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Cu-Catalyzed Hydroboration of Benzyldenecyclopropanes: Reaction Optimization, (Hetero)Aryl Scope, and Origins of Pathway Selectivity

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Copper catalysis, hydroborations, benzyldenecyclopropanes, cyclopropylboronic esters, β -carbon elimination, heterocycles.

ABSTRACT: The copper-catalyzed hydroboration of benzyldenecyclopropanes, conveniently accessed in one step from readily available benzaldehydes, is reported. Under otherwise identical reaction conditions, two distinct phosphine ligands grant access to different products by either suppressing or promoting cyclopropane opening via β -carbon elimination. Computational studies provide insight into how the rigidity and steric environment of these different bis-phosphine ligands influence the relative activation energies of β -carbon elimination versus protodecupration from the key benzylcopper intermediate. The method tolerates a wide variety of heterocycles prevalent in clinical and pre-clinical drug development, giving access to valuable synthetic intermediates. The versatility of the tertiary cyclopropylboronic ester products is demonstrated through several derivatization reactions.

Conformationally constrained small carbo- and heterocyclic ring systems are among the most important motifs in modern organic chemistry and drug discovery.^[1] Cyclopropane substructures are of special importance as they can imbue a molecule with unique properties, including increased potency, metabolic stability, and brain permeability as well as attenuated pK_a and lipophilicity.^[2] Indeed, cyclopropyl groups are found in a wide range of secondary metabolites, insecticides, pharmaceutical products, for example a TRPV1 agonist,^[3] GSK1360707F,^[4] and foretinib^[5] (Figure 1A). Accessing cyclopropane motifs with diverse substitution patterns is often a challenging aspect of the synthesis of such compounds.^[6]

Tertiary cyclopropylboronic esters have emerged as a versatile family of building blocks that can be further elaborated to prepare multi-substituted cyclopropane motifs. As a consequence, chemists have developed many important synthetic methods for their preparation (Figure 1B). For example, traditional cyclopropanation of vinyl boronates has been used to afford desired tertiary cyclopropylboronic esters.^[7] More recently, the Baran and Aggarwal groups independently demonstrated that decarboxylative borylation of cyclopropyl carboxylic acids produces the corresponding cyclopropylboronic esters.^[8] In addition, Harris and coworkers published a method for selective Suzuki–Miyaura coupling of *gem*-bis(boryl)cyclopropanes which gives tertiary cyclopropylboronic esters as products.^[9] This impressive progress notwithstanding, existing methods also have some limitations in terms of restricted scope, harsh reaction conditions, cost of reagents, and requirement of pre-functionalized precursors.

Figure 1. Overview of Proposed Approach to Preparation of Cyclopropylboronic Esters.

For ongoing programs in drug discovery at Pfizer, we sought a convenient and reliable method to access tertiary cyclopropylboronates bearing diverse $-\text{CH}_2\text{Ar}/\text{Het}$ substitution at the α -position. In this context, we were attracted to copper–boryl chemistry, which has emerged as a powerful reactivity paradigm for hydroboration and borylative difunctionalization of alkenes.^[10] This class of reactions

often proceeds under mild conditions and exhibits broad functional group tolerance, making it well suited for our purposes. In particular, we envisioned highly strained benzylidenecyclopropanes (BCPs) **1** would be ideal tertiary cyclopropylboronic esters precursors upon Cu-catalyzed hydroboration.^[11] The utility of the alkylidene/benzylidenecyclopropane substrate class stems largely from the relief of strain energy, which provides a thermodynamic driving force for engaging a wide array of reaction partners in complexity-generating transformations.^[12]

In considering the integration of BCP substrates into copper–boryl catalysis, we envisioned two potential competitive reaction pathways (Figure 1C) from the common intermediate **2** which is generated by migratory insertion of copper–boryl complex to BCP **1**.^[12] Direct protodecupration of **2** would generate cyclopropylboronic esters **3** (path A). On the other hand, alkenylboronates **4** could also be generated if β -carbon elimination of **2** is preferred over protodecupration (path B). We envisioned that by tuning the ligand sphere around the metal we could control the pathway selectivity of this process and enable straightforward access to these coveted building blocks. At the outset, we took inspiration from the work of Shi, who described a method for 1,2-aminoboration of BCPs using BINAP as ligand.^[11e]

We began our study by preparing several representative BCPs (**1a–1c**, Table 1). All BCP substrates were derived from the corresponding aldehydes through Wittig reactions with commercially available and inexpensive starting materials (see SI for details).^[13] The heterocycles were chosen based on their prevalence in bioactive compounds and their different electronic properties, which we thought might play a role in stabilizing intermediate **2** thereby impacting the innate tendency to undergo ring opening (Figure 1C).^[14] We explored various mono- and bis-phosphine ligands with different electronic and steric properties under conditions similar to those developed for the copper-catalyzed hydroboration of styrenes.^[15] For ease of visualization, the results in Table 1 are color-coded to highlight outcomes where the ¹H NMR yield for one of the two isomers was higher than 70% (**3** in blue and **4** in red). Entries 1–5 show results obtained with mono-phosphine ligands arranged from most electron-donating (entry 1) to most electron-withdrawing (entry 5). Although results varied from substrate to substrate, we observed a clear correlation between the electron-donating character of the ligand and the propensity for β -carbon elimination, which leads to formation of alkenylboronates **4**. Notably, use of tris(pentafluorophenyl)phosphine (entry 5), a ligand not commonly used in copper–boryl catalysis, provided cyclopropylboronic esters **3** exclusively, albeit in variable yields, showing that β -carbon elimination could be fully suppressed with ligands that deplete electron density at the metal center.

We then turned our attention to bis-phosphine ligands containing two –PPh₂ arms with varied natural bite angles (β_n) (entries 6–10).^[16] Using dppm (entry 6, $\beta_n = 72^\circ$), all three substrates preferentially formed cyclopropylboronic esters **3**. With dppbz as the ligand (entry 7, $\beta_n = 83^\circ$), most substrates gave **4** preferentially. In similar fashion, dppe (entry 8), which is known to bind copper with a larger bite-angle than dppm and dppbz ($\beta_n = 85^\circ$), favored formation of alkenylboronates **4**. Larger bite angle ligands (entries 9 and 10) such as *rac*-BINAP ($\beta_n = 92^\circ$) and xantphos ($\beta_n = 111^\circ$) switched the selectivity to favor product **3**. The lack of a clear trend between bite angle and selectivity points to a complex interplay of steric and conformational factors (vide infra). With the insights gained from this study, we opted to use *rac*-BINAP and dppe as the ligands for selective formation of products **3** and **4**, respectively.

Table 1. Ligand optimization with representative substrates

entry ^a	ligand	β_n^b	product ratio (3 : 4) in % yield ^c		
1	P(<i>t</i> -Bu) ₃ ·HBF ₄	---	8 : 82	22 : 62	62 : 20
2	PCy ₃	---	7 : 78	41 : 30	55 : 18
3	PPh ₃	---	53 : 27	65 : 6	68 : 0
4	(<i>p</i> -CF ₃ -C ₆ H ₄) ₃ P	---	42 : 23	67 : 10	41 : 0
5	(C ₆ F ₅) ₃ P	---	57 : 0	84 : 0	18 : 0
6	dppm	72°	70 : 21	93 : 6	55 : 0
7	dppbz	83°	0 : 88	2 : 72	21 : 66
8	dppe	85°	0 : 93	6 : 76	16 : 70
9	<i>rac</i> -BINAP	92°	79 : 0	83 : 6	91 : 0
10	xantphos	111°	71 : 0	34 : 0	41 : 0

^aReaction conditions: **1** (0.2 mmol), CuCl (10 mol%), ligand (10 mol%), B₂pin₂ (0.3 mmol), NaOt-Bu (0.2 mmol), MeOH (0.2 mmol) in THF (0.5 mL) at room temperature. ^bNatural bite angle (β_n) ^cYield determined by ¹H NMR.

We turned our attention to exploring the scope with respect to arene substituents (Scheme 1). The protocol to prepare cyclopropylboronic esters **3** was first examined and found to tolerate a number of electron-withdrawing groups relevant to medicinal chemistry. For example, BCPs containing fluoride at the *ortho* and *para* positions gave boronic esters **3d** and **3e** in good yields. A substrate with a bromide at the *para* position gave the desired cyclopropylboronic ester **3f** in 36%. As demonstrated by the synthesis of **3g** and **3h**, substrates containing trifluoromethyl groups can also be utilized in the reaction. Additionally, the cyano group was well-tolerated, as shown by the synthesis of product **3i**. BCPs bearing electron-donating groups also worked well under the optimized reaction conditions. With certain electron-poor substrates **1d**, **1e**, and **1g**, we found that tris(pentafluorophenyl)phosphine offered moderately higher yields (yield with this ligand in parentheses). Substrates with dimethylamine and methoxy substituents at the *para* position gave products **3j** and **3k**, respectively. A particularly electron-rich BCP bearing three methoxy groups gave the desired product **3l** in 88%. Moreover, cyclopropylboronic ester **3m**, containing the difluoro benzodioxole moiety, could be formed in excellent yield.

Scheme 1. Hydroboration of BCPs with substituted arenes

^aReaction conditions: **1** (0.2 mmol), CuCl (10 mol%), *rac*-BINAP (10 mol%), B₂pin₂ (0.3 mmol), NaOt-Bu (0.2 mmol), MeOH (0.2 mmol) in THF (0.5 mL) at room temperature. ^bThe values in parentheses

correspond to NMR yields with (C₆F₅)₃P as ligand in place of *rac*-BINAP

We then shifted our focus to more challenging BCPs containing heterocycles prevalent in biologically active molecules (Scheme 2). Many heterocyclic motifs are known to present problems in catalysis, as they can bind strongly to the metal center and inhibit progress. The transformation proved to be tolerant of diverse 5-membered heterocycles, including thiophene, Ts-protected pyrroles, oxazole, and thiazole to give the corresponding products **3n–3s** in good to excellent yields. 6-membered heterocycles, including various substituted pyridines, performed well in the reaction, as exemplified by formation of boronic esters **3t–3z**. It is worth mentioning that pyridine is the most common aromatic nitrogen-containing heterocycle in drug molecules. Synthetic methods that allow access to building blocks resembling **3t–3z** are highly sought-after. We also explored other heterocycles of interest, namely pyrimidine, quinoxaline, quinoline, pyrazolo pyrimidine, benzimidazole, and benzofuran, which gave products **3za–3zf** in synthetically useful to good yields.^[17]

Scheme 2. Hydroboration of BCPs with heterocycles

^aReaction conditions: **1** (0.2 mmol), CuCl (10 mol%), *rac*-BINAP (10 mol%), B₂pin₂ (0.3 mmol), NaOt-Bu (0.2 mmol), MeOH (0.2 mmol) in THF (0.5 mL) at room temperature. n.d. = not detected. ^bThe values in parentheses correspond to NMR yields with (C₆F₅)₃P as ligand in place of *rac*-BINAP.

Next, we explored the feasibility of β-carbon elimination on a number of substrates containing various substituents and heterocyclic motifs (Scheme 3). The system developed utilizing dppe as the ligand served to give alkenylboronates in good to excellent yields.

Scheme 3. Synthesis of vinyl boronates via β-C elimination

^aReaction conditions: **1** (0.2 mmol), CuCl (10 mol%), dppe (10 mol%), B₂pin₂ (0.3 mmol), NaOt-Bu (0.2 mmol), MeOH (0.2 mmol) in THF (0.5 mL) at room temperature.

Having established access to various tertiary cyclopropylboronic esters, we set out to demonstrate their synthetic utility through derivatization reactions (Scheme 4). We chose to focus our efforts on derivatizations of the tertiary cyclopropylboronic esters, as vinyl-boronates are widely known to be versatile building blocks. Compound **3a** was chosen as the model substrate for select C–X and C–C bond forming transformations. Exposure of **3a** to sodium perborate gave tertiary alcohol **5** in 99%.^[18] A modified amination protocol developed by Morken furnished primary amine **6** in modest yield.^[19] A Matteson–Aggarwal homologation delivered boronic ester **7**;^[20] and lastly, the gram-scale conversion of **3a** to tertiary trifluoroborate **8** occurred in 81%.^[21]

Furthermore, as illustrated in Scheme 5, facile access to trifluoroborate **8** enabled several Suzuki–Miyaura couplings. Under conditions developed by Harris and coworkers, use of alkenyl triflate electrophiles gave alkenyl cyclopropanes **9–11** in good yields.^[22] Likewise, use of heteroaryl bromides efficiently delivered products **12–14** containing nitrogen-based heterocycles and substituents (e.g. fluorine, trifluoromethyl, and methyl) critical in drug development.^[23]

Scheme 4. Select derivatization reactions with tertiary boronic ester 3a

Scheme 5. Enabling Suzuki–Miyaura couplings with tertiary trifluoroborate 8

Given the wide discrepancy between outcomes obtained with seemingly related bis-phosphine ligands under otherwise identical reaction conditions, we pursued further understanding of the ligand effects with computational studies. We performed DFT calculations at the M06/6-311+G(d,p)-SDD/SMD(THF)//M06L/6-31G(d)-LANL2DZ level of theory to investigate the reaction energy profiles leading to the alkenylboronate and cyclopropylboronic ester products with dppe and BINAP ligands (see Figure S1). The calculations suggest that the pathway selectivity is determined by the activation energy difference between β -carbon elimination (**TS1**) and protodecupration (**TS2**) from the benzylic copper intermediate **2** formed via the irreversible migratory insertion of the BCP **1a** (Scheme 6).^[24] Consistent with the experimental observations, with the dppe ligand the β -carbon elimination is favored over protodecupration by 3.2 kcal/mol, leading to the formation of the alkenylboronate product **4a**. The use of BINAP ligand completely reverses the pathway selectivity. β -Carbon elimination from the benzylic copper complex with BINAP as ligand requires a much higher barrier ($\Delta G^\ddagger = 22.4$ kcal/mol) than that with dppe as ligand ($\Delta G^\ddagger = 13.9$ kcal/mol). On the other hand, ligand effects have a much smaller impact on the barrier of protodecupration (**TS2**). Therefore, the reaction using BINAP as ligand forms the cyclopropylboronic ester **3a** via favorable protodecupration.

Scheme 6. Activation energies of the selectivity-determining steps.

The origin of ligand effects on the β -carbon elimination barrier can be visualized in the quadrant diagrams in Figure 2. The β -carbon elimination TS with the Cu(I) center prefers a tetrahedral geometry that places the benzylic (C_α) and γ -carbons (C_γ) within the vertical region perpendicular to the P–Cu–P plane. With dppe, this vertical region is not occupied by the PPh_2 arms. Thus, no unfavorable steric repulsions are observed in **TS1a**. On the other hand, the more rigid BINAP is confined to a C_2 -symmetric conformation, in which the vertical region is blocked by the pseudo-axial phenyl groups (Ph_{ax}) of the PPh_2 arms. The benzylic and γ -carbons in **TS1b** are significantly distorted to be placed in the less occupied diagonal regions in quadrants II and IV to avoid repulsions with the BINAP ligand. Consequently, the distorted tetrahedral **TS1b** is energetically disfavored. An isomer of **TS1b** that places C_α and C_γ in the more occupied I and III quadrants was also located and requires an even higher activation energy (26.7 kcal/mol).

Figure 2. Origin of ligand effects on β -carbon elimination barriers.

In summary, we have developed conditions for the hydroboration of benzylicenecyclopropanes that lead to formation of two distinct products, namely cyclopropylboronic esters and alkenylboronates. Both products represent highly versatile building blocks that enable access to diverse derivatives based on downstream manipulation of boronic ester functionality. This work should be of particular interest to the pharmaceutical industry and represents an example of an emerging concept in catalysis, whereby pathway selectivity can be tuned through ligand space.^[25] Computational analysis reveals the origins of ligand effects affecting a key β -carbon elimination step, providing a conceptual framework for strategically employing this family of strained alkenes in a broader range of catalytic transformations.

ASSOCIATED CONTENT

Supporting Information

Detailed experimental and computational procedures, compound characterization, Cartesian coordinates of the calculated structures. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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Notes

The authors declare no competing financial interest.

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Cu-Catalyzed Hydroboration of Benzyldenecyclopropanes: Reaction Optimization, (Hetero)Aryl Scope, and Origins of Pathway Selectivity

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Materials and Methods.

Unless stated otherwise, reactions were conducted in flame-dried glassware under an atmosphere of nitrogen using anhydrous solvents (freshly distilled or passed through activated alumina columns). All commercially obtained reagents were used as received unless otherwise specified. Potassium tert-butoxide (KOt-Bu) and sodium tert-butoxide (NaOt-Bu) were obtained from Oakwood Products, Inc. (3-Bromopropyl) triphenylphosphonium bromide (CAS number: 3607-17-8) was obtained from Astatech. Copper chloride (CuCl) was obtained from Sigma Aldrich. Racemic 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (*rac*-BINAP) was obtained from Strem Chemicals. Bis(pinacolato)diboron (B₂pin₂) was obtained from Combi-Blocks. All aldehyde starting materials were provided by Pfizer or purchased from Alfa Aesar, Sigma Aldrich, Oakwood Products, and Combi-Blocks. Reaction temperatures were controlled using an IKAmag temperature modulator and, unless stated otherwise, reactions were performed at room temperature (rt, approximately 23 °C). Thin layer chromatography (TLC) was conducted with EMD gel 60 F254 pre-coated plates (0.25 mm) and visualized using a combination of UV light and potassium permanganate staining. Preparative thin layer chromatography (TLC) was conducted with Analtech silica gel GF UV254 pre-coated plates (1.0 mm) and visualized using UV light. Silicycle Siliaflash P60 (particle size 0.040–0.063 mm) was used for flash column chromatography. ¹H and ¹³C NMR spectra were recorded on Bruker spectrometers (400 MHz, 600 MHz) and are reported relative to deuterated solvent signals or SiMe₄. The following abbreviations (or combinations thereof) were used to explain multiplicities: b = broad, s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septet, and m = multiplet. High-resolution mass spectra (HRMS) for new compounds were obtained on an Agilent LC/MSD TOF mass spectrometer.

Experimental Procedures.**A. Synthesis of Benzyldenecyclopropanes (BCPs).**

Note on BCP substrates: Some of the BCP substrates were found to decompose over time at room temperature. Some substrates were particularly unstable and showed significant decomposition within hours of being isolated. Solid substrates were generally more stable than oil substrates. We recommend that the BCPs be used soon after being made or alternatively that they be stored as frozen as stock solutions in benzene. Old BCP samples that were not appropriately stored generally gave lower product yields in hydroboration; upon re-purification by flash chromatography, the yields generally improved to reported levels.

Representative Procedure.¹

BCP substrate 1a. A flame-dried scintillation vial equipped with a stir bar was charged with (3-bromopropyl)triphenylphosphonium bromide (1.40 g, 3.0 mmol, 1.2 equiv) and KO*t*-Bu (700 mg, 6.0 mmol, 2.4 equiv). The solids were suspended in THF (10 mL), and the mixture was allowed to stir at 60 °C for 1 h. After the solution had cooled to room temperature, benzaldehyde (265 mg, 2.5 mmol, 1.0 equiv) was added to the suspension dropwise over 2 min. The vial was sealed, and the suspension was allowed to stir at 60 °C for 12 h. The reaction mixture was cooled to room temperature and filtered through a celite pad, which was subsequently rinsed with Et₂O (3 × 20 mL). The filtrate was concentrated, and the resulting crude mixture was purified by flash chromatography (hexanes) to provide BCP substrate **1a** (218 mg, 67% yield) as a colorless oil. Spectral data match those previously reported.²

Any modifications from this representative procedure are specified in the following schemes.

BCP substrate 1b. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1b** (235 mg, 72% yield) as a colorless oil. **1b**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.66 (s, 1H), 8.36 (d, $J = 5.0$ Hz, 1H), 7.76 (d, $J = 7.8$ Hz, 1H), 7.16 (dd, $J = 8.0, 4.9$ Hz, 1H), 6.66 (s, 1H), 1.36 (td, $J = 8.0, 4.0$ Hz, 2H), 1.14 (dd, $J = 9.3, 6.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 148.21, 147.57, 133.68, 132.93, 127.03, 123.29, 114.91, 4.08, 0.72; **HRMS-ESI** (m/z) [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_9\text{H}_9\text{N}$, 132.0813; found 132.0810.

BCP substrate 1c. Purification by flash chromatography (hexanes) afforded BCP substrate **1c** (88.3 mg, 30% yield) as a colorless oil. **1c**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.47 (s, 1H), 7.37 (s, 1H), 6.67 (s, 1H), 6.63–6.59 (m, 1H), 1.30–1.27 (m, 2H), 1.21–1.18 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 143.30, 139.56, 124.90, 123.38, 108.63, 108.58, 3.40, 1.76; **HRMS-ESI** (m/z) [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_8\text{H}_8\text{O}$, 121.0653; found 121.0657.

BCP substrate 1d. Purification by flash chromatography (hexanes) afforded BCP substrate **1d** (204 mg, 55% yield) as a colorless oil. **1d**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.74 (td, $J = 7.7, 1.8$ Hz, 1H), 7.16 (tdd, $J = 7.4, 5.1, 1.8$ Hz, 1H), 7.08 (td, $J = 7.5, 1.2$ Hz, 1H), 7.03 (ddd, $J = 10.6, 8.1, 1.3$ Hz, 1H), 6.98 (p, $J = 2.2$ Hz, 1H), 1.43–1.38 (m, 2H), 1.21–1.16 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 159.89 (d, $J = 248.3$ Hz), 128.03 (d, $J = 8.2$ Hz), 127.24 (d, $J = 3.9$ Hz), 126.74 (d, $J = 2.7$ Hz), 125.90 (d, $J = 12.2$ Hz), 124.00 (d, $J = 3.7$ Hz), 115.61 (d, $J = 22.0$ Hz), 110.39 (d, $J = 5.8$ Hz), 4.28, 1.01; **HRMS-ESI** (m/z) [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{10}\text{H}_9\text{F}$, 149.0767; found 149.0761.

BCP substrate 1e. Purification by flash chromatography (hexanes) afforded BCP substrate **1e** (233 mg, 63% yield) as a colorless oil. **1e**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.46 (dd, $J = 8.8, 5.6$ Hz, 2H), 7.02–6.96 (m, 2H), 6.71–6.65 (m, 1H), 1.37 (ddd, $J = 9.9, 5.7, 2.3$ Hz, 2H), 1.18–1.11 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 161.89 (d, $J = 245.5$ Hz), 134.53 (d, $J = 3.3$ Hz), 128.06 (d, $J = 7.8$ Hz), 123.90 (d, $J = 2.7$ Hz), 117.26, 115.39 (d, $J = 21.5$ Hz), 4.14, 0.69; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_9\text{F}$, 149.0767; found 149.0766.

BCP substrate 1f. Purification by flash chromatography (99:1 hexanes:EtOAc) afforded BCP substrate **1f** (287 mg, 55% yield) as a colorless oil. **1f**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.46–7.40 (m, 2H), 7.42–7.36 (m, 2H), 6.68 (p, $J = 2.1$ Hz, 1H), 1.39 (ddd, $J = 9.8, 5.7, 2.3$ Hz, 2H), 1.17 (ddd, $J = 9.8, 5.7, 1.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 137.16, 131.51, 128.09, 125.38, 120.34, 117.26, 4.19, 0.63.; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_9\text{Br}$, 208.9966; found 208.9958.

BCP substrate 1g. Purification by flash chromatography (hexanes) afforded BCP substrate **1g** (347 mg, 70% yield) as a colorless oil. **1g**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.60 (d, $J = 8.3$ Hz, 2H), 7.55 (d, $J = 8.3$ Hz, 2H), 6.79–6.75 (m, 1H), 1.44 (ddd, $J = 10.1, 5.9, 2.2$ Hz, 2H), 1.21 (td, $J = 7.8, 1.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 141.79 (d, $J = 1.7$ Hz), 128.59 (q, $J = 32.2$ Hz), 127.93, 126.77, 125.51 (q, $J = 3.8$ Hz), 124.52 (q, $J = 271.8$ Hz), 117.43, 4.46, 0.87; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_9\text{F}_3$, 199.0735; found 199.0737.

BCP substrate 1h. Purification by flash chromatography (hexanes) afforded BCP substrate **1h** (339 mg, 51% yield) as a colorless oil. **1h**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.92 (s, 2H), 7.69 (s, 1H), 6.82 (p, $J = 2.1$ Hz, 1H), 1.50 (ddd, $J = 8.2, 7.0, 2.3$ Hz, 2H), 1.30–1.24 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 140.35, 131.87 (q, $J = 33.0$ Hz), 129.65, 126.33 (d, $J = 3.8$ Hz), 123.62 (q, $J = 271.7$ Hz), 120.15 (m), 116.29, 4.45, 1.03; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_8\text{F}_6$, 267.0608; found 267.0614.

BCP substrate 1i. Purification by flash chromatography (98:2 hexanes:EtOAc) afforded BCP substrate **1i** (380 mg, 98% yield) as a colorless oil. **1i**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.81 (s, 1H), 7.71 (d, $J = 7.7$ Hz, 1H), 7.48 (d, $J = 7.7$ Hz, 1H), 7.41 (t, $J = 7.7$ Hz, 1H), 6.73 (t, $J = 2.1$ Hz, 1H), 1.46 (ddd, $J = 8.1, 6.9, 2.2$ Hz, 2H), 1.25–1.21 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 139.48, 130.92, 130.06, 129.95, 129.34, 127.99, 119.21, 116.60, 112.69, 4.42, 0.88; **HRMS-APCI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_9\text{N}$, 156.0813; found 156.0809.

BCP substrate 1j. Purification by flash chromatography (95:5 hexanes:EtOAc) afforded BCP substrate **1j** (169 mg, 39% yield) as a colorless oil. **1j**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.43 (d, $J = 8.7$ Hz, 2H), 6.71 (d, $J = 8.8$ Hz, 2H), 6.66 (t, $J = 2.1$ Hz, 1H), 2.95 (s, 6H), 1.42–1.31 (m, 2H), 1.13 (td, $J = 7.2, 1.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 149.69, 127.60, 127.40, 119.60, 118.02, 112.77, 40.80, 4.11, 0.56; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{15}\text{N}$, 174.1283; found 174.1285.

BCP substrate 1k. Purification by flash chromatography (98:2 hexanes:EtOAc) afforded BCP substrate **1k** (192 mg, 48% yield) as a colorless oil. **1k**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.46 (d, $J = 8.7$ Hz, 2H), 6.87 (d, $J = 8.8$ Hz, 2H), 6.69 (s, 1H), 3.80 (s, 3H), 1.38 (ddd, $J = 9.7, 5.5, 2.3$ Hz, 2H), 1.15 (ddd, $J = 9.5, 5.5, 1.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 158.64, 131.35, 127.80, 121.82, 117.69, 114.02, 55.41, 4.14, 0.63; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_{12}\text{O}$, 161.1966; found 161.1965.

BCP substrate 1l. Purification by flash chromatography (6:1 hexanes:EtOAc) afforded BCP substrate **1l** (551 mg, 71% yield) as a white solid. **1l**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 6.78 (s, 2H), 6.67 (q, $J = 1.9$ Hz, 1H), 3.89 (s, 6H), 3.85 (s, 3H), 1.42 (tt, $J = 7.4, 1.7$ Hz, 2H), 1.19 (tt, $J = 7.5, 1.5$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 153.41, 137.32, 134.22, 123.83, 118.29, 103.79, 61.07, 56.17, 4.18, 0.73; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{16}\text{O}_3$, 221.1178; found 221.1176.

BCP substrate 1m. Purification by flash chromatography (98:2 hexanes:EtOAc) afforded BCP substrate **1m** (399 mg, 76% yield) as a white solid. **1m**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.32 (d, $J = 1.6$ Hz, 1H), 7.13 (dd, $J = 8.3, 1.6$ Hz, 1H), 6.99 (d, $J = 8.3$ Hz, 1H), 6.71–6.68 (m, 1H), 1.40 (ddd, $J = 9.9, 5.8, 2.2$ Hz, 2H), 1.22–1.17 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 144.31, 142.60, 135.03, 131.77 (t, $J = 254.5$ Hz), 124.87, 122.41, 117.30, 109.34, 107.06, 4.23, 0.80; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_8\text{F}_2\text{O}_2$, 211.0571; found 211.0566.

