	-0.35343220
C	-3.72507650	3.32849770	-1.35671110
C	-3.27661410	2.87979940	0.97518620
C	-4.04523970	4.64515100	-1.03674980
H	-3.78404400	3.01102020	-2.39563260
C	-3.59246350	4.19617770	1.28613760
H	-2.96660050	2.19777940	1.76291520
C	-3.97632070	5.08306590	0.28178350
H	-4.34985970	5.32978410	-1.82597450
H	-3.54199860	4.53067280	2.32060980
H	-4.22670300	6.11299870	0.52843760
C	1.10697610	-1.89021110	-2.51517490
C	1.77556510	-3.09914140	-2.28732170

C	1.68549710	-0.94567900	-3.37598620
C	2.98244050	-3.36611430	-2.92912420
H	1.34292660	-3.84141030	-1.61699440
C	2.88303650	-1.22158820	-4.02764390
H	1.19455910	0.01582650	-3.53875280
C	3.53115670	-2.43671230	-3.80820600
H	3.49308300	-4.30896300	-2.74228910
H	3.31351010	-0.48382320	-4.70187910
H	4.46664980	-2.65487780	-4.31907020
C	-1.21886120	-3.05086680	-1.16171680
C	-1.29655250	-4.18982070	-1.97698590
C	-1.81369870	-3.07614780	0.10332000
C	-1.95522640	-5.32787880	-1.52626680
H	-0.83183170	-4.18856200	-2.96394640
C	-2.49045260	-4.20871240	0.54640750
H	-1.73502230	-2.20608310	0.75705650
C	-2.55935490	-5.33468750	-0.26795780
H	-2.00436720	-6.21071430	-2.16049020
H	-2.95299130	-4.20742130	1.53201540
H	-3.08321420	-6.22451340	0.07487000

MECP1

Co	0.16546865	0.38057089	0.75591504
P	-1.66921643	0.16406502	-0.56771604
P	1.43060412	-0.79845885	-0.62672127
C	1.10735229	-0.57957799	-2.42555562
H	1.78645391	-1.23384484	-2.98905046
H	1.41308653	0.44881069	-2.66358804
C	-1.31250820	0.28482670	-2.37885665
H	-0.88558450	1.27705432	-2.58055463
H	-2.25950044	0.22257175	-2.93168648
C	-0.34402020	-0.79552143	-2.85796368
H	-0.36828059	-0.82057126	-3.95468840
H	-0.69949420	-1.78552225	-2.53248137
C	-0.20202138	-0.34018010	2.43573450
C	0.85766393	0.41933564	2.47869419
O	0.75206061	2.15606582	-0.25602079
C	0.85795272	3.20864290	0.40024783
N	1.27936597	4.37303267	-0.10224173
H	0.59614409	3.24957790	1.47162001
C	1.41213719	5.55121140	0.73233307
H	0.79555210	6.36793873	0.33988162
H	2.45652852	5.88344852	0.76230629
H	1.08610769	5.32135048	1.74993327
C	1.67788976	4.49366718	-1.49179712
H	1.20276031	5.37417123	-1.93743069
H	1.36704230	3.59736278	-2.03181973
H	2.76677580	4.60738557	-1.57017261
C	1.95885546	0.99147299	3.28042560
H	2.76807908	1.39283039	2.65695172
H	2.39277151	0.24459045	3.95806487
H	1.59006223	1.81264752	3.91066563
C	-1.13085964	-1.22308389	3.16640123
H	-0.79923722	-2.26919215	3.08723447
H	-2.14735961	-1.19038852	2.75770974
H	-1.17544516	-0.97635956	4.23545035
C	3.19052657	-0.34910816	-0.44584559
C	4.10268071	-1.17670838	0.22040550

C	3.62110324	0.90621405	-0.90269423
C	5.41597500	-0.75909413	0.41926562
H	3.79288444	-2.15895441	0.57303104
C	4.93432511	1.31684663	-0.70466968
H	2.92141696	1.56697163	-1.41177855
C	5.83465685	0.48704335	-0.03874333
H	6.11626899	-1.41774741	0.92863451
H	5.25854973	2.28805595	-1.07517631
H	6.86167626	0.80987707	0.11787709
C	-2.83715382	1.53040096	-0.25961414
C	-3.84896412	1.38061909	0.70003743
C	-2.66662848	2.78048030	-0.87038014
C	-4.68007204	2.44759550	1.02414596
H	-3.99369159	0.41606514	1.18618830
C	-3.50431009	3.84441809	-0.54826335
H	-1.87783583	2.92840497	-1.60787023
C	-4.51252854	3.68099980	0.39883926
H	-5.46603271	2.31182553	1.76413995
H	-3.37481143	4.80380014	-1.04614594
H	-5.16728301	4.51302136	0.64804190
C	-2.68498852	-1.34695296	-0.48891883
C	-3.94486151	-1.40989348	-1.10245715
C	-2.17630500	-2.48543133	0.14440224
C	-4.67797937	-2.59053600	-1.07615631
H	-4.35704261	-0.52613696	-1.59101038
C	-2.90927809	-3.66972731	0.16333994
H	-1.19966663	-2.43447839	0.62578483
C	-4.16018211	-3.72197954	-0.44487767
H	-5.65760518	-2.63065256	-1.54807806
H	-2.50431630	-4.54932889	0.66053568
H	-4.73719173	-4.64427672	-0.42540752
C	1.33311120	-2.58542713	-0.30962412
C	1.17469412	-3.53396299	-1.32642476
C	1.37245561	-3.02050913	1.02434557
C	1.04592769	-4.88579741	-1.01410932
H	1.14972271	-3.22916007	-2.37114922
C	1.25783844	-4.37101308	1.33214378
H	1.48893946	-2.28550011	1.82179387
C	1.08498369	-5.30615200	0.31220004
H	0.91734705	-5.61169886	-1.81404744
H	1.29816994	-4.69346910	2.37104406
H	0.98318781	-6.36233005	0.55262621

TS1_t

C	-0.506190000	-0.920316000	2.540304000
C	0.217698000	0.116908000	2.371729000
Co	0.055186000	-0.787830000	0.619663000
P	1.502090000	0.473631000	-0.573601000
P	-1.836984000	-0.168273000	-0.633347000
C	-1.438957000	-0.020480000	-2.424090000
H	-1.237742000	-1.046813000	-2.757976000
H	-2.342200000	0.309373000	-2.955422000
C	1.118952000	0.331172000	-2.374762000
H	1.910375000	0.873399000	-2.909788000
H	1.185739000	-0.725913000	-2.656546000
C	-0.252831000	0.885077000	-2.762108000
H	-0.390088000	1.887475000	-2.327068000
H	-0.252392000	1.036517000	-3.849164000
O	0.380083000	-2.564472000	-1.332791000
C	0.865132000	-2.391901000	-0.207353000
H	-0.741909000	-1.959386000	1.117993000
N	1.809233000	-3.175034000	0.345444000
C	2.374660000	-4.290245000	-0.397044000
H	2.317725000	-5.206909000	0.201137000
H	1.811871000	-4.421111000	-1.322693000
H	3.429410000	-4.090108000	-0.631267000
C	2.453753000	-2.844774000	1.596634000
H	3.517229000	-2.620877000	1.427690000
H	1.975674000	-1.964454000	2.037343000

H	2.378621000	-3.682311000	2.301769000
C	-1.307309000	-1.814110000	3.391938000
H	-2.337039000	-1.900643000	3.021821000
H	-0.890475000	-2.828886000	3.406528000
H	-1.337226000	-1.437067000	4.420657000
C	0.854033000	1.292508000	2.988956000
H	1.756038000	1.621013000	2.461280000
H	0.163237000	2.146002000	2.985086000
H	1.118393000	1.084586000	4.033336000
C	-3.210002000	-1.362628000	-0.569042000
C	-4.541140000	-0.964540000	-0.395329000
C	-2.908435000	-2.726061000	-0.703703000
C	-5.554404000	-1.918913000	-0.356302000
H	-4.788997000	0.090547000	-0.289800000
C	-3.927358000	-3.671900000	-0.672476000
H	-1.873294000	-3.037672000	-0.845767000
C	-5.250327000	-3.270550000	-0.494501000
H	-6.586287000	-1.601967000	-0.220100000
H	-3.687236000	-4.727143000	-0.785593000
H	-6.045208000	-4.012824000	-0.464282000
C	3.219910000	-0.107714000	-0.412597000
C	3.703831000	-1.148695000	-1.215770000
C	4.038002000	0.402077000	0.605308000
C	4.984337000	-1.656541000	-1.011865000
H	3.079020000	-1.574967000	-2.000611000
C	5.315689000	-0.109841000	0.808240000
H	3.681320000	1.222279000	1.228870000
C	5.791560000	-1.140628000	0.000292000
H	5.355362000	-2.453195000	-1.654337000
H	5.943444000	0.302608000	1.595214000
H	6.792749000	-1.536983000	0.154618000
C	1.592197000	2.277871000	-0.342101000
C	0.521181000	2.963631000	0.239495000
C	2.682009000	3.006344000	-0.841691000
C	0.536321000	4.353215000	0.326866000
H	-0.325884000	2.402876000	0.632577000
C	2.697249000	4.393577000	-0.747405000
H	3.523886000	2.485716000	-1.298077000
C	1.625273000	5.068176000	-0.163954000
H	-0.303375000	4.873893000	0.783372000
H	3.548846000	4.950552000	-1.132167000
H	1.641931000	6.153624000	-0.091856000
C	-2.576879000	1.418514000	-0.144230000
C	-2.857558000	2.446576000	-1.051492000
C	-2.837032000	1.627096000	1.219689000
C	-3.377933000	3.658916000	-0.603425000
H	-2.675937000	2.309404000	-2.116031000
C	-3.362081000	2.835406000	1.663514000
H	-2.624889000	0.832448000	1.936228000
C	-3.628007000	3.856881000	0.751625000
H	-3.592225000	4.449197000	-1.319809000
H	-3.566964000	2.980794000	2.722294000
H	-4.035478000	4.804326000	1.097985000

TS1_s

C	-0.589271000	-0.735135000	2.482671000
C	0.295948000	0.196719000	2.318065000
Co	-0.090159000	-0.695740000	0.675717000
P	1.485730000	0.308897000	-0.586288000
P	-1.710269000	-0.044236000	-0.652381000
C	-1.356591000	0.049089000	-2.449489000
H	-1.265661000	-0.990536000	-2.782403000
H	-2.252109000	0.460014000	-2.934578000
C	1.201135000	0.181106000	-2.403085000
H	2.054031000	0.657560000	-2.903872000
H	1.193061000	-0.878348000	-2.681425000
C	-0.106312000	0.837850000	-2.837906000
H	-0.154370000	1.866889000	-2.448835000
H	-0.098586000	0.934247000	-3.930902000

O	-0.024725000	-2.545678000	-1.528945000
C	0.313359000	-2.370225000	-0.358483000
H	-0.856857000	-1.993875000	0.664490000
N	1.131243000	-3.239794000	0.302227000
C	1.614413000	-4.428500000	-0.385189000
H	1.360754000	-5.324970000	0.192780000
H	1.144829000	-4.482984000	-1.367317000
H	2.705509000	-4.384245000	-0.503222000
C	1.635352000	-3.008496000	1.642645000
H	2.383056000	-3.774276000	1.864832000
H	2.119401000	-2.027231000	1.726576000
H	0.842013000	-3.075096000	2.397793000
C	-1.511272000	-1.483767000	3.351006000
H	-2.545191000	-1.380111000	2.995045000
H	-1.295277000	-2.559054000	3.327218000
H	-1.467216000	-1.145961000	4.393818000
C	1.059979000	1.257283000	3.000072000
H	0.417794000	2.136985000	3.150833000
H	1.387516000	0.924842000	3.993487000
H	1.934301000	1.601067000	2.438002000
C	-3.211302000	-1.070227000	-0.540497000
C	-4.387928000	-0.592845000	0.052168000
C	-3.177268000	-2.378679000	-1.049195000
C	-5.511874000	-1.411357000	0.131105000
H	-4.437678000	0.422532000	0.439789000
C	-4.306375000	-3.185051000	-0.970613000
H	-2.263353000	-2.761288000	-1.501299000
C	-5.474199000	-2.705597000	-0.378517000
H	-6.422186000	-1.029095000	0.588026000
H	-4.274147000	-4.194211000	-1.375859000
H	-6.355226000	-3.340922000	-0.317924000
C	-2.239944000	1.630330000	-0.159771000
C	-2.442750000	2.644835000	-1.104025000
C	-2.447939000	1.922147000	1.197236000
C	-2.822603000	3.922213000	-0.698511000
H	-2.309122000	2.450388000	-2.165444000
C	-2.836728000	3.194746000	1.598780000
H	-2.295203000	1.145474000	1.945480000
C	-3.015010000	4.201968000	0.650719000
H	-2.970371000	4.699209000	-1.445246000
H	-3.000124000	3.401415000	2.654533000
H	-3.309840000	5.201019000	0.964572000
C	1.840902000	2.089816000	-0.403007000
C	2.999461000	2.633128000	-0.979116000
C	0.929223000	2.943038000	0.224566000
C	3.236986000	4.001411000	-0.919246000
H	3.724369000	1.979552000	-1.465210000
C	1.165776000	4.314689000	0.278102000
H	0.034564000	2.527311000	0.684333000
C	2.319195000	4.844328000	-0.292631000
H	4.141374000	4.412059000	-1.363097000
H	0.446591000	4.966193000	0.771224000
H	2.508083000	5.914883000	-0.248103000
C	3.096595000	-0.500040000	-0.326097000
C	3.451611000	-1.645140000	-1.050698000
C	3.951861000	-0.043505000	0.687415000
C	4.642921000	-2.310669000	-0.772818000
H	2.793952000	-2.028527000	-1.830591000
C	5.137708000	-0.714597000	0.965664000
H	3.697217000	0.856196000	1.247483000
C	5.484536000	-1.851215000	0.237448000
H	4.916569000	-3.188663000	-1.355457000
H	5.796612000	-0.344344000	1.748168000
H	6.414807000	-2.372967000	0.451329000

INT1_t

C	-0.345991000	0.153977000	2.810129000
C	0.165103000	-0.962120000	2.255762000
Co	-0.024716000	-0.968215000	0.360097000

P	1.880092000	-0.237434000	-0.743943000
P	-1.468645000	0.539950000	-0.747847000
C	-1.031644000	0.475756000	-2.545414000
H	-1.135131000	-0.565841000	-2.879345000
H	-1.775771000	1.065539000	-3.097545000
C	1.522008000	0.029933000	-2.531714000
H	2.449315000	0.354076000	-3.024411000
H	1.303657000	-0.970150000	-2.933308000
C	0.375432000	0.990261000	-2.858283000
H	0.534075000	1.962346000	-2.366279000
H	0.421334000	1.196695000	-3.935262000
O	-0.799659000	-2.602027000	-0.826529000
C	-1.308144000	-2.339302000	0.288241000
H	-1.138107000	0.682479000	2.267087000
N	-2.322429000	-2.955448000	0.873877000
C	-3.008870000	-4.054327000	0.204042000
H	-4.041618000	-3.761151000	-0.021201000
H	-2.485093000	-4.292628000	-0.722826000
H	-3.022863000	-4.934462000	0.856133000
C	-2.905235000	-2.478801000	2.112704000
H	-3.927382000	-2.122897000	1.930132000
H	-2.940225000	-3.291423000	2.847762000
H	-2.297588000	-1.659772000	2.503784000
C	0.090471000	0.817522000	4.077709000
H	0.393625000	1.856281000	3.883099000
H	-0.733183000	0.869328000	4.802156000
H	0.930666000	0.306065000	4.558317000
C	1.104694000	-1.944736000	2.868560000
H	0.600938000	-2.909947000	3.018363000
H	1.976028000	-2.149504000	2.230167000
H	1.476276000	-1.620678000	3.851427000
C	-3.237547000	0.114837000	-0.700964000
C	-4.091234000	0.733507000	0.223374000
C	-3.736070000	-0.930769000	-1.491058000
C	-5.417701000	0.328221000	0.339522000
H	-3.719690000	1.548422000	0.844804000
C	-5.064389000	-1.330773000	-1.373078000
H	-3.085268000	-1.443063000	-2.199503000
C	-5.908134000	-0.703413000	-0.458520000
H	-6.072198000	0.826127000	1.052079000
H	-5.442885000	-2.131862000	-2.005734000
H	-6.947325000	-1.013517000	-0.372557000
C	3.192237000	-1.497457000	-0.735684000
C	4.550858000	-1.161597000	-0.710173000
C	2.811079000	-2.846781000	-0.766581000
C	5.514628000	-2.165491000	-0.720865000
H	4.854453000	-0.115631000	-0.676666000
C	3.780244000	-3.844753000	-0.783946000
H	1.751529000	-3.111836000	-0.782946000
C	5.131374000	-3.504426000	-0.758539000
H	6.569511000	-1.900226000	-0.699841000
H	3.480088000	-4.890101000	-0.811565000
H	5.888463000	-4.285649000	-0.765004000
C	2.650257000	1.283597000	-0.124041000
C	3.003041000	2.358356000	-0.947189000
C	2.867913000	1.380729000	1.259253000
C	3.558537000	3.511130000	-0.396120000
H	2.849732000	2.304214000	-2.023934000
C	3.426729000	2.530351000	1.805068000
H	2.589975000	0.549504000	1.909559000
C	3.769094000	3.599591000	0.977135000
H	3.829798000	4.341070000	-1.044995000
H	3.595876000	2.592596000	2.878423000
H	4.203838000	4.501057000	1.403812000
C	-1.395352000	2.321164000	-0.380311000
C	-2.270129000	3.222782000	-1.005252000
C	-0.413029000	2.811843000	0.486916000
C	-2.160216000	4.586700000	-0.761142000
H	-3.047639000	2.852505000	-1.674228000
C	-0.301474000	4.179868000	0.725508000

H	0.270233000	2.117780000	0.976473000
C	-1.175057000	5.066307000	0.102916000
H	-2.844948000	5.279465000	-1.245747000
H	0.469325000	4.548220000	1.400210000
H	-1.092811000	6.134875000	0.290661000