BCP substrate 1n. Purification by flash chromatography (hexanes) afforded BCP substrate **1n** (227 mg, 67% yield) as a colorless oil. **1n**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.43 (d, J = 5.1 Hz, 1H), 7.32 (dd, J = 5.1, 3.0 Hz, 1H), 7.24 (s, 1H), 6.85 (s, 1H), 1.38 (ddd, J = 8.1, 5.9, 2.3 Hz, 2H), 1.28 (dt, J = 10.8, 4.2 Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 140.78, 126.01, 125.64, 123.71, 120.69, 113.16, 3.93, 1.82; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_8\text{H}_8\text{S}$, 137.0475; found 137.0479.

BCP substrate 1o. Purification by flash chromatography (9:1 hexanes:EtOAc) afforded BCP substrate **1o** (359 mg, 53% yield) as a colorless oil. **1o**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.74 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 8.2 Hz, 2H), 7.19–7.06 (m, 2H), 6.55 (s, 2H), 2.39 (s, 3H), 1.27–1.20 (m, 2H), 1.20–1.13 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 144.88, 136.08, 129.95, 128.17, 126.83, 123.59, 121.42, 117.25, 112.19, 110.24, 21.61, 3.39, 1.48; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$, 274.0902; found 274.0905.

BCP substrate 1p. Purification by flash chromatography (9:1 hexanes:EtOAc) afforded BCP substrate **1p** (152 mg, 22% yield) as a colorless oil. **1p**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.72 (d, J = 8.1 Hz, 2H), 7.34–7.28 (m, 3H), 7.19 (s, 1H), 6.51 (s, 1H), 6.28 (t, J = 3.4 Hz, 1H), 2.41 (s, 3H), 1.22 (td, J = 7.5, 7.1, 3.7 Hz, 4H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 144.77, 136.29, 133.60, 129.89, 126.86, 125.56, 122.03, 112.29, 111.34, 107.52, 21.62, 3.51, 2.21; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_2\text{S}$, 274.0902; found 274.0907.

BCP substrate 1q. Purification by flash chromatography (4:1 hexanes:Et₂O) afforded BCP substrate **1q** (143 mg, 47% yield) as a colorless oil. **1q**: ¹H NMR (600 MHz, CDCl₃): δ 7.86 (s, 1H), 7.69 (s, 1H), 6.65 (s, 1H), 1.34 (ddd, *J* = 9.4, 5.7, 1.8 Hz, 2H), 1.24 (tt, *J* = 7.2, 1.7 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 151.10, 139.17, 134.37, 127.05, 108.19, 3.85, 2.17; **HRMS-ESI** (*m/z*) [M + H]⁺ calcd for C₇H₇NO, 122.0606; found 122.0599.

BCP substrate 1r. Purification by flash chromatography (9:1 hexanes:Et₂O) afforded BCP substrate **1r** (199 mg, 58% yield) as a colorless oil. **1r**: ¹H NMR (600 MHz, CDCl₃): δ 8.79 (d, *J* = 2.1 Hz, 1H), 7.29 (d, *J* = 2.0 Hz, 1H), 6.99 (s, 1H), 1.41–1.38 (m, 2H), 1.28 (dd, *J* = 7.9, 2.0 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 155.61, 152.29, 127.33, 112.61, 112.57, 4.04, 2.07. **HRMS-APCI** (*m/z*) [M + H]⁺ calcd for C₇H₇NS, 138.0377; found 138.0378.

BCP substrate 1s. Purification by flash chromatography (9:1 hexanes:Et₂O) afforded BCP substrate **1s** (141 mg, 41% yield) as a colorless oil. **1s**: ¹H NMR (600 MHz, CDCl₃): δ 8.62 (s, 1H), 7.76 (s, 1H), 6.96 (s, 1H), 1.36–1.33 (m, 2H), 1.30 (dt, *J* = 6.6, 2.2 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 151.37, 139.87, 138.61, 128.00, 109.29, 4.15, 3.62; **HRMS-ESI** (*m/z*) [M + H]⁺ calcd for C₇H₇NS, 138.0377; found 138.0376.

BCP substrate 1t. Purification by flash chromatography (6:1 hexanes:EtOAc) afforded BCP substrate **1t** (197 mg, 48% yield) as an orange oil. **1t**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 9.00 (s, 1H), 8.31 (d, $J = 5.4$ Hz, 1H), 7.31 (d, $J = 5.4$ Hz, 1H), 7.08 (s, 1H), 1.48 (td, $J = 8.2, 2.2$ Hz, 2H), 1.31–1.26 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 148.52, 147.57, 141.78, 132.19, 130.33, 124.72, 111.70, 4.45, 1.66; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_8\text{ClN}$, 166.0424; found 166.0423.

BCP substrate 1u. Purification by flash chromatography (9:1 hexanes:EtOAc) afforded BCP substrate **1u** (159 mg, 43% yield) as a colorless oil. **1u**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.11 (ddd, $J = 9.5, 7.4, 1.9$ Hz, 1H), 8.04 (d, $J = 4.9$ Hz, 1H), 7.15 (ddd, $J = 7.0, 4.8, 1.6$ Hz, 1H), 6.88 (s, 1H), 1.43 (td, $J = 8.0, 2.2$ Hz, 2H), 1.24 (td, $J = 7.9, 1.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 160.37 (d, $J = 240.9$ Hz), 145.20 (d, $J = 14.5$ Hz), 136.94 (d, $J = 5.0$ Hz), 129.59, 121.54 (d, $J = 4.1$ Hz), 120.83 (d, $J = 26.9$ Hz), 109.45, 4.16, 1.16; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_8\text{FN}$, 150.0719; found 150.0716.

BCP substrate 1v. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1v** (211 mg, 52% yield) as a colorless oil. **1v**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.23 (s, 1H), 7.83 (dd, $J = 8.6, 2.5$ Hz, 1H), 6.72 (d, $J = 8.6$ Hz, 1H), 6.68 (t, $J = 2.1$ Hz, 1H), 3.94 (s, 3H), 1.38 (ddd, $J = 10.0, 5.7, 2.3$ Hz, 2H), 1.18 (ddd, $J = 9.8, 5.5, 1.9$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 163.12, 145.22, 136.29, 127.73, 123.62, 114.66, 110.86, 53.56, 4.06, 0.85; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_{11}\text{NO}$, 162.0919; found 162.0921.

BCP substrate 1w. Purification by flash chromatography (80g of SiO₂, Isco, 0–15% EtOAc/Heptanes) afforded BCP substrate **1w** (227 mg, 10% yield) as a white solid. **1w**: ¹H NMR (400 MHz, CDCl₃): δ 8.81 (d, *J* = 2.1 Hz, 1H), 7.94 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 6.78 (m, 1H), 1.56–1.37 (m, 2H), 1.37–1.17 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 148.46, 146.00 (q, *J* = 34.6 Hz), 136.80, 134.20, 130.99, 121.95 (q, *J* = 273.6 Hz), 120.49 (q, *J* = 2.8 Hz), 114.36, 4.54, 1.34; **HRMS-ESI** (*m/z*) [*M* + *H*]⁺ calcd for C₁₀H₉F₃N, 200.0682; found 200.0678.

BCP substrate 1x. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1x** (125 mg, 38% yield) as a colorless oil. **1x**: ¹H NMR (600 MHz, CDCl₃): δ 8.53 (d, *J* = 5.0 Hz, 2H), 7.38 (d, *J* = 4.6 Hz, 2H), 6.70 (s, 1H), 1.48 (td, *J* = 8.2, 4.3 Hz, 2H), 1.25–1.21 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 150.01, 145.48, 130.94, 121.23, 116.57, 4.54, 0.82; **HRMS-ESI** (*m/z*) [*M* + *H*]⁺ calcd for C₉H₉N, 132.0813; found 132.0817.

BCP substrate 1y. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1y** (157 mg, 48% yield) as a colorless oil. **1y**: ¹H NMR (600 MHz, CDCl₃): δ 8.55 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.70 (dt, *J* = 8.1, 1.1 Hz, 1H), 7.63 (td, *J* = 7.7, 1.8 Hz, 1H), 7.10 (ddd, *J* = 7.4, 4.9, 1.2 Hz, 1H), 6.96 (p, *J* = 2.1 Hz, 1H), 1.49–1.43 (m, 2H), 1.29–1.23 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 157.10, 149.24, 136.05, 129.56, 121.35, 120.37, 119.84, 4.29, 1.16; **HRMS-ESI** (*m/z*) [*M* + *H*]⁺ calcd for C₉H₉N, 132.0813; found 132.0812.

BCP substrate 1z. Purification by flash chromatography (9:1 hexanes:EtOAc) afforded BCP substrate **1z** (157 mg, 48% yield) as a colorless oil. **1z**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.27 (d, J = 5.1 Hz, 1H), 7.55 (s, 1H), 7.34 (dd, J = 5.2, 1.4 Hz, 1H), 6.66 (p, J = 2.0 Hz, 1H), 1.50 (ddd, J = 8.5, 7.3, 2.2 Hz, 2H), 1.29–1.24 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 150.19, 148.42, 142.83, 133.14, 125.21, 120.40, 115.51, 4.71, 1.12; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_8\text{BrN}$, 209.9918; found 209.9918.

BCP substrate 1za. Reaction performed with 1.5 mmol of aldehyde substrate due to limited material. Purification by flash chromatography (3:1 hexanes:EtOAc) afforded BCP substrate **1za** (104 mg, 48% yield) as a colorless oil. **1za**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.78 (s, 2H), 6.67 (t, J = 2.1 Hz, 1H), 2.74 (s, 3H), 1.46 (ddd, J = 8.2, 7.0, 2.3 Hz, 2H), 1.27 (td, J = 7.8, 1.7 Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 165.77, 154.50, 128.87, 128.73, 111.87, 25.65, 4.27, 1.31; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_{10}\text{N}_2$, 147.0922; found 147.0917.

BCP substrate 1zb. Purification by flash chromatography (80g of SiO_2 , Isco, 0–33% EtOAc/Heptanes) afforded BCP substrate **1zb** (117 mg, 32% yield) as a brown solid. **1zb**: $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 9.28 (s, 1H), 8.03–7.94 (m, 2H), 7.71–7.58 (m, 2H), 7.10 (m, 1H), 1.61–1.52 (m, 2H), 1.38–1.29 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 151.85, 144.02, 142.39,

141.21, 134.90, 130.12, 129.25, 129.20, 129.09, 118.76, 5.12, 2.26; **HRMS-ESI** (m/z) [$M + H$]⁺ calcd for C₁₂H₁₀N₂, 183.0917; found 183.0915.

BCP substrate 1zc. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1zc** (284 mg, 77% yield) as a colorless oil. **1zc**: ¹H NMR (600 MHz, CDCl₃): δ 8.84 (d, J = 4.8 Hz, 1H), 8.12 (d, J = 8.3 Hz, 1H), 8.09–8.01 (m, 2H), 7.77 (s, 1H), 7.37 (dd, J = 8.2, 4.2 Hz, 1H), 6.93 (s, 1H), 1.54 (td, J = 7.8, 2.1 Hz, 2H), 1.27–1.23 (m, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 149.89, 147.79, 136.72, 136.01, 129.56, 128.69, 128.27, 126.64, 125.27, 121.41, 117.96, 4.59, 0.90; **HRMS-ESI** (m/z) [$M + H$]⁺ calcd for C₁₃H₁₁N, 182.0970; found 182.0971.

BCP substrate 1zd. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1zd** (108 mg, 29% yield) as a colorless oil. **1zd**: ¹H NMR (600 MHz, CDCl₃): δ 8.80 (d, J = 2.2 Hz, 1H), 8.71 (s, 1H), 8.09 (d, J = 2.4 Hz, 1H), 6.72 (s, 1H), 6.68 (d, J = 2.4 Hz, 1H), 1.52–1.46 (m, 2H), 1.29 (td, J = 7.7, 1.8 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 149.17, 147.61, 145.12, 131.21, 127.36, 120.17, 111.62, 97.06, 4.44, 1.55; **HRMS-ESI** (m/z) [$M + H$]⁺ calcd for C₁₀H₉N₃, 172.0875; found 172.0876.

BCP substrate 1ze. Purification by flash chromatography (4:1 hexanes:EtOAc) afforded BCP substrate **1ze** (272 mg, 52% yield) as a colorless oil. **1ze**: ¹H NMR (600 MHz, CDCl₃): δ 7.78–7.72 (m, 1H), 7.51 (dd, J = 6.4, 2.9 Hz, 1H), 7.25–7.20 (m, 2H), 7.20–7.14 (m, 1H), 3.30 (tt, J = 7.2, 3.8 Hz, 1H), 1.67 (td, J = 8.6, 2.3 Hz, 2H), 1.33 (td, J = 8.5, 1.8 Hz, 2H), 1.25 (dt, J = 7.0,

3.4 Hz, 2H), 1.09 (p, $J = 4.9$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 152.43, 143.26, 136.05, 135.86, 122.34, 122.22, 119.78, 110.48, 107.29, 24.64, 7.63, 5.21, 2.41; **HRMS-ESI** (m/z) [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{14}\text{H}_{14}\text{N}_2$, 211.1235; found 211.1239.

BCP substrate 1zf. Purification by flash chromatography (98:2 hexanes:EtOAc) afforded BCP substrate **1zf** (374 mg, 88% yield) as a white solid. **1zf**: ^1H NMR (600 MHz, CDCl_3): δ 7.71 (s, 1H), 7.59 (d, $J = 2.2$ Hz, 1H), 7.53 (dd, $J = 8.6, 1.7$ Hz, 1H), 7.45 (d, $J = 8.5$ Hz, 1H), 6.83 (t, $J = 2.1$ Hz, 1H), 6.75 (d, $J = 1.3$ Hz, 1H), 1.45 (ddd, $J = 9.8, 5.6, 2.3$ Hz, 2H), 1.22–1.17 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 154.30, 145.39, 133.55, 127.79, 123.40, 122.80, 119.15, 118.43, 111.38, 106.83, 4.35, 0.79; **HRMS-ESI** (m/z) [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{12}\text{H}_{10}\text{O}$, 171.0810; found 171.0808.

B. Hydroboration Reactions. **Representative Procedure.**

Boronic ester 3a. A flame-dried 10-mL reaction vial equipped with a magnetic stir bar was charged with CuCl (2.0 mg, 0.02 mmol, 0.1 equiv), *rac*-BINAP (12.5 mg, 0.02 mmol, 0.1 equiv), B₂pin₂ (76.2 mg, 0.30 mmol, 1.5 equiv), and NaOt-Bu (19.2 mg, 0.20 mmol, 1.0 equiv). The vial was capped, evacuated for 1 min, and backfilled with N₂. The solids were suspended in THF (500 μL), and the reaction mixture was allowed to pre-stir for 10 min at room temperature. Next, BCP substrate **1a** (26.0 mg, 0.20 mmol, 1.0 equiv) and MeOH (8.1 μL, 0.20 mmol, 1.0 equiv) were added, and the reaction was allowed to stir at room temperature for 15–18 h. The reaction mixture was then filtered through a pad of silica gel, which was subsequently rinsed with EtOAc (15 mL). The filtrate was concentrated, and the resulting crude mixture was purified by preparative thin layer chromatography (95:5 hexanes:EtOAc) to provide boronic ester **3a** (40.7 mg, 79% yield) as a colorless oil. **3a**: ¹H NMR (600 MHz, CDCl₃): δ 7.31–7.25 (m, 4H), 7.20–7.15 (m, 1H), 2.65 (s, 2H), 1.19 (s, 12H), 0.76 (q, *J* = 3.6 Hz, 2H), 0.48 (q, *J* = 3.6 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 142.12, 128.99, 127.82, 125.53, 83.08, 41.10, 24.55, 11.31; **HRMS-ESI** (*m/z*) [*M* + OH][−] calcd for C₁₆H₂₃BO₂, 274.1855; found 274.1854.

Note: We recommend using solid NaOt-Bu in this reaction. In our hands, NaOt-Bu stock solution in THF generally gave lower yields of the desired product and led to formation of unknown side products. The origin of this effect is unclear at the present time.

Any modifications from this representative procedure are specified in the following schemes.

Figure S1. Picture of reagents and reaction mixture at different points of the reaction. a) CuCl, b) *rac*-BINAP, c) NaOt-Bu, d) B₂pin₂, e) reaction mixture after addition of THF before 10 min pre-stir, f) reaction mixture after 10 min pre-stir, g) reaction mixture after completion (15–18 h).

Boronic ester 3b. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester 3b (43.3 mg, 83% yield) as a colorless oil. **3b:** ¹H NMR (600 MHz, CDCl₃): δ 8.48 (d, *J* = 64.1 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.18 (t, *J* = 6.1 Hz, 1H), 2.58 (s, 2H), 1.14 (d, *J* = 2.6 Hz, 12H), 0.78 (t, *J* = 2.9 Hz, 2H), 0.47 (t, *J* = 3.0 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 150.47, 147.15, 137.73, 136.43, 123.03, 83.37, 38.74, 24.67, 11.75; **HRMS-ESI** (*m/z*) [*M* + H]⁺ calcd for C₁₅H₂₂BNO₂, 259.1858; found 259.1863.

Boronic ester 3c. Purification by preparative thin layer chromatography (9:1 hexanes:EtOAc) afforded boronic ester **3c** (45.1 mg, 91% yield) as a colorless oil. **3c**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.30 (t, $J = 1.7$ Hz, 1H), 7.23 (t, $J = 1.3$ Hz, 1H), 6.35 (s, 1H), 2.36 (s, 2H), 1.18 (s, 12H), 0.71 (q, $J = 3.6$ Hz, 2H), 0.40 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 142.23, 139.43, 124.97, 111.85, 83.24, 30.90, 24.74, 11.52; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{14}\text{H}_{21}\text{BO}_3$, 248.1698; found 248.1702.

Boronic ester 3d. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3d** (39.2 mg, 71% yield) as a colorless oil. **3d**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.41 (td, $J = 7.7, 1.7$ Hz, 1H), 7.13 (tdd, $J = 7.4, 5.1, 1.8$ Hz, 1H), 7.03 (td, $J = 7.5, 1.2$ Hz, 1H), 6.96 (ddd, $J = 9.6, 8.1, 1.2$ Hz, 1H), 2.68 (s, 2H), 1.17 (s, 12H), 0.74 (q, $J = 3.6$ Hz, 2H), 0.47 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 161.29 (d, $J = 244.4$ Hz), 131.14 (d, $J = 5.0$ Hz), 128.86 (d, $J = 16.0$ Hz), 127.24 (d, $J = 7.8$ Hz), 123.51 (d, $J = 3.4$ Hz), 114.89 (d, $J = 22.7$ Hz), 83.28, 33.34, 24.69, 11.38; **HRMS-ESI** (m/z) $[\text{M} + \text{OH}]^-$ calcd for $\text{C}_{16}\text{H}_{22}\text{BFO}_2$, 292.1761; found 292.1766.

Boronic ester 3e. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3e** (43.1 mg, 78% yield) as a colorless oil. **3e**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.25–7.20 (m, 2H), 6.96–6.89 (m, 2H), 2.57 (s, 2H), 1.15 (s, 12H), 0.74 (q, $J = 3.6$ Hz, 2H), 0.44 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 161.37 (d, $J = 241.7$ Hz), 137.96 (d, $J = 3.3$ Hz), 130.36 (d, $J = 7.8$ Hz), 114.60 (d, $J = 21.0$ Hz), 83.27, 40.54, 24.69, 11.47; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{22}\text{BFO}_2$, 277.1775; found 277.1774.

Boronic ester 3f. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3f** (24.5 mg, 36% yield) as a colorless oil. **3f**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.38–7.33 (m, 2H), 7.17–7.13 (m, 2H), 2.55 (s, 2H), 1.15 (s, 12H), 0.76–0.72 (m, 2H), 0.46–0.42 (m, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 141.24, 130.84, 130.72, 119.32, 83.18, 40.64, 24.56, 11.43; **HRMS-ESI** (m/z) $[\text{M} + \text{OH}]^-$ calcd for $\text{C}_{16}\text{H}_{22}\text{BBrO}_2$, 352.0960; found 352.0964.

Boronic ester 3g. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3g** (48.7 mg, 75% yield) as a colorless oil. **3g**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.49 (d, $J = 8.0$ Hz, 2H), 7.39 (d, $J = 8.0$ Hz, 2H), 2.65 (s, 2H), 1.15 (s, 12H), 0.78 (q, $J = 3.6$ Hz, 2H), 0.46 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 146.61, 129.29, 128.04 (q, $J = 31.8$ Hz), 124.87, 124.85, 83.39, 41.28, 24.68, 11.73; **HRMS-ESI** (m/z) $[\text{M} + \text{OH}]^-$ calcd for $\text{C}_{17}\text{H}_{22}\text{BF}_3\text{O}_2$, 342.1729; found 342.1737.

Boronic ester 3h. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3h** (51.6 mg, 65% yield) as a colorless oil. **3h**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.77 (s, 2H), 7.69 (s, 1H), 2.67 (s, 2H), 1.15 (s, 12H), 0.82 (q, $J = 3.9$ Hz, 2H), 0.50 (q, $J = 3.9$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 145.11, 131.09 (q, $J = 32.7$ Hz), 129.30 (d, $J = 3.9$ Hz), 123.77 (q, $J = 272.6$ Hz), 119.78 (p, $J = 4.0$ Hz), 83.61, 41.58, 24.65, 12.18; **HRMS-ESI** (m/z) $[\text{M} + \text{OH}]^-$ calcd for $\text{C}_{18}\text{H}_{21}\text{BF}_6\text{O}_2$, 410.1603; found 410.1601.

Boronic ester 3i. Purification by preparative thin layer chromatography (9:1 hexanes:EtOAc) afforded boronic ester **3i** (34.5 mg, 61% yield) as a colorless oil. **3i**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.65 (s, 1H), 7.48 (dd, $J = 22.2, 8.3$ Hz, 2H), 7.33 (t, $J = 7.7$ Hz, 1H), 2.60 (s, 2H), 1.15 (s, 12H), 0.79 (q, $J = 3.7$ Hz, 2H), 0.47 (q, $J = 3.7$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 143.97, 133.65, 132.69, 129.52, 128.70, 119.43, 111.89, 83.46, 41.20, 24.67, 11.84; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{22}\text{BNO}_2$, 283.1858; found 283.1858.

Boronic ester 3j. Purification by preparative thin layer chromatography (9:1 hexanes:EtOAc) afforded boronic ester **3j** (42.2 mg, 70% yield) as a colorless oil. **3j**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.13 (d, $J = 8.2$ Hz, 2H), 6.66 (d, $J = 8.3$ Hz, 2H), 2.89 (s, 6H), 2.54 (s, 2H), 1.17 (s, 12H), 0.68 (q, $J = 3.7$ Hz, 2H), 0.40 (q, $J = 3.7$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 149.08, 130.55, 129.79, 112.87, 83.12, 41.16, 39.98, 24.74, 11.15; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{28}\text{BNO}_2$, 301.2328; found 301.2331.

Boronic ester 3k. Purification by preparative thin layer chromatography (18:1:1 hexanes:EtOAc:PhH) afforded boronic ester **3k** (51.8 mg, 90% yield) as a colorless oil. **3k**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.18 (d, $J = 8.6$ Hz, 2H), 6.79 (d, $J = 8.6$ Hz, 2H), 3.77 (s, 3H), 2.56 (s, 2H), 1.16 (s, 12H), 0.71 (q, $J = 3.6$ Hz, 2H), 0.42 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 157.74, 134.37, 130.01, 113.36, 83.17, 55.34, 40.27, 24.70, 11.29; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{25}\text{BO}_3$, 288.2011; found 288.2008.

Boronic ester 3l. Purification by preparative thin layer chromatography (3:1 hexanes:EtOAc) afforded boronic ester **3l** (61.3 mg, 88% yield) as a white solid. **3l**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 6.51 (s, 2H), 3.85 (s, 6H), 3.82 (s, 3H), 2.56 (s, 2H), 1.17 (s, 12H), 0.76 (q, $J = 3.5$ Hz, 2H), 0.46 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 152.76, 138.15, 136.04, 106.04, 83.18, 60.94, 56.09, 41.65, 24.76, 11.71; **HRMS-ESI** (m/z) [$\text{M} + \text{H}$] $^+$ calcd for $\text{C}_{19}\text{H}_{29}\text{BO}_5$, 348.2223; found 348.2215.

Boronic ester 3m. Purification by preparative thin layer chromatography (9:1 hexanes:EtOAc) afforded boronic ester **3m** (62.9 mg, 93% yield) as a white solid. **3m**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.07 (d, $J = 1.6$ Hz, 1H), 6.94 (dd, $J = 8.2, 1.6$ Hz, 1H), 6.90 (d, $J = 8.2$ Hz, 1H), 2.57 (s, 2H), 1.16 (s, 12H), 0.76 (q, $J = 3.6$ Hz, 2H), 0.44 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 143.64, 141.94, 138.70, 131.78 (t, $J = 253.7$ Hz), 123.77, 110.25, 108.67, 83.40, 41.31, 24.70, 11.69; **HRMS-ESI** (m/z) [$\text{M} + \text{OH}$] $^-$ calcd for $\text{C}_{17}\text{H}_{21}\text{BF}_2\text{O}_4$, 354.1565; found 354.1566.

Boronic ester 3n. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3n** (46.4 mg, 88% yield) as a colorless oil. **3n**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.18 (dd, $J = 4.9, 3.0$ Hz, 1H), 7.04–6.96 (m, 2H), 2.59 (s, 2H), 1.16 (s, 12H), 0.73 (q, $J = 3.5$ Hz, 2H), 0.43 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 142.83, 129.06,

124.51, 120.61, 83.22, 36.17, 24.70, 11.58; **HRMS-ESI** (m/z) $[M + H]^+$ calcd for $C_{14}H_{21}BO_2S$, 264.1470; found 264.1468.

Boronic ester 3o. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3o** (83.3 mg, 99% yield) as a white amorphous solid. **3o**: 1H NMR (600 MHz, $CDCl_3$): δ 7.70 (d, $J = 8.3$ Hz, 2H), 7.25 (d, $J = 8.4$ Hz, 2H), 7.03 (t, $J = 2.7$ Hz, 1H), 6.94 (s, 1H), 6.21 (d, $J = 1.5$ Hz, 1H), 2.38 (s, 3H), 2.31 (s, 2H), 1.11 (s, 12H), 0.68 (q, $J = 3.6$ Hz, 2H), 0.35 (q, $J = 3.6$ Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.63, 136.60, 129.92, 129.79, 126.82, 120.44, 117.86, 115.47, 83.16, 32.95, 24.63, 21.68, 11.50; **HRMS-ESI** (m/z) $[M + H]^+$ calcd for $C_{21}H_{28}BNO_4S$, 401.1947; found 401.1948.

Boronic ester 3p. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3p** (75.7 mg, 94% yield) as a yellow amorphous solid. **3p**: 1H NMR (600 MHz, $CDCl_3$): δ 7.62 (d, $J = 8.2$ Hz, 2H), 7.27 (d, $J = 7.7$ Hz, 2H), 7.23 (t, $J = 2.4$ Hz, 1H), 6.19–6.14 (m, 2H), 2.66 (s, 2H), 2.40 (s, 3H), 1.07 (s, 12H), 0.74 (q, $J = 3.7$ Hz, 2H), 0.36 (q, $J = 3.7$ Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.38, 136.89, 136.41, 129.91, 126.81, 122.04, 112.21, 111.45, 83.10, 33.69, 24.58, 21.72, 11.38; **HRMS-ESI** (m/z) $[M + H]^+$ calcd for $C_{21}H_{28}BNO_4S$, 401.1947; found 401.1944.

Boronic ester 3q. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3q** (32.8 mg, 66% yield) as a white solid. **3q**: 1H NMR (600 MHz, $CDCl_3$): δ 7.77 (s, 1H), 7.47 (s, 1H), 2.53 (s, 2H), 1.18 (s, 12H), 0.75 (q, $J = 3.6$ Hz, 2H), 0.49

(q, $J = 3.6$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 150.41, 140.79, 134.88, 83.31, 32.30, 24.72, 11.33; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{20}\text{BNO}_3$, 249.1651; found 249.1654.

Boronic ester 3r. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3r** (30.6 mg, 58% yield) as a colorless oil. **3r**: ^1H NMR (600 MHz, CDCl_3): δ 8.70 (d, $J = 2.0$ Hz, 1H), 7.08 (d, $J = 2.0$ Hz, 1H), 2.83 (s, 2H), 1.17 (s, 12H), 0.78 (q, $J = 3.6$ Hz, 2H), 0.52 (q, $J = 3.6$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 158.55, 151.64, 113.05, 83.27, 37.15, 24.68, 11.48; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{20}\text{BNO}_2\text{S}$, 265.1422; found 265.1428.

Boronic ester 3s. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3s** (46.0 mg, 87% yield) as a colorless oil. **3s**: ^1H NMR (600 MHz, CDCl_3): δ 8.61 (s, 1H), 7.63 (s, 1H), 2.77 (s, 2H), 1.17 (s, 12H), 0.80 (q, $J = 3.7$ Hz, 2H), 0.50 (q, $J = 3.7$ Hz, 2H). ^{13}C NMR (150 MHz, CDCl_3): δ 151.37, 140.71, 139.40, 83.51, 33.03, 24.67, 12.15; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{20}\text{BNO}_2\text{S}$, 265.1422; found 265.1428.

Boronic ester 3t. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3t** (29.5 mg, 50% yield) as a colorless oil. **3t**: ^1H NMR (600 MHz, CDCl_3): δ 8.70 (s, 1H), 8.32 (d, $J = 5.3$ Hz, 1H), 7.26 (d, $J = 5.3$ Hz, 1H), 2.78 (s, 2H), 1.19 (s, 12H), 0.86 (q, $J = 3.7$ Hz, 2H), 0.51 (t, $J = 3.1$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 151.33, 147.81, 144.15, 135.52, 124.14, 83.52, 35.54, 24.69, 11.87; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{21}\text{BClNO}_2$, 293.1468; found 293.1472.

Boronic ester 3u. Purification by preparative thin layer chromatography (6:1 hexanes:EtOAc) afforded boronic ester **3u** (51.8 mg, 93% yield) as a colorless oil. **3u**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.02 (d, $J = 4.0$ Hz, 1H), 7.86 (ddd, $J = 9.5, 7.3, 1.9$ Hz, 1H), 7.09 (ddd, $J = 7.0, 4.8, 1.8$ Hz, 1H), 2.62 (s, 2H), 1.15 (s, 12H), 0.80 (q, $J = 3.7$ Hz, 2H), 0.52 (q, $J = 3.7$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 162.23 (d, $J = 238.0$ Hz), 144.69 (d, $J = 14.5$ Hz), 141.12 (d, $J = 5.9$ Hz), 124.09 (d, $J = 31.0$ Hz), 121.01 (d, $J = 4.1$ Hz), 83.39, 33.70, 24.65, 11.68; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{21}\text{BFNO}_2$, 277.1764; found 277.1770.

Boronic ester 3v. Purification by preparative thin layer chromatography (9:1 hexanes:EtOAc) afforded boronic ester **3v** (26.0 mg, 45% yield) as a colorless oil. **3v**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.01 (s, 1H), 7.56 (dd, $J = 8.5, 2.4$ Hz, 1H), 6.64 (d, $J = 8.4$ Hz, 1H), 3.91 (s, 3H), 2.50 (s, 2H), 1.16 (s, 12H), 0.74 (q, $J = 3.6$ Hz, 2H), 0.44 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 162.68, 146.64, 139.77, 130.28, 109.92, 83.32, 53.39, 37.69, 24.72, 11.56; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{24}\text{BNO}_3$, 289.1964; found 289.1969.

Boronic ester 3w. Purification by preparative thin layer chromatography (4g of SiO_2 , Isco, 0–20% EtOAc/Heptanes) afforded boronic ester **3w** (156.0 mg, 95% yield) as a colorless oil. **3w**: $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.64–8.52 (m, 1H), 7.78 (dd, $J = 8.1, 2.1$ Hz, 1H), 7.53 (d, $J = 8.1$ Hz, 1H), 2.61 (s, 2H), 1.11 (s, 12H), 0.83–0.71 (m, 2H), 0.51–0.42 (m, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 150.83, 145.89 (q, $J = 34.4$ Hz), 141.39, 137.56, 122.05 (q, $J = 273.7$ Hz),

119.84 (q, $J = 2.9$ Hz), 83.63, 38.82, 24.74, 12.11; **HRMS-ESI** (m/z) [$M + H$] $^+$ calcd for $C_{16}H_{22}BF_3NO_2$, 322.1727; found 322.1727.

Boronic ester 3x. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3x** (24.7 mg, 48% yield) as a colorless oil. **3x**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.45 (d, $J = 5.1$ Hz, 2H), 7.22 (d, $J = 6.1$ Hz, 2H), 2.58 (s, 2H), 1.15 (s, 12H), 0.81 (q, $J = 3.7$ Hz, 2H), 0.47 (q, $J = 3.7$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 151.57, 149.31, 124.46, 83.45, 40.90, 24.66, 11.84; **HRMS-ESI** (m/z) [$M + H$] $^+$ calcd for $C_{15}H_{22}BNO_2$, 259.1858; found 259.1860.

Boronic ester 3z. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3z** (60.4 mg, 89% yield) as a colorless oil. **3z**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.21 (d, $J = 5.1$ Hz, 1H), 7.48 (s, 1H), 7.15 (d, $J = 5.0$ Hz, 1H), 2.53 (s, 2H), 1.17 (s, 12H), 0.82 (q, $J = 3.7$ Hz, 2H), 0.47 (q, $J = 3.7$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 154.89, 149.53, 142.12, 128.49, 123.63, 83.58, 40.75, 24.68, 12.01; **HRMS-ESI** (m/z) [$M + H$] $^+$ calcd for $C_{15}H_{21}BBrNO_2$, 337.0963; found 337.0962.

Boronic ester 3za. Purification by preparative thin layer chromatography (3:1 hexanes:EtOAc) afforded boronic ester **3za** (26.5 mg, 48% yield) as a colorless oil. **3za**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.57 (s, 2H), 2.70 (s, 3H), 2.50 (s, 2H), 1.16 (s, 12H), 0.80 (t, $J = 3.0$ Hz, 2H), 0.48 (q, $J = 3.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 165.55, 157.31, 131.86, 83.55, 36.09, 25.62, 24.72, 12.03; **HRMS-ESI** (m/z) [$M + H$] $^+$ calcd for $C_{15}H_{23}BN_2O_2$, 274.1967; found 274.1970.

Boronic ester 3zb. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3zb** (48.0 mg, 84% yield) as a white solid. **3zb**: $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 8.96 (s, 1H), 8.11–7.94 (m, 2H), 7.75–7.62 (m, 2H), 2.99 (s, 2H), 1.16 (s, 12H), 0.86–0.79 (m, 2H), 0.64–0.58 (m, 2H); $^{13}\text{C NMR}$ (101 MHz, CDCl_3): δ 157.62, 146.52, 145.88, 141.35, 129.88, 129.28, 129.12, 128.99, 83.63, 42.37, 41.39, 24.84, 12.18; **HRMS-ESI** (m/z) [$M + \text{H}$] $^+$ calcd for $\text{C}_{18}\text{H}_{23}\text{BN}_2\text{O}_2$, 310.1962; found 310.1967.

Boronic ester 3zc. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3zc** (48.0 mg, 78% yield) as a white solid. **3zc**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.84 (dd, $J = 4.2, 1.8$ Hz, 1H), 8.08 (d, $J = 8.3$ Hz, 1H), 7.99 (d, $J = 8.2$ Hz, 1H), 7.69 (d, $J = 9.9$ Hz, 2H), 7.35 (dd, $J = 8.2, 4.1$ Hz, 1H), 2.80 (s, 2H), 1.14 (s, 12H), 0.81 (q, $J = 3.5$ Hz, 2H), 0.53 (t, $J = 2.9$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 149.58, 147.26, 140.98, 135.73, 131.90, 128.76, 128.26, 126.63, 120.99, 83.32, 41.39, 24.68, 11.74; **HRMS-ESI** (m/z) [$M + \text{H}$] $^+$ calcd for $\text{C}_{19}\text{H}_{24}\text{BNO}_2$, 309.2015; found 309.2020.

Boronic ester 3zd. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded boronic ester **3zd** (12.6 mg, 21% yield) as a colorless oil. **3zd**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.64 (s, 1H), 8.48 (s, 1H), 8.06 (s, 1H), 6.64 (s, 1H), 2.60 (s, 2H), 1.16 (s, 12H), 0.85 (q, $J = 3.7$ Hz, 2H), 0.54 (q, $J = 3.7$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 152.18, 147.62, 144.46, 133.52, 122.49, 96.29, 83.69, 36.08, 24.76, 12.13; **HRMS-ESI** (m/z) [$M + \text{H}$] $^+$ calcd for $\text{C}_{16}\text{H}_{22}\text{BN}_3\text{O}_2$, 299.1920; found 299.1925.

Boronic ester 3ze. Purification by preparative thin layer chromatography (2:1 hexanes:EtOAc) afforded boronic ester **3ze** (44.7 mg, 66% yield) as a colorless oil. **3ze**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.71 (d, $J = 7.0$ Hz, 1H), 7.50 (d, $J = 7.5$ Hz, 1H), 7.20 (p, $J = 7.2$ Hz, 2H), 3.24 (tt, $J = 7.2, 3.9$ Hz, 1H), 3.04 (s, 2H), 1.21 (t, $J = 6.5$ Hz, 2H), 1.15 (s, 12H), 1.10 (q, $J = 5.4, 4.4$ Hz, 2H), 0.90 (q, $J = 3.8$ Hz, 2H), 0.58 (q, $J = 3.8$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 156.84, 142.58, 136.27, 121.66, 121.42, 119.42, 110.16, 83.26, 33.38, 24.99, 24.64, 11.31, 7.08; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{20}\text{H}_{27}\text{BN}_2\text{O}_2$, 338.2280; found 338.2285.

Boronic ester 3zf. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **3zf** (49.4 mg, 83% yield) as a white solid. **3zf**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.56 (d, $J = 2.3$ Hz, 1H), 7.48 (s, 1H), 7.36 (d, $J = 8.5$ Hz, 1H), 7.22 (dd, $J = 8.5, 1.8$ Hz, 1H), 6.69 (dd, $J = 2.3, 1.0$ Hz, 1H), 2.71 (s, 2H), 1.15 (s, 12H), 0.74 (q, $J = 3.6$ Hz, 2H), 0.47 (q, $J = 3.6$ Hz, 2H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 153.56, 144.76, 136.57, 127.10, 125.65, 121.01, 110.44, 106.44, 83.09, 40.96, 24.58, 11.31; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{18}\text{H}_{23}\text{BO}_3$, 298.1855; found 298.1854.

Boronic ester 4a. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **4a** (48.0 mg, 93% yield) as a colorless oil. **4a**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.32 (m, 4H), 7.26 – 7.21 (m, 1H), 7.20 (s, 1H), 2.39 (q, $J = 7.5$, 2H), 1.31 (s, 12H), 1.10 (t, $J = 7.5$ Hz, 3H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 141.37, 137.91, 128.95, 128.08,

127.01, 83.38, 24.80, 22.68, 14.66.; Note: The signal corresponding to the carbon atom bonded to boron was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) $[M + OH]^-$ calcd for $C_{16}H_{23}BO_2$, 274.1855; found 274.1852.

Boronic ester 4b. Purification by preparative thin layer chromatography (7:1 hexanes:EtOAc) afforded boronic ester **4b** (39.4 mg, 76% yield) as a colorless oil. **4b**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.55 (s, 1H), 8.45 (d, $J = 4.2$ Hz, 1H), 7.59 (d, $J = 7.9$ Hz, 1H), 7.24 (dd, $J = 7.9$ Hz, 4.2 Hz, 1H), 2.34 (q, $J = 7.5$ Hz, 2H), 1.29 (s, 12H), 1.08 (t, $J = 7.5$ Hz, 3H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 151.18, 148.12, 137.57, 136.12, 133.72, 123.30, 83.84, 25.00, 22.99, 14.74; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) $[M + H]^+$ calcd for $C_{15}H_{22}BNO_2$, 259.1858; found 259.1859.

Boronic ester 4f. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded boronic ester **4f** (53.0 mg, 79% yield) as a colorless oil. **4f**: $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.45 (d, $J = 8.4$ Hz, 2H), 7.18 (d, $J = 8.4$ Hz, 2H), 7.11 (s, 1H), 2.35 (q, $J = 7.5$ Hz, 3H), 1.31 (s, 12H), 1.08 (t, $J = 7.5$ Hz, 3H); $^{13}\text{C NMR}$ (150 MHz, CDCl_3): δ 139.99, 136.73, 131.24, 130.53, 120.97, 83.49, 24.78, 22.66, 14.51; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) $[M + OH]^-$ calcd for $C_{16}H_{22}BBrO_2$, 352.0960; found 352.0968.

Boronic ester 4j. Purification by preparative thin layer chromatography (9:1 hexanes:EtOAc) afforded boronic ester **4j** (55.1 mg, 91% yield) as a colorless oil. **4j**: $^1\text{H NMR}$ (600 MHz,

CDCl₃): δ 7.28 (d, J = 8.6 Hz, 2H), 7.09 (s, 1H), 6.67 (d, J = 8.6 Hz, 2H), 2.95 (s, 6H), 2.43 (q, J = 7.5 Hz, 2H), 1.28 (s, 12H), 1.10 (t, J = 7.5 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 149.75, 141.81, 130.72, 126.45, 112.04, 83.31, 40.58, 25.01, 22.91, 14.81; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) [$M + H$]⁺ calcd for C₁₈H₂₈BN₂O₂, 301.2328; found 301.2327.

Boronic ester 4k. Purification by preparative thin layer chromatography (10:1 hexanes:EtOAc) afforded boronic ester **4k** (52.3 mg, 91% yield) as a colorless oil. **4k**: ¹H NMR (600 MHz, CDCl₃): δ 7.29 (d, J = 8.6 Hz, 2H), 7.14 (s, 1H), 6.87 (d, J = 8.6 Hz, 2H), 3.81 (s, 3H), 2.40 (q, J = 7.4 Hz, 2H), 1.30 (s, 12H), 1.11 (q, J = 7.4 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 158.66, 140.95, 130.55, 130.44, 113.52, 83.27, 55.20, 24.79, 22.62, 14.58; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) [$M + H$]⁺ calcd for C₁₇H₂₅BO₃, 288.2011; found 288.2010.

Boronic ester 4l. Purification by preparative thin layer chromatography (5:1 hexanes:EtOAc) afforded boronic ester **4l** (65.0 mg, 93% yield) as a white solid. **4l**: ¹H NMR (600 MHz, CDCl₃): δ 7.26 (s, 1H), 6.58 (s, 2H), 3.86 (s, 3H), 3.84 (s, 6H), 2.42 (q, J = 7.5 Hz, 2H), 1.31 (s, 12H), 1.13 (t, J = 7.5 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ 152.82, 141.34, 137.20, 133.43, 106.14, 83.42, 60.91, 56.00, 24.80, 22.88, 14.61; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) [$M + H$]⁺ calcd for C₁₉H₂₉BO₅, 348.2223; found 348.2225.

Boronic ester 4r. Purification by preparative thin layer chromatography (10:1 hexanes:EtOAc) afforded boronic ester **4r** (34.7 mg, 65% yield) as a colorless oil. **4r**: ^1H NMR (600 MHz, CDCl_3): δ 8.80 (d, $J = 1.9$ Hz, 1H), 7.29 (d, $J = 1.9$ Hz, 1H), 7.23 (s, 1H) 2.70 (q, $J = 7.5$ Hz, 2H), 1.30 (s, 12H), 1.10 (q, $J = 7.5$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 154.66, 151.75, 132.95, 117.98, 83.49, 24.78, 23.15, 14.17; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{20}\text{BNO}_2\text{S}$, 265.1422; found 265.1422.

Boronic ester 4zc. Purification by preparative thin layer chromatography (10:1 hexanes:EtOAc) afforded boronic ester **4zc** (52.0 mg, 84% yield) as a white solid. **4zc**: ^1H NMR (600 MHz, CDCl_3): δ 8.86 (d, $J = 3.0$ Hz, 1H), 8.10 (d, $J = 8.1$ Hz, 1H), 8.03 (d, $J = 8.7$ Hz, 1H), 7.71 (s, 1H), 7.67 (dd, $J = 8.7, 1.9$ Hz, 1H), 7.36 (dd, $J = 8.1$ Hz, 3.0 Hz, 1H) 7.33 (s, 1H), 2.44 (q, $J = 7.5$ Hz, 2H) 2.80 (s, 2H), 1.31 (s, 12H), 1.13 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ 150.51, 147.61, 140.65, 136.48, 136.40, 131.10, 129.26, 128.32, 127.75, 121.45, 83.76, 25.02, 23.01, 14.85; Note: The carbon signal bound to the boron atom was not observed, likely due to quadrupolar relaxation. **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{24}\text{BNO}_2$, 309.2015; found 309.2015.

C. Exceptional pathway selectivity of thiazole-BCP.

entry	ligand	product ratio (3 : 4) in % yield
1	P(<i>t</i> -Bu) ₃ •HBF ₄	60 : 16
2	PCy ₃	77 : 6
3	PPh ₃	79 : 0
4	(<i>p</i> -CF ₃ -C ₆ H ₄) ₃ P	97 : 0
5	(C ₆ F ₅) ₃ P	78 : 0
<hr/>		
6	dppm	77 : 0
7	dppbz	49 : 15
8	dppe	70 : 6
9	<i>rac</i> -BINAP	87 : 0
10	xantphos	45 : 0

D. Derivatization Experiments.

Alcohol 5. Alcohol **5** was prepared according to a modified procedure.³ A 10-mL reaction vial with a magnetic stir bar was charged with NaBO₃ (29.9 mg, 0.30 mmol, 3.0 equiv), THF (1.0 mL), H₂O (1.0 mL), and boronic ester **3a** (25.8 mg, 0.10 mmol, 1.0 equiv). The mixture was allowed to stir at room temperature for 2 h. The reaction was then diluted with H₂O (2.0 mL) and extracted with EtOAc (4 × 3 mL). The combined organic layers were combined, dried over Na₂SO₄, concentrated, and purified by preparative thin layer chromatography (4:1 hexanes:EtOAc) to give alcohol **5** as a colorless oil (16.0 mg, 99% yield). Spectral data match those previously reported.⁴

Amine 6. Amine **6** was prepared according to a modified procedure.⁵ A flame-dried 10-mL reaction vial with a magnetic stir bar was charged with MeONH₂ (500 μ L, 1.0 M solution in THF, 0.50 mmol, 5.0 equiv) and THF (1.0 mL). The vial was cooled to -78 $^\circ\text{C}$, and *n*-BuLi (200 μ L, 2.5 M solution in hexane, 0.50 mmol, 5.0 equiv) was added dropwise over 1 min. The reaction was allowed to stir at -78 $^\circ\text{C}$ for 30 min. Then, a solution of boronic ester **3a** (25.8 mg, 0.10 mmol, 1.0 equiv) in 200 μ L of THF was added dropwise over 1 min. The reaction mixture was allowed to warm to room temperature and was then heated to 60 $^\circ\text{C}$ for 15 h. The reaction mixture was cooled to room temperature and quenched with H₂O (3.0 mL). The mixture were extracted with EtOAc (4 × 3 mL), and the combined organic layers were dried over Na₂SO₄, concentrated, and purified by preparative thin layer chromatography (9:1 EtOAc:MeOH) to give amine **6** (5.3 mg, 36% yield) as a colorless oil. Spectral data match those previously reported.⁶

Boronic ester 7. Boronic ester **7** was prepared according to a modified procedure.⁷ A flame-dried 10-mL reaction vial with a magnetic stir bar was charged with boronic ester **3a** (25.8 mg, 0.10 mmol, 1.0 equiv), THF (1.0 mL), and CH₂BrCl (7.8 μL, 0.12 mmol, 1.2 equiv). The vial was cooled to −78 °C, and *n*-BuLi (48 μL, 2.5 M solution in hexane, 0.12 mmol, 1.2 equiv) was added dropwise over 1 min. The reaction mixture was allowed to stir at −78 °C for 15 min and then at room temperature for 16 h. The reaction was quenched with saturated NH₄Cl (1.0 mL) and diluted with H₂O (2.0 mL). The mixture was extracted with EtOAc (4 × 2 mL), and the combined organic layers were dried over Na₂SO₄, concentrated, and purified by preparative thin layer chromatography (95:5 hexanes:EtOAc) to give boronic ester **7** (24.2 mg, 89% yield) as a colorless oil. **7**: ¹H NMR (600 MHz, CDCl₃): δ 7.29 (t, *J* = 7.4 Hz, 2H), 7.25 (d, *J* = 7.4 Hz, 2H), 7.21 (t, *J* = 7.3 Hz, 1H), 2.65 (s, 2H), 1.27 (s, 12H), 0.87 (s, 2H), 0.47 (q, *J* = 3.5, 3.1 Hz, 2H), 0.44 (d, *J* = 4.1 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃): δ 140.83, 129.69, 128.11, 125.95, 83.01, 45.18, 25.01, 24.69, 17.69, 12.36; **HRMS-ESI** (*m/z*) [*M* + *H*]⁺ calcd for C₁₇H₂₅BO₂, 272.2062; found 272.2065.

Trifluoroborate 8. Trifluoroborate **8** was prepared according to a modified procedure.⁸ A flame-dried 100-mL round-bottom flask with a stir bar was charged with KHF₂ (2.79 g, 35.8 mmol, 7.0 equiv), MeOH (40 mL), and boronic ester **3a** (1.31 g, 5.11 mmol, 1.0 equiv). The mixture was heated to 70 °C and allowed to stir vigorously for 4 h. The reaction mixture was then cooled to room temperature and concentrated. The remaining solids were triturated with a heptane:Et₂O (4:1) solvent mixture (60 mL) for 15 min. The solids were collected by filtration, and further washed with cold Et₂O (30 mL). The heptane/Et₂O filtrate was then discarded. The precipitate was then washed with hot MeCN (300 mL), and the filtrate was collected in a clean round-bottom flask. Upon concentration trifluoroborate **8** (988 mg, 81% yield) was obtained as a white solid. **8**: ¹H NMR (600 MHz, DMSO-*d*₆) δ 7.15 (t, *J* = 7.5 Hz, 2H), 7.10–7.07 (m, 2H), 7.07–

7.03 (m, 1H), 2.53 (s, 2H), 0.01 (q, $J = 2.6$ Hz, 2H), -0.42 (s, 2H); ^{13}C NMR (150 MHz, DMSO- d_6) δ 142.54, 129.89, 127.00, 124.44, 40.73, 6.70. **HRMS-ESI** (m/z) $[\text{M} - \text{K}]^+$ calcd for $\text{C}_{10}\text{H}_{11}\text{BF}_3$, 198.0942; found 198.0942.

Representative Procedure for Suzuki Couplings.

Suzuki product 9. Suzuki product **9** was prepared according to a modified procedure.⁹ A 10-mL reaction vial equipped with a magnetic stir bar was charged with trifluoroborate **8** (23.8 mg, 0.10 mmol, 1.0 equiv), $\text{Pd}(\text{dppf})\text{Cl}_2$ (7.3 mg, 0.01 mmol, 0.1 equiv), Cs_2CO_3 (97.8 mg, 0.30 mmol, 3.0 equiv), alkenyl triflate (46.0 mg, 0.20 mmol, 2.0 equiv), toluene (2.5 mL), and H_2O (250 μL). The vial was capped and purged with N_2 for 10 min at room temperature. The reaction vial was then placed in an aluminum heating block, which was kept at 90°C for 15 h. The reaction vial was then cooled to room temperature, and the crude mixture filtered through a pad of silica gel that was subsequently rinsed with 1:1 hexanes:EtOAc (15 mL). The filtrate was concentrated, and the resulting crude mixture was purified by preparative thin layer chromatography (hexanes) to provide Suzuki product **9** (11.3 mg, 53% yield) as a colorless oil. **9**: ^1H NMR (600 MHz, CDCl_3): δ 7.23 (t, $J = 7.5$ Hz, 2H), 7.16 (t, $J = 7.3$ Hz, 1H), 7.13 (d, $J = 7.5$ Hz, 2H), 5.29 (s, 1H), 2.67 (s, 2H), 2.02–1.99 (m, 2H), 1.89–1.85 (m, 2H), 1.57 (dd, $J = 7.6, 4.3$ Hz, 2H), 1.49–1.45 (m, 2H), 0.54 (d, $J = 4.1$ Hz, 2H), 0.49 (d, $J = 3.7$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 140.68, 139.08, 129.45, 127.84, 125.83, 123.58, 42.68, 27.70, 27.05, 25.36, 23.27, 22.80, 11.41; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{20}$, 213.1643; found 213.1639.

Any modifications from this representative procedure are specified in the following schemes.

Suzuki product 10. Purification by preparative thin layer chromatography (98:2 hexanes:EtOAc) afforded Suzuki product **10** (13.4 mg, 63% yield) as a colorless oil. **10**: ^1H NMR (600 MHz, CDCl_3): δ 7.26–7.23 (m, 2H), 7.17 (dd, $J = 20.4, 7.4$ Hz, 3H), 5.30 (s, 1H), 4.02 (d, $J = 2.7$ Hz, 2H), 3.72 (t, $J = 5.5$ Hz, 2H), 2.72 (s, 2H), 2.10 (s, 2H), 0.63 (q, $J = 4.2$ Hz, 2H), 0.57 (q, $J = 4.1$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 140.11, 137.37, 129.31, 128.05, 126.07, 121.84, 65.65, 64.58, 42.22, 27.06, 26.65, 11.38; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{15}\text{H}_{18}\text{O}$, 215.1436; found 215.1436.

Suzuki product 11. Purification by preparative thin layer chromatography (95:5 hexanes:EtOAc) afforded Suzuki product **11** (16.4 mg, 53% yield) as a colorless oil. **11**: ^1H NMR (600 MHz, CDCl_3): δ 7.24 (t, $J = 7.5$ Hz, 2H), 7.17 (t, $J = 7.5$ Hz, 1H), 7.12 (d, $J = 7.2$ Hz, 2H), 5.22 (s, 1H), 3.74 (s, 2H), 3.41 (s, 2H), 2.70 (s, 2H), 2.09 (s, 2H), 1.45 (s, 9H), 0.57 (d, $J = 4.1$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 155.10, 140.08, 138.38, 129.30, 128.05, 126.09, 120.08, 79.52, 43.63, 42.43, 41.26, 40.04, 28.62, 26.96, 11.44; **HRMS-ESI** (m/z) $[\text{M} + \text{Na}]^+$ calcd for $\text{C}_{20}\text{H}_{27}\text{NO}_2$, 336.1939; found 336.1941.

Suzuki product 12. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded Suzuki product **12** (24.9 mg, 84% yield) as a colorless oil. **12**: ^1H NMR (600 MHz, CDCl_3): δ 8.31 (s, 1H), 7.46 (dd, $J = 8.5, 2.5$ Hz, 1H), 7.19 (q, $J = 7.4, 6.8$ Hz, 3H), 6.95–6.90 (m, 2H), 2.90 (s, 2H), 1.05–1.00 (m, 2H), 0.89–0.86 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 164.70 (d, $J = 247.4$ Hz), 143.30 (dd, $J = 17.3, 4.6$ Hz), 139.96 (dd, $J = 7.1, 3.5$ Hz), 138.41, 129.30, 128.39, 127.65 (d, $J = 28.7$ Hz), 126.80, 124.67 (qd, $J = 33.4, 4.6$ Hz), 123.10 (q, $J = 271.7$ Hz), 44.01, 22.82 (d, $J = 3.6$ Hz), 11.98; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{13}\text{F}_4\text{N}$, 296.1062; found 296.1064.