INT1_s

C	0.246980000	-0.651603000	2.770977000
C	1.110918000	-1.259054000	1.934609000
Co	0.070524000	-0.587757000	0.572958000
P	1.655174000	0.130391000	-0.730043000
P	-1.623603000	0.347863000	-0.598091000
C	-1.329551000	0.327126000	-2.416987000
H	-1.270569000	-0.720832000	-2.734699000
H	-2.205745000	0.771752000	-2.906773000
C	1.235498000	0.312762000	-2.507523000
H	2.096557000	0.793324000	-2.991736000
H	1.185850000	-0.709553000	-2.899879000
C	-0.056834000	1.063134000	-2.824943000
H	-0.048141000	2.067821000	-2.375647000
H	-0.087386000	1.224918000	-3.910037000
O	0.162319000	-2.394752000	-1.500077000
C	-0.279351000	-2.206346000	-0.365619000
H	-0.488497000	0.072731000	2.322913000
N	-1.046541000	-3.134570000	0.271810000
C	-1.289985000	-4.424543000	-0.358573000
H	-2.350371000	-4.517232000	-0.632426000
H	-0.675083000	-4.505141000	-1.254657000
H	-1.038612000	-5.234631000	0.336408000
C	-1.740884000	-2.913700000	1.521982000
H	-2.718014000	-3.409644000	1.474151000
H	-1.184310000	-3.313351000	2.382265000
H	-1.922490000	-1.846660000	1.682420000
C	0.026145000	-0.828628000	4.239033000
H	0.142056000	0.118497000	4.780486000
H	-0.992254000	-1.183993000	4.445179000
H	0.731964000	-1.551661000	4.660226000
C	2.212477000	-2.200029000	2.210022000
H	2.298696000	-2.463261000	3.273642000
H	2.089397000	-3.123790000	1.629729000
H	3.175091000	-1.775186000	1.892166000
C	-3.216707000	-0.519973000	-0.412526000
C	-4.141210000	-0.105866000	0.555864000
C	-3.477170000	-1.682962000	-1.150580000
C	-5.307645000	-0.833942000	0.771930000
H	-3.953389000	0.799202000	1.134004000
C	-4.647036000	-2.405467000	-0.933562000
H	-2.763225000	-2.035112000	-1.895150000
C	-5.562910000	-1.984230000	0.028444000
H	-6.022789000	-0.496388000	1.519176000
H	-4.846355000	-3.297633000	-1.524674000
H	-6.477802000	-2.548857000	0.194529000
C	-1.998165000	2.093681000	-0.241687000
C	-3.034247000	2.758124000	-0.914317000
C	-1.233699000	2.794706000	0.696409000
C	-3.290318000	4.099037000	-0.654223000
H	-3.652421000	2.218460000	-1.632497000
C	-1.490599000	4.139052000	0.955492000
H	-0.421908000	2.287362000	1.220933000
C	-2.517167000	4.790820000	0.278840000
H	-4.096984000	4.607190000	-1.178240000
H	-0.887334000	4.674630000	1.685907000
H	-2.720624000	5.840606000	0.479406000
C	2.072493000	1.805289000	-0.139188000
C	2.185487000	2.899142000	-1.007237000
C	2.275109000	2.010726000	1.234937000
C	2.480052000	4.166407000	-0.510848000
H	2.056598000	2.771284000	-2.079711000
C	2.580090000	3.275188000	1.726564000

H	2.196483000	1.167780000	1.922592000
C	2.674531000	4.358242000	0.854119000
H	2.564652000	5.005282000	-1.198179000
H	2.745032000	3.415160000	2.792927000
H	2.906213000	5.349580000	1.237682000
C	3.229339000	-0.786380000	-0.740305000
C	3.271859000	-2.078083000	-1.287743000
C	4.390072000	-0.243983000	-0.171519000
C	4.456187000	-2.806526000	-1.262474000
H	2.372471000	-2.514696000	-1.716373000
C	5.570357000	-0.982494000	-0.149013000
H	4.380165000	0.759917000	0.248260000
C	5.605432000	-2.264393000	-0.690441000
H	4.480191000	-3.805617000	-1.692803000
H	6.466195000	-0.548828000	0.290381000
H	6.528924000	-2.839217000	-0.671290000

MECP2

C	0.55970944	-0.40751304	2.75841181
C	1.07745349	-1.34205750	1.93969557
Co	0.04495239	-0.61739236	0.56340479
P	1.73272552	0.19441303	-0.76226392
P	-1.63071506	0.42042508	-0.55771689
C	-1.33580701	0.40568274	-2.37834424
H	-1.28852552	-0.64142811	-2.70327296
H	-2.20692048	0.86517400	-2.86400299
C	1.23269392	0.33744310	-2.52397318
H	2.07504216	0.76363978	-3.08527063
H	1.11464682	-0.69448368	-2.87880823
C	-0.05118966	1.12799321	-2.78332447
H	-0.00587444	2.11564869	-2.29772118
H	-0.10336584	1.33292359	-3.86004089
O	-0.05327553	-2.45077006	-1.29086046
C	-0.53552570	-2.30995895	-0.16223252
H	-0.05392976	0.40555063	2.27969488
N	-1.33414756	-3.20143292	0.45226498
C	-1.72950805	-4.42799786	-0.22301540
H	-2.80537370	-4.40318985	-0.44508356
H	-1.16476665	-4.52241250	-1.15178618
H	-1.52648052	-5.29206064	0.42050920
C	-2.00917607	-2.91401840	1.69809762
H	-3.09757743	-2.91411931	1.54450895
H	-1.75823154	-3.66475092	2.45876231
H	-1.70706504	-1.92749519	2.06356021
C	0.64145835	-0.24858878	4.24301854
H	1.02630159	0.74153924	4.51968878
H	-0.34759101	-0.34183540	4.70998583
H	1.29779297	-1.00609059	4.68279080
C	1.95660482	-2.49031862	2.22688778
H	1.46340479	-3.43421735	1.95858513
H	2.86443843	-2.44176791	1.61020436
H	2.26456990	-2.54939511	3.28060128
C	-3.23549145	-0.41600411	-0.35009727
C	-4.09926207	-0.03903647	0.68748176
C	-3.56015014	-1.53171311	-1.13431047
C	-5.27165087	-0.75122531	0.92194189
H	-3.85887263	0.82544130	1.30702458
C	-4.73308465	-2.24244161	-0.89552656
H	-2.89213022	-1.85858078	-1.93132672
C	-5.59137881	-1.85382758	0.13153544
H	-5.93903079	-0.44001732	1.72250898
H	-4.98089861	-3.09817251	-1.52167753
H	-6.50978498	-2.40719405	0.31402282
C	-1.95524218	2.17410014	-0.19741072
C	-3.11584935	2.80408342	-0.66958197
C	-1.00471404	2.92595211	0.50148528
C	-3.31339520	4.16137725	-0.44555372
H	-3.87070341	2.22422462	-1.20129303
C	-1.19879232	4.28904559	0.71248563

H	-0.10016649	2.44364306	0.87482807
C	-2.35299536	4.90573339	0.23957843
H	-4.21913324	4.64241496	-0.80769289
H	-0.44801823	4.86647729	1.24819456
H	-2.50872742	5.96941102	0.40681034
C	3.21134763	-0.86672829	-0.78247315
C	4.39032503	-0.49133385	-0.12636330
C	3.13718639	-2.12915289	-1.39249916
C	5.47678517	-1.36065052	-0.08586914
H	4.46830457	0.48568660	0.34688702
C	4.23008024	-2.98830753	-1.35254761
H	2.21798321	-2.44912068	-1.87844545
C	5.40040838	-2.60898042	-0.69764192
H	6.38875131	-1.05405328	0.42175418
H	4.16421200	-3.96233381	-1.83335958
H	6.25223990	-3.28508765	-0.66477834
C	2.29848579	1.84729721	-0.25193657
C	2.45124357	2.90475449	-1.15732318
C	2.54385801	2.08122338	1.11102788
C	2.83507894	4.16600196	-0.70841006
H	2.27832992	2.75342624	-2.22123720
C	2.93728046	3.33918697	1.55386485
H	2.42707184	1.26547841	1.82666232
C	3.07616539	4.38720052	0.64484554
H	2.94972838	4.97835950	-1.42296769
H	3.13347275	3.50279199	2.61154000
H	3.37827711	5.37318120	0.99178114

TS2_t

C	-0.215623000	-0.600623000	3.010366000
C	0.146593000	-1.516906000	2.093301000
Co	0.006005000	-0.907854000	0.230546000
P	1.872438000	-0.095170000	-0.859084000
P	-1.485305000	0.518794000	-0.800701000
C	-1.017782000	0.697535000	-2.588669000
H	-1.092884000	-0.296738000	-3.051928000
H	-1.789032000	1.316843000	-3.065666000
C	1.551080000	0.376059000	-2.610195000
H	2.470209000	0.810533000	-3.027600000
H	1.401156000	-0.571923000	-3.145883000
C	0.361116000	1.307502000	-2.841056000
H	0.472421000	2.227678000	-2.247278000
H	0.394397000	1.629717000	-3.889975000
O	-0.656516000	-2.968782000	-0.209524000
C	-1.230767000	-2.283005000	0.661897000
H	-1.014098000	0.104329000	2.768077000
N	-2.426398000	-2.535017000	1.198282000
C	-3.140452000	-3.754671000	0.847938000
H	-4.059058000	-3.507285000	0.300628000
H	-2.499517000	-4.374548000	0.219861000
H	-3.405734000	-4.304230000	1.758283000
C	-3.096293000	-1.596016000	2.072703000
H	-4.172909000	-1.645976000	1.878950000
H	-2.907849000	-1.819824000	3.130928000
H	-2.763971000	-0.577761000	1.852334000
C	0.428525000	-0.399523000	4.343091000
H	0.851336000	0.612254000	4.420902000
H	-0.302580000	-0.485864000	5.158091000
H	1.236252000	-1.113300000	4.532604000
C	1.174609000	-2.593104000	2.276848000
H	1.026046000	-3.414630000	1.567542000
H	2.192735000	-2.213515000	2.103625000
H	1.148537000	-3.017484000	3.289118000
C	-3.245732000	0.062104000	-0.912648000
C	-4.274861000	0.834759000	-0.362280000
C	-3.561785000	-1.160869000	-1.523606000
C	-5.596808000	0.401597000	-0.441301000
H	-4.045521000	1.778256000	0.131146000
C	-4.884013000	-1.584333000	-1.608914000

H	-2.767322000	-1.794057000	-1.923726000
C	-5.904639000	-0.803042000	-1.067853000
H	-6.389071000	1.013023000	-0.014310000
H	-5.117885000	-2.527498000	-2.099653000
H	-6.938586000	-1.134528000	-1.135029000
C	3.238169000	-1.290216000	-0.964993000
C	4.578535000	-0.888440000	-1.011353000
C	2.917673000	-2.653447000	-1.025480000
C	5.584781000	-1.842720000	-1.123387000
H	4.834036000	0.169715000	-0.952492000
C	3.928957000	-3.601825000	-1.144183000
H	1.873207000	-2.968756000	-0.973148000
C	5.261102000	-3.196786000	-1.191525000
H	6.625699000	-1.528120000	-1.157097000
H	3.676509000	-4.658959000	-1.192115000
H	6.051712000	-3.939246000	-1.276861000
C	2.552845000	1.379265000	-0.043479000
C	2.886554000	2.557616000	-0.719222000
C	2.716381000	1.321037000	1.349485000
C	3.372421000	3.657265000	-0.014716000
H	2.773656000	2.626566000	-1.800312000
C	3.208594000	2.416573000	2.048649000
H	2.450419000	0.407167000	1.885398000
C	3.533533000	3.588974000	1.366293000
H	3.629252000	4.568782000	-0.550096000
H	3.340876000	2.356614000	3.127394000
H	3.916155000	4.448682000	1.912366000
C	-1.415833000	2.235822000	-0.205267000
C	-2.082769000	3.272016000	-0.876702000
C	-0.617383000	2.544558000	0.901755000
C	-1.955498000	4.585682000	-0.440599000
H	-2.711237000	3.048220000	-1.739416000
C	-0.486451000	3.862142000	1.334152000
H	-0.081570000	1.747027000	1.420487000
C	-1.155801000	4.881447000	0.663863000
H	-2.479359000	5.382595000	-0.964090000
H	0.143230000	4.089290000	2.192051000
H	-1.055748000	5.911467000	0.999649000

TS2_s

C	-2.125783000	0.027264000	2.183572000
C	-0.786281000	-0.122331000	2.081780000
Co	0.183106000	-0.486469000	0.402813000
P	1.898478000	0.188685000	-0.865205000
P	-1.338561000	0.179543000	-0.978722000
C	-0.808476000	0.332091000	-2.746479000
H	-0.510682000	-0.662882000	-3.106987000
H	-1.695507000	0.620443000	-3.325418000
C	1.700116000	0.809376000	-2.591832000
H	2.475708000	1.564721000	-2.779827000
H	1.943719000	-0.046144000	-3.236501000
C	0.316540000	1.340652000	-2.960205000
H	0.088292000	2.266411000	-2.410785000
H	0.338631000	1.628183000	-4.019064000
O	1.153959000	-1.740365000	1.602528000
C	-0.108833000	-1.861065000	1.577234000
H	-2.761908000	-0.510073000	1.481351000
N	-0.776380000	-2.959113000	1.957653000
C	-0.065435000	-4.020198000	2.660001000
H	-0.317435000	-4.988335000	2.214709000
H	1.008211000	-3.850973000	2.576115000
H	-0.348722000	-4.036283000	3.720553000
C	-2.219439000	-3.045631000	1.918659000
H	-2.502031000	-4.101522000	1.874159000
H	-2.674893000	-2.595241000	2.813386000
H	-2.609943000	-2.550596000	1.026882000
C	-2.852144000	0.935785000	3.111620000
H	-3.390975000	1.703548000	2.535909000
H	-3.617003000	0.397078000	3.687087000

H	-2.193793000	1.454727000	3.814069000
C	0.191800000	0.563415000	2.999139000
H	1.131891000	0.011530000	3.074445000
H	0.444731000	1.570608000	2.635005000
H	-0.215010000	0.675296000	4.013296000
C	-2.720460000	-1.006583000	-1.135706000
C	-4.021008000	-0.744025000	-0.686495000
C	-2.430770000	-2.270850000	-1.672542000
C	-5.009666000	-1.721575000	-0.780627000
H	-4.263007000	0.229306000	-0.259950000
C	-3.421441000	-3.241607000	-1.772406000
H	-1.416555000	-2.502657000	-2.001596000
C	-4.713365000	-2.968728000	-1.324571000
H	-6.016478000	-1.503576000	-0.430490000
H	-3.184121000	-4.214373000	-2.198106000
H	-5.488452000	-3.728147000	-1.400900000
C	3.330676000	-0.920642000	-0.967263000
C	4.620667000	-0.411743000	-1.169872000
C	3.133204000	-2.304558000	-0.905210000
C	5.696614000	-1.281066000	-1.310291000
H	4.783016000	0.665732000	-1.206786000
C	4.213604000	-3.170187000	-1.051063000
H	2.132458000	-2.697018000	-0.724536000
C	5.493064000	-2.659196000	-1.253019000
H	6.696955000	-0.882409000	-1.464800000
H	4.057106000	-4.245568000	-0.999742000
H	6.337453000	-3.336541000	-1.362100000
C	2.440810000	1.609099000	0.133817000
C	2.068303000	2.921976000	-0.182209000
C	3.161677000	1.365484000	1.313120000
C	2.413206000	3.972194000	0.664399000
H	1.506601000	3.132523000	-1.091773000
C	3.513862000	2.419280000	2.148357000
H	3.444804000	0.344296000	1.570616000
C	3.136165000	3.723081000	1.828716000
H	2.122745000	4.988842000	0.406675000
H	4.083158000	2.221988000	3.054318000
H	3.409831000	4.545775000	2.485781000
C	-2.070026000	1.826557000	-0.696153000
C	-3.130819000	2.308551000	-1.476308000
C	-1.477002000	2.675958000	0.245455000
C	-3.599843000	3.606081000	-1.298714000
H	-3.598541000	1.663668000	-2.221344000
C	-1.937979000	3.979191000	0.412199000
H	-0.644223000	2.307632000	0.845691000
C	-3.003625000	4.442412000	-0.355316000
H	-4.429551000	3.968228000	-1.902069000
H	-1.463740000	4.630651000	1.144104000
H	-3.369860000	5.458314000	-0.222923000

INT2_t

C	-1.737333000	-0.738745000	1.951815000
C	-1.218526000	-1.983873000	1.619104000
Co	-0.142098000	-0.610843000	0.477050000
P	1.866880000	-0.416292000	-0.572556000
P	-1.137762000	1.107817000	-0.660070000
C	-0.675878000	1.027958000	-2.450354000
H	-1.028148000	0.062121000	-2.839618000
H	-1.233822000	1.806121000	-2.988277000
C	1.683353000	-0.029146000	-2.367297000
H	2.685549000	0.069601000	-2.807341000
H	1.249034000	-0.935949000	-2.813087000
C	0.822591000	1.187579000	-2.709873000
H	1.195552000	2.082016000	-2.186978000
H	0.957699000	1.396089000	-3.779236000
O	-1.110479000	-2.284806000	-0.695521000
C	-1.728400000	-2.608935000	0.349921000
H	-2.641439000	-0.417874000	1.428249000
N	-2.781565000	-3.439721000	0.349669000

C	-3.259555000	-4.020381000	-0.892671000
H	-4.274258000	-3.663447000	-1.107295000
H	-2.590256000	-3.730976000	-1.702777000
H	-3.285211000	-5.112576000	-0.808190000
C	-3.551860000	-3.751163000	1.537974000
H	-3.552002000	-4.832565000	1.719549000
H	-3.135887000	-3.240966000	2.408053000
H	-4.590060000	-3.421604000	1.404702000
C	-1.388117000	0.044208000	3.178725000
H	-1.519290000	1.118540000	3.003562000
H	-2.040289000	-0.221996000	4.022968000
H	-0.354000000	-0.117905000	3.507767000
C	-0.254013000	-2.798217000	2.437464000
H	0.498001000	-3.295433000	1.811000000
H	0.273790000	-2.183674000	3.174141000
H	-0.777595000	-3.590767000	2.994251000
C	-2.959149000	1.065507000	-0.686580000
C	-3.729231000	1.970537000	0.054922000
C	-3.600220000	-0.007669000	-1.325706000
C	-5.111559000	1.818954000	0.135630000
H	-3.246144000	2.802732000	0.566415000
C	-4.981742000	-0.151678000	-1.245721000
H	-3.012783000	-0.740048000	-1.880745000
C	-5.741020000	0.761254000	-0.515226000
H	-5.698793000	2.535002000	0.707042000
H	-5.470345000	-0.975502000	-1.763710000
H	-6.821431000	0.648793000	-0.455436000
C	2.920343000	-1.905917000	-0.589100000
C	4.308725000	-1.848724000	-0.424374000
C	2.299111000	-3.146923000	-0.791207000
C	5.063928000	-3.017714000	-0.464552000
H	4.800397000	-0.890161000	-0.261541000
C	3.060692000	-4.310224000	-0.839287000
H	1.215191000	-3.193285000	-0.915500000
C	4.442996000	-4.246782000	-0.672904000
H	6.142925000	-2.966648000	-0.334193000
H	2.574322000	-5.269903000	-1.003090000
H	5.037099000	-5.157665000	-0.704117000
C	2.911069000	0.900392000	0.124026000
C	3.591281000	1.846588000	-0.649467000
C	3.015641000	0.964425000	1.521615000
C	4.352902000	2.839682000	-0.036702000
H	3.533741000	1.814680000	-1.736610000
C	3.786798000	1.946280000	2.132095000
H	2.484419000	0.229115000	2.132691000
C	4.453034000	2.890253000	1.350797000
H	4.874368000	3.572802000	-0.648422000
H	3.867340000	1.978281000	3.216805000
H	5.052107000	3.664574000	1.825384000
C	-0.687301000	2.808547000	-0.197149000
C	-1.139056000	3.921438000	-0.921221000
C	0.174772000	3.006211000	0.886955000
C	-0.729917000	5.201655000	-0.565840000
H	-1.823034000	3.785279000	-1.759696000
C	0.590164000	4.288130000	1.238844000
H	0.532848000	2.142971000	1.451601000
C	0.137719000	5.385064000	0.511428000
H	-1.086840000	6.060523000	-1.130414000
H	1.269244000	4.426263000	2.077962000
H	0.459210000	6.388389000	0.783169000