Suzuki product 13. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded Suzuki product **13** (18.7 mg, 89% yield) as a colorless oil. **13**: ^1H NMR (600 MHz, CDCl_3): δ 8.99 (s, 1H), 8.43 (s, 2H), 7.20 (dq, $J = 14.1, 7.0$ Hz, 3H), 6.99 (d, $J = 7.1$ Hz, 2H), 2.92 (s, 2H), 1.06–1.00 (m, 2H), 0.92 (d, $J = 5.7$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ 157.82, 156.58, 138.35, 138.04, 129.32, 128.52, 126.80, 45.16, 22.69, 12.26; **HRMS-ESI** (m/z) $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{14}\text{H}_{14}\text{N}_2$, 211.1235; found 211.1239.

Suzuki product 14. Purification by preparative thin layer chromatography (4:1 hexanes:EtOAc) afforded Suzuki product **14** (15.7 mg, 70% yield) as a colorless oil. **14**: ¹H NMR (600 MHz, CDCl₃): δ 8.28 (d, *J* = 5.3 Hz, 1H), 7.23–7.12 (m, 3H), 7.05 (d, *J* = 6.8 Hz, 2H), 6.95–6.78 (m, 2H), 3.00 (s, 2H), 2.46 (s, 3H), 0.94 (s, 4H); ¹³C NMR (150 MHz, CDCl₃): δ 158.06, 154.69, 148.84, 139.02, 129.30, 128.22, 126.35, 122.67, 120.45, 43.66, 24.62, 24.51, 14.25; HRMS-ESI (*m/z*) [M + H]⁺ calcd for C₁₆H₁₇N, 224.1439; found 224.1444.

Computational Methods

All DFT calculations were performed with Gaussian 16.¹⁰ Geometry optimizations were performed in the gas phase with the M06L functional¹¹ with a mixed basis set of LANL2DZ for Cu and 6-31G(d) for other atoms. Single point calculations were performed at the M06 level of theory with a mixed basis set of SDD for Cu and 6-311+G(d,p) for other atoms in THF using the SMD solvation model.¹² Gibbs free energies were calculated at the standard conditions (298K, 1 mol/L) using Cramer and Truhlar's quasiharmonic approximation¹³ using Goodvibes v2.0.1.¹⁴ Images of structures were generated using CYLview.¹⁵

Additional Computational Results

The proposed mechanisms of the Cu-catalyzed hydroboration of benzyldenecyclopropane (BCP) are presented in Scheme S1. The [L]Cu(I)—OR complex first undergoes borylation with B₂(pin)₂ to form the [L]Cu(I)—B(pin) intermediate **IM2**. Subsequent migratory insertion of the BCP substrate **1a** into Cu-Bpin forms benzylic copper(I) complex **2**, a key common intermediate to form both alkenyl boronates (**4a**) and boronic esters (**3a**). The two different products are generated through distinct transition states. Protodecupration (**TS2**) of **2** releases the boronic ester product **3a** and regenerates **IM1**. Conversely, β-carbon elimination (**TS1**) may take place to cleave the cyclopropane ring. A subsequent protodecupration (**TS3**) would then form the alkenyl boronate product **4a**.

Scheme S1. Proposed reaction mechanisms.

The computed energy profiles for the two competing pathways with the (*S*)-BINAP and dppe-supported Cu(I)-B(pin) complexes are shown in Figure S1. In reactions using both (*S*)-BINAP and dppe ligands, the key intermediates **16** and **20** are generated via an irreversible BCP migratory insertion (**TS4** and **TS6**). In reaction with the (*S*)-BINAP ligand, the Cu-Bpin complex preferentially adds to the *Re*-face of the BCP double bond, leading to the (*R*)-benzylic Cu(I) complex **16**. Addition to the opposite face of BCP (*vide infra*) requires higher barrier. Nonetheless, this newly formed benzylic chiral center is ablated in subsequent steps, eventually leading to achiral products in both pathways depicted in Scheme S1. The benzylic Cu(I) intermediates **16** and **20** adopt a distorted tetrahedral conformation with one of the oxygen atoms on Bpin datively bonded onto the Cu center, where the distortion from the tetrahedral geometry is more substantial in the (*S*)-BINAP-bound species **16**. From the dppe-supported complex **20**, the β -carbon elimination transition state (**TS1a**) is more favorable over protodecupration (**TS2a**) by 3.2 kcal/mol, leading to the formation of the alkenyl boronate product **4a**. The most favorable β -carbon elimination transition state (**TS1a**) places the Ph and Bpin groups on the opposite sides

of the double bond, leading to the experimentally observed *Z* stereoisomer of the alkenyl boronate. Another β -carbon elimination transition state (**TS8**), which would eventually lead to the *E*-stereoisomer of the alkenyl boronate, is 3.5 kcal/mol less stable than **TS1a**.

In contrast, the (*S*)-BINAP-supported complex **16** favors the protodecupration (**TS2b**) over β -carbon elimination (**TS1b**) by 3.2 kcal/mol, leading to the formation of the boronic ester. This less favorable β -carbon elimination transition state, **TS1b**, would eventually lead to the *Z*-alkenyl boronate. The β -carbon elimination to form the *E*-double bond is expected to be even less favorable, because of the steric repulsions between Ph and BPin groups. However, after multiple attempts, this β -carbon elimination transition state still cannot be located, because of the unfavorable steric interactions in this transition state.

Overall, the computational studies indicated the hydroboration reaction with the dppe-support Cu catalyst favors the *Z*-alkenyl boronate **4a**, while the use of BINAP-supported Cu catalyst leads to the cyclopropylboronic ester **3a**. This reversal of product selectivity is in good agreement with experiment.

Figure S1. Computed reaction energy profiles of the hydroboration of benzylidenecyclopropane **1** with (S)-BINAP (top) and dppe (bottom)-supported Cu catalysts.

We also considered the alternative pathway with the (*S*)-BINAP ligand that initiates via the Cu-Bpin complex adding to the opposite face of the BCP π bond. The computed energy profile in this pathway is shown in Figure S2. The calculations suggest this pathway is much less favorable because the initial migratory insertion (**TS1BINAP2**) is much less favorable than the competing pathway via **TS4**.

Figure S2. Alternative diastereomeric TS with the (*S*)-BINAP-supported Cu catalyst.

Two β -carbon elimination transition states with (*S*)-BINAP as ligand were located (Figure S3). In the more favorable transition state **TS1b**, the γ - and benzylic carbons (highlighted in pink) are placed in the less occupied quadrants II and IV. In **TS1b'**, the γ - and benzylic carbons are placed in the more occupied quadrants I and III. Therefore, greater steric repulsions with the ligand are observed in **TS1b'**.

Figure S3. β -Carbon elimination transition states for (*S*)-BINAP.

The optimized geometries of the protodecupration transition states with both dppe and BINAP ligands (**TS2a** and **TS2b**, respectively) are shown in Figure S4. These transition states are less crowded than the β -carbon elimination transition states due to a smaller substrate bite

angle. Therefore, both **TS2a** and **TS2b** experience smaller ligand-substrate steric repulsions and are less distorted from the tetrahedral geometry.

Figure S4. Protodecupration transition states.

Cartesian Coordinates

Cartesian coordinates of the structures shown in **Figure S1**:

Filename: MeOH

SCF Energy (M06L/LANL2DZ-6-31g(d))

-115.692955 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-115.692635 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-115.636826 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-115.660729 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.655483	-0.019172	0.000011
2	1	0	1.073330	0.991638	-0.000567
3	1	0	1.037223	-0.542427	-0.892708
4	1	0	1.037279	-0.541438	0.893289
5	8	0	-0.744772	0.121744	-0.000020
6	1	0	-1.122555	-0.766697	0.000080

Filename: 1

SCF Energy (M06L/LANL2DZ-6-31g(d))

-386.969332 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-386.818925 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-386.642267 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-386.682117 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.793223	1.016397	0.000010
2	6	0	3.579178	-0.291321	-0.000002
3	6	0	2.122609	-0.279178	-0.000001
4	6	0	0.988214	-0.976357	-0.000005
5	1	0	1.058229	-2.067300	-0.000016
6	6	0	-0.365631	-0.431439	-0.000003
7	6	0	-1.459696	-1.310037	0.000003
8	6	0	-0.628022	0.949125	-0.000006
9	6	0	-2.765756	-0.833723	0.000005
10	1	0	-1.271639	-2.384289	0.000004
11	6	0	-1.931716	1.424755	-0.000004
12	1	0	0.206472	1.648057	-0.000009
13	6	0	-3.008426	0.537313	0.000002
14	1	0	-3.597669	-1.536277	0.000007
15	1	0	-2.112985	2.498625	-0.000005
16	1	0	-4.029652	0.914105	0.000004
17	1	0	4.109104	-0.568119	-0.912145
18	1	0	4.109105	-0.568136	0.912136
19	1	0	2.792586	1.615074	-0.912255
20	1	0	2.792587	1.615058	0.912285

Filename: 2

SCF Energy (M06L/LANL2DZ-6-31g(d))

-798.849867 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-798.605633 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-798.221136 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-798.282519 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.394919	-0.468984	0.031782
2	1	0	-0.983311	-1.462711	0.232762
3	6	0	-2.855867	-0.436269	0.016079
4	6	0	-3.543861	-1.623182	-0.293149
5	6	0	-3.623789	0.699530	0.327924
6	6	0	-4.931053	-1.666651	-0.336003
7	1	0	-2.964806	-2.520098	-0.514446
8	6	0	-5.012906	0.653897	0.296628
9	1	0	-3.128245	1.616226	0.638497
10	6	0	-5.673719	-0.523846	-0.045299
11	1	0	-5.436317	-2.597138	-0.589831
12	1	0	-5.584731	1.544859	0.551328
13	1	0	-6.761558	-0.555021	-0.069972
14	6	0	-0.489064	0.509501	-0.211365
15	5	0	1.009154	0.135216	-0.116035
16	8	0	1.480666	-1.126841	0.172152
17	8	0	2.017496	1.052839	-0.316204
18	6	0	2.903000	-0.992282	0.417223
19	6	0	3.257993	0.303659	-0.376987
20	6	0	-0.824599	1.929223	-0.587772
21	1	0	-0.129721	2.254298	-1.375198
22	1	0	-1.832899	1.997328	-1.017596
23	6	0	-0.686928	2.896201	0.585934
24	1	0	-1.359113	2.628352	1.411765
25	1	0	0.335782	2.881203	0.981244
26	1	0	-0.914825	3.925955	0.286120
27	6	0	3.078889	-0.829687	1.921167
28	1	0	2.618223	-1.680752	2.433348
29	1	0	4.137318	-0.789793	2.204750
30	1	0	2.591745	0.084023	2.281305
31	6	0	3.602442	-2.246483	-0.066905
32	1	0	4.691273	-2.147717	0.029392
33	1	0	3.289453	-3.106773	0.534634
34	1	0	3.366334	-2.463762	-1.112542
35	6	0	4.364663	1.141070	0.231770
36	1	0	5.303624	0.574484	0.274971
37	1	0	4.539539	2.033458	-0.378980
38	1	0	4.113560	1.470712	1.244031
39	6	0	3.538977	0.036557	-1.849486
40	1	0	2.754359	-0.584522	-2.296927
41	1	0	3.566108	0.987862	-2.391051
42	1	0	4.501594	-0.468070	-1.994278

Filename: 3

SCF Energy (M06L/LANL2DZ-6-31g(d))

-798.840914 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-798.601016 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-798.217012 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-798.276646 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.596563	1.647217	-0.930343
2	6	0	-0.288519	1.960468	-0.228475
3	6	0	0.273973	3.363027	-0.385880
4	6	0	-0.317233	2.956512	0.914288
5	1	0	-0.287953	4.050699	-1.016024
6	1	0	0.350037	2.787518	1.756658
7	5	0	0.735032	0.804192	-0.144256
8	8	0	1.784969	0.777591	0.745283
9	8	0	0.686793	-0.297459	-0.963697
10	6	0	2.622586	-0.343524	0.355925
11	6	0	1.614565	-1.261307	-0.403517
12	6	0	3.224770	-0.957720	1.602897
13	1	0	3.798988	-1.859352	1.354124
14	1	0	3.907074	-0.247042	2.081996
15	1	0	2.455039	-1.229006	2.331051
16	6	0	3.711802	0.214045	-0.549732
17	1	0	3.284926	0.643285	-1.464000
18	1	0	4.249925	1.008841	-0.022329
19	1	0	4.435850	-0.557169	-0.838214
20	6	0	2.217666	-2.073498	-1.531191
21	1	0	2.985842	-2.758859	-1.150586
22	1	0	1.441479	-2.675464	-2.015873
23	1	0	2.672372	-1.433637	-2.293141
24	6	0	0.802736	-2.150958	0.528536
25	1	0	-0.041041	-2.576624	-0.025380
26	1	0	1.404165	-2.972744	0.935607
27	1	0	0.389134	-1.575252	1.365185
28	1	0	1.354037	3.480136	-0.448602
29	1	0	-1.288625	3.370491	1.181786
30	1	0	-1.409981	1.465753	-1.999159
31	6	0	-2.324759	0.453166	-0.360907
32	6	0	-2.991415	-0.437968	-1.206451
33	6	0	-2.348315	0.198578	1.015001
34	6	0	-3.670158	-1.542157	-0.699543
35	1	0	-2.966993	-0.263514	-2.282850
36	6	0	-3.023501	-0.906390	1.527255
37	1	0	-1.822387	0.871605	1.692038
38	6	0	-3.689057	-1.781428	0.672527
39	1	0	-4.179404	-2.223385	-1.379935
40	1	0	-3.027138	-1.085558	2.601787
41	1	0	-4.215436	-2.646530	1.072463
42	1	0	-2.250625	2.535396	-0.890336

Filename: 4

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2985.837834 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2986.317682 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2985.462819 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2985.582906 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	1.675047	0.018982	-0.028453
2	15	0	0.001472	1.700649	0.147385
3	15	0	0.030479	-1.689812	-0.182273
4	6	0	-1.429178	1.175167	1.168017
5	6	0	-0.676999	2.229345	-1.464803
6	6	0	0.591409	3.250713	0.920575
7	6	0	0.617382	-3.237558	-0.960963
8	6	0	-0.597876	-2.219373	1.450436
9	6	0	-1.430426	-1.183894	-1.167568
10	6	0	-2.357005	0.227309	0.720559
11	6	0	-1.435935	1.559472	2.536355
12	6	0	-0.040313	1.749306	-2.615373
13	6	0	-1.785021	3.073881	-1.603118
14	6	0	-0.244814	4.324625	1.257672
15	6	0	1.968816	3.359570	1.147694
16	6	0	1.998037	-3.357645	-1.162073
17	6	0	-0.221958	-4.301074	-1.322773
18	6	0	0.024220	-1.678962	2.581972
19	6	0	-1.654406	-3.121776	1.620809
20	6	0	-1.452817	-1.550775	-2.540763
21	6	0	-2.369631	-0.261726	-0.692093
22	6	0	-3.332670	-0.294404	1.628186
23	6	0	-2.344353	1.042478	3.422471
24	1	0	-0.694534	2.274286	2.887893
25	1	0	0.817017	1.080355	-2.508426
26	6	0	-0.499451	2.108633	-3.879797
27	6	0	-2.245072	3.429880	-2.865645
28	1	0	-2.313100	3.427653	-0.717509
29	1	0	-1.321716	4.243429	1.108668
30	6	0	0.287757	5.486431	1.803872
31	6	0	2.499145	4.528176	1.691977
32	1	0	2.623705	2.521478	0.897057
33	1	0	2.654993	-2.525526	-0.897432
34	6	0	2.528260	-4.528096	-1.702159
35	6	0	0.310754	-5.464445	-1.865738
36	1	0	-1.301283	-4.208719	-1.198855
37	1	0	0.842912	-0.967251	2.449401
38	6	0	-0.401356	-2.032410	3.859591
39	6	0	-2.081522	-3.471589	2.896626
40	1	0	-2.165416	-3.532148	0.749880
41	1	0	-0.700142	-2.241744	-2.915270
42	6	0	-2.389207	-1.044726	-3.403420
43	6	0	-3.378164	0.242776	-1.573571

44	6	0	-4.315716	-1.234599	1.223867
45	6	0	-3.316680	0.109019	3.000466
46	1	0	-2.325031	1.346545	4.469310
47	1	0	0.000321	1.722696	-4.766698
48	6	0	-1.602654	2.948545	-4.005379
49	1	0	-3.120871	4.069795	-2.961342
50	1	0	-0.370146	6.314035	2.064523
51	6	0	1.662643	5.590807	2.018164
52	1	0	3.572026	4.599917	1.862663
53	1	0	3.603470	-4.608648	-1.853105
54	6	0	1.688653	-5.580934	-2.051763
55	1	0	-0.349608	-6.283543	-2.146305
56	1	0	0.085609	-1.598537	4.731345
57	6	0	-1.455834	-2.927646	4.017364
58	1	0	-2.918204	-4.157924	3.017532
59	1	0	-2.380455	-1.333028	-4.454822
60	6	0	-3.378077	-0.143407	-2.950858
61	6	0	-4.378132	1.151473	-1.139386
62	1	0	-4.341066	-1.557593	0.184915
63	6	0	-5.225002	-1.745672	2.120733
64	6	0	-4.258723	-0.441952	3.900319
65	1	0	-1.971205	3.222374	-4.992774
66	1	0	2.077457	6.502673	2.445058
67	1	0	2.103532	-6.493797	-2.476420
68	1	0	-1.798849	-3.197330	5.015044
69	6	0	-4.351087	0.393313	-3.826015
70	6	0	-5.318060	1.648237	-2.012484
71	1	0	-4.393066	1.461554	-0.096371
72	1	0	-5.969244	-2.465099	1.783007
73	6	0	-5.197509	-1.351460	3.473997
74	1	0	-4.223514	-0.127480	4.943596
75	1	0	-4.327082	0.092674	-4.873682
76	6	0	-5.305824	1.271722	-3.370920
77	1	0	-6.075003	2.342739	-1.651523
78	1	0	-5.918488	-1.766475	4.176077
79	1	0	-6.050783	1.675716	-4.054145
80	6	0	5.870553	0.464374	0.626497
81	6	0	5.876731	-0.433328	-0.641474
82	8	0	4.503345	0.936044	0.662527
83	8	0	4.507620	-0.897544	-0.696202
84	5	0	3.695954	0.021211	-0.022040
85	6	0	6.105195	-0.323508	1.909770
86	1	0	7.144670	-0.664236	1.999439
87	1	0	5.877479	0.313479	2.771353
88	1	0	5.447733	-1.199242	1.956478
89	6	0	6.800784	1.660705	0.567369
90	1	0	6.722664	2.242987	1.492923
91	1	0	7.846976	1.343871	0.458800
92	1	0	6.553283	2.323610	-0.267142
93	6	0	6.799270	-1.634931	-0.569699
94	1	0	6.730600	-2.216660	-1.496349
95	1	0	7.845662	-1.324135	-0.446586
96	1	0	6.536468	-2.296503	0.261216
97	6	0	6.133245	0.353087	-1.921422
98	1	0	7.175680	0.688183	-1.996807
99	1	0	5.913924	-0.282792	-2.785984
100	1	0	5.481234	1.232339	-1.977179

Filename: 5

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.880431 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.204726 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.170267 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.306074 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.846739	1.732619	0.659259
2	1	0	3.076922	1.383800	1.678641
3	6	0	3.856632	1.112014	-0.287666
4	6	0	2.531545	3.168747	0.736375
5	5	0	4.105612	-0.382824	-0.012677
6	6	0	2.782820	4.151576	-0.247474
7	6	0	1.848072	3.627563	1.891617
8	8	0	5.192889	-1.093217	-0.477445
9	8	0	3.225030	-1.182728	0.701709
10	6	0	2.357122	5.470636	-0.094197
11	1	0	3.303412	3.888382	-1.164647
12	6	0	1.418839	4.935742	2.040101
13	1	0	1.636085	2.899272	2.679949
14	6	0	4.910250	-2.495640	-0.265514
15	6	0	3.891011	-2.453442	0.915223
16	6	0	1.663946	5.881932	1.039478
17	1	0	2.583855	6.191061	-0.882117
18	1	0	0.890481	5.224602	2.949606
19	6	0	6.208069	-3.215702	0.042208
20	6	0	4.302861	-3.025122	-1.556828
21	6	0	2.847555	-3.552402	0.913458
22	6	0	4.574138	-2.373786	2.273704
23	1	0	1.335693	6.913488	1.152223
24	1	0	6.021975	-4.268371	0.291844
25	1	0	6.867463	-3.189567	-0.832123
26	1	0	6.740518	-2.750983	0.876801
27	1	0	5.002400	-2.856735	-2.382508
28	1	0	4.091540	-4.100478	-1.499253
29	1	0	3.371396	-2.500442	-1.800312
30	1	0	3.318147	-4.542953	0.965674
31	1	0	2.196737	-3.443773	1.790519
32	1	0	2.214335	-3.514477	0.019224
33	1	0	3.825296	-2.149393	3.040957
34	1	0	5.062427	-3.319388	2.538539
35	1	0	5.329466	-1.579299	2.290183
36	29	0	1.090270	0.775138	0.321693
37	15	0	-0.449784	-0.295387	1.705198
38	15	0	-0.262773	0.619426	-1.596666
39	6	0	-1.353300	-1.624784	0.827373
40	6	0	-1.692565	0.913084	2.285444
41	6	0	0.148956	-1.077424	3.246387
42	6	0	0.189343	1.874802	-2.842060
43	6	0	-0.229762	-0.976642	-2.469803

44	6	0	-2.032796	0.935472	-1.199686
45	6	0	-2.298293	-1.363234	-0.170549
46	6	0	-0.875693	-2.953373	0.995644
47	6	0	-1.482905	2.259738	1.964267
48	6	0	-2.824280	0.558332	3.029163
49	6	0	-0.614654	-1.944717	4.040406
50	6	0	1.439610	-0.732876	3.664293
51	6	0	0.496444	3.154641	-2.355216
52	6	0	0.363970	1.609785	-4.204520
53	6	0	0.711770	-1.923921	-2.050669
54	6	0	-1.122224	-1.308033	-3.497473
55	6	0	-2.568295	2.223361	-1.462659
56	6	0	-2.791109	0.016355	-0.464920
57	6	0	-2.828219	-2.444066	-0.947047
58	6	0	-1.340662	-3.989068	0.229647
59	1	0	-0.116635	-3.148325	1.749854
60	1	0	-0.598816	2.546076	1.387952
61	6	0	-2.389523	3.233304	2.374705
62	6	0	-3.732900	1.530127	3.432350
63	1	0	-3.009254	-0.487765	3.273687
64	1	0	-1.610322	-2.244772	3.712480
65	6	0	-0.100481	-2.447496	5.230418
66	6	0	1.948373	-1.228158	4.863754
67	1	0	2.044859	-0.084362	3.027487
68	1	0	0.425153	3.359842	-1.284581
69	6	0	0.932778	4.155210	-3.215740
70	6	0	0.819699	2.609294	-5.061377
71	1	0	0.162404	0.614765	-4.597596
72	1	0	1.387049	-1.672088	-1.226349
73	6	0	0.764691	-3.177986	-2.653854
74	6	0	-1.067728	-2.561228	-4.098172
75	1	0	-1.878848	-0.586352	-3.808484
76	1	0	-1.983553	2.932913	-2.043647
77	6	0	-3.803148	2.594931	-0.997923
78	6	0	-4.094913	0.380888	-0.002641
79	6	0	-3.823916	-2.247482	-1.939110
80	6	0	-2.333266	-3.772296	-0.752381
81	1	0	-0.949527	-4.997037	0.373026
82	1	0	-2.212353	4.275671	2.114316
83	6	0	-3.517281	2.868213	3.105027
84	1	0	-4.621422	1.240747	3.991389
85	1	0	-0.700864	-3.123439	5.837128
86	6	0	1.180121	-2.084428	5.647123
87	1	0	2.951805	-0.947963	5.181021
88	1	0	1.171604	5.137729	-2.811828
89	6	0	1.097287	3.883310	-4.572805
90	1	0	0.961468	2.387347	-6.117871
91	1	0	1.494378	-3.912832	-2.313668
92	6	0	-0.124795	-3.497146	-3.676988
93	1	0	-1.778274	-2.816973	-4.882484
94	1	0	-4.189252	3.593082	-1.205277
95	6	0	-4.596049	1.697299	-0.250215
96	6	0	-4.913674	-0.514816	0.733229
97	1	0	-4.211157	-1.244783	-2.107926
98	6	0	-4.300899	-3.297631	-2.689574
99	6	0	-2.834405	-4.828296	-1.547976
100	1	0	-4.234627	3.625483	3.417723

101	1	0	1.579057	-2.475058	6.581720
102	1	0	1.457346	4.659391	-5.245947
103	1	0	-0.093336	-4.482231	-4.139680
104	6	0	-5.864799	2.066685	0.254863
105	6	0	-6.147400	-0.129258	1.203533
106	1	0	-4.548383	-1.520242	0.933829
107	1	0	-5.067547	-3.117412	-3.441463
108	6	0	-3.801736	-4.601740	-2.498976
109	1	0	-2.437140	-5.830854	-1.387544
110	1	0	-6.224375	3.077646	0.062479
111	6	0	-6.629580	1.174792	0.968664
112	1	0	-6.754826	-0.835945	1.766716
113	1	0	-4.182694	-5.423989	-3.102019
114	1	0	-7.605275	1.470371	1.350212
115	6	0	3.881528	1.416940	-1.785224
116	6	0	5.017864	1.858899	-0.928787
117	1	0	5.108432	2.917209	-0.696391
118	1	0	5.969288	1.339829	-1.033635
119	1	0	3.168960	2.153897	-2.153785
120	1	0	4.052960	0.593173	-2.479961

Filename: 6

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.887308 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.205401 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.170309 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.306164 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.295149	0.344999	-0.074633
2	1	0	-4.441025	0.623305	0.974965
3	6	0	-3.480160	1.137298	-0.813124
4	6	0	-4.987481	-0.884407	-0.458400
5	6	0	-1.533080	1.297308	-2.369874
6	6	0	-2.998186	0.860990	-2.219376
7	5	0	-2.880409	2.430046	-0.184121
8	6	0	-5.357748	-1.194635	-1.780074
9	6	0	-5.333045	-1.811906	0.541306
10	1	0	-1.073063	0.778992	-3.227959
11	1	0	-1.502883	2.373092	-2.607282
12	1	0	-3.662810	1.359975	-2.951679
13	1	0	-3.094195	-0.213107	-2.435195
14	8	0	-2.976663	3.663680	-0.788119
15	8	0	-2.221165	2.483231	1.029965
16	6	0	-5.984813	-2.397740	-2.086150
17	1	0	-5.182923	-0.466533	-2.567994
18	6	0	-5.950698	-3.017591	0.236532
19	1	0	-5.106715	-1.570150	1.580548
20	6	0	-2.095542	4.560206	-0.070153
21	6	0	-1.991560	3.882274	1.334554
22	6	0	-6.269567	-3.324170	-1.085090
23	1	0	-6.264296	-2.608427	-3.117813
24	1	0	-6.187309	-3.720824	1.034107
25	6	0	-2.710872	5.945306	-0.058833
26	6	0	-0.771619	4.568331	-0.821186
27	6	0	-0.631101	4.022748	1.989986
28	6	0	-3.097646	4.300979	2.292031
29	1	0	-6.757224	-4.266636	-1.329338
30	1	0	-2.104897	6.636444	0.541417
31	1	0	-2.759003	6.341174	-1.079107
32	1	0	-3.727171	5.935394	0.346061
33	1	0	-0.946301	4.867426	-1.861065
34	1	0	-0.047808	5.264276	-0.379153
35	1	0	-0.324584	3.564437	-0.838887
36	1	0	-0.358359	5.080288	2.102387
37	1	0	-0.642181	3.568540	2.987049
38	1	0	0.145304	3.524853	1.395936
39	1	0	-3.082044	3.638784	3.165402
40	1	0	-2.971066	5.334679	2.636551
41	1	0	-4.083273	4.213186	1.819891
42	29	0	-0.447666	0.920142	-0.709924
43	15	0	1.937253	1.324822	-0.692048

44	15	0	-0.498523	-0.667656	1.008268
45	6	0	1.907550	-0.297944	-1.580193
46	6	0	3.358065	1.200312	0.457997
47	6	0	2.496346	2.565991	-1.921711
48	6	0	-1.329339	-0.163122	2.549629
49	6	0	-1.356450	-2.195295	0.492001
50	6	0	1.137029	-1.300024	1.563218
51	6	0	1.789980	-1.502242	-0.874135
52	6	0	1.733979	-0.302872	-2.989030
53	6	0	3.184141	1.598113	1.787643
54	6	0	4.605756	0.701641	0.059467
55	6	0	1.558083	2.995639	-2.874511
56	6	0	3.753817	3.182623	-1.897063
57	6	0	-0.728344	0.797838	3.374392
58	6	0	-2.628524	-0.581229	2.850080
59	6	0	-1.834742	-2.263820	-0.819120
60	6	0	-1.515602	-3.298892	1.340674
61	6	0	1.462071	-1.465394	2.933699
62	6	0	2.081295	-1.615376	0.587347
63	6	0	1.459366	-2.707601	-1.573554
64	6	0	1.435519	-1.452879	-3.671911
65	1	0	1.832753	0.631284	-3.537405
66	1	0	2.212099	1.978932	2.106209
67	6	0	4.229771	1.498394	2.701769
68	6	0	5.652192	0.604949	0.970268
69	1	0	4.748535	0.371555	-0.970490
70	1	0	0.561728	2.551458	-2.874125
71	6	0	1.881876	3.984142	-3.797118
72	6	0	4.070025	4.181893	-2.814584
73	1	0	4.491522	2.891316	-1.152385
74	1	0	0.277701	1.151878	3.141938
75	6	0	-1.398511	1.306434	4.480218
76	6	0	-3.309250	-0.056133	3.945871
77	1	0	-3.114917	-1.315580	2.211081
78	1	0	-1.683980	-1.405376	-1.477428
79	6	0	-2.478053	-3.410757	-1.275772
80	6	0	-2.162302	-4.442589	0.884896
81	1	0	-1.137023	-3.255097	2.363314
82	1	0	0.713203	-1.239453	3.689653
83	6	0	2.703117	-1.901045	3.321794
84	6	0	3.360635	-2.125839	0.974763
85	6	0	1.275146	-3.942057	-0.898936
86	6	0	1.264611	-2.678529	-2.989823
87	1	0	1.309930	-1.429210	-4.754419
88	1	0	4.076299	1.800955	3.736367
89	6	0	5.464472	1.000186	2.293543
90	1	0	6.610978	0.198754	0.651934
91	1	0	1.139714	4.298343	-4.529391
92	6	0	3.140602	4.581100	-3.770659
93	1	0	5.052298	4.650564	-2.778645
94	1	0	-0.909764	2.044303	5.115848
95	6	0	-2.696617	0.884826	4.767620
96	1	0	-4.324421	-0.389867	4.158059
97	1	0	-2.856814	-3.448504	-2.295837
98	6	0	-2.646447	-4.497016	-0.422695
99	1	0	-2.290351	-5.294975	1.550653
100	1	0	2.941859	-2.010652	4.380030

101	6	0	3.685280	-2.236535	2.363263
102	6	0	4.344163	-2.507993	0.026768
103	1	0	1.396174	-3.978615	0.182169
104	6	0	0.910094	-5.077557	-1.583409
105	6	0	0.903087	-3.866904	-3.666808
106	1	0	6.280338	0.909452	3.008865
107	1	0	3.391879	5.362869	-4.485505
108	1	0	-3.226290	1.291254	5.627539
109	1	0	-3.160703	-5.390236	-0.775004
110	6	0	4.971392	-2.688330	2.742521
111	6	0	5.581411	-2.956868	0.426892
112	1	0	4.110872	-2.436535	-1.033968
113	1	0	0.752116	-6.006747	-1.038393
114	6	0	0.725829	-5.045096	-2.980679
115	1	0	0.760550	-3.825546	-4.746691
116	1	0	5.204362	-2.757064	3.805322
117	6	0	5.904607	-3.041656	1.796667
118	1	0	6.318273	-3.246242	-0.320557
119	1	0	0.439115	-5.951022	-3.511805
120	1	0	6.888682	-3.393366	2.101709

Filename: 7

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2689.759104 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2690.310960 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2689.603710 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2689.710851 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-0.367398	-2.042628	-1.198566
2	15	0	-1.784744	-0.297183	-0.813291
3	15	0	1.626758	-1.091125	-0.578622
4	6	0	-0.894971	1.303717	-0.841906
5	6	0	-2.382729	-0.553467	0.897008
6	6	0	-3.329065	-0.013805	-1.748585
7	6	0	2.891566	-2.368114	-0.241618
8	6	0	2.502764	0.272592	-1.412621
9	6	0	1.162709	-0.440631	1.083756
10	6	0	0.094566	1.628042	0.093339
11	6	0	-1.065989	2.129749	-1.986489
12	6	0	-2.121877	-1.789602	1.502857
13	6	0	-3.095677	0.422088	1.602957
14	6	0	-4.092644	1.158943	-1.665097
15	6	0	-3.801543	-1.076902	-2.527334
16	6	0	2.431341	-3.692145	-0.160525
17	6	0	4.254407	-2.100260	-0.066347
18	6	0	2.204749	0.521258	-2.757619
19	6	0	3.436446	1.090173	-0.762427
20	6	0	1.411491	-1.269434	2.209175
21	6	0	0.419015	0.734829	1.246831
22	6	0	0.833292	2.847083	-0.052825
23	6	0	-0.322279	3.265626	-2.168455
24	1	0	-1.799629	1.846209	-2.738718
25	1	0	-1.570357	-2.558580	0.951321
26	6	0	-2.557416	-2.033109	2.803519
27	6	0	-3.524585	0.175417	2.901750
28	1	0	-3.293931	1.390991	1.143387
29	1	0	-3.729989	2.001444	-1.075844
30	6	0	-5.299926	1.263250	-2.346803
31	6	0	-5.015603	-0.973946	-3.202409
32	1	0	-3.209628	-1.991038	-2.594698
33	1	0	1.372133	-3.917080	-0.325923
34	6	0	3.328167	-4.720811	0.119564
35	6	0	5.144119	-3.136107	0.200988
36	1	0	4.627611	-1.081033	-0.153407
37	1	0	1.458394	-0.095381	-3.260042
38	6	0	2.834437	1.557071	-3.441901
39	6	0	4.067137	2.123100	-1.447339
40	1	0	3.641900	0.937639	0.297961
41	1	0	1.972582	-2.191770	2.073008
42	6	0	0.951862	-0.937676	3.457030
43	6	0	-0.028209	1.113502	2.553360

44	6	0	1.791904	3.272472	0.903017
45	6	0	0.629716	3.668910	-1.205257
46	1	0	-0.463999	3.878875	-3.058556
47	1	0	-2.344845	-2.993670	3.269789
48	6	0	-3.252833	-1.051920	3.504584
49	1	0	-4.058099	0.948931	3.451971
50	1	0	-5.882714	2.180316	-2.277920
51	6	0	-5.764680	0.195482	-3.114002
52	1	0	-5.372478	-1.809254	-3.801941
53	1	0	2.963984	-5.744770	0.182118
54	6	0	4.681337	-4.446741	0.300840
55	1	0	6.203208	-2.918560	0.330452
56	1	0	2.586677	1.745561	-4.485122
57	6	0	3.767348	2.357651	-2.787703
58	1	0	4.776046	2.763862	-0.925506
59	1	0	1.147240	-1.593246	4.305743
60	6	0	0.228540	0.256776	3.669106
61	6	0	-0.748900	2.312808	2.788097
62	1	0	1.967480	2.659535	1.784585
63	6	0	2.499018	4.440621	0.733926
64	6	0	1.385906	4.853966	-1.360486
65	1	0	-3.582511	-1.239438	4.525457
66	1	0	-6.711210	0.278927	-3.645203
67	1	0	5.379941	-5.255539	0.509837
68	1	0	4.252376	3.175738	-3.317795
69	6	0	-0.247199	0.620779	4.950857
70	6	0	-1.185195	2.647444	4.048992
71	1	0	-0.960774	2.973592	1.949682
72	1	0	3.222727	4.745938	1.487963
73	6	0	2.302125	5.239505	-0.410238
74	1	0	1.221131	5.460185	-2.251472
75	1	0	-0.048866	-0.050543	5.786490
76	6	0	-0.938386	1.793507	5.143001
77	1	0	-1.733363	3.575799	4.201396
78	1	0	2.872823	6.157587	-0.538080
79	1	0	-1.294851	2.064335	6.135260
80	8	0	-0.680677	-3.881004	-0.975049
81	6	0	-1.940884	-4.409348	-1.153760
82	1	0	-2.243321	-4.486619	-2.221348
83	1	0	-2.006407	-5.436876	-0.744380
84	1	0	-2.749753	-3.827267	-0.649814

Filename: 8

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2295.142921 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2295.918339 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2295.273692 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2295.371443 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	15	0	0.369694	1.895746	-0.121231
2	15	0	-2.061206	-0.114350	-0.024363
3	6	0	-1.359094	2.591457	-0.197275
4	6	0	-2.343663	1.654687	0.488989
5	6	0	-3.138862	-0.994014	1.153696
6	6	0	-4.196588	-1.821528	0.762103
7	6	0	-4.944131	-2.507541	1.716541
8	6	0	-4.645134	-2.378472	3.069551
9	6	0	-3.583906	-1.567016	3.468137
10	6	0	-2.831200	-0.886658	2.518603
11	6	0	-2.896822	-0.191268	-1.643940
12	6	0	-4.198018	0.285069	-1.855949
13	6	0	-4.765844	0.240712	-3.124754
14	6	0	-4.037850	-0.274325	-4.197281
15	6	0	-2.744270	-0.748551	-3.998461
16	6	0	-2.176274	-0.709691	-2.727183
17	6	0	0.665295	1.815256	1.684614
18	6	0	1.404550	0.733958	2.187600
19	6	0	1.608113	0.600973	3.560496
20	6	0	1.081632	1.540316	4.441947
21	6	0	0.353729	2.624438	3.950483
22	6	0	0.149057	2.761461	2.581532
23	6	0	1.356936	3.328138	-0.677521
24	6	0	1.065552	3.921980	-1.914563
25	6	0	1.831077	4.979827	-2.391769
26	6	0	2.911489	5.453345	-1.649784
27	6	0	3.219578	4.860187	-0.428567
28	6	0	2.449808	3.806421	0.056170
29	1	0	-1.408706	3.601216	0.232207
30	1	0	-1.612573	2.691892	-1.262030
31	1	0	-3.382466	1.953803	0.294919
32	1	0	-2.200265	1.690677	1.577570
33	1	0	-4.437689	-1.930680	-0.294424
34	1	0	-5.765789	-3.146704	1.397588
35	1	0	-5.231261	-2.915528	3.812958
36	1	0	-3.335341	-1.470449	4.523553
37	1	0	-1.985501	-0.274426	2.839447
38	1	0	-4.774716	0.679986	-1.018327
39	1	0	-5.778852	0.608551	-3.279137
40	1	0	-4.483593	-0.306297	-5.190019
41	1	0	-2.174126	-1.152403	-4.832802
42	1	0	-1.164316	-1.088252	-2.559668
43	1	0	1.818476	-0.012122	1.504722

44	1	0	2.179001	-0.246904	3.934653
45	1	0	1.238629	1.432894	5.514094
46	1	0	-0.053370	3.365511	4.636632
47	1	0	-0.415364	3.615869	2.205690
48	1	0	0.233432	3.551076	-2.513899
49	1	0	1.585202	5.433638	-3.350445
50	1	0	3.513246	6.278786	-2.025412
51	1	0	4.063612	5.221973	0.156442
52	1	0	2.694940	3.354836	1.016748
53	29	0	0.228991	-0.533010	-0.404182
54	5	0	1.716309	-1.881129	-0.523452
55	8	0	2.141549	-2.659856	-1.598299
56	8	0	2.553502	-2.111849	0.580586
57	6	0	3.139684	-3.592056	-1.125999
58	6	0	3.698370	-2.873034	0.132379
59	6	0	4.154168	-3.826475	-2.228942
60	1	0	4.974747	-4.468831	-1.881099
61	1	0	3.675820	-4.325634	-3.079391
62	1	0	4.581353	-2.886297	-2.590393
63	6	0	2.416684	-4.891290	-0.790406
64	1	0	1.868434	-5.236599	-1.673636
65	1	0	3.112741	-5.683807	-0.486554
66	1	0	1.690914	-4.737582	0.016299
67	6	0	4.798780	-1.871390	-0.198611
68	1	0	4.995817	-1.248132	0.681022
69	1	0	5.735724	-2.366601	-0.484256
70	1	0	4.492097	-1.210153	-1.017200
71	6	0	4.146526	-3.794773	1.250143
72	1	0	4.965342	-4.448229	0.919325
73	1	0	4.512150	-3.206105	2.099764
74	1	0	3.326014	-4.424202	1.607339

Filename: 9

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2682.184444 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2682.805762 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2681.981657 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2682.095468 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.211471	-1.187942	-2.194710
2	1	0	-0.415818	-0.358630	-2.891137
3	6	0	1.205403	-1.665508	-2.425530
4	6	0	-1.408577	-2.044663	-2.137187
5	6	0	1.790709	-2.907633	-1.743863
6	6	0	1.565991	-2.902479	-3.219989
7	5	0	2.264839	-0.550272	-2.328965
8	6	0	-1.452883	-3.442048	-1.927139
9	6	0	-2.674249	-1.404412	-2.209679
10	1	0	1.140833	-3.485526	-1.090048
11	1	0	2.824782	-2.866078	-1.396857
12	1	0	2.441086	-2.880492	-3.867849
13	1	0	0.733340	-3.485659	-3.608151
14	8	0	3.502634	-0.586212	-2.935020
15	8	0	2.124840	0.551230	-1.495945
16	6	0	-2.659284	-4.122409	-1.755990
17	1	0	-0.534438	-4.021811	-1.892156
18	6	0	-3.869863	-2.078133	-2.033920
19	1	0	-2.688427	-0.325437	-2.382666
20	6	0	4.340004	0.376387	-2.254834
21	6	0	3.297582	1.384571	-1.670549
22	6	0	-3.879578	-3.456370	-1.790405
23	1	0	-2.634487	-5.201887	-1.597723
24	1	0	-4.806364	-1.520763	-2.085679
25	6	0	5.310333	0.975377	-3.253080
26	6	0	5.089926	-0.390947	-1.173806
27	6	0	3.676885	1.970708	-0.324601
28	6	0	2.915101	2.483685	-2.651748
29	1	0	-4.815733	-3.993891	-1.650907
30	1	0	5.917547	1.761187	-2.785334
31	1	0	5.990832	0.201414	-3.624446
32	1	0	4.790968	1.405881	-4.114111
33	1	0	5.647359	-1.211976	-1.637822
34	1	0	5.797935	0.245148	-0.627923
35	1	0	4.392446	-0.821588	-0.445328
36	1	0	4.597199	2.564958	-0.400424
37	1	0	2.880781	2.632593	0.039739
38	1	0	3.826804	1.192697	0.430702
39	1	0	2.041778	3.025447	-2.269485
40	1	0	3.729426	3.204018	-2.796980
41	1	0	2.645368	2.066192	-3.628624
42	29	0	-0.322235	-0.167235	-0.458613
43	15	0	0.435993	-0.334304	1.725466

44	15	0	-2.009642	1.233967	0.401672
45	6	0	-0.606994	0.803231	2.764901
46	6	0	-0.106090	-1.974014	2.321727
47	6	0	2.119087	-0.138594	2.380818
48	6	0	-2.031947	0.827788	2.220061
49	6	0	-3.768524	1.419994	-0.018912
50	6	0	-1.365107	2.945080	0.433771
51	1	0	-0.589655	0.501486	3.821213
52	1	0	-0.178444	1.813075	2.700781
53	6	0	-0.961683	-2.724000	1.504159
54	6	0	0.271022	-2.485964	3.570348
55	6	0	2.545229	1.005869	3.066840
56	6	0	3.066934	-1.125487	2.064914
57	1	0	-2.654810	1.544469	2.773269
58	1	0	-2.490135	-0.165338	2.333769
59	6	0	-4.777463	0.739873	0.674730
60	6	0	-4.117973	2.163275	-1.157121
61	6	0	-2.118856	4.035034	0.886581
62	6	0	-0.036350	3.151382	0.037273
63	1	0	-1.241223	-2.349782	0.514975
64	6	0	-1.437714	-3.961798	1.930265
65	6	0	-0.198515	-3.726467	3.989337
66	1	0	0.946461	-1.914297	4.208279
67	1	0	1.836094	1.793579	3.316981
68	6	0	3.880991	1.155844	3.432871
69	6	0	4.397419	-0.976060	2.438146
70	1	0	2.752151	-2.016719	1.519326
71	1	0	-4.534263	0.142287	1.551823
72	6	0	-6.101286	0.812648	0.249417
73	6	0	-5.440506	2.236829	-1.576830
74	1	0	-3.342946	2.688965	-1.716052
75	1	0	-3.157487	3.885022	1.183522
76	6	0	-1.554099	5.305528	0.944690
77	6	0	0.528896	4.423025	0.104082
78	1	0	0.548894	2.303598	-0.335712
79	1	0	-2.098136	-4.530359	1.277612
80	6	0	-1.054895	-4.463752	3.171327
81	1	0	0.105388	-4.121514	4.957479
82	1	0	4.194172	2.051311	3.967174
83	6	0	4.810854	0.167911	3.120629
84	1	0	5.117959	-1.752502	2.185433
85	1	0	-6.872796	0.279043	0.801802
86	6	0	-6.437835	1.561221	-0.874683
87	1	0	-5.693837	2.821584	-2.459381
88	1	0	-2.149153	6.147758	1.293916
89	6	0	-0.229111	5.500210	0.557204
90	1	0	1.561408	4.575595	-0.209827
91	1	0	-1.417847	-5.435481	3.502250
92	1	0	5.854060	0.287413	3.406874
93	1	0	-7.472867	1.615162	-1.206628
94	1	0	0.210278	6.495187	0.602506

Filename: 10

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2682.191660 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2682.806587 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2681.982093 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2681.982093 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.097722	-1.132579	-1.588281
2	1	0	3.243598	-1.924809	-0.844796
3	6	0	1.877500	-1.074123	-2.177242
4	6	0	4.300184	-0.329541	-1.800720
5	6	0	0.655420	1.053444	-2.458427
6	6	0	1.401863	-0.072269	-3.196447
7	5	0	0.755042	-2.049987	-1.730093
8	6	0	4.310399	0.960588	-2.366482
9	6	0	5.533200	-0.850759	-1.367555
10	1	0	1.385728	1.814801	-2.126889
11	1	0	-0.029746	1.567528	-3.149842
12	1	0	0.690459	-0.584452	-3.859974
13	1	0	2.219933	0.280856	-3.845000
14	8	0	-0.071438	-2.711724	-2.607490
15	8	0	0.439522	-2.305367	-0.409656
16	6	0	5.498462	1.666360	-2.520728
17	1	0	3.373039	1.432151	-2.651553
18	6	0	6.719987	-0.144691	-1.518083
19	1	0	5.547467	-1.839898	-0.908189
20	6	0	-1.183738	-3.235795	-1.841875
21	6	0	-0.596754	-3.320120	-0.391854
22	6	0	6.711524	1.119170	-2.104332
23	1	0	5.473409	2.662517	-2.961110
24	1	0	7.656498	-0.582183	-1.174854
25	6	0	-1.599477	-4.568819	-2.431582
26	6	0	-2.307735	-2.219078	-1.974393
27	6	0	-1.579779	-2.967740	0.708044
28	6	0	0.094043	-4.642574	-0.094893
29	1	0	7.638306	1.677524	-2.224893
30	1	0	-2.404357	-5.022368	-1.838825
31	1	0	-1.973598	-4.425022	-3.450862
32	1	0	-0.764043	-5.273641	-2.476626
33	1	0	-2.562114	-2.094837	-3.032660
34	1	0	-3.213062	-2.519450	-1.432148
35	1	0	-1.988913	-1.236690	-1.597547
36	1	0	-2.464454	-3.617964	0.674280
37	1	0	-1.107956	-3.078517	1.691904
38	1	0	-1.915881	-1.926994	0.606211
39	1	0	0.632254	-4.558502	0.856153
40	1	0	-0.624406	-5.466956	-0.011995
41	1	0	0.819657	-4.895785	-0.876745
42	29	0	-0.218383	0.484699	-0.734770
43	15	0	-2.388263	1.039347	0.150720

44	15	0	0.491642	0.505921	1.548803
45	6	0	-2.193480	1.108124	1.998825
46	6	0	-2.677448	2.805141	-0.236997
47	6	0	-4.025501	0.278336	-0.093302
48	6	0	-0.784687	1.582738	2.358465
49	6	0	2.070117	1.361055	1.879018
50	6	0	0.605247	-0.934839	2.670005
51	1	0	-2.960911	1.751903	2.451326
52	1	0	-2.351113	0.090370	2.382881
53	6	0	-1.672208	3.519095	-0.899504
54	6	0	-3.848554	3.471522	0.149439
55	6	0	-4.550051	-0.690175	0.773613
56	6	0	-4.713380	0.547975	-1.287638
57	1	0	-0.649924	1.634945	3.448022
58	1	0	-0.619627	2.599933	1.975092
59	6	0	2.911873	1.618083	0.792414
60	6	0	2.485491	1.714158	3.169850
61	6	0	-0.246800	-1.159989	3.757406
62	6	0	1.583947	-1.896318	2.375442
63	1	0	-0.770590	2.991455	-1.220384
64	6	0	-1.831922	4.878285	-1.162914
65	6	0	-4.009086	4.825474	-0.122842
66	1	0	-4.642750	2.919298	0.653658
67	1	0	-4.037347	-0.933135	1.703519
68	6	0	-5.730656	-1.359580	0.460579
69	6	0	-5.892378	-0.119288	-1.596180
70	1	0	-4.316106	1.291802	-1.978815
71	1	0	2.586949	1.325668	-0.207942
72	6	0	4.154832	2.216657	0.989712
73	6	0	3.717740	2.327744	3.363489
74	1	0	1.847454	1.491784	4.026461
75	1	0	-1.008287	-0.427829	4.024060
76	6	0	-0.132083	-2.319419	4.523495
77	6	0	1.705741	-3.044828	3.147131
78	1	0	2.246086	-1.739377	1.524628
79	1	0	-1.044735	5.424065	-1.679815
80	6	0	-2.998981	5.530959	-0.777013
81	1	0	-4.924602	5.333801	0.175453
82	1	0	-6.125174	-2.103130	1.151406
83	6	0	-6.406058	-1.077806	-0.723672
84	1	0	-6.412455	0.108518	-2.525053
85	1	0	4.810314	2.386278	0.136242
86	6	0	4.553619	2.575931	2.273723
87	1	0	4.034968	2.603267	4.368151
88	1	0	-0.804628	-2.476913	5.365341
89	6	0	0.841332	-3.266134	4.219729
90	1	0	2.476278	-3.776095	2.906895
91	1	0	-3.126914	6.591096	-0.989474
92	1	0	-7.327991	-1.602586	-0.966698
93	1	0	5.524249	3.043632	2.431336
94	1	0	0.930693	-4.170916	4.818246

Filename: 11

SCF Energy (M06L/LANL2DZ-6-31g(d))

-1999.061407 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-1999.907344 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-1999.410310 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-1999.495345 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	0.112109	-1.544294	1.022128
2	15	0	-1.465370	-0.163129	-0.274888
3	15	0	1.663555	-0.406074	-0.137819
4	6	0	-0.585632	-0.463671	-1.885487
5	6	0	-3.075129	-0.976024	-0.531567
6	6	0	-1.856165	1.614495	-0.282540
7	6	0	0.927301	-0.204624	-1.846755
8	6	0	3.405453	-0.806797	-0.517552
9	6	0	1.696772	1.327922	0.444149
10	1	0	-0.765292	-1.530226	-2.073722
11	1	0	-1.060916	0.083988	-2.711528
12	6	0	-3.304754	-2.189192	0.132718
13	6	0	-4.061429	-0.440352	-1.371567
14	6	0	-1.162323	2.537154	-1.075638
15	6	0	-2.789977	2.099775	0.647033
16	1	0	1.169461	0.807630	-2.196422
17	1	0	1.445378	-0.893154	-2.525314
18	6	0	3.684322	-1.905184	-1.343779
19	6	0	4.474831	-0.125033	0.076017
20	6	0	2.336383	2.343867	-0.279813
21	6	0	0.983141	1.664666	1.598948
22	1	0	-2.540425	-2.591359	0.809492
23	6	0	-4.511762	-2.859255	-0.063107
24	6	0	-5.262663	-1.115732	-1.555885
25	1	0	-3.887890	0.513145	-1.872207
26	1	0	-0.427153	2.191617	-1.801612
27	6	0	-1.393994	3.903904	-0.944765
28	6	0	-3.027891	3.463350	0.768126
29	1	0	-3.338147	1.396202	1.274354
30	1	0	2.866560	-2.475420	-1.786356
31	6	0	4.995939	-2.290518	-1.594697
32	6	0	5.787794	-0.516360	-0.172810
33	1	0	4.280237	0.720414	0.734188
34	1	0	2.907043	2.093089	-1.175611
35	6	0	2.256611	3.666760	0.141335
36	6	0	0.894753	2.990000	2.015534
37	1	0	0.469112	0.876137	2.153463
38	1	0	-4.692445	-3.799537	0.455210
39	6	0	-5.486458	-2.328117	-0.903277
40	1	0	-6.026752	-0.696708	-2.208924
41	1	0	-0.839038	4.604606	-1.567171
42	6	0	-2.326580	4.372129	-0.024100
43	1	0	-3.763479	3.820026	1.487287

44	1	0	5.192839	-3.142113	-2.243461
45	6	0	6.053442	-1.594365	-1.012079
46	1	0	6.607338	0.027896	0.293365
47	1	0	2.757732	4.448428	-0.427438
48	6	0	1.529339	3.991314	1.286166
49	1	0	0.319309	3.240108	2.904754
50	1	0	-6.428788	-2.854805	-1.047377
51	1	0	-2.508116	5.440621	0.076862
52	1	0	7.080472	-1.897404	-1.206308
53	1	0	1.454449	5.029101	1.606587
54	8	0	-0.791250	-2.808925	2.014988
55	6	0	-0.196221	-3.945812	2.528255
56	1	0	0.745610	-3.751373	3.081996
57	1	0	-0.875132	-4.449774	3.243314
58	1	0	0.053484	-4.702973	1.754394

Filename: 12

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2682.198806 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2682.810894 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2681.987005 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2682.101211 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.808487	0.405026	-2.534060
2	1	0	2.979639	1.366560	-3.033273
3	6	0	1.654600	-0.248752	-2.793726
4	6	0	3.852139	-0.005753	-1.597652
5	6	0	-0.496175	1.000566	-2.922150
6	6	0	0.626042	0.326632	-3.733858
7	5	0	1.139088	-1.511613	-2.040375
8	6	0	4.167411	-1.357056	-1.377187
9	6	0	4.575761	0.959466	-0.876780
10	1	0	-0.268368	2.080029	-2.856691
11	1	0	-1.453810	0.931694	-3.461045
12	1	0	0.200453	-0.494312	-4.329745
13	1	0	1.107536	1.013678	-4.450639
14	8	0	0.552078	-2.583086	-2.673651
15	8	0	1.118910	-1.643123	-0.663170
16	6	0	5.127481	-1.730355	-0.444060
17	1	0	3.660157	-2.118160	-1.970905
18	6	0	5.535269	0.588851	0.058769
19	1	0	4.350806	2.014869	-1.035972
20	6	0	-0.138287	-3.357371	-1.658900
21	6	0	0.634948	-2.975153	-0.355122
22	6	0	5.814134	-0.758464	0.284024
23	1	0	5.351566	-2.786589	-0.293812
24	1	0	6.065497	1.358181	0.619124
25	6	0	-0.064063	-4.824576	-2.030840
26	6	0	-1.584148	-2.880347	-1.653412
27	6	0	-0.224227	-2.881456	0.889886
28	6	0	1.858111	-3.844035	-0.102085
29	1	0	6.569916	-1.049344	1.012201
30	1	0	-0.518801	-5.447110	-1.249517
31	1	0	-0.611729	-5.002341	-2.962575
32	1	0	0.967999	-5.155507	-2.179492
33	1	0	-2.015092	-3.016485	-2.651165
34	1	0	-2.198247	-3.430989	-0.929251
35	1	0	-1.646951	-1.808229	-1.413277
36	1	0	-0.746939	-3.826850	1.088187
37	1	0	0.395675	-2.640170	1.762004
38	1	0	-0.976970	-2.090981	0.777629
39	1	0	2.466740	-3.384715	0.685751
40	1	0	1.575637	-4.853357	0.221120
41	1	0	2.479313	-3.933794	-1.001344
42	29	0	-0.641310	0.450298	-0.989742
43	15	0	-2.589739	0.433653	0.394899