INT2_s

C	-1.559421000	-1.102337000	1.827586000
C	-0.265529000	-1.245213000	2.297974000
Co	0.123803000	-0.549570000	0.410767000
P	1.627221000	0.443068000	-0.851315000
P	-1.502237000	0.211596000	-0.808891000
C	-1.161773000	0.480686000	-2.608398000
H	-0.904026000	-0.493470000	-3.048770000

H	-2.111215000	0.785987000	-3.067258000
C	1.321502000	0.984785000	-2.584034000
H	2.095895000	1.718681000	-2.846495000
H	1.527128000	0.099963000	-3.202536000
C	-0.075486000	1.507972000	-2.890274000
H	-0.284664000	2.429514000	-2.326473000
H	-0.114364000	1.790298000	-3.950274000
O	1.630158000	-1.684127000	1.097636000
C	0.616263000	-2.242139000	1.647534000
H	-1.973517000	-1.909670000	1.220718000
N	0.386385000	-3.564597000	1.578385000
C	1.194296000	-4.396806000	0.704712000
H	0.598225000	-4.740768000	-0.152033000
H	2.049080000	-3.820763000	0.348080000
H	1.550255000	-5.273826000	1.255588000
C	-0.739531000	-4.204666000	2.227966000
H	-0.408778000	-5.146572000	2.678836000
H	-1.140456000	-3.560329000	3.012761000
H	-1.540181000	-4.428204000	1.508172000
C	-2.550116000	-0.155477000	2.417494000
H	-3.282739000	0.190617000	1.681020000
H	-3.118245000	-0.666573000	3.208503000
H	-2.081410000	0.725341000	2.867078000
C	0.336397000	-0.373677000	3.365719000
H	1.421780000	-0.497072000	3.407824000
H	0.123476000	0.690399000	3.204262000
H	-0.073873000	-0.640803000	4.349940000
C	-2.913808000	-0.947559000	-0.952621000
C	-4.241052000	-0.627167000	-0.653890000
C	-2.605252000	-2.254660000	-1.361166000
C	-5.240531000	-1.592639000	-0.769733000
H	-4.501048000	0.378006000	-0.324567000
C	-3.604188000	-3.214136000	-1.480816000
H	-1.565195000	-2.519582000	-1.571137000
C	-4.926081000	-2.883240000	-1.183757000
H	-6.269896000	-1.330668000	-0.534098000
H	-3.352616000	-4.221929000	-1.805914000
H	-5.709119000	-3.632849000	-1.274471000
C	3.209720000	-0.437403000	-1.038574000
C	4.442462000	0.158773000	-0.761224000
C	3.172543000	-1.748988000	-1.529000000
C	5.622731000	-0.550656000	-0.975454000
H	4.483697000	1.177941000	-0.378977000
C	4.351432000	-2.450604000	-1.748596000
H	2.206969000	-2.221286000	-1.724586000
C	5.579280000	-1.851225000	-1.468601000
H	6.579659000	-0.080959000	-0.757915000
H	4.315008000	-3.468146000	-2.133313000
H	6.503116000	-2.401238000	-1.634768000
C	1.983673000	1.952727000	0.097150000
C	1.794362000	3.243685000	-0.406691000
C	2.360665000	1.790078000	1.439860000
C	1.969716000	4.351463000	0.420497000
H	1.507682000	3.396861000	-1.445782000
C	2.539635000	2.897180000	2.260481000
H	2.520636000	0.782892000	1.827393000
C	2.335465000	4.180971000	1.752743000
H	1.819647000	5.351499000	0.018906000
H	2.840454000	2.760043000	3.297587000
H	2.470036000	5.048483000	2.395477000
C	-2.146871000	1.849912000	-0.326701000
C	-3.175966000	2.495603000	-1.028018000
C	-1.509724000	2.528495000	0.719968000
C	-3.571972000	3.780234000	-0.670215000
H	-3.673212000	1.992752000	-1.858114000
C	-1.901506000	3.816918000	1.072223000
H	-0.688117000	2.036769000	1.248449000
C	-2.936167000	4.440910000	0.380502000
H	-4.375251000	4.269989000	-1.216631000
H	-1.393460000	4.334111000	1.883981000

H	-3.245781000	5.447393000	0.654235000
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DMF

C	0.862160000	-0.646835000	-0.000177000
H	0.737308000	-1.753446000	0.000259000
O	1.947466000	-0.097225000	0.000069000
N	-0.349002000	-0.018992000	-0.000046000
C	-0.415351000	1.422413000	-0.000021000
C	-1.587130000	-0.751786000	0.000070000
H	-0.944612000	1.789099000	-0.889968000
H	-0.943191000	1.789228000	0.890722000
H	0.607926000	1.803830000	-0.000852000
H	-2.189392000	-0.516664000	0.889158000
H	-2.188870000	-0.517995000	-0.889733000
H	-1.373954000	-1.826060000	0.000945000

2-butyne

C	0.000000000	0.000000000	0.605713000
C	0.000000000	0.000000000	-0.605713000
C	0.000000000	0.000000000	2.055653000
H	0.103782000	1.014855000	2.461036000
H	-0.930781000	-0.417550000	2.461036000
H	0.826999000	-0.597305000	2.461036000
C	0.000000000	0.000000000	-2.055653000
H	-0.103782000	1.014855000	-2.461036000
H	0.930781000	-0.417550000	-2.461036000
H	-0.826999000	-0.597305000	-2.461036000

(E)-N,N,2-trimethylbut-2-enamide

C	-1.486162000	-0.710612000	-0.428955000
C	-0.909659000	0.381657000	0.101100000
O	0.906155000	1.765231000	-0.496508000
C	0.547289000	0.648272000	-0.128832000
H	-0.830743000	-1.425769000	-0.933009000
N	1.446182000	-0.385949000	0.022798000
C	2.824875000	-0.152826000	-0.348405000
H	3.205642000	-1.004732000	-0.926865000
H	2.878534000	0.757957000	-0.945281000
H	3.460820000	-0.032576000	0.541392000
C	1.218180000	-1.599482000	0.775085000
H	0.237385000	-1.579484000	1.251514000
H	1.278062000	-2.492180000	0.134266000
H	1.985826000	-1.698618000	1.556640000
C	-2.932528000	-1.061774000	-0.449442000
H	-3.301855000	-1.150181000	-1.480232000
H	-3.107773000	-2.039564000	0.020105000
H	-3.560515000	-0.329637000	0.066682000
C	-1.630451000	1.512372000	0.763547000
H	-1.295923000	1.643573000	1.801573000
H	-1.396101000	2.448213000	0.244912000
H	-2.715132000	1.377145000	0.776188000

TS3_s

Co	0.015961000	-0.734950000	0.793220000
P	1.588259000	0.301645000	-0.485420000
P	-1.617152000	-0.104352000	-0.479019000
C	-1.270032000	-0.060976000	-2.294150000
H	-2.166035000	0.349502000	-2.779957000
H	-1.218305000	-1.108089000	-2.619555000
C	1.286568000	0.043253000	-2.286590000
H	1.264420000	-1.039385000	-2.477053000
H	2.136582000	0.456954000	-2.845574000
C	-0.016968000	0.680811000	-2.753676000
H	-0.025800000	0.704725000	-3.850934000
H	-0.043137000	1.732933000	-2.433264000
O	1.553590000	-2.285500000	1.396125000

C	0.825345000	-2.401177000	0.402874000
H	-0.691382000	-2.065765000	0.816608000
N	0.887147000	-3.379074000	-0.514527000
C	1.921150000	-4.400431000	-0.416458000
H	1.479342000	-5.371111000	-0.159481000
H	2.634972000	-4.106594000	0.354582000
H	2.439855000	-4.493162000	-1.378084000
C	-0.092593000	-3.531180000	-1.563594000
H	0.355061000	-3.372373000	-2.555181000
H	-0.905567000	-2.815544000	-1.412533000
H	-0.517465000	-4.542495000	-1.539552000
C	-0.043656000	0.451485000	2.409655000
C	-0.777450000	-0.564553000	2.595588000
C	0.520657000	1.717094000	2.902383000
C	-1.680532000	-1.443044000	3.347431000
H	0.616065000	1.685109000	3.995218000
H	-0.139535000	2.560598000	2.655706000
H	1.503343000	1.950305000	2.478530000
H	-1.278124000	-2.461060000	3.420570000
H	-2.662448000	-1.519643000	2.860206000
H	-1.839048000	-1.066546000	4.366059000
C	3.214740000	-0.455663000	-0.196411000
C	3.771511000	-1.397209000	-1.067941000
C	3.879765000	-0.155357000	0.999889000
C	4.978212000	-2.018738000	-0.752459000
H	3.273258000	-1.650897000	-2.002928000
C	5.083072000	-0.774544000	1.310669000
H	3.446138000	0.564843000	1.694362000
C	5.633277000	-1.710777000	0.435852000
H	5.407701000	-2.742871000	-1.442401000
H	5.591552000	-0.531410000	2.241009000
H	6.574523000	-2.197922000	0.681103000
C	1.922953000	2.096195000	-0.435606000
C	0.920660000	2.985940000	-0.037610000
C	3.149628000	2.606672000	-0.885145000
C	1.131447000	4.361130000	-0.090046000
H	-0.025736000	2.596142000	0.331881000
C	3.361385000	3.980473000	-0.929108000
H	3.943203000	1.925741000	-1.192461000
C	2.353104000	4.859156000	-0.534446000
H	0.340687000	5.039620000	0.225590000
H	4.318620000	4.367310000	-1.272187000
H	2.524367000	5.933033000	-0.569355000
C	-2.277904000	1.564466000	-0.117033000
C	-2.368155000	2.568551000	-1.090468000
C	-2.723175000	1.844918000	1.183193000
C	-2.863107000	3.828754000	-0.763320000
H	-2.051319000	2.385193000	-2.114357000
C	-3.216775000	3.103766000	1.506445000
H	-2.676347000	1.073374000	1.949154000
C	-3.278214000	4.102883000	0.536246000
H	-2.922356000	4.596888000	-1.531501000
H	-3.558563000	3.303621000	2.519845000
H	-3.659652000	5.089218000	0.791351000
C	-3.145264000	-1.124181000	-0.442664000
C	-3.221973000	-2.393602000	0.137966000
C	-4.287450000	-0.600237000	-1.069911000
C	-4.405394000	-3.127345000	0.088145000
H	-2.356281000	-2.816250000	0.647487000
C	-5.465629000	-1.334666000	-1.123036000
H	-4.259040000	0.397871000	-1.507728000
C	-5.527257000	-2.600795000	-0.543646000
H	-4.448698000	-4.110852000	0.551073000
H	-6.340780000	-0.913356000	-1.612831000
H	-6.452073000	-3.172347000	-0.579203000

INT3_s

Co	-0.048417000	-0.598630000	0.841076000
P	1.608791000	0.259782000	-0.490596000

P	-1.663672000	-0.063429000	-0.500169000
C	-1.308079000	0.017776000	-2.315319000
H	-2.173328000	0.506643000	-2.784636000
H	-1.337359000	-1.021714000	-2.668532000
C	1.250728000	-0.036426000	-2.277091000
H	1.158168000	-1.121649000	-2.428558000
H	2.120662000	0.301593000	-2.855439000
C	-0.007479000	0.669849000	-2.771227000
H	-0.000314000	0.666330000	-3.868819000
H	0.027199000	1.730321000	-2.483163000
O	1.255024000	-2.122957000	1.570770000
C	0.643503000	-2.300250000	0.501208000
H	-1.153203000	-1.402184000	1.407854000
N	0.751334000	-3.365120000	-0.292113000
C	1.682491000	-4.438141000	0.039898000
H	1.139127000	-5.346374000	0.326321000
H	2.316650000	-4.112729000	0.866340000
H	2.307238000	-4.659963000	-0.833068000
C	-0.037065000	-3.530294000	-1.491059000
H	0.610694000	-3.590364000	-2.376599000
H	-0.720079000	-2.683386000	-1.592281000
H	-0.632511000	-4.450633000	-1.437134000
C	0.088013000	0.855788000	2.330091000
C	-0.700461000	-0.026640000	2.745369000
C	0.802684000	2.117851000	2.569693000
C	-1.568925000	-0.746326000	3.680406000
H	0.869830000	2.302898000	3.648845000
H	0.267144000	2.964083000	2.120930000
H	1.816343000	2.132289000	2.155147000
H	-1.169285000	-1.742498000	3.904305000
H	-2.582262000	-0.887300000	3.281621000
H	-1.646207000	-0.189186000	4.622382000
C	3.170148000	-0.627782000	-0.201549000
C	3.794270000	-1.416394000	-1.174146000
C	3.736463000	-0.547895000	1.078511000
C	4.971343000	-2.100606000	-0.874266000
H	3.374566000	-1.500464000	-2.175419000
C	4.912551000	-1.225256000	1.372634000
H	3.236472000	0.033192000	1.854203000
C	5.531862000	-2.004379000	0.395654000
H	5.452881000	-2.704874000	-1.640529000
H	5.342734000	-1.153620000	2.369136000
H	6.451407000	-2.537872000	0.626763000
C	2.086273000	2.022062000	-0.531216000
C	1.082065000	2.994443000	-0.455438000
C	3.414271000	2.427363000	-0.714985000
C	1.391066000	4.345305000	-0.570659000
H	0.051537000	2.688931000	-0.272936000
C	3.723073000	3.781321000	-0.817807000
H	4.209418000	1.685436000	-0.773461000
C	2.715186000	4.740553000	-0.749358000
H	0.597969000	5.088598000	-0.506431000
H	4.758379000	4.087112000	-0.952923000
H	2.963004000	5.796815000	-0.829530000
C	-2.404612000	1.560089000	-0.109097000
C	-2.366070000	2.650148000	-0.987364000
C	-3.027001000	1.718441000	1.137489000
C	-2.918721000	3.875003000	-0.618095000
H	-1.901937000	2.557930000	-1.968083000
C	-3.581531000	2.938864000	1.502262000
H	-3.087538000	0.872225000	1.820734000
C	-3.521071000	4.023190000	0.627605000
H	-2.883036000	4.711755000	-1.312802000
H	-4.066972000	3.043757000	2.470138000
H	-3.952859000	4.979576000	0.914272000
C	-3.124951000	-1.169518000	-0.513053000
C	-3.078452000	-2.477490000	-0.020071000
C	-4.312191000	-0.706747000	-1.100432000
C	-4.193571000	-3.307267000	-0.111756000
H	-2.165711000	-2.848223000	0.445646000

C	-5.424255000	-1.536219000	-1.189339000
H	-4.372000000	0.315716000	-1.474543000
C	-5.366581000	-2.838315000	-0.695586000
H	-4.145631000	-4.320700000	0.281364000
H	-6.340954000	-1.162223000	-1.640147000
H	-6.239143000	-3.484627000	-0.761384000

TS4_s

Co	-0.036034000	-0.591214000	0.832446000
P	1.611611000	0.262330000	-0.493806000
P	-1.653702000	-0.064030000	-0.509653000
C	-1.297966000	0.015152000	-2.324013000
H	-2.164620000	0.498887000	-2.795861000
H	-1.318989000	-1.024429000	-2.677253000
C	1.259953000	-0.029217000	-2.281866000
H	1.170291000	-1.114106000	-2.437844000
H	2.130480000	0.313377000	-2.856712000
C	0.000462000	0.676055000	-2.774229000
H	0.009545000	0.680612000	-3.871764000
H	0.030510000	1.734466000	-2.477332000
O	1.266343000	-2.128513000	1.552573000
C	0.641396000	-2.303286000	0.490411000
H	-1.139102000	-1.361101000	1.453515000
N	0.741474000	-3.369573000	-0.303210000
C	1.674767000	-4.442974000	0.021444000
H	1.133414000	-5.351447000	0.310946000
H	2.314753000	-4.118094000	0.843616000
H	2.293382000	-4.664501000	-0.856031000
C	-0.054074000	-3.533894000	-1.497330000
H	0.587902000	-3.589801000	-2.387447000
H	-0.740514000	-2.689133000	-1.591861000
H	-0.646578000	-4.456070000	-1.442081000
C	0.091281000	0.830598000	2.318855000
C	-0.710136000	-0.050060000	2.726790000
C	0.802852000	2.085547000	2.609275000
C	-1.591439000	-0.727015000	3.684649000
H	0.873972000	2.229314000	3.694510000
H	0.261749000	2.946362000	2.195964000
H	1.814294000	2.121750000	2.190557000
H	-1.214106000	-1.726002000	3.933681000
H	-2.609838000	-0.855690000	3.294250000
H	-1.651747000	-0.143232000	4.611329000
C	3.176438000	-0.617046000	-0.201539000
C	3.797639000	-1.414805000	-1.168464000
C	3.745593000	-0.525709000	1.076408000
C	4.974869000	-2.097122000	-0.864979000
H	3.375324000	-1.507785000	-2.167878000
C	4.921462000	-1.201646000	1.374169000
H	3.247964000	0.063120000	1.847722000
C	5.537871000	-1.990254000	0.402957000
H	5.454338000	-2.708641000	-1.626768000
H	5.353848000	-1.121522000	2.369066000
H	6.457240000	-2.522736000	0.637046000
C	2.072605000	2.027970000	-0.520749000
C	1.062644000	2.990213000	-0.406529000
C	3.391981000	2.445742000	-0.736318000
C	1.357642000	4.344895000	-0.515148000
H	0.040580000	2.671950000	-0.199262000
C	3.686958000	3.803091000	-0.832374000
H	4.190830000	1.710536000	-0.824432000
C	2.673159000	4.752793000	-0.725818000
H	0.561154000	5.081256000	-0.420865000
H	4.715614000	4.119325000	-0.992005000
H	2.910139000	5.811923000	-0.800985000
C	-2.402591000	1.557945000	-0.125478000
C	-2.371837000	2.643426000	-1.009796000
C	-3.023191000	1.720125000	1.121512000
C	-2.931533000	3.866820000	-0.646655000
H	-1.907661000	2.549399000	-1.990178000