44	15	0	0.553760	1.143046	0.971713
45	6	0	-2.024512	1.046389	2.058185
46	6	0	-3.664235	1.816917	-0.139519
47	6	0	-3.765534	-0.900791	0.797227
48	6	0	-0.819956	1.977039	1.907065
49	6	0	1.747880	2.499461	0.699078
50	6	0	1.369237	0.110606	2.238237
51	1	0	-2.848892	1.545445	2.586414
52	1	0	-1.744042	0.166663	2.652362
53	6	0	-3.225743	2.635522	-1.186298
54	6	0	-4.875966	2.114985	0.499707
55	6	0	-3.535814	-1.797444	1.850830
56	6	0	-4.837822	-1.157301	-0.072473
57	1	0	-0.479045	2.351745	2.882696
58	1	0	-1.098184	2.860620	1.314132
59	6	0	1.670783	3.181953	-0.521758
60	6	0	2.728851	2.869202	1.626826
61	6	0	0.871791	-0.070904	3.535348
62	6	0	2.530129	-0.585007	1.863332
63	1	0	-2.290556	2.389357	-1.693871
64	6	0	-3.982009	3.736913	-1.582925
65	6	0	-5.632848	3.209288	0.096072
66	1	0	-5.231534	1.475251	1.308641
67	1	0	-2.700776	-1.643235	2.533685
68	6	0	-4.358090	-2.904710	2.036906
69	6	0	-5.658868	-2.263223	0.116676
70	1	0	-5.030050	-0.478045	-0.902996
71	1	0	0.934383	2.858624	-1.260857
72	6	0	2.542646	4.230604	-0.800654
73	6	0	3.608753	3.908909	1.340229
74	1	0	2.811844	2.330079	2.570704
75	1	0	-0.011697	0.470785	3.869955
76	6	0	1.504800	-0.934204	4.428152
77	6	0	3.168986	-1.431772	2.761944
78	1	0	2.931791	-0.466511	0.858108
79	1	0	-3.632292	4.365991	-2.399506
80	6	0	-5.184769	4.023404	-0.944423
81	1	0	-6.575465	3.429846	0.594515
82	1	0	-4.164365	-3.583685	2.865821
83	6	0	-5.423122	-3.142451	1.172042
84	1	0	-6.487950	-2.439557	-0.566563
85	1	0	2.475024	4.751775	-1.754286
86	6	0	3.515052	4.593664	0.129496
87	1	0	4.372104	4.186261	2.065818
88	1	0	1.100259	-1.061824	5.431133
89	6	0	2.653615	-1.619275	4.044246
90	1	0	4.074446	-1.950708	2.448564
91	1	0	-5.779149	4.879949	-1.258225
92	1	0	-6.065193	-4.009009	1.317795
93	1	0	4.206613	5.404906	-0.092203
94	1	0	3.148728	-2.292181	4.742277

Filename: TS5

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.828200 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.148312 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.116458 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.251669 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.393632	0.675657	2.376422
2	6	0	-2.668782	-0.684418	2.005328
3	6	0	-2.582197	-1.855416	2.917950
4	6	0	-3.907949	-1.476573	2.309204
5	1	0	-2.403039	-1.667093	3.976534
6	1	0	-2.124888	-2.767513	2.534537
7	1	0	-4.333263	-2.172154	1.589386
8	1	0	-4.637863	-0.956305	2.928806
9	29	0	-1.149104	-0.125122	0.817017
10	15	0	-0.315683	1.197380	-0.853973
11	15	0	0.976130	-0.948756	1.552491
12	6	0	0.858220	0.038763	-1.656338
13	6	0	0.598836	2.699347	-0.344984
14	6	0	-1.339602	1.832937	-2.227637
15	6	0	0.931395	-1.220853	3.358385
16	6	0	1.575980	-2.531452	0.864457
17	6	0	2.393868	0.194770	1.256948
18	6	0	2.159993	-0.199465	-1.217276
19	6	0	0.293036	-0.806450	-2.652695
20	6	0	0.597395	3.028671	1.013941
21	6	0	1.247817	3.542669	-1.253677
22	6	0	-0.893262	1.956939	-3.549202
23	6	0	-2.624016	2.277082	-1.896134
24	6	0	0.565838	-0.145896	4.185010
25	6	0	1.082621	-2.486579	3.936112
26	6	0	0.728181	-3.264687	0.028738
27	6	0	2.876103	-2.994856	1.105453
28	6	0	3.038333	0.849495	2.336708
29	6	0	2.755342	0.522335	-0.054689
30	6	0	2.956402	-1.201817	-1.869737
31	6	0	1.027137	-1.791542	-3.256608
32	1	0	-0.751111	-0.659581	-2.928612
33	1	0	0.074041	2.365585	1.709287
34	6	0	1.254143	4.170570	1.463103
35	6	0	1.910917	4.678827	-0.803395
36	1	0	1.242125	3.302871	-2.317577
37	1	0	0.104079	1.610918	-3.822781
38	6	0	-1.725697	2.502774	-4.522718
39	6	0	-3.448133	2.835358	-2.867770
40	1	0	-2.983930	2.169011	-0.873477
41	1	0	0.419042	0.841504	3.742943
42	6	0	0.384401	-0.325133	5.551151
43	6	0	0.883781	-2.668188	5.303256

44	1	0	1.348554	-3.338207	3.311985
45	1	0	-0.283134	-2.897495	-0.157095
46	6	0	1.182010	-4.437464	-0.570339
47	6	0	3.323110	-4.168659	0.509844
48	1	0	3.544308	-2.418428	1.747602
49	1	0	2.784338	0.570674	3.356656
50	6	0	3.980101	1.823996	2.123359
51	6	0	3.743419	1.526680	-0.291414
52	6	0	4.307189	-1.447109	-1.516511
53	6	0	2.383349	-1.998407	-2.909988
54	1	0	0.573378	-2.426817	-4.018609
55	1	0	1.251404	4.415086	2.524609
56	6	0	1.916934	4.992586	0.555077
57	1	0	2.433567	5.317834	-1.513536
58	1	0	-1.372318	2.587443	-5.549254
59	6	0	-3.003533	2.943669	-4.183776
60	1	0	-4.444147	3.178960	-2.591128
61	1	0	0.107276	0.522751	6.175213
62	6	0	0.538833	-1.591314	6.114413
63	1	0	1.000932	-3.660798	5.735052
64	1	0	0.524401	-4.992645	-1.238305
65	6	0	2.478157	-4.887260	-0.335373
66	1	0	4.340254	-4.514555	0.688218
67	1	0	4.460810	2.316586	2.968923
68	6	0	4.345554	2.205313	0.813637
69	6	0	4.130774	1.907046	-1.601845
70	1	0	4.758310	-0.867874	-0.713627
71	6	0	5.054426	-2.400975	-2.170388
72	6	0	3.170946	-2.980410	-3.552353
73	1	0	2.439084	5.882199	0.904242
74	1	0	-3.651318	3.371852	-4.947269
75	1	0	0.383488	-1.737244	7.181820
76	1	0	2.837161	-5.795277	-0.817641
77	6	0	5.287518	3.232244	0.568487
78	6	0	5.053068	2.906164	-1.808278
79	1	0	3.675680	1.401450	-2.452058
80	1	0	6.092151	-2.561733	-1.882669
81	6	0	4.485624	-3.177217	-3.198004
82	1	0	2.711907	-3.578515	-4.339860
83	1	0	5.731705	3.743711	1.422593
84	6	0	5.636374	3.579781	-0.715116
85	1	0	5.331558	3.183073	-2.823688
86	1	0	5.083934	-3.932188	-3.705052
87	1	0	6.362462	4.371598	-0.890630
88	5	0	-2.477082	-1.397677	-0.086997
89	8	0	-3.097122	-0.742322	-1.138384
90	8	0	-2.760327	-2.753494	-0.096329
91	6	0	-3.995916	-1.669776	-1.796116
92	6	0	-3.439719	-3.059734	-1.344043
93	6	0	-3.930461	-1.407611	-3.288973
94	6	0	-5.391840	-1.365185	-1.271563
95	6	0	-4.502851	-4.105391	-1.069511
96	6	0	-2.379145	-3.619316	-2.282365
97	1	0	-4.562687	-2.112917	-3.844766
98	1	0	-4.283976	-0.392603	-3.503093
99	1	0	-2.907548	-1.488344	-3.671513
100	1	0	-5.624480	-0.312983	-1.476768

101	1	0	-6.159497	-1.988318	-1.747070
102	1	0	-5.451336	-1.511457	-0.186002
103	1	0	-5.074200	-4.331049	-1.979719
104	1	0	-4.036096	-5.035115	-0.726134
105	1	0	-5.205535	-3.777992	-0.297010
106	1	0	-1.934429	-4.511083	-1.826019
107	1	0	-2.797437	-3.904766	-3.255425
108	1	0	-1.574307	-2.891361	-2.445365
109	6	0	-3.216289	1.784584	1.941406
110	6	0	-4.344127	1.599423	1.110141
111	6	0	-2.921460	3.109121	2.331357
112	6	0	-5.123143	2.674961	0.700051
113	1	0	-4.591265	0.592966	0.777128
114	6	0	-3.693913	4.180533	1.908409
115	1	0	-2.057081	3.284143	2.975673
116	6	0	-4.804909	3.976403	1.086081
117	1	0	-5.989261	2.492466	0.061847
118	1	0	-3.429504	5.189702	2.223530
119	1	0	-5.412388	4.817906	0.758014
120	1	0	-1.716901	0.848931	3.214913

Filename: TS6

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.854343 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.168245 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.135793 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.270537 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.429547	1.004396	-0.843564
2	6	0	3.019726	1.681529	0.376672
3	29	0	1.294565	0.636231	-0.461505
4	15	0	-0.880472	1.140731	-1.281921
5	15	0	0.373632	-0.742463	1.221908
6	6	0	-2.356094	1.113516	-0.188008
7	6	0	-1.323177	-0.022155	-2.620324
8	6	0	-0.893833	2.795572	-2.055211
9	6	0	1.193905	-1.836537	2.447945
10	6	0	-0.460550	0.387652	2.403750
11	6	0	-0.884056	-1.793612	0.415672
12	6	0	-2.766870	-0.085160	0.406550
13	6	0	-3.003581	2.325815	0.162585
14	6	0	-0.414208	-1.028871	-2.960379
15	6	0	-2.566817	0.021038	-3.263712
16	6	0	-1.173778	3.018610	-3.409211
17	6	0	-0.504786	3.883530	-1.257932
18	6	0	2.358820	-1.331811	3.042339
19	6	0	0.691130	-3.064910	2.892825
20	6	0	-0.138275	1.747512	2.369999
21	6	0	-1.331642	-0.085932	3.391976
22	6	0	-0.372275	-3.033040	-0.066371
23	6	0	-2.170085	-1.397176	0.029499
24	6	0	-3.822412	-0.067104	1.373672
25	6	0	-4.022961	2.352555	1.077571
26	1	0	-2.691912	3.252935	-0.311908
27	1	0	0.541094	-1.071940	-2.431671
28	6	0	-0.741166	-1.979795	-3.922294
29	6	0	-2.888658	-0.923624	-4.232227
30	1	0	-3.292948	0.785845	-2.983530
31	1	0	-1.444180	2.184179	-4.053562
32	6	0	-1.102428	4.303596	-3.941352
33	6	0	-0.458457	5.168530	-1.787083
34	1	0	-0.224261	3.722193	-0.214387
35	1	0	2.757144	-0.374548	2.708219
36	6	0	3.011327	-2.040919	4.043886
37	6	0	1.356009	-3.783201	3.884624
38	1	0	-0.227516	-3.464974	2.464943
39	1	0	0.567665	2.110655	1.619415
40	6	0	-0.699722	2.627570	3.293054
41	6	0	-1.899863	0.793932	4.305432
42	1	0	-1.576443	-1.148227	3.435821
43	1	0	0.642876	-3.318483	0.207337

44	6	0	-1.110997	-3.871099	-0.853619
45	6	0	-2.968466	-2.278208	-0.782567
46	6	0	-4.242248	-1.239321	2.052973
47	6	0	-4.450470	1.169331	1.720591
48	1	0	-4.511990	3.294428	1.326218
49	1	0	-0.034746	-2.774496	-4.159701
50	6	0	-1.977746	-1.926516	-4.560550
51	1	0	-3.863700	-0.892843	-4.715896
52	1	0	-1.320182	4.460403	-4.996523
53	6	0	-0.758382	5.382264	-3.130671
54	1	0	-0.161520	5.997090	-1.146992
55	1	0	3.913829	-1.630432	4.494256
56	6	0	2.516690	-3.275387	4.462499
57	1	0	0.954078	-4.739695	4.215440
58	1	0	-0.434445	3.683511	3.255104
59	6	0	-1.587011	2.152913	4.254756
60	1	0	-2.594847	0.419106	5.055537
61	1	0	-0.688845	-4.813992	-1.203242
62	6	0	-2.432463	-3.526758	-1.228197
63	6	0	-4.283605	-1.945250	-1.195435
64	1	0	-3.762311	-2.186832	1.814340
65	6	0	-5.228060	-1.193521	3.012210
66	6	0	-5.465287	1.183659	2.705427
67	1	0	-2.240838	-2.676471	-5.304799
68	1	0	-0.708757	6.386265	-3.548498
69	1	0	3.030141	-3.836158	5.241713
70	1	0	-2.031892	2.839175	4.973923
71	6	0	-3.215020	-4.377870	-2.038895
72	6	0	-5.029335	-2.800705	-1.976675
73	1	0	-4.708567	-0.991330	-0.891638
74	1	0	-5.527476	-2.107703	3.521963
75	6	0	-5.850882	0.027225	3.342239
76	1	0	-5.932220	2.136707	2.954359
77	1	0	-2.780904	-5.322733	-2.367000
78	6	0	-4.495569	-4.029216	-2.406037
79	1	0	-6.038167	-2.516309	-2.271639
80	1	0	-6.630310	0.051952	4.101701
81	1	0	-5.090698	-4.696535	-3.026889
82	5	0	3.813347	-0.500960	-0.761887
83	8	0	4.286837	-1.185840	-1.862203
84	8	0	3.747054	-1.282344	0.368040
85	6	0	4.224167	-2.589606	-1.513368
86	6	0	4.379155	-2.548061	0.036644
87	6	0	5.323126	-3.332187	-2.243051
88	6	0	2.847346	-3.074954	-1.951692
89	6	0	3.676535	-3.672568	0.768029
90	6	0	5.828967	-2.444598	0.487503
91	1	0	5.351529	-4.385362	-1.935495
92	1	0	5.146639	-3.302482	-3.323794
93	1	0	6.304665	-2.889377	-2.050265
94	1	0	2.724075	-2.888059	-3.024902
95	1	0	2.703035	-4.147007	-1.767546
96	1	0	2.056781	-2.524235	-1.420984
97	1	0	4.073425	-4.644507	0.446445
98	1	0	3.826103	-3.584324	1.849503
99	1	0	2.597658	-3.662833	0.586112
100	1	0	5.853480	-2.194023	1.553851

101	1	0	6.367023	-3.389325	0.344313
102	1	0	6.361026	-1.657160	-0.058629
103	6	0	3.786002	1.613519	-2.154777
104	6	0	2.395039	1.111859	-2.396851
105	1	0	1.649826	1.900082	-2.531692
106	1	0	2.295326	0.251427	-3.058264
107	1	0	3.928004	2.692369	-2.168093
108	1	0	4.576190	1.099088	-2.702536
109	1	0	3.196184	1.075045	1.266423
110	6	0	2.850367	3.089216	0.639856
111	6	0	2.618300	4.090534	-0.335012
112	6	0	2.847662	3.529768	1.989321
113	6	0	2.450934	5.424897	0.016684
114	1	0	2.524610	3.818544	-1.384676
115	6	0	2.655395	4.857296	2.334861
116	1	0	3.000997	2.785087	2.773384
117	6	0	2.466048	5.830895	1.350047
118	1	0	2.292775	6.159635	-0.773804
119	1	0	2.663719	5.140603	3.387768
120	1	0	2.332325	6.877272	1.617300

Filename: TS7

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3488.570200 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3488.881408 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3487.794350A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3487.936427 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.844670	1.942601	-0.279417
2	6	0	4.548068	2.800906	-1.308811
3	6	0	4.883674	2.995177	0.126195
4	5	0	4.399727	0.516601	-0.089547
5	1	0	3.952957	3.567071	-1.804774
6	1	0	5.287550	2.328099	-1.954058
7	1	0	5.857629	2.658177	0.478424
8	1	0	4.504351	3.881619	0.631177
9	8	0	5.644989	0.123713	-0.535821
10	8	0	3.766969	-0.472260	0.645482
11	6	0	5.780550	-1.281572	-0.213552
12	6	0	4.801092	-1.434092	0.985865
13	6	0	7.232278	-1.570325	0.108683
14	6	0	5.324084	-2.068219	-1.434185
15	6	0	4.193264	-2.811581	1.140007
16	6	0	5.408932	-0.972535	2.304485
17	1	0	7.358423	-2.606539	0.448444
18	1	0	7.851538	-1.432381	-0.784546
19	1	0	7.612571	-0.901940	0.887022
20	1	0	5.893682	-1.742631	-2.311653
21	1	0	5.474924	-3.147427	-1.305538
22	1	0	4.259678	-1.895151	-1.637036
23	1	0	4.979885	-3.558957	1.309620
24	1	0	3.512670	-2.837545	1.999290
25	1	0	3.627878	-3.102194	0.250700
26	1	0	4.615714	-0.890241	3.055939
27	1	0	6.160639	-1.679878	2.675148
28	1	0	5.882023	0.011875	2.202592
29	8	0	1.378745	1.960365	-2.436464
30	6	0	2.324063	1.469900	-3.340508
31	1	0	2.934819	2.279998	-3.774598
32	1	0	3.024227	0.742280	-2.880218
33	1	0	1.822848	0.957016	-4.180407
34	1	0	1.875274	2.111643	-1.367468
35	6	0	1.842190	3.333088	0.678405
36	6	0	0.983944	3.230706	1.792066
37	6	0	2.103056	4.637675	0.212357
38	6	0	0.422736	4.345092	2.403270
39	1	0	0.763382	2.232226	2.181721
40	6	0	1.560247	5.757051	0.835918
41	1	0	2.736541	4.776887	-0.663627
42	6	0	0.713556	5.625448	1.935157
43	1	0	-0.238365	4.214961	3.262205

44	1	0	1.793232	6.748639	0.446598
45	1	0	0.278552	6.503079	2.410114
46	6	0	2.358396	2.106013	0.038854
47	1	0	2.116573	1.272090	0.724215
48	29	0	0.587085	0.796108	-0.763469
49	15	0	0.294952	-1.455475	-0.426595
50	15	0	-1.565746	1.543917	-0.321605
51	6	0	-1.424421	-1.975672	-0.853177
52	6	0	0.547497	-2.095756	1.260215
53	6	0	1.316057	-2.468919	-1.554725
54	6	0	-2.010329	3.283998	-0.014021
55	6	0	-2.723316	1.115643	-1.673195
56	6	0	-2.060548	0.607152	1.172799
57	6	0	-2.522557	-1.526730	-0.113066
58	6	0	-1.644327	-2.716926	-2.043445
59	6	0	1.102369	-1.235481	2.214906
60	6	0	0.147762	-3.380720	1.649192
61	6	0	1.766786	-3.768628	-1.302620
62	6	0	1.625989	-1.872028	-2.783636
63	6	0	-3.108912	3.701311	0.747748
64	6	0	-1.235406	4.236868	-0.685228
65	6	0	-2.183665	0.672486	-2.885584
66	6	0	-4.109628	1.270561	-1.557002
67	6	0	-1.876808	1.264658	2.421213
68	6	0	-2.368167	-0.756019	1.157725
69	6	0	-3.848766	-1.824989	-0.560345
70	6	0	-2.910149	-2.992501	-2.491853
71	1	0	-0.791447	-3.069765	-2.618417
72	1	0	1.408625	-0.233434	1.915918
73	6	0	1.262227	-1.654665	3.532073
74	6	0	0.322535	-3.803461	2.962955
75	1	0	-0.336270	-4.039494	0.926592
76	1	0	1.548798	-4.246461	-0.348302
77	6	0	2.515415	-4.450351	-2.259617
78	6	0	2.359705	-2.558276	-3.746111
79	1	0	1.283759	-0.853478	-2.974806
80	1	0	-3.713751	2.966711	1.280723
81	6	0	-3.421223	5.053946	0.840641
82	6	0	-1.562672	5.586581	-0.602594
83	1	0	-0.366568	3.911648	-1.260267
84	1	0	-1.098935	0.576814	-2.981306
85	6	0	-3.019577	0.368185	-3.957380
86	6	0	-4.942915	0.960473	-2.625241
87	1	0	-4.538971	1.623964	-0.619016
88	1	0	-1.601610	2.317879	2.421981
89	6	0	-2.030401	0.601666	3.609969
90	6	0	-2.585748	-1.448369	2.394448
91	6	0	-4.999382	-1.390724	0.147467
92	6	0	-4.043920	-2.550055	-1.777087
93	1	0	-3.054795	-3.556738	-3.413369
94	1	0	1.681032	-0.970412	4.268408
95	6	0	0.876862	-2.940214	3.906183
96	1	0	-0.002803	-4.799549	3.258796
97	1	0	2.871798	-5.457047	-2.046790
98	6	0	2.809038	-3.850474	-3.482778
99	1	0	2.594789	-2.074092	-4.692757
100	1	0	-4.271616	5.372553	1.441681

101	6	0	-2.652462	5.996790	0.160560
102	1	0	-0.947060	6.320348	-1.119642
103	1	0	-2.590607	0.020245	-4.895733
104	6	0	-4.398661	0.505851	-3.825817
105	1	0	-6.021585	1.064502	-2.518499
106	1	0	-1.880704	1.126475	4.553755
107	6	0	-2.403285	-0.761756	3.635699
108	6	0	-2.978047	-2.810860	2.442001
109	1	0	-4.871131	-0.831546	1.072203
110	6	0	-6.265143	-1.651955	-0.323074
111	6	0	-5.358424	-2.798330	-2.237902
112	1	0	0.992254	-3.266200	4.938624
113	1	0	3.396451	-4.387212	-4.225626
114	1	0	-2.899772	7.054628	0.234290
115	1	0	-5.053633	0.260613	-4.660569
116	6	0	-2.605358	-1.453722	4.852423
117	6	0	-3.184765	-3.452550	3.641495
118	1	0	-3.116615	-3.353752	1.509109
119	1	0	-7.131271	-1.305024	0.237934
120	6	0	-6.450877	-2.359740	-1.528388
121	1	0	-5.485473	-3.345606	-3.172049
122	1	0	-2.454322	-0.912977	5.786792
123	6	0	-2.992693	-2.773214	4.860751
124	1	0	-3.491939	-4.497205	3.647626
125	1	0	-7.457421	-2.556678	-1.893056
126	1	0	-3.153146	-3.292310	5.804028

Filename: TS8

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3488.579879 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3488.888207A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3487.800112 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3487.942743 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.710500	2.079021	0.579688
2	6	0	-4.060713	0.912909	1.176461
3	6	0	-2.092814	0.065860	2.515802
4	6	0	-3.587683	0.438753	2.529142
5	5	0	-4.892496	-0.088502	0.335437
6	1	0	-1.499293	0.997075	2.596295
7	1	0	-1.847634	-0.531141	3.406614
8	1	0	-4.159540	-0.461524	2.792532
9	1	0	-3.831256	1.172659	3.315211
10	8	0	-5.472020	-1.223587	0.859364
11	8	0	-5.192214	0.089901	-1.004301
12	6	0	-6.347843	-1.766943	-0.152078
13	6	0	-5.779885	-1.148305	-1.470799
14	6	0	-7.753081	-1.277630	0.175553
15	6	0	-6.286556	-3.280528	-0.087803
16	6	0	-4.651486	-1.971475	-2.078500
17	6	0	-6.828659	-0.826687	-2.518382
18	1	0	-8.502201	-1.695654	-0.507870
19	1	0	-8.011149	-1.581484	1.195547
20	1	0	-7.812246	-0.184179	0.125821
21	1	0	-6.674954	-3.629789	0.875527
22	1	0	-6.897318	-3.731540	-0.880954
23	1	0	-5.260160	-3.645264	-0.189784
24	1	0	-5.012647	-2.931760	-2.467007
25	1	0	-4.208865	-1.414970	-2.913881
26	1	0	-3.861297	-2.146915	-1.338965
27	1	0	-6.354063	-0.393182	-3.406510
28	1	0	-7.354796	-1.736573	-2.835352
29	1	0	-7.568963	-0.110827	-2.149090
30	1	0	-2.281334	-0.858688	1.398184
31	8	0	-2.436069	-1.577977	0.443668
32	6	0	-2.500189	-2.876154	0.955941
33	1	0	-2.320463	-3.623185	0.163564
34	1	0	-1.739932	-3.053574	1.745135
35	1	0	-3.491835	-3.088431	1.395838
36	29	0	-0.624407	-0.217459	0.871669
37	15	0	0.235775	1.105132	-0.777395
38	15	0	1.241284	-1.523065	1.324175
39	6	0	1.386545	0.084411	-1.793942
40	6	0	1.220654	2.511800	-0.170178
41	6	0	-0.939346	1.783233	-1.999942
42	6	0	1.272727	-2.264515	2.992387
43	6	0	1.499858	-2.891491	0.153568

44	6	0	2.741582	-0.462891	1.223406
45	6	0	2.613889	-0.380502	-1.309604
46	6	0	0.905212	-0.394497	-3.041555
47	6	0	1.070918	2.869635	1.174214
48	6	0	2.127569	3.223666	-0.966236
49	6	0	-0.675497	2.896768	-2.807248
50	6	0	-2.180781	1.142261	-2.099917
51	6	0	0.797191	-1.467267	4.045471
52	6	0	1.641381	-3.586651	3.262401
53	6	0	0.465422	-3.154821	-0.753554
54	6	0	2.680299	-3.643258	0.088673
55	6	0	3.338844	-0.011725	2.429481
56	6	0	3.186659	0.054064	0.001763
57	6	0	3.386300	-1.294449	-2.099316
58	6	0	1.618676	-1.294838	-3.788628
59	1	0	-0.055877	-0.040473	-3.408571
60	1	0	0.362471	2.318103	1.797323
61	6	0	1.808002	3.920690	1.711590
62	6	0	2.856203	4.279931	-0.430907
63	1	0	2.293473	2.921743	-2.000970
64	1	0	0.272708	3.424193	-2.718066
65	6	0	-1.635135	3.358785	-3.701533
66	6	0	-3.138793	1.606090	-3.000145
67	1	0	-2.412230	0.298021	-1.443537
68	1	0	0.464915	-0.448879	3.834569
69	6	0	0.730664	-1.966302	5.341083
70	6	0	1.557652	-4.090034	4.558625
71	1	0	1.980991	-4.233022	2.455146
72	1	0	-0.443476	-2.548453	-0.714300
73	6	0	0.606747	-4.164406	-1.701584
74	6	0	2.817599	-4.650024	-0.861092
75	1	0	3.503873	-3.417923	0.767902
76	1	0	2.994401	-0.419031	3.377437
77	6	0	4.341988	0.921791	2.426930
78	6	0	4.270769	0.990526	-0.016393
79	6	0	4.652638	-1.777365	-1.677788
80	6	0	2.873333	-1.768668	-3.346704
81	1	0	1.225088	-1.652244	-4.740382
82	1	0	1.678242	4.189143	2.758937
83	6	0	2.698469	4.628611	0.909368
84	1	0	3.571292	4.813982	-1.054642
85	1	0	-1.423901	4.231181	-4.318099
86	6	0	-2.867561	2.712609	-3.800003
87	1	0	-4.111918	1.120385	-3.030076
88	1	0	0.361807	-1.332827	6.145723
89	6	0	1.110608	-3.282079	5.600258
90	1	0	1.842756	-5.122656	4.753068
91	1	0	-0.199118	-4.356815	-2.408248
92	6	0	1.781028	-4.911592	-1.755607
93	1	0	3.745158	-5.217415	-0.918481
94	1	0	4.782101	1.257041	3.366229
95	6	0	4.836650	1.449316	1.213937
96	6	0	4.807086	1.506040	-1.225122
97	1	0	5.059710	-1.437006	-0.728046
98	6	0	5.366395	-2.671585	-2.441531
99	6	0	3.625288	-2.697735	-4.103879
100	1	0	3.280630	5.447359	1.329550

101	1	0	-3.621848	3.083280	-4.492421
102	1	0	1.044587	-3.680524	6.611085
103	1	0	1.897394	-5.692454	-2.505691
104	6	0	5.879664	2.404995	1.189893
105	6	0	5.832501	2.422853	-1.217399
106	1	0	4.392239	1.169534	-2.173086
107	1	0	6.335998	-3.023664	-2.093084
108	6	0	4.849965	-3.142489	-3.665430
109	1	0	3.210839	-3.051336	-5.048150
110	1	0	6.290253	2.747159	2.139962
111	6	0	6.372504	2.885371	-0.000087
112	1	0	6.226153	2.798811	-2.160398
113	1	0	5.420696	-3.854304	-4.259235
114	1	0	7.179306	3.616108	-0.005526
115	6	0	-2.869704	3.194337	1.006897
116	6	0	-2.468015	3.463169	2.329558
117	6	0	-2.434978	4.086212	0.007264
118	6	0	-1.678568	4.568577	2.625686
119	1	0	-2.793324	2.813428	3.136851
120	6	0	-1.620694	5.172890	0.298378
121	1	0	-2.744688	3.899543	-1.022405
122	6	0	-1.243677	5.425369	1.615216
123	1	0	-1.394860	4.760764	3.660320
124	1	0	-1.282264	5.825718	-0.506090
125	1	0	-0.608187	6.277458	1.852558
126	1	0	-4.082542	2.214314	-0.439623

Filename: TS9

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2682.135243 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2682.752177 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2681.930660 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2682.042938 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.007776	0.600335	2.513592
2	6	0	0.075784	-0.354778	2.634080
3	6	0	1.079309	-0.371876	3.735475
4	6	0	0.095015	-1.509381	3.575035
5	5	0	1.294540	-1.292957	1.014276
6	1	0	0.930037	0.329748	4.556081
7	1	0	2.124013	-0.577141	3.505390
8	1	0	0.475456	-2.476555	3.252553
9	1	0	-0.743992	-1.573193	4.267891
10	8	0	2.650411	-1.022514	1.123002
11	8	0	1.062295	-2.629477	0.757850
12	6	0	3.342503	-2.143072	0.518987
13	6	0	2.347626	-3.313452	0.771379
14	6	0	4.697794	-2.290746	1.179615
15	6	0	3.501842	-1.810711	-0.960838
16	6	0	2.333331	-4.379419	-0.305162
17	6	0	2.517454	-3.940239	2.147090
18	1	0	5.225346	-3.176777	0.802452
19	1	0	5.316188	-1.412667	0.960357
20	1	0	4.610289	-2.378033	2.266979
21	1	0	4.014224	-0.845949	-1.059309
22	1	0	4.086988	-2.571347	-1.492689
23	1	0	2.520709	-1.728843	-1.448182
24	1	0	3.319604	-4.853698	-0.398930
25	1	0	1.606893	-5.160685	-0.053179
26	1	0	2.048492	-3.965759	-1.277784
27	1	0	1.656828	-4.582761	2.363921
28	1	0	3.424817	-4.554805	2.202003
29	1	0	2.575174	-3.174548	2.930020
30	29	0	-0.050406	0.204019	0.704899
31	15	0	1.117449	1.845080	-0.476658
32	15	0	-1.215302	-0.322981	-1.229369
33	6	0	0.818284	1.350542	-2.242115
34	6	0	0.415497	3.540249	-0.453346
35	6	0	2.924634	2.072129	-0.409845
36	6	0	-0.643783	0.960453	-2.443050
37	6	0	-3.030400	-0.182487	-1.362170
38	6	0	-0.828778	-1.921435	-2.015360
39	1	0	1.088061	2.162543	-2.932440
40	1	0	1.488858	0.503591	-2.450957
41	6	0	-0.806899	3.718838	0.205023
42	6	0	1.015206	4.634370	-1.088124
43	6	0	3.717668	2.344117	-1.532374

44	6	0	3.546867	1.911404	0.834887
45	1	0	-0.841475	0.643183	-3.476502
46	1	0	-1.286595	1.833774	-2.259750
47	6	0	-3.628378	0.860959	-0.645003
48	6	0	-3.835083	-1.039265	-2.120293
49	6	0	-1.316397	-3.086606	-1.404851
50	6	0	-0.019158	-2.047269	-3.149020
51	1	0	-1.252087	2.863352	0.721471
52	6	0	-1.429683	4.964602	0.212000
53	6	0	0.396442	5.880387	-1.072994
54	1	0	1.978533	4.512024	-1.585621
55	1	0	3.257260	2.460548	-2.513552
56	6	0	5.100447	2.458482	-1.411142
57	6	0	4.926515	2.036496	0.956947
58	1	0	2.940923	1.651207	1.702131
59	1	0	-3.006461	1.501739	-0.017190
60	6	0	-5.002965	1.056592	-0.699240
61	6	0	-5.213779	-0.847473	-2.162911
62	1	0	-3.384534	-1.859991	-2.676984
63	1	0	-1.928478	-3.003286	-0.505459
64	6	0	-1.031229	-4.337667	-1.935630
65	6	0	0.283711	-3.304920	-3.669801
66	1	0	0.381217	-1.160744	-3.640371
67	1	0	-2.381394	5.091357	0.725759
68	6	0	-0.828536	6.045642	-0.427139
69	1	0	0.871654	6.727733	-1.564793
70	1	0	5.705605	2.665564	-2.292301
71	6	0	5.706112	2.307052	-0.166046
72	1	0	5.396654	1.904196	1.929927
73	1	0	-5.455326	1.860495	-0.121342
74	6	0	-5.799054	0.200137	-1.456490
75	1	0	-5.832853	-1.520225	-2.754513
76	1	0	-1.426913	-5.230634	-1.454548
77	6	0	-0.228682	-4.451519	-3.070845
78	1	0	0.915239	-3.384246	-4.553316
79	1	0	-1.309892	7.022133	-0.417137
80	1	0	6.787313	2.394076	-0.072367
81	1	0	-6.878038	0.342643	-1.487105
82	1	0	0.003321	-5.433033	-3.480656
83	6	0	-2.394077	0.175917	2.450110
84	6	0	-2.756322	-1.135523	2.065649
85	6	0	-3.444384	1.063085	2.763832
86	6	0	-4.086749	-1.524701	1.993149
87	1	0	-1.961634	-1.840578	1.811339
88	6	0	-4.774070	0.664663	2.700926
89	1	0	-3.195073	2.081638	3.070031
90	6	0	-5.110997	-0.632165	2.313121
91	1	0	-4.330657	-2.540222	1.678284
92	1	0	-5.559476	1.376226	2.958470
93	1	0	-6.153310	-0.940273	2.253332
94	1	0	-0.815474	1.620390	2.856091

Filename: TS10

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2682.169540 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2682.783287 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2681.961006 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2682.073331 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.446497	-2.262539	-0.494413
2	6	0	0.404229	-1.837455	-1.605589
3	6	0	0.029259	-0.312057	-2.628333
4	6	0	0.047127	-1.753288	-3.047945
5	5	0	1.931396	-1.813536	-1.300358
6	1	0	0.886282	0.283123	-2.937638
7	1	0	-0.939651	0.186139	-2.715839
8	1	0	-0.915741	-2.185487	-3.324732
9	1	0	0.830380	-2.043979	-3.752360
10	8	0	2.850343	-1.094469	-2.029438
11	8	0	2.508134	-2.602019	-0.331730
12	6	0	4.159430	-1.610891	-1.688043
13	6	0	3.918120	-2.268602	-0.287363
14	6	0	5.146219	-0.460962	-1.684015
15	6	0	4.517819	-2.624167	-2.767118
16	6	0	4.707397	-3.540078	-0.042086
17	6	0	4.106222	-1.301237	0.870334
18	1	0	6.144436	-0.803819	-1.381515
19	1	0	5.227143	-0.033366	-2.689916
20	1	0	4.832841	0.339302	-1.006199
21	1	0	4.483861	-2.134508	-3.746192
22	1	0	5.523463	-3.037032	-2.623987
23	1	0	3.803641	-3.456233	-2.783173
24	1	0	5.786246	-3.340021	-0.071378
25	1	0	4.467692	-3.943682	0.947652
26	1	0	4.478668	-4.311394	-0.782933
27	1	0	3.768574	-1.772072	1.800198
28	1	0	5.155804	-1.006287	0.992613
29	1	0	3.514818	-0.390747	0.720829
30	29	0	-0.180272	-0.148903	-0.417861
31	15	0	-2.074332	1.082210	0.153412
32	15	0	1.125098	1.296104	0.788279
33	6	0	-1.408072	2.347896	1.339744
34	6	0	-2.944146	2.062120	-1.113991
35	6	0	-3.410998	0.301990	1.118475
36	6	0	0.011410	2.775717	0.981722
37	6	0	2.644441	2.107300	0.166754
38	6	0	1.461719	0.838539	2.527575
39	1	0	-2.084331	3.211042	1.415495
40	1	0	-1.410435	1.860951	2.325266
41	6	0	-2.655256	3.410371	-1.359944
42	6	0	-3.848418	1.405407	-1.964558
43	6	0	-4.724568	0.784145	1.154881

44	6	0	-3.071918	-0.823057	1.878662
45	1	0	0.416031	3.467478	1.733949
46	1	0	0.036933	3.305013	0.018646
47	6	0	2.623074	2.528313	-1.171551
48	6	0	3.816323	2.287931	0.910472
49	6	0	1.802105	1.762969	3.524506
50	6	0	1.298267	-0.507583	2.877714
51	1	0	-1.957219	3.947797	-0.718329
52	6	0	-3.260951	4.086370	-2.416413
53	6	0	-4.456831	2.084055	-3.013899
54	1	0	-4.087728	0.356977	-1.779377
55	1	0	-4.999911	1.656243	0.562236
56	6	0	-5.681867	0.146608	1.938194
57	6	0	-4.030218	-1.453256	2.665565
58	1	0	-2.053551	-1.214198	1.819522
59	1	0	1.728002	2.353592	-1.772071
60	6	0	3.731720	3.144970	-1.739809
61	6	0	4.931604	2.893764	0.334660
62	1	0	3.863653	1.940926	1.942304
63	1	0	1.934071	2.815417	3.269392
64	6	0	1.981867	1.348183	4.840698
65	6	0	1.484317	-0.923387	4.193598
66	1	0	1.018967	-1.221495	2.097515
67	1	0	-3.028713	5.136484	-2.586843
68	6	0	-4.163644	3.427152	-3.246025
69	1	0	-5.164670	1.560582	-3.654582
70	1	0	-6.702570	0.525526	1.958581
71	6	0	-5.336220	-0.971451	2.694516
72	1	0	-3.759763	-2.340331	3.235951
73	1	0	3.696745	3.467877	-2.778851
74	6	0	4.890413	3.330321	-0.986847
75	1	0	5.837210	3.024626	0.925045
76	1	0	2.243617	2.074893	5.608033
77	6	0	1.823796	0.004204	5.175600
78	1	0	1.357465	-1.972965	4.453103
79	1	0	-4.636363	3.956755	-4.071016
80	1	0	-6.089380	-1.472641	3.300494
81	1	0	5.762975	3.803305	-1.433809
82	1	0	1.961439	-0.318236	6.206318
83	1	0	0.121407	-2.737271	0.307351
84	6	0	-1.835906	-2.665031	-0.580508
85	6	0	-2.775786	-2.056590	-1.445260
86	6	0	-2.341424	-3.658036	0.288278
87	6	0	-4.120159	-2.410281	-1.428869
88	1	0	-2.447907	-1.258036	-2.111969
89	6	0	-3.684610	-4.005462	0.305966
90	1	0	-1.645484	-4.152399	0.968844
91	6	0	-4.593901	-3.384646	-0.551887
92	1	0	-4.811776	-1.909276	-2.108625
93	1	0	-4.029860	-4.773110	0.999451
94	1	0	-5.648623	-3.652021	-0.534397

Filename: TS11

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2797.876979 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2798.484900 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2797.608252 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2797.728914 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.881922	-2.996141	-0.995168
2	6	0	-0.736598	-3.800178	-2.266325
3	6	0	-0.720337	-4.518284	-0.964762
4	5	0	-2.294431	-2.506399	-0.622472
5	1	0	0.210740	-3.706137	-2.797373
6	1	0	-1.607014	-3.910118	-2.911375
7	1	0	-1.579279	-5.132942	-0.699468
8	1	0	0.238196	-4.889547	-0.603733
9	8	0	-3.455999	-3.118863	-1.050098
10	8	0	-2.545388	-1.453185	0.244764
11	6	0	-4.557419	-2.307834	-0.578661
12	6	0	-3.931375	-1.592216	0.653696
13	6	0	-5.730707	-3.212537	-0.261006
14	6	0	-4.913372	-1.338749	-1.698512
15	6	0	-4.514264	-0.230944	0.971840
16	6	0	-3.934379	-2.466615	1.901637
17	1	0	-6.555633	-2.641855	0.184977
18	1	0	-6.104063	-3.681703	-1.177890
19	1	0	-5.447233	-4.010370	0.431627
20	1	0	-5.147795	-1.902883	-2.607401
21	1	0	-5.780344	-0.716926	-1.442595
22	1	0	-4.067150	-0.677035	-1.925132
23	1	0	-5.589202	-0.314345	1.180171
24	1	0	-4.032283	0.189861	1.862221
25	1	0	-4.379497	0.479585	0.150269
26	1	0	-3.295956	-2.003611	2.662654
27	1	0	-4.942403	-2.574833	2.320079
28	1	0	-3.540105	-3.467330	1.687176
29	8	0	0.288985	-0.441864	-2.641880
30	6	0	-0.998742	-0.334851	-3.166696
31	1	0	-1.152810	-1.012120	-4.025608
32	1	0	-1.772975	-0.588305	-2.408701
33	1	0	-1.208572	0.693961	-3.504917
34	1	0	0.248177	-1.235479	-1.734175
35	29	0	0.313073	0.155644	-0.504375
36	15	0	2.300940	1.009293	0.351513
37	15	0	-0.827641	1.933360	0.298640
38	6	0	1.706540	2.470930	1.344116
39	6	0	3.484345	0.209564	1.480216
40	6	0	3.312527	1.786598	-0.949348
41	6	0	0.519519	3.160174	0.672719
42	6	0	-1.524505	1.631629	1.964290
43	6	0	-2.100170	2.908476	-0.564741

44	1	0	1.405329	2.094562	2.332339
45	1	0	2.524134	3.184702	1.513217
46	6	0	4.749704	-0.201887	1.045562
47	6	0	3.073552	-0.129967	2.778020
48	6	0	4.379528	2.649215	-0.661341
49	6	0	2.978355	1.520630	-2.283335
50	1	0	0.826609	3.604073	-0.285619
51	1	0	0.149575	3.976034	1.309734
52	6	0	-1.196577	0.430452	2.604651
53	6	0	-2.360235	2.545615	2.616270
54	6	0	-2.223970	4.300910	-0.486416
55	6	0	-2.999572	2.192537	-1.365757
56	1	0	5.072818	0.021833	0.029793
57	6	0	5.592372	-0.909724	1.897468
58	6	0	3.920554	-0.830910	3.628427
59	1	0	2.076474	0.145723	3.126173
60	1	0	4.655753	2.843424	0.376311
61	6	0	5.100701	3.240535	-1.692258
62	6	0	3.704831	2.118664	-3.312551
63	1	0	2.147335	0.845806	-2.509604
64	1	0	-0.579966	-0.301494	2.077534
65	6	0	-1.679906	0.157031	3.881845
66	6	0	-2.855919	2.264501	3.886082
67	1	0	-2.640638	3.474490	2.117652
68	1	0	-1.527468	4.880461	0.119323
69	6	0	-3.234924	4.957482	-1.184415
70	6	0	-4.016916	2.846573	-2.051765
71	1	0	-2.879081	1.110876	-1.449066
72	1	0	6.571081	-1.226803	1.540708
73	6	0	5.185874	-1.219832	3.191910
74	1	0	3.589105	-1.078928	4.635505
75	1	0	5.930442	3.907233	-1.462758
76	6	0	4.761371	2.975776	-3.019590
77	1	0	3.441681	1.908967	-4.347735
78	1	0	-1.417886	-0.780472	4.370077
79	6	0	-2.513863	1.071626	4.521691
80	1	0	-3.513780	2.976980	4.381021
81	1	0	-3.319816	6.040950	-1.119971
82	6	0	-4.134992	4.232304	-1.961928
83	1	0	-4.709253	2.274263	-2.667676
84	1	0	5.847312	-1.772726	3.856587
85	1	0	5.327301	3.439586	-3.826063
86	1	0	-2.903620	0.852555	5.514259
87	1	0	-4.923487	4.749333	-2.505761
88	6	0	1.643034	-2.640142	-0.532895
89	6	0	2.228888	-3.127762	0.647521
90	6	0	2.435316	-2.656078	-1.695044
91	6	0	3.534909	-3.606368	0.674020
92	1	0	1.637612	-3.116908	1.566132
93	6	0	3.739054	-3.145028	-1.675838
94	1	0	2.022014	-2.241082	-2.615046
95	6	0	4.297667	-3.622781	-0.491972
96	1	0	3.961536	-3.963584	1.611358
97	1	0	4.328331	-3.140472	-2.592766
98	1	0	5.321486	-3.994931	-0.475271
99	6	0	0.256175	-2.082175	-0.536728
100	1	0	0.012116	-1.823811	0.513895

Filename: TS12

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2797.890458 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2798.493603 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2797.616797 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2797.737829 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.246346	0.834158	2.675103
2	6	0	-1.690099	0.402784	2.975738
3	1	0	-0.283240	1.689804	1.972461
4	1	0	0.216384	1.277530	3.572664
5	1	0	0.649002	-0.310036	2.753212
6	8	0	1.399593	-1.268196	2.692489
7	6	0	2.684926	-0.826221	2.998472
8	1	0	3.439495	-1.322867	2.361356
9	1	0	2.801730	0.267334	2.828220
10	1	0	2.956766	-1.026601	4.050000
11	29	0	0.624126	-0.139493	0.886792
12	15	0	-0.043028	-1.236204	-1.023697
13	15	0	2.355107	0.834844	-0.351631
14	6	0	0.714393	-0.195960	-2.375334
15	6	0	0.991728	-2.740136	-1.132745
16	6	0	-1.632636	-1.717805	-1.771433
17	6	0	2.169423	0.121698	-2.052455
18	6	0	4.159978	0.730978	-0.101579
19	6	0	2.009415	2.616988	-0.529194
20	1	0	0.633819	-0.710059	-3.343008
21	1	0	0.127217	0.731003	-2.451747
22	6	0	1.727658	-3.114369	-0.001104
23	6	0	1.127207	-3.476368	-2.317562
24	6	0	-2.123808	-3.022907	-1.643376
25	6	0	-2.438329	-0.748470	-2.383502
26	1	0	2.624944	0.763917	-2.817957
27	1	0	2.757163	-0.807481	-2.047038
28	6	0	4.970078	1.849093	0.121673
29	6	0	4.740321	-0.546166	-0.073090
30	6	0	1.741900	3.323575	0.653713
31	6	0	1.957197	3.299602	-1.749514
32	1	0	1.607712	-2.552568	0.932180
33	6	0	2.595959	-4.204141	-0.063261
34	6	0	1.993174	-4.563342	-2.373332
35	1	0	0.542070	-3.201790	-3.196686
36	1	0	-1.524127	-3.782514	-1.142067
37	6	0	-3.384441	-3.351245	-2.132683
38	6	0	-3.698493	-1.078553	-2.868062
39	1	0	-2.095212	0.282737	-2.450144
40	1	0	4.534509	2.847534	0.107103
41	6	0	6.334482	1.692667	0.355852
42	6	0	6.103430	-0.696720	0.150446
43	1	0	4.114717	-1.430554	-0.215262

44	1	0	1.757896	2.791426	1.606789
45	6	0	1.446295	4.682036	0.616478
46	6	0	1.642877	4.656213	-1.787076
47	1	0	2.157539	2.774731	-2.682857
48	1	0	3.163476	-4.488900	0.821769
49	6	0	2.732103	-4.925116	-1.246399
50	1	0	2.092924	-5.131488	-3.296836
51	1	0	-3.754843	-4.368619	-2.015574
52	6	0	-4.174812	-2.382805	-2.746535
53	1	0	-4.315298	-0.309847	-3.331219
54	1	0	6.954343	2.571422	0.525937
55	6	0	6.904946	0.423339	0.367322
56	1	0	6.540206	-1.693744	0.165462
57	1	0	1.241912	5.216293	1.542712
58	6	0	1.388538	5.349587	-0.606446
59	1	0	1.597064	5.173116	-2.744346
60	1	0	3.410293	-5.775803	-1.293194
61	1	0	-5.163496	-2.640854	-3.122151
62	1	0	7.971337	0.304642	0.549943
63	1	0	1.137907	6.408701	-0.638412
64	6	0	-2.506043	0.276554	1.716697
65	6	0	-2.964316	-0.877521	1.173597
66	1	0	-3.602561	-0.786016	0.288024
67	6	0	-2.726093	-2.262024	1.580886
68	6	0	-1.492080	-2.691034	2.096778
69	6	0	-3.717227	-3.231750	1.352749
70	6	0	-1.264170	-4.034516	2.378670
71	1	0	-0.684784	-1.976988	2.243711
72	6	0	-3.496609	-4.570493	1.650461
73	1	0	-4.669619	-2.918467	0.922970
74	6	0	-2.265059	-4.979432	2.163452
75	1	0	-0.289951	-4.336136	2.762057
76	1	0	-4.283585	-5.302352	1.471203
77	1	0	-2.085925	-6.030551	2.384915
78	5	0	-2.819820	1.591950	0.967934
79	8	0	-2.681961	2.841320	1.535085
80	8	0	-3.216738	1.655992	-0.356967
81	6	0	-3.205418	3.798549	0.584872
82	6	0	-3.052570	3.033843	-0.764444
83	6	0	-2.397304	5.076538	0.688298
84	1	0	-2.561770	5.546477	1.664326
85	1	0	-1.325385	4.881022	0.583558
86	1	0	-2.698120	5.794434	-0.086302
87	6	0	-4.660347	4.050455	0.956077
88	1	0	-4.715665	4.378635	1.999199
89	1	0	-5.111310	4.827446	0.326854
90	1	0	-5.257969	3.136820	0.857697
91	6	0	-1.648192	3.160278	-1.343397
92	1	0	-1.535524	2.467077	-2.186802
93	1	0	-1.442386	4.172524	-1.712218
94	1	0	-0.884793	2.909239	-0.593476
95	6	0	-4.096245	3.360826	-1.812780
96	1	0	-4.051477	4.420491	-2.095490
97	1	0	-3.918828	2.765808	-2.716776
98	1	0	-5.107207	3.139045	-1.458648
99	1	0	-2.187134	1.156808	3.609850
100	1	0	-1.701451	-0.534729	3.550311

Filename: TS13

SCF Energy (M06L/LANL2DZ-6-31g(d))

-2682.163645 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-2682.777106 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-2681.955265 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-2682.067739 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.218883	-0.375962	-2.425945
2	1	0	0.494917	-0.655928	-3.207120
3	6	0	-1.044832	-1.464911	-1.918227
4	6	0	-0.561803	1.027547	-2.389972
5	6	0	-0.300385	-2.867841	-0.949826
6	6	0	-0.805305	-2.872352	-2.358355
7	5	0	-2.516260	-1.304367	-1.418255
8	6	0	0.146034	1.940722	-3.211412
9	6	0	-1.548817	1.599843	-1.548829
10	1	0	-0.952602	-3.293689	-0.190523
11	1	0	0.758251	-3.119547	-0.851281
12	1	0	-0.039060	-2.980449	-3.130778
13	1	0	-1.678198	-3.491437	-2.585297
14	8	0	-2.986760	-1.751302	-0.204906
15	8	0	-3.513135	-0.864852	-2.253292
16	6	0	-0.096606	3.307058	-3.176478
17	1	0	0.901172	1.543462	-3.893555
18	6	0	-1.803575	2.962819	-1.534163
19	1	0	-2.103040	0.956732	-0.863549
20	6	0	-4.428889	-1.862189	-0.340437
21	6	0	-4.736443	-0.834783	-1.473749
22	6	0	-1.077344	3.842329	-2.339428
23	1	0	0.483355	3.965795	-3.824552
24	1	0	-2.581293	3.348592	-0.871439
25	6	0	-5.071580	-1.553167	0.994653
26	6	0	-4.711904	-3.299858	-0.755601
27	6	0	-5.891001	-1.213114	-2.379949
28	6	0	-4.916024	0.584352	-0.952426
29	1	0	-1.272202	4.912286	-2.316390
30	1	0	-6.166050	-1.555092	0.907732
31	1	0	-4.790860	-2.313024	1.733022
32	1	0	-4.753646	-0.580936	1.382608
33	1	0	-4.274385	-3.982557	-0.019040
34	1	0	-5.787897	-3.502470	-0.815764
35	1	0	-4.267071	-3.526074	-1.732383
36	1	0	-6.824641	-1.294418	-1.808467
37	1	0	-6.031861	-0.443596	-3.146579
38	1	0	-5.712200	-2.164697	-2.888976