C	-3.584079000	2.939390000	1.480518000
H	-3.077445000	0.877790000	1.809954000
C	-3.532282000	4.018823000	0.599353000
H	-2.901765000	4.699760000	-1.346184000
H	-4.068025000	3.046980000	2.448853000
H	-3.969301000	4.974251000	0.881255000
C	-3.109091000	-1.177158000	-0.509980000
C	-3.057003000	-2.475431000	0.007472000
C	-4.298338000	-0.729843000	-1.105232000
C	-4.168622000	-3.311493000	-0.068756000
H	-2.141693000	-2.833456000	0.478278000
C	-5.406625000	-1.565731000	-1.179233000
H	-4.362641000	0.285679000	-1.497173000
C	-5.343363000	-2.858332000	-0.661500000
H	-4.116505000	-4.317328000	0.342921000
H	-6.324858000	-1.204218000	-1.637052000
H	-6.213137000	-3.509460000	-0.715713000

INT1_s'

Co	0.095855000	-0.530963000	0.700361000
P	1.685575000	0.316914000	-0.510834000
P	-1.546587000	-0.038744000	-0.628783000
C	-1.169883000	0.045605000	-2.435758000
H	-2.019503000	0.532873000	-2.933262000
H	-1.170138000	-0.994114000	-2.790405000
C	1.389617000	0.025058000	-2.307057000
H	1.311355000	-1.060778000	-2.461638000
H	2.279292000	0.371456000	-2.850280000
C	0.140018000	0.717672000	-2.842233000
H	0.187485000	0.720183000	-3.938626000
H	0.148987000	1.777117000	-2.547060000
O	1.263904000	-2.094882000	1.415947000
C	0.620694000	-2.319372000	0.357540000
H	-0.493945000	-1.337912000	2.578258000
N	0.680968000	-3.461056000	-0.328172000
C	1.547187000	-4.553946000	0.096057000
H	0.951140000	-5.432534000	0.369817000
H	2.134718000	-4.225538000	0.954755000
H	2.222106000	-4.829359000	-0.723564000
C	-0.097262000	-3.671401000	-1.527617000
H	0.559467000	-3.828627000	-2.394513000
H	-0.731910000	-2.798109000	-1.700765000
H	-0.743149000	-4.552018000	-1.419850000
C	-0.145450000	0.697290000	2.122787000
C	-0.766911000	-0.293506000	2.799945000
C	-0.148972000	2.138180000	2.454983000
C	-1.858933000	-0.161739000	3.819209000
H	-0.502202000	2.337668000	3.476266000
H	-0.775127000	2.714547000	1.759395000
H	0.861660000	2.558825000	2.364636000
H	-1.543744000	-0.570471000	4.787976000
H	-2.750938000	-0.728885000	3.519362000
H	-2.154871000	0.882527000	3.968006000
C	3.233848000	-0.545022000	-0.131065000
C	3.771898000	-1.528942000	-0.967061000
C	3.839860000	-0.287614000	1.106735000
C	4.909486000	-2.232261000	-0.576764000
H	3.313849000	-1.751933000	-1.929999000
C	4.975571000	-0.987947000	1.490053000
H	3.408856000	0.459315000	1.774913000
C	5.510534000	-1.964027000	0.649440000
H	5.328389000	-2.988898000	-1.237259000
H	5.441014000	-0.779110000	2.450694000
H	6.397929000	-2.515591000	0.952352000
C	2.098926000	2.088830000	-0.462373000
C	1.057597000	3.019930000	-0.388924000
C	3.416981000	2.547750000	-0.592613000
C	1.317830000	4.384659000	-0.445732000
H	0.034956000	2.666249000	-0.268138000

C	3.676102000	3.914485000	-0.640880000
H	4.240807000	1.838539000	-0.654566000
C	2.630850000	4.833347000	-0.568498000
H	0.495094000	5.095056000	-0.382029000
H	4.702296000	4.262782000	-0.736184000
H	2.841610000	5.900048000	-0.604144000
C	-2.433756000	1.515039000	-0.264399000
C	-2.349553000	2.655125000	-1.071984000
C	-3.200989000	1.569674000	0.908331000
C	-3.003867000	3.829643000	-0.704634000
H	-1.770336000	2.639006000	-1.995003000
C	-3.853854000	2.740855000	1.272318000
H	-3.290714000	0.682012000	1.534818000
C	-3.751043000	3.876320000	0.468974000
H	-2.933905000	4.707033000	-1.344471000
H	-4.448051000	2.767124000	2.183640000
H	-4.261033000	4.793852000	0.753916000
C	-2.911774000	-1.256497000	-0.558455000
C	-2.835821000	-2.395822000	0.248437000
C	-4.070827000	-1.030831000	-1.315626000
C	-3.892280000	-3.303170000	0.288258000
H	-1.939705000	-2.573152000	0.844166000
C	-5.119551000	-1.942072000	-1.281718000
H	-4.159718000	-0.129906000	-1.923537000
C	-5.031207000	-3.079630000	-0.479769000
H	-3.825064000	-4.184283000	0.923180000
H	-6.012214000	-1.760758000	-1.876491000
H	-5.856047000	-3.788308000	-0.449685000

INT3_q

C	-0.229434000	-0.848734000	2.821749000
C	0.925511000	-0.433579000	2.597767000
Co	0.205244000	-1.131817000	0.746447000
P	1.378970000	0.668189000	-0.659633000
P	-1.807302000	-0.287627000	-0.569547000
C	-1.474250000	-0.180365000	-2.384664000
H	-1.198157000	-1.200126000	-2.684333000
H	-2.432601000	0.034362000	-2.877590000
C	1.022768000	0.469035000	-2.458338000
H	1.728896000	1.094401000	-3.020254000
H	1.251006000	-0.574188000	-2.708456000
C	-0.409922000	0.809835000	-2.852274000
H	-0.652462000	1.827810000	-2.513370000
H	-0.456106000	0.845138000	-3.948792000
O	0.718188000	-2.510177000	-1.332085000
C	1.177602000	-2.683126000	-0.189826000
H	-1.012811000	-2.238672000	1.048822000
N	1.986528000	-3.680504000	0.179807000
C	2.461789000	-4.665793000	-0.781716000
H	2.258566000	-5.678391000	-0.415806000
H	1.945177000	-4.508922000	-1.730118000
H	3.544193000	-4.557973000	-0.931863000
C	2.531172000	-3.749040000	1.518498000
H	3.609506000	-3.536697000	1.512360000
H	2.023371000	-3.016506000	-2.153293000
H	2.375263000	-4.748665000	1.940201000
C	-1.457888000	-1.267995000	3.492650000
H	-2.347653000	-1.107270000	2.875227000
H	-1.417688000	-2.340696000	3.710695000
H	-1.574452000	-0.725361000	4.439953000
C	2.264255000	0.133114000	2.766633000
H	3.035208000	-0.470386000	2.270692000
H	2.322096000	1.139710000	2.331985000
H	2.515466000	0.208829000	3.831692000
C	-3.240750000	-1.403810000	-0.516346000
C	-4.531120000	-0.962336000	-0.205426000
C	-3.022224000	-2.758110000	-0.808168000
C	-5.591625000	-1.865755000	-0.195628000
H	-4.711842000	0.086619000	0.025313000

C	-4.087690000	-3.650612000	-0.809105000
H	-2.013376000	-3.108352000	-1.029641000
C	-5.372631000	-3.206286000	-0.499410000
H	-6.593154000	-1.516602000	0.046975000
H	-3.914110000	-4.698579000	-1.044630000
H	-6.203759000	-3.908351000	-0.492995000
C	3.181724000	0.410241000	-0.573656000
C	3.717482000	-0.796913000	-1.051210000
C	4.033170000	1.333573000	0.047412000
C	5.073939000	-1.070381000	-0.905326000
H	3.073379000	-1.518483000	-1.553435000
C	5.389241000	1.054289000	0.189657000
H	3.634332000	2.278758000	0.415484000
C	5.911518000	-0.149271000	-0.279159000
H	5.480507000	-2.003537000	-1.291761000
H	6.041689000	1.783997000	0.664781000
H	6.971731000	-0.364692000	-0.165750000
C	1.119971000	2.437969000	-0.334723000
C	0.534004000	2.827747000	0.875334000
C	1.490400000	3.424164000	-1.260703000
C	0.321389000	4.174415000	1.157992000
H	0.221561000	2.065330000	1.591269000
C	1.269682000	4.768005000	-0.980901000
H	1.960410000	3.142443000	-2.202789000
C	0.685278000	5.143970000	0.228280000
H	-0.140094000	4.464096000	2.099952000
H	1.557542000	5.525571000	-1.706730000
H	0.514331000	6.196575000	0.443998000
C	-2.450486000	1.344604000	-0.088911000
C	-2.872974000	2.305663000	-1.016874000
C	-2.547570000	1.640123000	1.278370000
C	-3.368209000	3.533077000	-0.584618000
H	-2.835182000	2.095654000	-2.084310000
C	-3.060727000	2.857774000	1.709695000
H	-2.209295000	0.906535000	2.010971000
C	-3.464877000	3.810695000	0.776582000
H	-3.691683000	4.270177000	-1.316498000
H	-3.139408000	3.066773000	2.774940000
H	-3.859328000	4.768144000	1.110373000

TS4_q

C	-0.554892000	-0.913870000	2.639240000
C	0.600545000	-0.375628000	2.595298000
Co	0.193518000	-0.979920000	0.732432000
P	1.418940000	0.687743000	-0.692154000
P	-1.815271000	-0.248903000	-0.612955000
C	-1.434286000	-0.134085000	-2.416002000
H	-1.104936000	-1.140317000	-2.706581000
H	-2.383658000	0.041391000	-2.940173000
C	1.049748000	0.560889000	-2.492358000
H	1.739169000	1.221199000	-3.035736000
H	1.273798000	-0.468642000	-2.797784000
C	-0.395750000	0.904865000	-2.841513000
H	-0.650391000	1.897353000	-2.439847000
H	-0.459983000	1.005153000	-3.932831000
O	0.710365000	-2.449566000	-1.290906000
C	1.178257000	-2.547808000	-0.141222000
H	-0.944017000	-2.110349000	1.176644000
N	2.053785000	-3.472724000	0.262586000
C	2.583317000	-4.469416000	-0.656987000
H	2.434956000	-5.475346000	-0.248370000
H	2.059993000	-4.381391000	-1.610756000
H	3.658364000	-4.309974000	-0.811582000
C	2.631340000	-3.426829000	1.588788000
H	3.689701000	-3.134050000	1.540469000
H	2.083974000	-2.697227000	2.192703000
H	2.561197000	-4.410147000	2.068036000
C	-1.804300000	-1.277870000	3.322807000
H	-2.679419000	-1.164824000	2.672303000

H	-1.774558000	-2.330675000	3.626682000
H	-1.942891000	-0.663396000	4.222119000
C	1.719827000	0.368727000	3.191513000
H	2.685303000	-0.103013000	2.968556000
H	1.765620000	1.383203000	2.772705000
H	1.620053000	0.455435000	4.280890000
C	-3.171131000	-1.456490000	-0.554182000
C	-4.495040000	-1.098578000	-0.276296000
C	-2.849052000	-2.802637000	-0.783724000
C	-5.485927000	-2.076966000	-0.238772000
H	-4.754654000	-0.056935000	-0.091934000
C	-3.846213000	-3.770816000	-0.756793000
H	-1.814179000	-3.084363000	-0.982737000
C	-5.164366000	-3.409772000	-0.480699000
H	-6.513918000	-1.793162000	-0.023191000
H	-3.593060000	-4.812177000	-0.944715000
H	-5.941796000	-4.170361000	-0.452330000
C	3.178771000	0.245868000	-0.553487000
C	3.691185000	-0.857224000	-1.254752000
C	4.014052000	0.927479000	0.344036000
C	5.014579000	-1.248933000	-1.077911000
H	3.054491000	-1.413256000	-1.942247000
C	5.333605000	0.524729000	0.523571000
H	3.634179000	1.792158000	0.888197000
C	5.837712000	-0.562599000	-0.187320000
H	5.407130000	-2.090472000	-1.646118000
H	5.974304000	1.071098000	1.212719000
H	6.872466000	-0.870006000	-0.052506000
C	1.323172000	2.464665000	-0.330708000
C	0.473687000	2.905854000	0.689907000
C	2.057478000	3.406260000	-1.066881000
C	0.347085000	4.265263000	0.965622000
H	-0.098561000	2.175535000	1.264049000
C	1.934039000	4.762013000	-0.786621000
H	2.736865000	3.075557000	-1.852984000
C	1.076264000	5.192083000	0.226530000
H	-0.323416000	4.597480000	1.755832000
H	2.507743000	5.487377000	-1.359612000
H	0.980318000	6.254663000	0.439752000
C	-2.564984000	1.349571000	-0.173248000
C	-3.020652000	2.267249000	-1.128962000
C	-2.704159000	1.667844000	1.185834000
C	-3.591009000	3.474149000	-0.732798000
H	-2.945624000	2.041424000	-2.191222000
C	-3.287281000	2.866559000	1.580560000
H	-2.340127000	0.970100000	1.940567000
C	-3.726064000	3.775921000	0.619702000
H	-3.939318000	4.177041000	-1.486553000
H	-3.395475000	3.094058000	2.639299000
H	-4.176411000	4.717887000	0.925387000

INT1_q

C	-0.604769000	0.427576000	3.113925000
C	0.171740000	-0.511137000	2.543963000
Co	0.006306000	-0.844780000	0.612847000
P	1.895665000	-0.259726000	-0.677669000
P	-1.522698000	0.473052000	-0.671552000
C	-1.073154000	0.214172000	-2.445975000
H	-1.145901000	-0.860891000	-2.655304000
H	-1.843876000	0.717609000	-3.045789000
C	1.480351000	-0.195463000	-2.469621000
H	2.385293000	0.086221000	-3.024878000
H	1.253520000	-1.231889000	-2.753491000
C	0.314296000	0.723817000	-2.839946000
H	0.472972000	1.736902000	-2.439038000
H	0.322096000	0.837700000	-3.931482000
O	-0.310341000	-2.826083000	-1.224581000
C	-0.913946000	-2.523535000	-0.183046000
H	-1.224187000	1.056404000	2.461575000

N	-1.994256000	-3.162934000	0.290413000
C	-2.574376000	-4.293185000	-0.419723000
H	-3.616444000	-4.068386000	-0.682574000
H	-1.994654000	-4.476364000	-1.326142000
H	-2.559144000	-5.189143000	0.211653000
C	-2.679823000	-2.728504000	1.489069000
H	-3.712779000	-2.439448000	1.249843000
H	-2.703130000	-3.536543000	2.231014000
H	-2.158192000	-1.866653000	1.920160000
C	-0.749150000	0.730775000	4.571770000
H	-0.509770000	1.782563000	4.776766000
H	-1.785858000	0.582977000	4.901885000
H	-0.105956000	0.108012000	5.200464000
C	1.097053000	-1.466969000	3.228855000
H	1.171062000	-1.290188000	4.312043000
H	0.771901000	-2.508505000	3.092305000
H	2.117301000	-1.411100000	2.822136000
C	-3.269073000	-0.010369000	-0.566005000
C	-4.091593000	0.577237000	0.406076000
C	-3.783441000	-1.043320000	-1.361494000
C	-5.404596000	0.147920000	0.569305000
H	-3.705581000	1.386267000	1.026651000
C	-5.098707000	-1.468637000	-1.194999000
H	-3.159099000	-1.524313000	-2.114292000
C	-5.910560000	-0.875946000	-0.229701000
H	-6.036303000	0.618455000	1.319621000
H	-5.493073000	-2.259926000	-1.830028000
H	-6.938983000	-1.207504000	-0.104506000
C	-1.498594000	2.276883000	-0.460110000
C	-2.410385000	3.093371000	-1.145983000
C	-0.523457000	2.864624000	0.353678000
C	-2.337304000	4.475470000	-1.020170000
H	-3.183961000	2.644420000	-1.769600000
C	-0.450873000	4.250595000	0.472373000
H	0.180343000	2.234467000	0.899059000
C	-1.356103000	5.054291000	-0.214271000
H	-3.047893000	5.104723000	-1.551778000
H	0.312808000	4.698409000	1.105126000
H	-1.303010000	6.136879000	-0.119879000
C	2.590210000	1.364671000	-0.257356000
C	2.951592000	2.312571000	-1.221683000
C	2.772870000	1.669659000	1.100302000
C	3.478498000	3.542819000	-0.835419000
H	2.829968000	2.097311000	-2.282073000
C	3.308124000	2.894570000	1.482297000
H	2.482950000	0.943241000	1.861075000
C	3.658198000	3.834917000	0.513804000
H	3.754585000	4.271939000	-1.594051000
H	3.451465000	3.116574000	2.537774000
H	4.074042000	4.795068000	0.812006000
C	3.282135000	-1.430877000	-0.547743000
C	2.997067000	-2.804190000	-0.589007000
C	4.606538000	-1.002766000	-0.393459000
C	4.028833000	-3.731719000	-0.491695000
H	1.967392000	-3.141821000	-0.711592000
C	5.631673000	-1.938782000	-0.290786000
H	4.837961000	0.060617000	-0.352500000
C	5.345402000	-3.300814000	-0.339839000
H	3.802916000	-4.795274000	-0.530608000
H	6.658894000	-1.600348000	-0.172928000
H	6.150007000	-4.028444000	-0.257731000

AlMe₃

Al	-0.000032000	-0.000091000	-0.000839000
C	-1.785536000	-0.810463000	0.000164000
H	-2.369645000	-0.501045000	0.877783000
H	-2.376645000	-0.489568000	-0.868527000
H	-1.775225000	-1.906600000	-0.006694000
C	1.594763000	-1.140868000	0.000190000

H	1.613509000	-1.812216000	-0.869265000
H	2.538584000	-0.583329000	-0.005350000
H	1.618527000	-1.802536000	0.876966000
C	0.190801000	1.951400000	0.000017000
H	0.741549000	2.303192000	0.883250000
H	0.773248000	2.302583000	-0.862739000
H	-0.763652000	2.490288000	-0.016735000

CP1a_t

Co	0.002738000	-0.464987000	0.332556000
P	-0.740553000	1.391955000	-0.873747000
P	2.115484000	-0.424446000	-0.596988000
C	2.112227000	0.052054000	-2.382664000
H	3.151156000	0.061622000	-2.738530000
H	1.624121000	-0.776098000	-2.916564000
C	-0.105102000	1.373155000	-2.614949000
H	-0.517858000	0.492813000	-3.126105000
H	-0.512902000	2.256365000	-3.125094000
C	1.420533000	1.374951000	-2.718719000
H	1.680476000	1.629019000	-3.754539000
H	1.832474000	2.190881000	-2.104484000
C	-0.640540000	0.112045000	2.195825000
C	0.158832000	-0.850478000	2.309960000
O	-2.434249000	-1.478578000	0.117249000
C	-3.416695000	-1.036326000	0.753621000
N	-3.849277000	-1.488261000	1.924260000
H	-3.982490000	-0.177788000	0.358078000
C	-4.993715000	-0.875359000	2.574486000
H	-5.798468000	-1.608363000	2.696224000
H	-4.705994000	-0.502359000	3.564388000
H	-5.359100000	-0.040554000	1.969326000
C	-3.202965000	-2.587742000	2.619136000
H	-3.902529000	-3.423118000	2.732589000
H	-2.331932000	-2.915866000	2.048807000
H	-2.883878000	-2.252088000	3.613235000
C	0.971331000	-1.880306000	2.974533000
H	1.895646000	-2.104249000	2.427285000
H	1.238441000	-1.568347000	3.992557000
H	0.417527000	-2.824345000	3.043929000
C	-1.581007000	1.160381000	2.601776000
H	-1.133020000	2.158067000	2.503924000
H	-2.489560000	1.166554000	1.983293000
H	-1.884146000	1.029022000	3.649720000
Al	-1.833223000	-3.151837000	-0.772127000
C	-3.573218000	-4.061449000	-0.910534000
C	-0.434337000	-3.884290000	0.431992000
C	-1.020143000	-2.286308000	-2.366589000
H	-4.326372000	-3.426418000	-1.400369000
H	-3.532291000	-4.987532000	-1.498112000
H	-3.992078000	-4.347248000	0.065396000
H	0.023119000	-4.758975000	-0.056331000
H	0.411760000	-3.204503000	0.623094000
H	-0.774368000	-4.246128000	1.412975000
H	-0.387679000	-2.962974000	-2.959463000
H	-1.756277000	-1.866192000	-3.066900000
H	-0.360863000	-1.449332000	-2.073822000
C	-0.165923000	3.021662000	-0.293858000
C	-0.532097000	4.196508000	-0.967097000
C	0.708670000	3.103943000	0.794506000
C	-0.029847000	5.425745000	-0.555733000
H	-1.222588000	4.149405000	-1.810121000
C	1.216935000	4.335751000	1.201279000
H	0.995434000	2.192360000	1.319865000
C	0.848262000	5.495630000	0.526196000
H	-0.321681000	6.332619000	-1.081190000
H	1.901476000	4.385654000	2.045833000
H	1.242777000	6.459017000	0.842598000
C	3.218692000	0.782847000	0.208863000
C	4.071465000	1.631382000	-0.506866000

C	3.232056000	0.838263000	1.610091000
C	4.909334000	2.519432000	0.163636000
H	4.093520000	1.604457000	-1.594761000
C	4.080076000	1.713951000	2.278938000
H	2.561893000	0.192927000	2.178501000
C	4.917953000	2.560876000	1.554944000
H	5.563510000	3.175615000	-0.406507000
H	4.085409000	1.737804000	3.366957000
H	5.578571000	3.250944000	2.075672000
C	3.068794000	-1.981197000	-0.610457000
C	2.496202000	-3.093436000	-1.243258000
C	4.322067000	-2.109858000	-0.000499000
C	3.171755000	-4.307689000	-1.278427000
H	1.508560000	-3.010798000	-1.700382000
C	4.990567000	-3.331386000	-0.031599000
H	4.781943000	-1.255203000	0.493470000
C	4.419787000	-4.428949000	-0.670352000
H	2.717907000	-5.163292000	-1.774673000
H	5.965953000	-3.421834000	0.442102000
H	4.946442000	-5.380613000	-0.693014000
C	-2.542253000	1.587136000	-1.097030000
C	-3.287381000	2.449221000	-0.279679000
C	-3.221798000	0.761975000	-2.004771000
C	-4.678102000	2.481604000	-0.366229000
H	-2.774991000	3.110914000	0.418728000
C	-4.610305000	0.797711000	-2.091876000
H	-2.665378000	0.066908000	-2.632345000
C	-5.343053000	1.653770000	-1.269203000
H	-5.241376000	3.165863000	0.265722000
H	-5.121353000	0.153369000	-2.804527000
H	-6.428340000	1.683035000	-1.340933000

CP1a_s

Co	-0.087515000	0.055946000	0.552121000
P	-0.059249000	-1.680734000	-0.853647000
P	-1.551105000	1.087998000	-0.657979000
C	-1.727474000	0.789614000	-2.472051000
H	-2.634381000	1.318243000	-2.794930000
H	-0.875121000	1.245417000	-2.990226000
C	-0.500038000	-1.443066000	-2.625353000
H	0.325825000	-0.882259000	-3.083486000
H	-0.512881000	-2.421155000	-3.122809000
C	-1.812709000	-0.689838000	-2.840454000
H	-2.085977000	-0.763342000	-3.900580000
H	-2.634607000	-1.172814000	-2.289119000
C	-0.897865000	-0.030593000	2.209097000
C	0.176445000	0.703322000	2.271940000
O	2.320149000	0.591156000	0.269224000
C	2.900918000	-0.233639000	1.021777000
N	3.947662000	-0.006541000	1.802770000
H	2.519878000	-1.263672000	1.082077000
C	4.563238000	-1.105826000	2.528362000
H	5.594911000	-1.245323000	2.185605000
H	4.575187000	-0.886056000	3.601722000
H	4.005650000	-2.029098000	2.351435000
C	4.565332000	1.297906000	1.974418000
H	5.572242000	1.299968000	1.544388000
H	3.966430000	2.065456000	1.480729000
H	4.630223000	1.518021000	3.046226000
C	1.068337000	1.584680000	3.046691000
H	1.794670000	2.103914000	2.409253000
H	0.490428000	2.349380000	3.583598000
H	1.621858000	1.014424000	3.806484000
C	-2.106583000	-0.487122000	2.919729000
H	-2.498496000	-1.436851000	2.539601000
H	-1.910542000	-0.586672000	3.995369000
H	-2.909127000	0.254082000	2.797981000
Al	3.005877000	2.046242000	-0.980816000
C	4.888440000	1.455640000	-1.197146000

C	2.515486000	3.670067000	0.032638000
C	1.784812000	1.620686000	-2.481672000
H	5.094735000	0.471148000	-0.747131000
H	5.143798000	1.350960000	-2.261039000
H	5.629124000	2.149310000	-0.776525000
H	2.508032000	4.550404000	-0.626268000
H	1.487069000	3.586041000	0.418169000
H	3.149489000	3.948541000	0.886431000
H	1.303946000	2.504033000	-2.923511000
H	2.240054000	1.059245000	-3.310099000
H	0.976647000	0.992493000	-2.077189000
C	1.602449000	-2.444107000	-0.945829000
C	1.935560000	-3.577895000	-0.192359000
C	2.607846000	-1.795061000	-1.678087000
C	3.246694000	-4.049955000	-0.173175000
H	1.167447000	-4.104359000	0.372020000
C	3.915470000	-2.269753000	-1.655968000
H	2.380122000	-0.892322000	-2.244224000
C	4.239586000	-3.394818000	-0.898350000
H	3.488294000	-4.940486000	0.404063000
H	4.682126000	-1.753542000	-2.230538000
H	5.262367000	-3.765938000	-0.882934000
C	-1.291753000	2.878214000	-0.476570000
C	-1.368767000	3.427333000	0.813125000
C	-0.991039000	3.715775000	-1.556004000
C	-1.158451000	4.784907000	1.015355000
H	-1.603831000	2.780538000	1.660035000
C	-0.768678000	5.075067000	-1.347314000
H	-0.931041000	3.317818000	-2.566492000
C	-0.850059000	5.610544000	-0.065896000
H	-1.228869000	5.200546000	2.018523000
H	-0.531695000	5.716016000	-2.193739000
H	-0.671938000	6.671775000	0.093186000
C	-3.264190000	0.791310000	-0.088736000
C	-3.680024000	-0.523896000	0.154627000
C	-4.192175000	1.832625000	0.040649000
C	-4.995489000	-0.798019000	0.513172000
H	-2.958855000	-1.337824000	0.094994000
C	-5.505396000	1.556064000	0.413314000
H	-3.890945000	2.861901000	-0.147930000
C	-5.910381000	0.243760000	0.647431000
H	-5.297361000	-1.827531000	0.699493000
H	-6.216151000	2.373193000	0.517816000
H	-6.937940000	0.034927000	0.937579000
C	-1.165501000	-3.011911000	-0.271260000
C	-2.034796000	-3.705425000	-1.122597000
C	-1.198329000	-3.295607000	1.102386000
C	-2.924043000	-4.646606000	-0.608536000
H	-2.036572000	-3.511608000	-2.193141000
C	-2.074401000	-4.247910000	1.611514000
H	-0.538411000	-2.746118000	1.775885000
C	-2.947979000	-4.918352000	0.756527000
H	-3.598685000	-5.170847000	-1.281990000
H	-2.082631000	-4.459551000	2.679096000
H	-3.644461000	-5.653245000	1.154318000

MECP1a

Co	-0.00817434	-0.20408789	0.66431305
P	1.72416843	-0.61824221	-0.81024105
P	-1.55713752	-0.91349402	-0.78160035
C	-1.22327932	-1.07061914	-2.59222861
H	-2.04783572	-1.65592517	-3.02142318
H	-1.25309822	-0.07283572	-3.04630328
C	1.34408161	-0.89014666	-2.59910761
H	1.22264404	0.11146343	-3.03517292
H	2.24065959	-1.31582088	-3.07119695
C	0.11125650	-1.74137144	-2.91180183
H	0.12461698	-1.96765400	-3.98584539
H	0.16520034	-2.71870710	-2.40926658

C	-0.05171624	-1.26474843	2.21685363
C	-0.60942135	-0.12199914	2.44773370
O	-0.09547065	2.16901417	0.55897538
C	0.81275748	2.45617471	1.38941142
N	0.73438071	3.37405413	2.33870800
H	1.77286714	1.91581929	1.35976631
C	1.90175577	3.71150719	3.13451028
H	2.20268026	4.74437163	2.92498160
H	1.66862357	3.61920050	4.20086754
H	2.73012420	3.04419327	2.88362901
C	-0.46720925	4.15444499	2.58505810
H	-0.28430241	5.20814775	2.35094599
H	-1.28278184	3.78710105	1.95968666
H	-0.73874980	4.06461402	3.64314202
C	-1.31184544	0.80898064	3.34930107
H	-1.77940969	1.63918760	2.80608589
H	-2.09730462	0.29352202	3.91833016
H	-0.61725222	1.23477125	4.08650669
C	0.28758256	-2.61545818	2.69986310
H	0.93591560	-3.17334029	2.01756369
H	0.79161350	-2.55223648	3.67355294
H	-0.63046825	-3.20073143	2.84123165
Al	-0.87641001	3.57338811	-0.77849421
C	0.50295991	4.98083663	-0.51539054
C	-2.71221777	3.85243237	-0.11772065
C	-0.63641838	2.45386875	-2.39499365
H	1.50366801	4.58112282	-0.28591247
H	0.62901825	5.56048363	-1.44164106
H	0.28168306	5.72613302	0.26127885
H	-3.40130860	4.01122367	-0.95877972
H	-3.10975041	2.97734230	0.41863861
H	-2.84024236	4.71969604	0.54434997
H	-1.55936103	2.30571750	-2.97267955
H	0.12128159	2.83299585	-3.09485321
H	-0.29377944	1.45663637	-2.08211074
C	-1.98160809	-2.63910635	-0.35315971
C	-3.30240047	-3.10269292	-0.31993365
C	-0.93786814	-3.54283925	-0.11566285
C	-3.56602641	-4.44159331	-0.04394538
H	-4.12748521	-2.41725398	-0.50839220
C	-1.20347213	-4.88320839	0.14522601
H	0.09373352	-3.18738321	-0.11642894
C	-2.52092858	-5.33380755	0.18722786
H	-4.59641101	-4.78915010	-0.01223272
H	-0.37750901	-5.56974706	0.32590743
H	-2.73518338	-6.37853114	0.40340074
C	-3.12400181	-0.00625672	-0.65130270
C	-3.75497064	0.58582694	-1.75068015
C	-3.72900566	0.07985187	0.61250020
C	-4.97183778	1.24376039	-1.58958603
H	-3.30824315	0.52676041	-2.74070682
C	-4.94852156	0.72770957	0.76655107
H	-3.24591364	-0.38680165	1.47251908
C	-5.57055039	1.31319573	-0.33585025
H	-5.45599528	1.69925044	-2.45062293
H	-5.41792915	0.77600139	1.74698626
H	-6.52359943	1.82378263	-0.21784128
C	3.05840041	0.63596472	-0.89901695
C	4.41148498	0.32447508	-0.71314207
C	2.70004065	1.95962787	-1.19696339
C	5.38129377	1.31858794	-0.82217406
H	4.71446557	-0.69708549	-0.49132152
C	3.67318482	2.94730041	-1.31196074
H	1.65137309	2.21887752	-1.34351855
C	5.01677481	2.62893698	-1.12099727
H	6.42946739	1.06118022	-0.68157416
H	3.37516265	3.96559597	-1.55667384
H	5.77893809	3.40022135	-1.21207770
C	2.58162495	-2.13496800	-0.27628981
C	2.65331390	-3.28792295	-1.06673383

C	3.14951179	-2.15932297	1.00665099
C	3.26516059	-4.44108710	-0.57987703
H	2.23234924	-3.29668471	-2.07028544
C	3.78140958	-3.30254637	1.48105236
H	3.09136567	-1.26902081	1.63656755
C	3.83132813	-4.45097551	0.69129977
H	3.30849589	-5.32994520	-1.20517058
H	4.22703016	-3.30297173	2.47357722
H	4.31592754	-5.35027826	1.06535045

TS1a_t

C	0.785747000	0.062944000	2.846671000
C	0.539122000	-1.130631000	2.470114000
Co	-0.017013000	0.074846000	1.005993000
P	-0.874294000	-1.442054000	-0.438482000
P	1.754847000	0.727053000	-0.393569000
C	1.211917000	0.796285000	-2.143535000
H	0.525260000	1.651059000	-2.188014000
H	2.077351000	1.072761000	-2.761507000
C	-0.874850000	-0.719080000	-2.138691000
H	-1.408950000	-1.433308000	-2.779999000
H	-1.459404000	0.210066000	-2.124952000
C	0.521756000	-0.449457000	-2.698551000
H	1.155264000	-1.342162000	-2.578979000
H	0.416980000	-0.305307000	-3.781680000
O	-1.570924000	1.850233000	-0.331014000
C	-1.644701000	1.174940000	0.727201000
H	0.235300000	1.353755000	1.744940000
N	-2.690830000	1.201694000	1.560519000
C	-3.871364000	2.026582000	1.343382000
H	-4.134735000	2.526275000	2.282020000
H	-3.675856000	2.781626000	0.582801000
H	-4.713106000	1.395528000	1.027501000
C	-2.803755000	0.268118000	2.663942000
H	-3.712555000	-0.336091000	2.539280000
H	-1.939640000	-0.400572000	2.683394000
H	-2.865355000	0.805678000	3.618464000
C	1.287917000	1.040323000	3.824947000
H	2.060188000	1.685690000	3.387109000
H	0.484197000	1.702120000	4.170857000
H	1.711795000	0.526735000	4.695352000
C	0.541326000	-2.567206000	2.790594000
H	0.329057000	-2.721646000	3.855814000
H	-0.186561000	-3.139426000	2.205078000
H	1.526270000	-3.004905000	2.582222000
Al	-2.318726000	3.248439000	-1.569153000
C	-0.949531000	3.427095000	-2.984291000
C	-2.406422000	4.767344000	-0.291011000
C	-3.963123000	2.327672000	-2.195470000
H	-0.826979000	2.550545000	-3.637857000
H	-1.278896000	4.235314000	-3.654827000
H	0.052574000	3.729149000	-2.646677000
H	-1.939168000	5.664339000	-0.721015000
H	-3.422847000	5.067152000	-0.000842000
H	-1.868319000	4.565021000	0.648779000
H	-4.690480000	2.039814000	-1.423505000
H	-4.511526000	2.977843000	-2.892336000
H	-3.737714000	1.418800000	-2.775419000
C	3.213778000	-0.350791000	-0.329386000
C	3.763098000	-0.659600000	0.925238000
C	3.782683000	-0.915956000	-1.476863000
C	4.855339000	-1.513598000	1.027419000
H	3.332357000	-0.222396000	1.826489000
C	4.873861000	-1.775322000	-1.370563000
H	3.383303000	-0.686233000	-2.462883000
C	5.409331000	-2.077744000	-0.121624000
H	5.278464000	-1.736966000	2.004627000
H	5.308604000	-2.205074000	-2.270421000
H	6.262578000	-2.747970000	-0.042190000

C	2.357702000	2.405798000	-0.043504000
C	3.718720000	2.711877000	0.071276000
C	1.404227000	3.425562000	0.099499000
C	4.116010000	4.023054000	0.322711000
H	4.469160000	1.930671000	-0.039919000
C	1.808918000	4.733803000	0.337389000
H	0.342392000	3.194232000	0.011039000
C	3.165903000	5.032805000	0.453550000
H	5.175246000	4.255344000	0.410469000
H	1.060449000	5.518118000	0.431459000
H	3.483144000	6.055633000	0.645089000
C	-2.616604000	-1.832738000	-0.092889000
C	-3.630878000	-0.975203000	-0.540950000
C	-2.953813000	-2.928542000	0.713609000
C	-4.957962000	-1.221502000	-0.200351000
H	-3.394185000	-0.104445000	-1.152647000
C	-4.281544000	-3.167217000	1.055888000
H	-2.177426000	-3.614014000	1.054473000
C	-5.285603000	-2.314867000	0.599816000
H	-5.736745000	-0.558822000	-0.574657000
H	-4.532961000	-4.026982000	1.673241000
H	-6.323818000	-2.507818000	0.861139000
C	-0.057034000	-3.047408000	-0.693353000
C	1.271009000	-3.236266000	-0.298164000
C	-0.718910000	-4.070984000	-1.388381000
C	1.929561000	-4.428862000	-0.586110000
H	1.789955000	-2.444915000	0.241463000
C	-0.060055000	-5.262449000	-1.669862000
H	-1.754058000	-3.937447000	-1.702576000
C	1.263658000	-5.442496000	-1.269562000
H	2.962843000	-4.563768000	-0.272201000
H	-0.581351000	-6.053186000	-2.204875000
H	1.775012000	-6.376744000	-1.491520000

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C	1.011901000	-0.033421000	2.724133000
C	0.945479000	-1.240745000	2.261930000
Co	0.147971000	0.011561000	1.055550000
P	-0.610842000	-1.514720000	-0.449770000
P	1.448509000	1.005402000	-0.405863000
C	0.860172000	1.045895000	-2.134378000
H	-0.001620000	1.721707000	-2.140465000
H	1.638337000	1.546657000	-2.726046000
C	-0.806684000	-0.894257000	-2.174688000
H	-1.140993000	-1.744000000	-2.784563000
H	-1.597996000	-0.136612000	-2.192341000
C	0.478737000	-0.302404000	-2.744194000
H	1.302397000	-1.027923000	-2.652157000
H	0.335549000	-0.150213000	-3.821492000
O	-1.750435000	1.458973000	-0.497802000
C	-1.525007000	0.968493000	0.633681000
H	-0.105066000	1.433882000	1.476780000
N	-2.480112000	0.891201000	1.584093000
C	-3.882105000	1.174612000	1.294808000
H	-4.201546000	2.078938000	1.825489000
H	-4.027973000	1.317396000	0.224593000
H	-4.489722000	0.323076000	1.622739000
C	-2.224146000	0.382785000	2.921021000
H	-2.137488000	-0.712736000	2.930915000
H	-1.311988000	0.818456000	3.333965000
H	-3.060428000	0.673140000	3.561704000
C	1.447965000	0.920416000	3.755267000
H	2.086774000	1.699428000	3.317601000
H	0.594061000	1.450779000	4.195972000
H	1.999433000	0.428868000	4.566206000
C	1.342866000	-2.638497000	2.510867000
H	1.303924000	-2.864882000	3.584020000
H	0.740918000	-3.376081000	1.969908000
H	2.382015000	-2.788954000	2.184926000

Al	-2.846339000	2.748276000	-1.581741000
C	-1.593409000	3.326167000	-3.004936000
C	-3.247655000	4.086116000	-0.174149000
C	-4.246049000	1.550915000	-2.326338000
H	-1.316920000	2.537461000	-3.721208000
H	-2.129117000	4.075911000	-3.607435000
H	-0.661847000	3.822429000	-2.697505000
H	-3.087108000	5.113516000	-0.529307000
H	-4.283597000	4.051551000	0.190190000
H	-2.606442000	3.970998000	0.714825000
H	-4.960970000	1.085821000	-1.633102000
H	-4.859991000	2.116605000	-3.042370000
H	-3.805542000	0.733366000	-2.919854000
C	3.083894000	0.196605000	-0.455043000
C	3.745088000	-0.146994000	0.733504000
C	3.707145000	-0.092791000	-1.677509000
C	4.986144000	-0.772422000	0.701974000
H	3.281196000	0.071132000	1.693623000
C	4.945786000	-0.728437000	-1.706339000
H	3.235142000	0.174187000	-2.619551000
C	5.585035000	-1.075133000	-0.519988000
H	5.486417000	-1.025382000	1.634422000
H	5.411329000	-0.948705000	-2.664360000
H	6.551084000	-1.574486000	-0.545763000
C	1.769712000	2.742628000	0.016980000
C	3.028351000	3.186753000	0.442420000
C	0.706801000	3.655728000	-0.068179000
C	3.216871000	4.527447000	0.770593000
H	3.866062000	2.494427000	0.503845000
C	0.905521000	4.991958000	0.253190000
H	-0.276981000	3.325149000	-0.397477000
C	2.160591000	5.429372000	0.676893000
H	4.198323000	4.866912000	1.094458000
H	0.075673000	5.690919000	0.168754000
H	2.315118000	6.475811000	0.930712000
C	-2.276692000	-2.043417000	0.056917000
C	-3.431300000	-1.619563000	-0.610796000
C	-2.403573000	-2.849621000	1.198721000
C	-4.687952000	-2.011976000	-0.153717000
H	-3.367677000	-0.975991000	-1.486233000
C	-3.659312000	-3.238804000	1.650846000
H	-1.509572000	-3.186324000	1.726491000
C	-4.804897000	-2.820376000	0.973637000
H	-5.576498000	-1.679459000	-0.687216000
H	-3.744759000	-3.874206000	2.529926000
H	-5.787414000	-3.128083000	1.325009000
C	0.314169000	-3.064024000	-0.713770000
C	1.712392000	-3.054535000	-0.651841000
C	-0.346522000	-4.247508000	-1.070793000
C	2.440260000	-4.204309000	-0.942262000
H	2.232893000	-2.146910000	-0.349125000
C	0.384230000	-5.398101000	-1.351331000
H	-1.434380000	-4.271258000	-1.125553000
C	1.776312000	-5.378381000	-1.289528000
H	3.527312000	-4.182916000	-0.888058000
H	-0.137363000	-6.313855000	-1.621012000
H	2.342797000	-6.280732000	-1.509451000

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C	1.117426000	-0.293559000	2.942829000
C	0.547890000	-1.233464000	2.144707000
Co	-0.017639000	-0.393216000	0.518530000
P	1.894620000	-0.179092000	-0.855831000
P	-1.168085000	1.184074000	-0.810012000
C	-0.810049000	1.108668000	-2.621371000
H	-1.162753000	0.138991000	-2.995703000
H	-1.431754000	1.879467000	-3.096008000
C	1.605298000	0.184763000	-2.640875000
H	2.588928000	0.351221000	-3.102335000

H	1.222186000	-0.754281000	-3.063801000
C	0.655157000	1.332055000	-2.984937000
H	0.999482000	2.276852000	-2.539523000
H	0.706959000	1.483144000	-4.070974000
O	-2.161699000	-2.054500000	0.784473000
C	-1.758411000	-0.958065000	1.237047000
H	1.005810000	0.767422000	2.680527000
N	-2.511917000	-0.262342000	2.099298000
C	-3.845025000	-0.713054000	2.480287000
H	-4.575033000	0.066686000	2.231739000
H	-4.085678000	-1.624952000	1.932920000
H	-3.884528000	-0.908889000	3.558211000
C	-2.054628000	0.969231000	2.698390000
H	-2.866859000	1.705428000	2.689579000
H	-1.729401000	0.812389000	3.736080000
H	-1.213890000	1.378272000	2.126331000
C	1.944883000	-0.544420000	4.158294000
H	2.930079000	-0.065966000	4.073756000
H	1.472207000	-0.103444000	5.047383000
H	2.098094000	-1.610862000	4.346020000
Al	-2.070298000	-3.405202000	-0.638593000
C	-1.012410000	-2.424150000	-2.034234000
C	-3.996473000	-3.616319000	-0.996978000
C	-1.124042000	-4.934384000	0.183105000
H	-0.271026000	-3.075950000	-2.520159000
H	-1.635917000	-2.008209000	-2.840641000
H	-0.432898000	-1.576101000	-1.628257000
H	-4.203453000	-4.165401000	-1.925372000
H	-4.506265000	-4.170256000	-0.196828000
H	-4.521249000	-2.654118000	-1.084165000
H	-1.507904000	-5.200395000	1.178068000
H	-1.280654000	-5.828077000	-0.438612000
H	-0.034293000	-4.834554000	0.287998000
C	-2.983335000	1.228430000	-0.734796000
C	-3.682991000	2.243368000	-0.070455000
C	-3.693376000	0.158528000	-1.298908000
C	-5.073343000	2.199195000	0.006633000
H	-3.143450000	3.075505000	0.380498000
C	-5.081981000	0.124032000	-1.223789000
H	-3.162844000	-0.659570000	-1.790205000
C	-5.773950000	1.144312000	-0.573501000
H	-5.609425000	2.998060000	0.515245000
H	-5.622491000	-0.706523000	-1.673142000
H	-6.859975000	1.115473000	-0.518059000
C	-0.582822000	2.851098000	-0.369125000
C	-1.064696000	3.987121000	-1.037754000
C	0.423551000	3.007072000	0.590053000
C	-0.550879000	5.244571000	-0.742281000
H	-1.853145000	3.886638000	-1.784155000
C	0.941688000	4.265767000	0.884232000
H	0.829212000	2.129185000	1.099178000
C	0.452899000	5.384718000	0.216967000
H	-0.933469000	6.119811000	-1.262771000
H	1.732371000	4.365766000	1.625019000
H	0.854041000	6.370610000	0.441684000
C	3.106236000	1.043447000	-0.271152000
C	3.452974000	2.188416000	-0.996462000
C	3.674606000	0.840434000	0.996163000
C	4.342727000	3.116846000	-0.460319000
H	3.039799000	2.362473000	-1.988204000
C	4.559969000	1.770083000	1.528717000
H	3.436490000	-0.067201000	1.551614000
C	4.890965000	2.914393000	0.802959000
H	4.610030000	3.999560000	-1.037354000
H	5.005060000	1.595541000	2.506553000
H	5.586887000	3.640394000	1.217764000
C	2.799688000	-1.755538000	-0.878753000
C	2.113832000	-2.944699000	-0.604020000
C	4.160840000	-1.802758000	-1.209167000
C	2.776552000	-4.167095000	-0.665631000

H	1.053720000	-2.921874000	-0.344575000
C	4.819386000	-3.026280000	-1.266387000
H	4.706393000	-0.881329000	-1.413538000
C	4.128847000	-4.207228000	-0.996040000
H	2.231973000	-5.085535000	-0.453739000
H	5.876072000	-3.058296000	-1.523006000
H	4.648830000	-5.161737000	-1.041210000
C	0.520875000	-2.692496000	2.449617000
H	1.474539000	-3.159471000	2.162603000
H	0.360314000	-2.896703000	3.516363000
H	-0.259260000	-3.215298000	1.886979000

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C	-0.230475000	0.850880000	3.030834000
C	0.944953000	0.580201000	2.433050000
Co	-0.038756000	0.125845000	0.943657000
P	0.997776000	1.360601000	-0.518199000
P	-1.713835000	-0.516926000	-0.453671000
C	-1.108152000	-0.798857000	-2.170692000
H	-0.363428000	-1.606474000	-2.146746000
H	-1.953613000	-1.157961000	-2.771935000
C	0.884108000	0.812861000	-2.257709000
H	1.354059000	1.595705000	-2.868864000
H	1.542032000	-0.060112000	-2.328592000
C	-0.498666000	0.452647000	-2.795104000
H	-1.198125000	1.296769000	-2.697434000
H	-0.390185000	0.277936000	-3.873165000
O	1.553780000	-1.665166000	-0.420327000
C	0.843638000	-1.503744000	0.600017000
H	-1.148199000	0.879281000	2.378290000
N	0.686764000	-2.473469000	1.527922000
C	1.495687000	-3.685423000	1.549444000
H	0.875561000	-4.560347000	1.317493000
H	2.311385000	-3.617724000	0.829862000
H	1.918956000	-3.808972000	2.553808000
C	-0.287535000	-2.396858000	2.600318000
H	-0.747488000	-3.384599000	2.724004000
H	0.177775000	-2.097723000	3.550246000
H	-1.085172000	-1.690083000	2.354134000
C	-0.565449000	1.080339000	4.469106000
H	-1.038767000	2.058851000	4.619678000
H	-1.278856000	0.329408000	4.833384000
H	0.331218000	1.035127000	5.095134000
Al	2.542737000	-2.909277000	-1.652835000
C	2.714622000	-1.881336000	-3.339229000
C	1.299893000	-4.439503000	-1.857104000
C	4.228017000	-3.082519000	-0.614320000
H	3.299316000	-0.950612000	-3.314184000
H	3.264036000	-2.539425000	-4.030566000
H	1.771145000	-1.656768000	-3.859094000
H	0.400667000	-4.184099000	-2.438805000
H	1.798405000	-5.225220000	-2.443802000
H	0.956248000	-4.933700000	-0.938389000
H	4.398195000	-4.075538000	-0.175989000
H	5.099193000	-2.885946000	-1.255551000
H	4.296015000	-2.363380000	0.217271000
C	-2.453355000	-2.112657000	0.018963000
C	-3.617037000	-2.159137000	0.798672000
C	-1.789455000	-3.306425000	-0.294654000
C	-4.112544000	-3.381226000	1.243911000
H	-4.145209000	-1.238051000	1.045558000
C	-2.292452000	-4.525983000	0.149021000
H	-0.872670000	-3.294614000	-0.883214000
C	-3.452563000	-4.565505000	0.920309000
H	-5.022977000	-3.408518000	1.838991000
H	-1.776977000	-5.446506000	-0.120074000
H	-3.846618000	-5.519517000	1.263923000
C	-3.123544000	0.613487000	-0.667780000
C	-4.197198000	0.259631000	-1.498647000

C	-3.140934000	1.852521000	-0.019513000
C	-5.260895000	1.135728000	-1.677937000
H	-4.207181000	-0.712162000	-1.993100000
C	-4.207309000	2.730181000	-0.201599000
H	-2.307964000	2.139536000	0.624912000
C	-5.265487000	2.372186000	-1.031437000
H	-6.091109000	0.853420000	-2.321688000
H	-4.208756000	3.692636000	0.306267000
H	-6.100148000	3.055214000	-1.174217000
C	0.190536000	2.993745000	-0.432707000
C	-0.238940000	3.655395000	-1.591556000
C	-0.029960000	3.603003000	0.813096000
C	-0.876922000	4.889494000	-1.503477000
H	-0.067436000	3.221180000	-2.573625000
C	-0.660042000	4.839978000	0.896584000
H	0.300827000	3.104399000	1.724095000
C	-1.092376000	5.482220000	-0.262314000
H	-1.200816000	5.391074000	-2.412633000
H	-0.812339000	5.303848000	1.868930000
H	-1.591162000	6.446846000	-0.198062000
C	2.772897000	1.650928000	-0.258222000
C	3.698045000	0.659316000	-0.618149000
C	3.232902000	2.828719000	0.348771000
C	5.053722000	0.844090000	-0.369621000
H	3.367575000	-0.260312000	-1.095244000
C	4.591734000	3.006607000	0.591587000
H	2.533663000	3.617570000	0.619926000
C	5.503118000	2.013898000	0.239137000
H	5.758263000	0.066792000	-0.658183000
H	4.938026000	3.928970000	1.052999000
H	6.564434000	2.155826000	0.431085000
C	2.314406000	0.497849000	2.972023000
H	2.353570000	0.602440000	4.065334000
H	2.786867000	-0.454402000	2.693779000
H	2.949984000	1.282831000	2.538928000

MECP2a

C	0.87150663	0.58465614	2.90671756
C	0.95924426	-0.64690198	2.37629182
Co	0.04953325	0.02511586	0.89022879
P	1.78936443	-0.12113008	-0.61694007
P	-1.28683643	1.27369025	-0.45731705
C	-1.21355101	0.64987682	-2.18634578
H	-1.52055720	-0.40655173	-2.17409930
H	-1.95431393	1.19842843	-2.78352531
C	1.18415970	-0.27024359	-2.33877842
H	2.05838633	-0.30170094	-3.00264030
H	0.72599509	-1.26514520	-2.39694498
C	0.17454837	0.77478711	-2.81283152
H	0.56230042	1.79571189	-2.67148133
H	0.06410743	0.64572264	-3.89668059
O	-0.84311967	-2.16512318	-0.26657206
C	-1.12873284	-1.50654560	0.76468977
H	0.47051141	1.40132499	2.23900433
N	-2.02428485	-1.88302307	1.68362786
C	-2.65031813	-3.20032275	1.70403348
H	-3.72302335	-3.12329568	1.49203909
H	-2.18315795	-3.85197803	0.96369023
H	-2.51355619	-3.63801602	2.70035735
C	-2.40920626	-1.00116076	2.76807888
H	-3.49888871	-0.87632350	2.77053545
H	-2.09529155	-1.41413690	3.73665749
H	-1.95022082	-0.01820273	2.63164528
C	1.21265853	1.09738746	4.26813542
H	1.92624429	1.92961823	4.21505636
H	0.32444811	1.47930914	4.78699127
H	1.65325577	0.30686538	4.88328320
C	1.45757507	-1.91527242	2.93671971
H	0.67098759	-2.68224162	2.92792269

H	2.27488608	-2.31667891	2.32258921
H	1.82770917	-1.81277073	3.96650023
Al	-1.52047898	-3.55736916	-1.56238665
C	-0.68207804	-3.06534662	-3.29122495
C	-3.47580053	-3.20957539	-1.47441275
C	-0.73456337	-5.15879316	-0.68640610
H	0.41022364	-3.17459563	-3.35690754
H	-1.07941649	-3.77517098	-4.03388458
H	-0.93432205	-2.07275504	-3.69305589
H	-3.87289365	-2.85326989	-2.43576405
H	-4.05220571	-4.11131500	-1.22339627
H	-3.75952627	-2.45641400	-0.72651551
H	-1.47329231	-5.85104177	-0.25864147
H	-0.15015916	-5.75009385	-1.40589445
H	-0.04215923	-4.90278821	0.13067882
C	-3.04400748	1.18929278	0.00213882
C	-3.50978123	1.97522646	1.06704763
C	-3.91476000	0.28238952	-0.61123638
C	-4.82669824	1.86157786	1.49816396
H	-2.84030774	2.69002244	1.54890710
C	-5.23094177	0.16517414	-0.17025669
H	-3.57714127	-0.34029423	-1.43795999
C	-5.68859824	0.95427340	0.88165024
H	-5.18282538	2.48193180	2.31814047
H	-5.89770056	-0.54103565	-0.66135029
H	-6.72028563	0.87093323	1.21605539
C	-0.94041445	3.05523509	-0.59541522
C	-1.84627418	3.90745189	-1.24399711
C	0.24734223	3.58312468	-0.07947161
C	-1.55720798	5.26033188	-1.37878881
H	-2.78574681	3.51125493	-1.62976142
C	0.53825003	4.93809068	-0.22169277
H	0.95604420	2.92908802	0.43041154
C	-0.36314872	5.77476304	-0.87267661
H	-2.26622850	5.91684076	-1.87860190
H	1.46800102	5.33666113	0.17976907
H	-0.13970718	6.83360779	-0.98399773
C	2.82496015	-1.59406445	-0.36496788
C	4.09191550	-1.50579334	0.22746517
C	2.30363783	-2.85798928	-0.68405306
C	4.82411825	-2.66056561	0.48972453
H	4.51667264	-0.53429903	0.47319672
C	3.04324113	-4.00618393	-0.42204473
H	1.31671096	-2.95572066	-1.13299319
C	4.30165845	-3.91104344	0.16910314
H	5.81066964	-2.57900992	0.94106046
H	2.62821128	-4.97768986	-0.68180891
H	4.87762721	-4.81102343	0.37326288
C	2.89171360	1.32233769	-0.55528147
C	3.23900717	2.03436440	-1.70973497
C	3.36312931	1.77213852	0.68875619
C	4.03940867	3.17025545	-1.62110558
H	2.89325105	1.70676910	-2.68773350
C	4.16888605	2.90250230	0.77236258
H	3.09637802	1.22645777	1.59471209
C	4.50300250	3.60744258	-0.38333752
H	4.30203267	3.71236227	-2.52657296
H	4.53594640	3.23520111	1.74143683
H	5.12815585	4.49541213	-0.31918130

TS2a_t

C	0.408665000	0.326707000	3.176344000
C	0.274710000	-0.744719000	2.372716000
Co	-0.004256000	-0.365518000	0.468340000
P	1.933558000	-0.274954000	-0.839614000
P	-1.145830000	1.210113000	-0.824232000
C	-0.727237000	1.077913000	-2.624531000
H	-1.099274000	0.109479000	-2.985992000
H	-1.315355000	1.851699000	-3.135963000

C	1.650657000	0.058998000	-2.628043000
H	2.632439000	0.167748000	-3.109875000
H	1.214789000	-0.865409000	-3.031899000
C	0.753341000	1.252328000	-2.958005000
H	1.133668000	2.169180000	-2.482077000
H	0.828570000	1.429820000	-4.038705000
O	-1.571282000	-2.242246000	0.906654000
C	-1.578268000	-1.068794000	1.362743000
H	-0.118692000	1.250510000	2.937809000
N	-2.643558000	-0.541166000	1.971820000
C	-3.875652000	-1.306242000	2.126250000
H	-4.655738000	-0.890419000	1.475364000
H	-3.698106000	-2.345681000	1.849484000
H	-4.208485000	-1.250314000	3.168429000
C	-2.658955000	0.813990000	2.475744000
H	-3.651680000	1.243169000	2.307429000
H	-2.432785000	0.840440000	3.550141000
H	-1.928425000	1.427912000	1.937086000
C	1.289705000	0.390686000	4.380549000
H	2.022353000	1.203161000	4.282060000
H	0.706978000	0.614686000	5.284189000
H	1.839284000	-0.539696000	4.551851000
Al	-1.866694000	-3.578654000	-0.536201000
C	-1.017780000	-2.555711000	-2.039858000
C	-3.834898000	-3.710110000	-0.591367000
C	-0.796005000	-5.075428000	0.177875000
H	-0.219503000	-3.122767000	-2.541507000
H	-1.718356000	-2.240037000	-2.827812000
H	-0.535952000	-1.632648000	-1.669100000
H	-4.182162000	-4.259903000	-1.477143000
H	-4.259103000	-4.240056000	0.272695000
H	-4.333040000	-2.730074000	-0.629705000
H	-1.362848000	-5.711720000	0.870106000
H	-0.435897000	-5.740862000	-0.619984000
H	0.100507000	-4.753662000	0.729758000
C	-2.965297000	1.210059000	-0.839340000
C	-3.740061000	2.286251000	-0.391586000
C	-3.603277000	0.038623000	-1.274310000
C	-5.130582000	2.198047000	-0.399100000
H	-3.259449000	3.194472000	-0.029783000
C	-4.992243000	-0.039894000	-1.290132000
H	-3.013019000	-0.823322000	-1.594731000
C	-5.757933000	1.040403000	-0.852892000
H	-5.724523000	3.041741000	-0.053564000
H	-5.474460000	-0.950802000	-1.639863000
H	-6.843925000	0.978019000	-0.864590000
C	-0.590097000	2.896493000	-0.428557000
C	-1.029321000	4.005455000	-1.168080000
C	0.374560000	3.083220000	0.568363000
C	-0.521300000	5.271502000	-0.900400000
H	-1.777033000	3.878213000	-1.951480000
C	0.889226000	4.350804000	0.829815000
H	0.745247000	2.224230000	1.132129000
C	0.438762000	5.444723000	0.097166000
H	-0.871701000	6.126547000	-1.474424000
H	1.646939000	4.478328000	1.600300000
H	0.837353000	6.436648000	0.298957000
C	3.076105000	1.009254000	-0.248788000
C	3.614175000	2.005323000	-1.070674000
C	3.397411000	1.004892000	1.117899000
C	4.453872000	2.979899000	-0.535198000
H	3.389366000	2.026210000	-2.135769000
C	4.240527000	1.974495000	1.647507000
H	2.987779000	0.227850000	1.765891000
C	4.766108000	2.967843000	0.821178000
H	4.869628000	3.747224000	-1.184664000
H	4.495803000	1.952123000	2.705322000
H	5.425940000	3.727508000	1.234787000
C	2.868932000	-1.830435000	-0.808933000
C	2.173926000	-3.023539000	-0.573012000

C	4.249522000	-1.865788000	-1.042589000
C	2.847946000	-4.240635000	-0.582080000
H	1.098288000	-3.003185000	-0.380931000
C	4.919696000	-3.084665000	-1.046207000
H	4.799169000	-0.939829000	-1.213638000
C	4.220646000	-4.269637000	-0.818704000
H	2.297216000	-5.161220000	-0.398750000
H	5.992251000	-3.110089000	-1.226463000
H	4.750621000	-5.219757000	-0.821269000
C	0.879648000	-2.096357000	2.596707000
H	1.939135000	-2.113773000	2.302651000
H	0.818508000	-2.396967000	3.650735000
H	0.373451000	-2.870202000	2.008846000

TS2a_s

C	-0.544700000	-0.301260000	2.977096000
C	-1.524003000	-0.260890000	2.042641000
Co	0.028915000	0.005870000	0.858299000
P	-0.290618000	-1.585068000	-0.560719000
P	1.460719000	1.011129000	-0.459646000
C	0.824540000	1.087814000	-2.185480000
H	-0.187746000	1.518048000	-2.135338000
H	1.435629000	1.796100000	-2.759639000
C	-0.326415000	-1.185840000	-2.339064000
H	-0.362766000	-2.134461000	-2.892152000
H	-1.299161000	-0.702800000	-2.493335000
C	0.770827000	-0.272098000	-2.872993000
H	1.753932000	-0.760922000	-2.817642000
H	0.571437000	-0.113759000	-3.940550000
O	-2.351581000	0.745865000	-0.221831000
C	-1.589660000	1.027351000	0.755023000
H	0.449004000	0.180013000	2.767367000
N	-1.658671000	2.263659000	1.358647000
C	-2.909617000	3.010879000	1.397972000
H	-2.731773000	4.060264000	1.138916000
H	-3.633007000	2.591163000	0.698458000
H	-3.328515000	2.965478000	2.414531000
C	-0.726706000	2.645104000	2.394937000
H	-0.699130000	3.737881000	2.455509000
H	-1.014921000	2.241159000	3.380162000
H	0.288136000	2.309807000	2.156678000
C	-0.579902000	-0.944668000	4.322721000
H	0.237045000	-1.667189000	4.444725000
H	-0.453151000	-0.201174000	5.120952000
H	-1.528861000	-1.461962000	4.493256000
Al	-3.380771000	1.610644000	-1.670519000
C	-3.072396000	0.601996000	-3.360069000
C	-2.602419000	3.424327000	-1.909187000
C	-5.204171000	1.324777000	-0.949870000
H	-3.289847000	-0.473401000	-3.422702000
H	-3.789338000	1.066641000	-4.056716000
H	-2.091357000	0.762689000	-3.832841000
H	-1.706118000	3.395583000	-2.549619000
H	-3.318123000	4.048399000	-2.465052000
H	-2.335281000	4.007688000	-1.018998000
H	-5.485531000	1.871606000	-0.039716000
H	-5.962234000	1.587372000	-1.701048000
H	-5.365921000	0.259118000	-0.724584000
C	1.662160000	2.760758000	0.005089000
C	2.712583000	3.165919000	0.839432000
C	0.687811000	3.690855000	-0.381788000
C	2.787674000	4.486177000	1.272807000
H	3.480144000	2.451332000	1.137246000
C	0.771240000	5.009967000	0.052406000
H	-0.146926000	3.391590000	-1.012828000
C	1.817186000	5.408486000	0.883233000
H	3.612243000	4.797855000	1.910464000
H	0.015745000	5.726188000	-0.266806000
H	1.881690000	6.440463000	1.221618000

C	3.151899000	0.349760000	-0.592923000
C	3.934778000	0.518734000	-1.742432000
C	3.689660000	-0.336085000	0.502508000
C	5.224864000	0.000326000	-1.793496000
H	3.541324000	1.059222000	-2.602731000
C	4.985754000	-0.839850000	0.456429000
H	3.076930000	-0.482529000	1.394594000
C	5.751596000	-0.677502000	-0.695401000
H	5.823985000	0.132747000	-2.691832000
H	5.393044000	-1.368709000	1.316089000
H	6.762258000	-1.077921000	-0.738459000
C	1.160748000	-2.627751000	-0.235679000
C	1.975283000	-3.115612000	-1.264893000
C	1.512298000	-2.895157000	1.097880000
C	3.115587000	-3.855149000	-0.964365000
H	1.718569000	-2.931378000	-2.306283000
C	2.643260000	-3.647546000	1.393648000
H	0.885135000	-2.512223000	1.906501000
C	3.449511000	-4.123182000	0.360947000
H	3.741804000	-4.228702000	-1.771525000
H	2.898206000	-3.860796000	2.429822000
H	4.339460000	-4.705599000	0.589921000
C	-1.760027000	-2.620902000	-0.309757000
C	-2.979997000	-2.256931000	-0.900742000
C	-1.705220000	-3.760549000	0.506675000
C	-4.116744000	-3.028231000	-0.685493000
H	-3.053736000	-1.363475000	-1.516955000
C	-2.848453000	-4.523258000	0.720576000
H	-0.764007000	-4.069099000	0.958224000
C	-4.055673000	-4.158004000	0.127522000
H	-5.054413000	-2.738903000	-1.155381000
H	-2.792076000	-5.413032000	1.344000000
H	-4.947549000	-4.758163000	0.294246000
C	-2.882087000	-0.856740000	2.194214000
H	-2.830181000	-1.921260000	2.456220000
H	-3.430511000	-0.345978000	2.997950000
H	-3.468802000	-0.761442000	1.276779000

INT2a_t

C	-0.729553000	0.789032000	2.337549000
C	-1.041965000	-0.561328000	2.248628000
Co	0.160741000	-0.137737000	0.587390000
P	1.991442000	-0.819978000	-0.622751000
P	-0.438461000	1.544688000	-0.861394000
C	0.056169000	1.226637000	-2.614978000
H	-0.489997000	0.345700000	-2.978171000
H	-0.273367000	2.083059000	-3.218422000
C	2.060386000	-0.391112000	-2.414199000
H	3.092619000	-0.537136000	-2.762521000
H	1.457267000	-1.152993000	-2.925908000
C	1.561775000	1.008480000	-2.784004000
H	2.116522000	1.779381000	-2.226104000
H	1.810614000	1.177009000	-3.839559000
O	-2.013384000	-1.368028000	0.279587000
C	-2.249129000	-0.938269000	1.448344000
H	-1.475037000	1.496209000	1.962238000
N	-3.474833000	-0.778857000	1.940208000
C	-4.653086000	-1.072789000	1.135030000
H	-5.440406000	-0.361057000	1.399698000
H	-4.412478000	-0.972150000	0.076679000
H	-5.007718000	-2.091784000	1.328786000
C	-3.737839000	-0.332707000	3.299403000
H	-4.397254000	-1.052090000	3.796770000
H	-2.811831000	-0.245477000	3.868028000
H	-4.237552000	0.643595000	3.278547000
C	0.334347000	1.373129000	3.212566000
H	0.757521000	2.283770000	2.774022000
H	-0.087710000	1.657344000	4.187651000
H	1.158184000	0.677852000	3.408876000

Al	-2.424503000	-2.930399000	-0.968560000
C	-1.007901000	-2.439397000	-2.268391000
C	-4.248377000	-2.743918000	-1.705013000
C	-2.144086000	-4.336040000	0.400094000
H	-0.297852000	-3.236328000	-2.528041000
H	-1.418368000	-2.060061000	-3.216324000
H	-0.410602000	-1.623257000	-1.832185000
H	-4.326537000	-3.387728000	-2.593532000
H	-5.072203000	-3.046313000	-1.045634000
H	-4.483429000	-1.731535000	-2.066318000
H	-2.910599000	-4.279724000	1.189195000
H	-2.226081000	-5.350196000	-0.014512000
H	-1.173662000	-4.300202000	0.916690000
C	-2.238781000	1.810455000	-0.932198000
C	-2.854873000	2.713531000	-0.051654000
C	-3.045710000	1.025666000	-1.768816000
C	-4.240670000	2.847643000	-0.029121000
H	-2.241949000	3.342425000	0.595340000
C	-4.429975000	1.175591000	-1.755059000
H	-2.597992000	0.288734000	-2.436335000
C	-5.030688000	2.085359000	-0.887224000
H	-4.701597000	3.566776000	0.645507000
H	-5.041065000	0.575802000	-2.427192000
H	-6.112386000	2.203254000	-0.883906000
C	0.287790000	3.185912000	-0.543606000
C	-0.221669000	4.353523000	-1.128929000
C	1.441806000	3.267213000	0.246135000
C	0.406803000	5.575645000	-0.916062000
H	-1.119187000	4.304710000	-1.746119000
C	2.075694000	4.490802000	0.450374000
H	1.853895000	2.360814000	0.695489000
C	1.555128000	5.645405000	-0.127396000
H	0.002081000	6.477669000	-1.370252000
H	2.974107000	4.539750000	1.062818000
H	2.044427000	6.603530000	0.034717000
C	3.363219000	0.114466000	0.139408000
C	4.252219000	0.928231000	-0.571239000
C	3.463577000	0.066957000	1.538702000
C	5.209482000	1.683344000	0.104130000
H	4.205335000	0.982199000	-1.657574000
C	4.420157000	0.817134000	2.212337000
H	2.785764000	-0.581498000	2.100508000
C	5.291692000	1.634680000	1.493097000
H	5.894243000	2.312272000	-0.460970000
H	4.488901000	0.763251000	3.297196000
H	6.039034000	2.227591000	2.015978000
C	2.483662000	-2.565864000	-0.537840000
C	1.509289000	-3.513217000	-0.203192000
C	3.793710000	-2.983377000	-0.804206000
C	1.833955000	-4.865346000	-0.148655000
H	0.485831000	-3.187338000	-0.005823000
C	4.116190000	-4.334775000	-0.743142000
H	4.562969000	-2.249780000	-1.048223000
C	3.137912000	-5.274446000	-0.418030000
H	1.067018000	-5.595568000	0.102644000
H	5.134872000	-4.657241000	-0.947949000
H	3.396081000	-6.330355000	-0.372336000
C	-0.380804000	-1.689327000	2.994690000
H	0.613124000	-1.413936000	3.362051000
H	-0.979403000	-1.987653000	3.869384000
H	-0.278565000	-2.583177000	2.365687000

INT2a_s

C	-0.388683000	1.198320000	-2.469191000
C	-1.160912000	1.674758000	-1.381340000
Co	0.144842000	0.209932000	-0.878254000
P	1.531567000	1.061860000	0.495781000
P	-0.046012000	-1.582311000	0.420954000
C	-0.317575000	-1.214076000	2.190720000

H	-1.206933000	-0.570168000	2.248710000
H	-0.553876000	-2.135757000	2.738425000
C	1.138277000	0.888023000	2.280981000
H	1.940026000	1.381403000	2.847975000
H	0.230344000	1.486923000	2.439909000
C	0.892158000	-0.520376000	2.811030000
H	1.788222000	-1.146172000	2.688319000
H	0.724064000	-0.439095000	3.892503000
O	-2.399468000	0.761830000	0.414132000
C	-2.335319000	0.927731000	-0.839295000
H	-0.737668000	0.238368000	-2.909383000
N	-3.297540000	0.467790000	-1.655196000
C	-4.407388000	-0.310908000	-1.125401000
H	-4.617084000	-1.137611000	-1.812510000
H	-4.145521000	-0.709135000	-0.144759000
H	-5.299635000	0.319579000	-1.031693000
C	-3.420981000	0.817306000	-3.060825000
H	-4.452420000	1.133480000	-3.251780000
H	-2.752929000	1.637293000	-3.324515000
H	-3.203620000	-0.050785000	-3.697834000
C	0.463269000	2.024922000	-3.378804000
H	1.270210000	1.431752000	-3.824225000
H	-0.121512000	2.444959000	-4.211096000
H	0.919855000	2.868647000	-2.848708000
Al	-3.571646000	1.325702000	1.894339000
C	-2.224379000	2.276428000	3.009493000
C	-4.182557000	-0.392628000	2.677798000
C	-4.881716000	2.430328000	0.893045000
H	-1.542628000	2.912287000	2.420046000
H	-2.684059000	2.948203000	3.747634000
H	-1.595338000	1.587542000	3.595784000
H	-3.374746000	-0.965179000	3.160169000
H	-4.916152000	-0.206715000	3.475661000
H	-4.681813000	-1.081270000	1.979750000
H	-5.821996000	1.901307000	0.682656000
H	-5.167063000	3.335343000	1.446160000
H	-4.502718000	2.788064000	-0.078253000
C	-1.536830000	-2.445085000	-0.171914000
C	-1.636309000	-2.712249000	-1.546061000
C	-2.561863000	-2.863186000	0.683370000
C	-2.728226000	-3.409596000	-2.052422000
H	-0.834384000	-2.397163000	-2.220148000
C	-3.653102000	-3.562357000	0.172826000
H	-2.523571000	-2.640638000	1.747856000
C	-3.734712000	-3.842489000	-1.189263000
H	-2.788449000	-3.626224000	-3.117311000
H	-4.442350000	-3.887493000	0.847760000
H	-4.585137000	-4.396838000	-1.580709000
C	1.276056000	-2.835910000	0.373658000
C	1.583221000	-3.652329000	1.468849000
C	1.992353000	-2.997960000	-0.818431000
C	2.592450000	-4.605394000	1.370911000
H	1.034615000	-3.552910000	2.404592000
C	2.992969000	-3.957839000	-0.918452000
H	1.770218000	-2.352659000	-1.671531000
C	3.296504000	-4.760235000	0.178949000
H	2.825100000	-5.233276000	2.228261000
H	3.543779000	-4.071799000	-1.850108000
H	4.083566000	-5.507620000	0.105755000
C	3.111116000	0.216469000	0.183239000
C	3.975012000	-0.178216000	1.210793000
C	3.456389000	-0.064076000	-1.147287000
C	5.160697000	-0.843120000	0.909041000
H	3.733091000	0.039023000	2.250141000
C	4.650243000	-0.710309000	-1.446429000
H	2.769964000	0.221537000	-1.949492000
C	5.501133000	-1.105149000	-0.415882000
H	5.825746000	-1.148336000	1.713954000
H	4.912565000	-0.915774000	-2.482452000
H	6.432056000	-1.619030000	-0.645697000

C	1.892306000	2.837773000	0.320071000
C	1.361759000	3.789168000	1.203292000
C	2.662900000	3.272374000	-0.768728000
C	1.604778000	5.143965000	1.001003000
H	0.745916000	3.485365000	2.048397000
C	2.897322000	4.628291000	-0.969866000
H	3.096167000	2.544109000	-1.454072000
C	2.366512000	5.566331000	-0.086154000
H	1.193391000	5.871797000	1.696752000
H	3.503862000	4.952087000	-1.812951000
H	2.551681000	6.626828000	-0.241891000
C	-1.109166000	3.088137000	-0.882785000
H	-0.182316000	3.598296000	-1.156272000
H	-1.944853000	3.662665000	-1.311318000
H	-1.226031000	3.129048000	0.207047000

TS3a_s

Co	0.167825000	-0.521040000	0.152769000
P	1.900481000	0.080902000	-0.996972000
P	-1.486305000	-0.146026000	-1.373117000
C	-0.898726000	-0.151390000	-3.113183000
H	-1.714606000	0.181387000	-3.767388000
H	-0.686196000	-1.192872000	-3.391446000
C	1.628671000	0.061130000	-2.816027000
H	1.652509000	-0.996062000	-3.112080000
H	2.519821000	0.511206000	-3.273591000
C	0.348556000	0.710212000	-3.328551000
H	0.463860000	0.891927000	-4.404836000
H	0.216109000	1.704697000	-2.873037000
O	-1.222893000	0.046908000	2.069767000
C	-0.558901000	0.813165000	1.305697000
H	0.886098000	0.256215000	1.241155000
N	-0.654978000	2.142494000	1.386830000
C	-1.420217000	2.772565000	2.457075000
H	-0.781699000	3.496590000	2.976126000
H	-1.765245000	2.019107000	3.166415000
H	-2.281754000	3.300480000	2.029300000
C	-0.212322000	3.038907000	0.338921000
H	-1.061431000	3.666031000	0.036379000
H	0.116874000	2.459373000	-0.525605000
H	0.606784000	3.682814000	0.681247000
C	0.956730000	-2.164625000	0.808700000
C	0.206371000	-2.437124000	-0.192474000
C	1.941153000	-2.545066000	1.825526000
C	-0.301544000	-3.477757000	-1.106130000
H	2.262618000	-3.585258000	1.683349000
H	1.523525000	-2.440609000	2.833881000
H	2.831767000	-1.904154000	1.776403000
H	-0.524876000	-3.096992000	-2.110693000
H	-1.238687000	-3.904777000	-0.726650000
H	0.423693000	-4.297038000	-1.199635000
C	-2.755223000	-1.447455000	-1.253667000
C	-3.038909000	-1.984184000	0.009769000
C	-3.449935000	-1.913466000	-2.375005000
C	-4.004312000	-2.976728000	0.145457000
H	-2.485355000	-1.642763000	0.885962000
C	-4.404322000	-2.917415000	-2.234884000
H	-3.249318000	-1.500633000	-3.363190000
C	-4.682265000	-3.448647000	-0.977203000
H	-4.215790000	-3.389792000	1.129715000
H	-4.934156000	-3.283209000	-3.111832000
H	-5.428843000	-4.232895000	-0.872453000
C	3.332321000	-1.048737000	-0.844080000
C	4.513344000	-0.672913000	-0.193445000
C	3.240828000	-2.338872000	-1.389188000
C	5.573577000	-1.571424000	-0.085144000
H	4.620952000	0.325445000	0.223157000
C	4.301505000	-3.228387000	-1.285321000
H	2.327409000	-2.660388000	-1.888344000

C	5.469871000	-2.848441000	-0.624633000
H	6.484560000	-1.263717000	0.423084000
H	4.215597000	-4.222890000	-1.717869000
H	6.297959000	-3.548051000	-0.536298000
C	-2.490248000	1.382198000	-1.267841000
C	-2.483567000	2.376023000	-2.254165000
C	-3.297029000	1.559738000	-0.134211000
C	-3.259627000	3.523926000	-2.106990000
H	-1.881794000	2.267073000	-3.154412000
C	-4.071771000	2.705763000	0.008767000
H	-3.324000000	0.792548000	0.641026000
C	-4.050881000	3.694248000	-0.974818000
H	-3.249401000	4.282763000	-2.886587000
H	-4.703031000	2.821052000	0.888019000
H	-4.660445000	4.588303000	-0.863781000
C	2.567403000	1.717953000	-0.571191000
C	2.771625000	2.714515000	-1.532482000
C	2.867142000	1.993724000	0.772403000
C	3.264770000	3.962155000	-1.156032000
H	2.544586000	2.532176000	-2.581357000
C	3.376005000	3.233380000	1.141128000
H	2.703079000	1.234580000	1.539903000
C	3.569428000	4.223039000	0.177031000
H	3.415691000	4.729852000	-1.911661000
H	3.614903000	3.427230000	2.184641000
H	3.958092000	5.196949000	0.466137000
Al	-0.767388000	-0.632431000	3.918030000
C	-1.072249000	-2.569291000	3.640700000
C	1.063323000	0.158088000	4.004218000
C	-2.123984000	0.295810000	5.018067000
H	-0.458382000	-3.221236000	4.277677000
H	-0.899962000	-2.898571000	2.605140000
H	-2.116339000	-2.823352000	3.874398000
H	1.011509000	1.252759000	3.874904000
H	1.784335000	-0.210227000	3.258701000
H	1.543640000	0.004886000	4.980627000
H	-1.850092000	1.311431000	5.336039000
H	-2.311747000	-0.265202000	5.944451000
H	-3.102253000	0.369954000	4.520376000

INT3a_s

Co	0.223242000	-0.459392000	0.234174000
P	2.005963000	-0.008435000	-0.887154000
P	-1.381423000	-0.155862000	-1.391919000
C	-0.729211000	-0.141770000	-3.111916000
H	-1.502465000	0.266681000	-3.775146000
H	-0.582360000	-1.184607000	-3.424125000
C	1.796677000	-0.099506000	-2.712798000
H	1.734340000	-1.166567000	-2.964529000
H	2.728399000	0.252867000	-3.173942000
C	0.581571000	0.632726000	-3.275765000
H	0.745590000	0.804287000	-4.347304000
H	0.499849000	1.635410000	-2.825695000
O	-1.147925000	0.171224000	1.793523000
C	-0.462837000	1.014435000	1.125984000
H	1.300692000	-0.281860000	1.260408000
N	-0.505370000	2.322355000	1.297122000
C	-1.283127000	2.933003000	2.371348000
H	-0.677857000	3.711606000	2.846993000
H	-1.556511000	2.181796000	3.112964000
H	-2.193324000	3.386151000	1.958132000
C	-0.015383000	3.243504000	0.287536000
H	-0.853372000	3.865101000	-0.052679000
H	0.375481000	2.682686000	-0.563564000
H	0.773478000	3.887062000	0.692669000
C	0.815581000	-2.359185000	0.919915000
C	0.195791000	-2.525396000	-0.153347000
C	1.605324000	-2.635068000	2.115284000
C	-0.284281000	-3.408976000	-1.228889000

H	1.722100000	-3.720411000	2.231405000
H	1.127449000	-2.241013000	3.019801000
H	2.605422000	-2.187448000	2.036916000
H	-0.335626000	-2.916852000	-2.207488000
H	-1.289024000	-3.790795000	-1.014465000
H	0.388844000	-4.271016000	-1.319833000
C	-2.699576000	-1.410056000	-1.353140000
C	-3.057266000	-1.950732000	-0.110402000
C	-3.360959000	-1.836780000	-2.509678000
C	-4.061433000	-2.910200000	-0.029394000
H	-2.529118000	-1.640849000	0.792815000
C	-4.356841000	-2.805861000	-2.423897000
H	-3.102174000	-1.420187000	-3.482666000
C	-4.706956000	-3.342679000	-1.186570000
H	-4.328240000	-3.328011000	0.939121000
H	-4.861652000	-3.141257000	-3.327364000
H	-5.484750000	-4.100743000	-1.124940000
C	3.365085000	-1.197107000	-0.596684000
C	4.464826000	-0.872260000	0.207099000
C	3.287954000	-2.485038000	-1.147219000
C	5.461241000	-1.814195000	0.453146000
H	4.557990000	0.123132000	0.635651000
C	4.284770000	-3.421370000	-0.901903000
H	2.437002000	-2.770034000	-1.764352000
C	5.372590000	-3.089290000	-0.096086000
H	6.311580000	-1.543606000	1.075090000
H	4.211518000	-4.414056000	-1.340998000
H	6.151335000	-3.823463000	0.097953000
C	-2.345046000	1.402502000	-1.296469000
C	-2.230409000	2.431077000	-2.239218000
C	-3.236009000	1.564990000	-0.224476000
C	-2.988237000	3.594198000	-2.113683000
H	-1.557298000	2.338113000	-3.089620000
C	-3.987627000	2.728168000	-0.099925000
H	-3.349659000	0.771468000	0.514235000
C	-3.864412000	3.747953000	-1.043524000
H	-2.895584000	4.378467000	-2.862137000
H	-4.681028000	2.830779000	0.733194000
H	-4.459220000	4.653923000	-0.950146000
C	2.732853000	1.622708000	-0.532920000
C	3.113821000	2.508042000	-1.548654000
C	2.921982000	2.003686000	0.804941000
C	3.673682000	3.744290000	-1.233106000
H	2.977474000	2.247065000	-2.596342000
C	3.505979000	3.226536000	1.115373000
H	2.603005000	1.339730000	1.609543000
C	3.877638000	4.102745000	0.096108000
H	3.959489000	4.423790000	-2.032983000
H	3.661443000	3.499486000	2.157063000
H	4.323927000	5.064545000	0.339032000
Al	-1.360040000	-0.488902000	3.719874000
C	-1.666527000	-2.416205000	3.388114000
C	0.418319000	0.160201000	4.321321000
C	-2.984434000	0.508293000	4.264296000
H	-1.200232000	-3.057983000	4.149164000
H	-1.294484000	-2.777662000	2.418762000
H	-2.740097000	-2.652102000	3.416933000
H	0.416491000	1.239963000	4.534301000
H	1.199936000	-0.001204000	3.560386000
H	0.785723000	-0.323803000	5.236412000
H	-2.817533000	1.462614000	4.781870000
H	-3.585584000	-0.104107000	4.950847000
H	-3.646137000	0.726104000	3.410839000

TS4a_s

Co	0.153465000	-0.507612000	0.171423000
P	1.845028000	-0.001433000	-1.074014000
P	-1.554815000	-0.255387000	-1.294344000
C	-1.014182000	-0.405438000	-3.040479000

H	-1.858212000	-0.165964000	-3.699685000
H	-0.769914000	-1.461083000	-3.224169000
C	1.520928000	-0.092518000	-2.884343000
H	1.582168000	-1.156810000	-3.145964000
H	2.370113000	0.378462000	-3.396228000
C	0.195502000	0.476507000	-3.374735000
H	0.252442000	0.582684000	-4.465606000
H	0.052260000	1.497340000	-2.987300000
O	-0.995909000	0.326834000	1.968901000
C	-0.381710000	1.031618000	1.101036000
H	1.272140000	-0.566001000	1.168711000
N	-0.405891000	2.357269000	1.111121000
C	-1.006141000	3.104723000	2.211544000
H	-0.290907000	3.856050000	2.565246000
H	-1.260638000	2.430128000	3.030119000
H	-1.912299000	3.613282000	1.857718000
C	-0.073911000	3.151026000	-0.055665000
H	-0.950400000	3.755295000	-0.325007000
H	0.163740000	2.492200000	-0.892643000
H	0.777496000	3.813442000	0.141543000
C	0.886175000	-2.250141000	0.944062000
C	0.070104000	-2.489742000	-0.001873000
C	1.871080000	-2.694281000	1.938616000
C	-0.540118000	-3.571847000	-0.799512000
H	1.962221000	-3.786316000	1.891571000
H	1.570310000	-2.410300000	2.954095000
H	2.861124000	-2.257922000	1.748192000
H	-0.803486000	-3.264694000	-1.819050000
H	-1.467684000	-3.927246000	-0.334391000
H	0.148072000	-4.425079000	-0.863839000
C	-2.869614000	-1.482367000	-1.021731000
C	-3.131190000	-1.873371000	0.298764000
C	-3.623738000	-2.023774000	-2.067490000
C	-4.135088000	-2.798047000	0.566454000
H	-2.527497000	-1.474037000	1.116123000
C	-4.616889000	-2.960897000	-1.794692000
H	-3.438220000	-1.724509000	-3.098727000
C	-4.873456000	-3.347186000	-0.480838000
H	-4.328187000	-3.099424000	1.594066000
H	-5.193102000	-3.388888000	-2.612182000
H	-5.650383000	-4.079743000	-0.273104000
C	3.215004000	-1.200283000	-0.888728000
C	4.401228000	-0.868380000	-0.223707000
C	3.059400000	-2.501851000	-1.388921000
C	5.409158000	-1.818486000	-0.067432000
H	4.551385000	0.135995000	0.166023000
C	4.066813000	-3.445052000	-1.233676000
H	2.135792000	-2.790154000	-1.890598000
C	5.244513000	-3.105591000	-0.568009000
H	6.327487000	-1.544219000	0.446817000
H	3.932636000	-4.448588000	-1.631874000
H	6.032459000	-3.845020000	-0.443745000
C	-2.498654000	1.316962000	-1.268340000
C	-2.572448000	2.188443000	-2.361601000
C	-3.194875000	1.645378000	-0.094925000
C	-3.313742000	3.365891000	-2.279457000
H	-2.064568000	1.959699000	-3.296238000
C	-3.932712000	2.821283000	-0.015957000
H	-3.163367000	0.973789000	0.763846000
C	-3.989861000	3.688309000	-1.106908000
H	-3.366371000	4.027784000	-3.141279000
H	-4.475341000	3.054013000	0.898489000
H	-4.571342000	4.605614000	-1.046198000
C	2.603565000	1.611872000	-0.718796000
C	2.951988000	2.529359000	-1.715901000
C	2.830480000	1.943402000	0.625970000
C	3.516349000	3.756269000	-1.372955000
H	2.781472000	2.303789000	-2.767195000
C	3.409317000	3.161361000	0.963070000
H	2.539578000	1.248857000	1.415956000

C	3.748275000	4.073141000	-0.036941000
H	3.778796000	4.464227000	-2.155993000
H	3.586896000	3.399659000	2.010115000
H	4.191837000	5.031065000	0.225780000
Al	-0.576442000	-0.233813000	3.870554000
C	-1.106517000	-2.138745000	3.778537000
C	1.326622000	0.359512000	3.874304000
C	-1.812493000	0.906106000	4.914881000
H	-0.591863000	-2.775702000	4.511584000
H	-0.953060000	-2.611780000	2.798155000
H	-2.178782000	-2.236721000	4.004340000
H	1.382028000	1.430553000	3.613793000
H	2.008554000	-0.161393000	3.184379000
H	1.791437000	0.277765000	4.866814000
H	-1.428956000	1.898206000	5.190110000
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H	-2.778365000	1.065500000	4.412370000

INT1a_s'

Co	0.054976000	-0.480023000	0.085025000
P	1.742891000	0.043055000	-1.178242000
P	-1.638592000	-0.189209000	-1.261638000
C	-1.167706000	-0.321931000	-3.027968000
H	-2.042027000	-0.080978000	-3.646460000
H	-0.929813000	-1.376461000	-3.227054000
C	1.370499000	0.006584000	-2.982534000
H	1.440748000	-1.046634000	-3.282296000
H	2.192702000	0.510488000	-3.506252000
C	0.020834000	0.568257000	-3.411573000
H	0.029080000	0.676653000	-4.503671000
H	-0.112874000	1.586983000	-3.016177000
O	-0.803225000	0.401934000	2.082784000
C	-0.252873000	1.061500000	1.135261000
H	1.004130000	-1.185631000	1.447810000
N	-0.230195000	2.392386000	1.145850000
C	-0.684612000	3.161956000	2.298278000
H	0.105930000	3.858639000	2.601834000
H	-0.918602000	2.492532000	3.126984000
H	-1.578433000	3.738336000	2.025673000
C	0.027315000	3.174544000	-0.045254000
H	-0.847899000	3.807294000	-0.246468000
H	0.173208000	2.507306000	-0.896725000
H	0.913121000	3.810099000	0.078268000
C	0.826576000	-2.231001000	1.029611000
C	-0.081824000	-2.371319000	0.065744000
C	1.803745000	-3.168112000	1.653248000
C	-0.615995000	-3.584948000	-0.582786000
H	1.684073000	-4.180461000	1.253521000
H	1.665305000	-3.193776000	2.741865000
H	2.834998000	-2.837371000	1.465839000
H	-0.842960000	-3.436999000	-1.646431000
H	-1.556586000	-3.895813000	-0.108058000
H	0.085020000	-4.428861000	-0.492294000
C	-2.964878000	-1.396179000	-0.956084000
C	-3.228535000	-1.750294000	0.374764000
C	-3.724918000	-1.958628000	-1.985755000
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C	-4.727124000	-2.878864000	-1.686187000
H	-3.538410000	-1.690732000	-3.025160000
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H	-4.436452000	-2.927392000	1.704333000
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C	3.703783000	-3.546138000	-1.454873000
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H	-4.235620000	3.205929000	1.186821000
H	-4.465183000	4.759070000	-0.744732000
C	2.622721000	1.591969000	-0.816207000
C	2.986423000	2.530721000	-1.786776000
C	2.910644000	1.853036000	0.531873000
C	3.626870000	3.710544000	-1.413021000
H	2.767744000	2.360863000	-2.839723000
C	3.561381000	3.024324000	0.900307000
H	2.610080000	1.137200000	1.299720000
C	3.915530000	3.958892000	-0.073411000
H	3.902111000	4.436809000	-2.174619000
H	3.784733000	3.208719000	1.949529000
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Al	-0.247316000	-0.285776000	3.886876000
C	-1.061177000	-2.090063000	3.845623000
C	1.717593000	0.020249000	3.701785000
C	-1.127746000	0.981273000	5.124597000
H	-0.662414000	-2.751725000	4.627498000
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H	-2.138973000	-2.007928000	4.052294000
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H	-0.585871000	1.921714000	5.295655000
H	-1.234073000	0.515744000	6.114907000
H	-2.149699000	1.250187000	4.820011000

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3aa

3ba

3ca

3da

3ea

3fa

3fa'

3ga

3ha

3ia

3ja

3ka

3la

3ma

3na

3ab

3ac

3ad

Chemical structure of compound 10: c1ccc(cc1)-c2nc(c3cc(F)cc(F)c3)c4cc(F)cc(F)c4n2

¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 0 to 8 ppm. Aromatic signals are observed between 6.6 and 7.4 ppm, with integration values of 4.00, 4.03, and 4.04. A singlet at ~7.2 ppm has an integration of 4.00. A doublet at ~7.3 ppm has an integration of 3.03. A multiplet at ~7.1 ppm has an integration of 14.04. A reference peak for TMS is at 0 ppm. A solvent peak for CDCl₃ is at 7.26 ppm. The chemical structure of compound 10 is shown in the top left corner.

3af

3ag

3ah

3ai

3aj

3ak

3al

3lm

3nn

30a

3ob

3oc

[D₃]-3oa

3pa

3qa

3ra

3sa

3ta

3ua

3va

3wa

3xa

3ya

3za

3aaa

3pl

8a

8b

8c

WCS_pyridine-azaPAH_SI.pdf (11.54 MiB)

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