39	1	0	-4.851314	1.288989	-1.788260
40	1	0	-5.889378	0.708670	-0.461411
41	1	0	-4.137245	0.849019	-0.227744
42	29	0	0.411734	-0.851863	-0.437351
43	15	0	2.572301	-0.812148	0.354604
44	15	0	-0.174055	0.446634	1.438636
45	6	0	2.451918	-0.158425	2.105887
46	6	0	3.601358	-2.308258	0.555502
47	6	0	3.675088	0.383520	-0.475753
48	6	0	1.033792	-0.259729	2.665856
49	6	0	-1.722557	0.574676	2.392914
50	6	0	0.419336	2.177203	1.397110
51	1	0	3.166158	-0.688087	2.749559
52	1	0	2.758793	0.896149	2.077248
53	6	0	3.203987	-3.275522	1.490667
54	6	0	4.704505	-2.578872	-0.263220
55	6	0	4.877253	0.828550	0.089795
56	6	0	3.254771	0.919656	-1.697704
57	1	0	0.962866	0.265485	3.629342
58	1	0	0.762704	-1.310683	2.840333
59	6	0	-2.073001	-0.355050	3.379536
60	6	0	-2.630040	1.597975	2.080495
61	6	0	0.360667	3.013921	2.520421
62	6	0	1.056502	2.631858	0.239975
63	1	0	2.328877	-3.094236	2.118246
64	6	0	3.909021	-4.466035	1.625325
65	6	0	5.404579	-3.775507	-0.131672
66	1	0	5.024334	-1.842505	-0.999624
67	1	0	5.220010	0.409627	1.036993
68	6	0	5.636021	1.801461	-0.553001
69	6	0	4.016358	1.891381	-2.341791
70	1	0	2.300386	0.588054	-2.115042
71	1	0	-1.393097	-1.169120	3.629008
72	6	0	-3.283824	-0.245830	4.058113
73	6	0	-3.841456	1.702574	2.756716
74	1	0	-2.368499	2.328273	1.312590
75	1	0	-0.146427	2.673192	3.424460
76	6	0	0.936939	4.279500	2.481703
77	6	0	1.636775	3.897216	0.202886
78	1	0	1.078149	1.991211	-0.641454
79	1	0	3.592004	-5.201351	2.363022
80	6	0	5.013758	-4.719639	0.813836
81	1	0	6.264800	-3.967539	-0.770957
82	1	0	6.566099	2.147495	-0.104996
83	6	0	5.205106	2.334853	-1.767872
84	1	0	3.670218	2.311672	-3.285082
85	1	0	-3.534647	-0.970413	4.831353
86	6	0	-4.169625	0.784962	3.753670
87	1	0	-4.530299	2.507801	2.504879
88	1	0	0.886982	4.924833	3.357515
89	6	0	1.579388	4.720202	1.324133
90	1	0	2.120297	4.236543	-0.711996

91	1	0	5.563593	-5.653392	0.915157
92	1	0	5.798346	3.101200	-2.264204
93	1	0	-5.114919	0.869676	4.286673
94	1	0	2.029451	5.711473	1.297857

Cartesian coordinates of the structures shown in **Figure S2**:

Filename: TS1BINAP2

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.822273 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.141072 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.108131 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.241524 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.690506	1.189118	-1.867301
2	6	0	-3.228223	-0.042693	-1.303745
3	6	0	-4.695097	-0.251209	-1.109839
4	6	0	-3.948535	-1.025912	-2.169023
5	1	0	-5.338003	0.575275	-1.412889
6	1	0	-5.062145	-0.797584	-0.242311
7	1	0	-3.809681	-2.093106	-2.012978
8	1	0	-4.091938	-0.743267	-3.212694
9	29	0	-1.367796	0.256968	-0.516678
10	15	0	0.373792	-1.080131	-1.455165
11	15	0	0.041685	1.531895	0.855574
12	6	0	1.289083	-1.550775	0.063945
13	6	0	1.574053	-0.344962	-2.631402
14	6	0	0.003247	-2.673253	-2.273809
15	6	0	-0.514129	3.262690	1.058700
16	6	0	0.376936	0.990358	2.567326
17	6	0	1.759218	1.692373	0.158716
18	6	0	2.238449	-0.728793	0.669448
19	6	0	0.841064	-2.715101	0.749096
20	6	0	1.328186	0.957850	-3.078366
21	6	0	2.685083	-1.038064	-3.125248
22	6	0	0.796037	-3.823301	-2.181072
23	6	0	-1.143098	-2.705656	-3.074264
24	6	0	-0.797152	4.009388	-0.095030
25	6	0	-0.730170	3.848851	2.310295
26	6	0	-0.409402	-0.019631	3.124732
27	6	0	1.414114	1.552315	3.322705
28	6	0	2.193590	2.933085	-0.373887
29	6	0	2.616189	0.588118	0.082990
30	6	0	2.861470	-1.140742	1.895032
31	6	0	1.386821	-3.092290	1.947489
32	1	0	0.041458	-3.304171	0.305813
33	1	0	0.456650	1.491839	-2.689190
34	6	0	2.191610	1.566885	-3.984832
35	6	0	3.548368	-0.428159	-4.028550
36	1	0	2.882064	-2.057206	-2.790887

37	1	0	1.690297	-3.819428	-1.557454
38	6	0	0.436284	-4.983813	-2.861520
39	6	0	-1.500050	-3.862611	-3.758502
40	1	0	-1.768542	-1.815453	-3.134431
41	1	0	-0.689817	3.543514	-1.075747
42	6	0	-1.219839	5.328736	0.001447
43	6	0	-1.185853	5.162443	2.403555
44	1	0	-0.543618	3.280564	3.219148
45	1	0	-1.223176	-0.440084	2.532322
46	6	0	-0.147388	-0.479071	4.413441
47	6	0	1.666814	1.098552	4.611915
48	1	0	2.033388	2.338581	2.887803
49	1	0	1.552099	3.805084	-0.286441
50	6	0	3.412059	3.066783	-0.989476
51	6	0	3.895109	0.715873	-0.546816
52	6	0	3.900835	-0.396457	2.508218
53	6	0	2.431788	-2.343268	2.538497
54	1	0	1.030645	-3.990800	2.454476
55	1	0	1.997908	2.586128	-4.315896
56	6	0	3.304453	0.875748	-4.457146
57	1	0	4.422378	-0.967287	-4.391079
58	1	0	1.057848	-5.873846	-2.775959
59	6	0	-0.713190	-5.007089	-3.648730
60	1	0	-2.402126	-3.872496	-4.369000
61	1	0	-1.432530	5.890965	-0.904950
62	6	0	-1.417536	5.908538	1.252993
63	1	0	-1.352945	5.603359	3.385047
64	1	0	-0.749719	-1.282559	4.835649
65	6	0	0.892317	0.074470	5.155042
66	1	0	2.485401	1.528468	5.187226
67	1	0	3.717575	4.033063	-1.391623
68	6	0	4.290118	1.968601	-1.108895
69	6	0	4.789946	-0.378835	-0.663608
70	1	0	4.230882	0.531868	2.046867
71	6	0	4.498032	-0.828177	3.670797
72	6	0	3.049337	-2.749357	3.743438
73	1	0	3.986213	1.353160	-5.159394
74	1	0	-0.994246	-5.917236	-4.176051
75	1	0	-1.770060	6.936040	1.327985
76	1	0	1.106398	-0.295553	6.156568
77	6	0	5.540960	2.077019	-1.761446
78	6	0	6.002679	-0.241858	-1.297810
79	1	0	4.500326	-1.343149	-0.250189
80	1	0	5.300959	-0.240935	4.113605
81	6	0	4.069962	-2.013225	4.299442
82	1	0	2.702333	-3.666496	4.219910
83	1	0	5.821451	3.039966	-2.188625
84	6	0	6.384205	0.995669	-1.855715
85	1	0	6.670701	-1.098014	-1.375844
86	1	0	4.544088	-2.341941	5.222592
87	1	0	7.344791	1.091253	-2.358907
88	5	0	-2.540528	-1.276785	0.279035

89	8	0	-3.311548	-1.234580	1.430366
90	8	0	-2.332514	-2.586221	-0.129097
91	6	0	-3.470022	-2.588673	1.932479
92	6	0	-3.140218	-3.473274	0.685007
93	6	0	-4.885236	-2.734979	2.459484
94	6	0	-2.475257	-2.767958	3.069799
95	6	0	-2.326553	-4.721991	0.974760
96	6	0	-4.366479	-3.856756	-0.133087
97	1	0	-5.072892	-3.761639	2.800583
98	1	0	-5.036561	-2.064203	3.312115
99	1	0	-5.632222	-2.483709	1.700475
100	1	0	-2.662227	-2.000119	3.829162
101	1	0	-2.577318	-3.751516	3.545283
102	1	0	-1.440172	-2.656946	2.721957
103	1	0	-2.904061	-5.439588	1.572087
104	1	0	-2.055471	-5.208189	0.029431
105	1	0	-1.401490	-4.498001	1.514327
106	1	0	-4.041442	-4.307333	-1.078483
107	1	0	-4.990168	-4.587911	0.396085
108	1	0	-4.988710	-2.987561	-0.371776
109	6	0	-3.235735	2.469982	-1.465913
110	6	0	-3.827241	2.662018	-0.196377
111	6	0	-3.241222	3.569641	-2.349038
112	6	0	-4.403587	3.874910	0.153245
113	1	0	-3.821390	1.833241	0.514591
114	6	0	-3.831148	4.777536	-1.999297
115	1	0	-2.792803	3.448819	-3.337280
116	6	0	-4.421110	4.942567	-0.745462
117	1	0	-4.843466	3.991908	1.143744
118	1	0	-3.835272	5.600065	-2.715438
119	1	0	-4.880467	5.890557	-0.469919
120	1	0	-2.308745	1.122281	-2.890167

Filename: TS2BINAP2

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.846433 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.166489 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.133817 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.268374 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.184337	-2.244830	0.649655
2	1	0	-1.798473	-3.086207	1.234457
3	6	0	-2.877368	-1.224842	1.419340
4	6	0	-2.400191	-2.522815	-0.751062
5	6	0	-1.981014	-0.203440	2.697882
6	6	0	-2.955926	-1.318548	2.907559
7	5	0	-4.017452	-0.309834	0.863038
8	6	0	-2.049785	-3.784344	-1.287501
9	6	0	-2.918513	-1.583838	-1.671383
10	1	0	-2.354241	0.813032	2.808661
11	1	0	-0.998703	-0.392238	3.134849
12	1	0	-2.528081	-2.236850	3.322196
13	1	0	-3.911973	-1.081342	3.384195
14	8	0	-3.984392	1.065390	0.868794
15	8	0	-5.233906	-0.817819	0.483059
16	6	0	-2.194498	-4.071834	-2.638070
17	1	0	-1.639285	-4.538766	-0.613585
18	6	0	-3.064900	-1.872498	-3.019178
19	1	0	-3.172487	-0.586120	-1.312574
20	6	0	-5.360615	1.510547	0.735026
21	6	0	-6.031364	0.300877	0.012712
22	6	0	-2.701827	-3.123135	-3.527280
23	1	0	-1.902699	-5.056777	-3.004210
24	1	0	-3.470228	-1.107133	-3.685282
25	6	0	-5.380468	2.811441	-0.039060
26	6	0	-5.883895	1.717528	2.150149
27	6	0	-7.476433	0.051879	0.395530
28	6	0	-5.886853	0.364065	-1.501198
29	1	0	-2.817786	-3.351595	-4.584655
30	1	0	-6.412388	3.137392	-0.224218
31	1	0	-4.876071	3.597629	0.534287
32	1	0	-4.864646	2.720018	-0.999574
33	1	0	-5.233550	2.424089	2.677170
34	1	0	-6.903410	2.121156	2.152649
35	1	0	-5.887966	0.776475	2.713801
36	1	0	-8.101672	0.917283	0.140662
37	1	0	-7.863648	-0.815344	-0.150096
38	1	0	-7.583476	-0.149799	1.465328

39	1	0	-6.117746	-0.616729	-1.930093
40	1	0	-6.566884	1.107732	-1.935135
41	1	0	-4.864891	0.628277	-1.796637
42	29	0	-0.924025	-0.485652	0.762494
43	15	0	-0.196880	1.383026	-0.408955
44	15	0	1.198279	-1.422805	1.085664
45	6	0	1.183639	0.898859	-1.539173
46	6	0	0.574971	2.614174	0.704302
47	6	0	-1.352811	2.386452	-1.431334
48	6	0	1.115840	-2.543784	2.522493
49	6	0	1.780612	-2.459471	-0.295385
50	6	0	2.570783	-0.241754	1.368787
51	6	0	2.440362	0.494615	-1.063847
52	6	0	0.897131	0.761144	-2.923615
53	6	0	0.473098	2.436332	2.087675
54	6	0	1.303492	3.704356	0.211261
55	6	0	-1.574681	3.753404	-1.221797
56	6	0	-2.134556	1.731203	-2.397415
57	6	0	0.871699	-2.028836	3.807422
58	6	0	1.046742	-3.932811	2.343027
59	6	0	0.999620	-2.538650	-1.452198
60	6	0	3.010286	-3.130187	-0.244963
61	6	0	3.182278	-0.111712	2.642253
62	6	0	2.914003	0.652270	0.346611
63	6	0	3.400746	-0.055837	-1.983995
64	6	0	1.806021	0.245567	-3.807995
65	1	0	-0.062524	1.095022	-3.304902
66	1	0	-0.077577	1.575315	2.468650
67	6	0	1.090583	3.326367	2.962009
68	6	0	1.910139	4.600451	1.084823
69	1	0	1.409998	3.837753	-0.866372
70	1	0	-1.018116	4.285330	-0.453963
71	6	0	-2.508150	4.449570	-1.987292
72	6	0	-3.054990	2.430357	-3.171390
73	1	0	-2.017902	0.658762	-2.548505
74	1	0	0.879346	-0.950675	3.970069
75	6	0	0.608710	-2.873297	4.880188
76	6	0	0.771174	-4.775727	3.416322
77	1	0	1.198940	-4.356733	1.351667
78	1	0	0.048963	-2.005390	-1.493595
79	6	0	1.442656	-3.274969	-2.547726
80	6	0	3.448563	-3.866834	-1.339358
81	1	0	3.627096	-3.062037	0.652721
82	1	0	2.960964	-0.842684	3.415418
83	6	0	4.071647	0.895344	2.912071
84	6	0	3.864163	1.692428	0.608841
85	6	0	4.680499	-0.505715	-1.565914
86	6	0	3.077036	-0.185563	-3.370010
87	1	0	1.556123	0.167976	-4.866173
88	1	0	1.017845	3.167630	4.036757
89	6	0	1.808465	4.409902	2.461353
90	1	0	2.489307	5.433303	0.689518

91	1	0	-2.659029	5.513030	-1.808145
92	6	0	-3.241449	3.797336	-2.973611
93	1	0	-3.636194	1.898964	-3.924443
94	1	0	0.430857	-2.449631	5.867153
95	6	0	0.557376	-4.252505	4.688457
96	1	0	0.722386	-5.851081	3.253309
97	1	0	0.824744	-3.322674	-3.443148
98	6	0	2.666572	-3.936238	-2.492499
99	1	0	4.410920	-4.375256	-1.300848
100	1	0	4.535060	0.970320	3.896133
101	6	0	4.421750	1.836889	1.918161
102	6	0	4.269923	2.618107	-0.387606
103	1	0	4.946959	-0.446535	-0.513119
104	6	0	5.584249	-1.029470	-2.462398
105	6	0	4.023625	-0.730817	-4.267377
106	1	0	2.300349	5.101663	3.143338
107	1	0	-3.965557	4.345717	-3.573706
108	1	0	0.341949	-4.914273	5.525219
109	1	0	3.019118	-4.503740	-3.352581
110	6	0	5.322404	2.894900	2.181989
111	6	0	5.157932	3.630170	-0.104353
112	1	0	3.858770	2.527047	-1.391005
113	1	0	6.556464	-1.368085	-2.107917
114	6	0	5.259697	-1.142830	-3.827780
115	1	0	3.749445	-0.816386	-5.318993
116	1	0	5.730173	2.988769	3.188783
117	6	0	5.686797	3.779041	1.193355
118	1	0	5.449472	4.325977	-0.889596
119	1	0	5.982167	-1.559086	-4.527656
120	1	0	6.385200	4.586053	1.407822

Filename: TS2BINAP3

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.843230 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.157696 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.125433 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.260482 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.243925	1.308510	-0.073606
2	6	0	-3.490722	0.142534	-0.917736
3	6	0	-2.604467	0.010338	-2.509986
4	6	0	-4.082737	0.117565	-2.282554
5	5	0	-3.627762	-1.187899	-0.116367
6	1	0	-2.225222	-0.910750	-2.953687
7	1	0	-2.137963	0.926794	-2.882628
8	1	0	-4.594361	1.011678	-2.633109
9	1	0	-4.646769	-0.786896	-2.512958
10	8	0	-4.010871	-2.389712	-0.668124
11	8	0	-3.514834	-1.239438	1.255200
12	6	0	-4.443790	-3.230473	0.437925
13	6	0	-3.652084	-2.630486	1.641158
14	6	0	-4.118257	-4.675050	0.122345
15	6	0	-5.948344	-3.036060	0.565728
16	6	0	-4.371249	-2.693945	2.973007
17	6	0	-2.245082	-3.190351	1.757690
18	1	0	-4.390654	-5.323668	0.964849
19	1	0	-4.690122	-5.006014	-0.752220
20	1	0	-3.055904	-4.817217	-0.096627
21	1	0	-6.428029	-3.282617	-0.387215
22	1	0	-6.375045	-3.682616	1.341564
23	1	0	-6.196957	-1.996586	0.809367
24	1	0	-4.567818	-3.734793	3.260064
25	1	0	-3.750976	-2.242495	3.755343
26	1	0	-5.322825	-2.155470	2.946957
27	1	0	-1.659758	-2.572008	2.448863
28	1	0	-2.241275	-4.223294	2.127295
29	1	0	-1.743532	-3.173010	0.781536
30	1	0	-3.244407	1.073439	0.990170
31	6	0	-3.523917	2.690278	-0.372451
32	6	0	-3.673476	3.244123	-1.668729
33	6	0	-3.654740	3.603294	0.704582
34	6	0	-4.015297	4.578256	-1.859105
35	1	0	-3.502822	2.627913	-2.548827
36	6	0	-3.972189	4.935984	0.509642
37	1	0	-3.503777	3.225746	1.718100
38	6	0	-4.181246	5.440105	-0.777805

39	1	0	-4.138919	4.952117	-2.876398
40	1	0	-4.063329	5.594734	1.373663
41	1	0	-4.444561	6.485172	-0.931550
42	29	0	-1.318893	0.291040	-0.661438
43	15	0	0.296546	1.699023	0.320218
44	15	0	0.336951	-1.493943	-0.850552
45	6	0	2.043478	1.608077	-0.238399
46	6	0	0.327171	1.291349	2.101170
47	6	0	-0.097258	3.479117	0.246574
48	6	0	0.027958	-3.253639	-1.279938
49	6	0	1.355800	-1.000983	-2.305210
50	6	0	1.472547	-1.588247	0.578019
51	6	0	2.834425	0.463336	-0.057251
52	6	0	2.510563	2.639614	-1.098685
53	6	0	-0.695156	0.493952	2.629588
54	6	0	1.342960	1.746406	2.952295
55	6	0	0.087706	4.359995	1.317044
56	6	0	-0.591893	3.980241	-0.964509
57	6	0	-1.185235	-3.564846	-1.905873
58	6	0	0.964848	-4.280012	-1.085025
59	6	0	0.981005	0.117529	-3.055731
60	6	0	2.477901	-1.736194	-2.706421
61	6	0	1.164692	-2.587119	1.544747
62	6	0	2.455961	-0.636086	0.871037
63	6	0	4.086776	0.350512	-0.745283
64	6	0	3.708910	2.546001	-1.753567
65	1	0	1.901965	3.531000	-1.233685
66	1	0	-1.486544	0.124410	1.972710
67	6	0	-0.700079	0.160885	3.981556
68	6	0	1.334388	1.415249	4.303076
69	1	0	2.161759	2.339256	2.542182
70	1	0	0.443367	3.986449	2.275470
71	6	0	-0.195716	5.715003	1.169766
72	6	0	-0.859722	5.335342	-1.115113
73	1	0	-0.777583	3.292482	-1.791894
74	1	0	-1.944138	-2.793223	-2.024473
75	6	0	-1.449021	-4.860728	-2.343474
76	6	0	0.694265	-5.576255	-1.510186
77	1	0	1.906990	-4.063640	-0.581592
78	1	0	0.114313	0.702090	-2.740530
79	6	0	1.718668	0.506114	-4.170794
80	6	0	3.215541	-1.349890	-3.819346
81	1	0	2.789020	-2.608789	-2.132655
82	1	0	0.396684	-3.321658	1.316381
83	6	0	1.815148	-2.659223	2.745249
84	6	0	3.164452	-0.716578	2.119832
85	6	0	4.907933	-0.801396	-0.635756
86	6	0	4.522545	1.397419	-1.615993
87	1	0	4.048067	3.358396	-2.396736
88	1	0	-1.499724	-0.464202	4.378125
89	6	0	0.312275	0.621391	4.820114
90	1	0	2.141167	1.759286	4.948322

91	1	0	-0.054446	6.389034	2.013234
92	6	0	-0.660899	6.205862	-0.046884
93	1	0	-1.259506	5.704747	-2.056949
94	1	0	-2.400850	-5.080091	-2.825037
95	6	0	-0.510601	-5.869643	-2.147467
96	1	0	1.430875	-6.361268	-1.346539
97	1	0	1.419855	1.387374	-4.736112
98	6	0	2.838007	-0.226806	-4.553497
99	1	0	4.098509	-1.919239	-4.105130
100	1	0	1.558237	-3.436819	3.464942
101	6	0	2.828155	-1.727543	3.072481
102	6	0	4.171019	0.215833	2.479171
103	1	0	4.588051	-1.618633	0.008141
104	6	0	6.088607	-0.908302	-1.336334
105	6	0	5.738152	1.258830	-2.322912
106	1	0	0.311286	0.356150	5.876283
107	1	0	-0.889595	7.264613	-0.158198
108	1	0	-0.717675	-6.884033	-2.483812
109	1	0	3.420334	0.077176	-5.421861
110	6	0	3.496092	-1.769492	4.316659
111	6	0	4.810770	0.147475	3.697242
112	1	0	4.435796	1.004679	1.778512
113	1	0	6.696729	-1.805676	-1.232788
114	6	0	6.513073	0.128979	-2.189266
115	1	0	6.049374	2.070533	-2.980983
116	1	0	3.218924	-2.549066	5.026636
117	6	0	4.472897	-0.851600	4.629549
118	1	0	5.580278	0.877957	3.941753
119	1	0	7.447226	0.034273	-2.740012
120	1	0	4.980654	-0.894706	5.591497

Filename: TS4BINAP2

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3488.574565 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3488.882789 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3487.795626 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3487.938792 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.432804	-1.291943	-1.682112
2	1	0	-2.680621	-1.703031	-2.367956
3	6	0	-3.525375	0.059551	-1.649678
4	6	0	-4.155846	-2.338760	-0.961010
5	6	0	-1.702686	1.854687	-1.984170
6	6	0	-2.674361	0.848314	-2.621739
7	5	0	-4.420153	0.927799	-0.718727
8	6	0	-5.489187	-2.225382	-0.537225
9	6	0	-3.495639	-3.558266	-0.730800
10	1	0	-0.770252	1.878047	-2.578611
11	1	0	-2.087114	2.881590	-2.103445
12	1	0	-3.354607	1.365624	-3.320155
13	1	0	-2.114522	0.130625	-3.242921
14	8	0	-4.663621	2.247161	-1.029818
15	8	0	-5.061187	0.528708	0.432487
16	6	0	-6.117884	-3.270834	0.127689
17	1	0	-6.036445	-1.309321	-0.742159
18	6	0	-4.120942	-4.601358	-0.059657
19	1	0	-2.464615	-3.669821	-1.073907
20	6	0	-5.709371	2.716312	-0.149199
21	6	0	-5.649302	1.704200	1.045587
22	6	0	-5.436521	-4.461256	0.377695
23	1	0	-7.154854	-3.159973	0.443062
24	1	0	-3.578400	-5.528253	0.123424
25	6	0	-7.008103	2.630545	-0.941422
26	6	0	-5.412985	4.154559	0.226059
27	6	0	-4.714773	2.139547	2.164217
28	6	0	-7.002057	1.310010	1.610387
29	1	0	-5.933102	-5.279722	0.897166
30	1	0	-7.862400	3.013412	-0.370227
31	1	0	-6.911943	3.224011	-1.856749
32	1	0	-7.226674	1.596764	-1.235547
33	1	0	-5.452754	4.789364	-0.666148
34	1	0	-6.152137	4.533524	0.943812
35	1	0	-4.416834	4.253177	0.667715
36	1	0	-5.088013	3.036892	2.673163
37	1	0	-4.644590	1.337777	2.909221
38	1	0	-3.705092	2.324510	1.779428

39	1	0	-6.868596	0.569647	2.407689
40	1	0	-7.513681	2.179405	2.043311
41	1	0	-7.654632	0.868840	0.850459
42	1	0	-1.868433	2.054441	-0.518143
43	8	0	-1.818507	2.266386	0.663348
44	6	0	-1.547985	3.625902	0.822083
45	1	0	-0.550209	3.811641	1.262285
46	1	0	-1.582135	4.164325	-0.146270
47	1	0	-2.290074	4.108358	1.485149
48	29	0	-0.298153	1.061966	-0.442093
49	15	0	0.079850	-1.055776	0.380268
50	15	0	1.872014	1.814446	-0.513208
51	6	0	1.579276	-1.092116	1.449676
52	6	0	0.391945	-2.262104	-0.957076
53	6	0	-1.227200	-1.803318	1.410430
54	6	0	2.314780	3.246148	-1.558721
55	6	0	2.615156	2.221942	1.105574
56	6	0	2.790275	0.404478	-1.244564
57	6	0	2.861597	-0.860507	0.941358
58	6	0	1.393583	-1.148520	2.856589
59	6	0	0.081329	-1.856357	-2.260268
60	6	0	0.909482	-3.546976	-0.753367
61	6	0	-1.124525	-3.080024	1.983800
62	6	0	-2.399534	-1.062772	1.594587
63	6	0	1.287167	4.150056	-1.852465
64	6	0	3.606448	3.504200	-2.038461
65	6	0	1.758297	2.222927	2.213026
66	6	0	3.963521	2.553961	1.282434
67	6	0	2.944699	0.408590	-2.658517
68	6	0	3.112732	-0.749288	-0.526086
69	6	0	3.970288	-0.727709	1.834960
70	6	0	2.443489	-0.997175	3.725126
71	1	0	0.392061	-1.303768	3.251768
72	1	0	-0.301541	-0.845252	-2.419392
73	6	0	0.261194	-2.721033	-3.336350
74	6	0	1.094675	-4.409465	-1.828466
75	1	0	1.206412	-3.862858	0.246650
76	1	0	-0.209483	-3.659813	1.865593
77	6	0	-2.180264	-3.607527	2.715405
78	6	0	-3.464924	-1.604821	2.312754
79	1	0	-2.481148	-0.064232	1.161050
80	1	0	0.276328	3.934316	-1.499969
81	6	0	1.548422	5.300821	-2.592477
82	6	0	3.863854	4.649280	-2.784098
83	1	0	4.409041	2.791549	-1.845765
84	1	0	0.707058	1.956252	2.072974
85	6	0	2.244894	2.543551	3.477888
86	6	0	4.448410	2.866641	2.547051
87	1	0	4.642237	2.550456	0.429586
88	1	0	2.644656	1.290869	-3.221560
89	6	0	3.447817	-0.676661	-3.326377
90	6	0	3.694322	-1.868819	-1.204310

91	6	0	5.292027	-0.503983	1.370314
92	6	0	3.755183	-0.784312	3.247470
93	1	0	2.274440	-1.034549	4.801584
94	1	0	0.012729	-2.389662	-4.343490
95	6	0	0.766141	-4.000405	-3.120167
96	1	0	1.515886	-5.399406	-1.660333
97	1	0	-2.093416	-4.600957	3.153488
98	6	0	-3.357086	-2.873446	2.869874
99	1	0	-4.389071	-1.037177	2.398501
100	1	0	0.740914	5.996315	-2.813539
101	6	0	2.836048	5.551689	-3.057153
102	1	0	4.869608	4.839093	-3.155383
103	1	0	1.571524	2.534385	4.333351
104	6	0	3.589567	2.862452	3.645589
105	1	0	5.503099	3.103004	2.679177
106	1	0	3.547609	-0.655583	-4.411700
107	6	0	3.851842	-1.835216	-2.625068
108	6	0	4.107670	-3.038635	-0.516910
109	1	0	5.472758	-0.452283	0.298131
110	6	0	6.337841	-0.343674	2.249468
111	6	0	4.850205	-0.609229	4.125913
112	1	0	0.917247	-4.677610	-3.959279
113	1	0	-4.195996	-3.301530	3.416676
114	1	0	3.040555	6.447516	-3.640983
115	1	0	3.973976	3.103817	4.635455
116	6	0	4.395326	-2.957289	-3.292778
117	6	0	4.648337	-4.108446	-1.192541
118	1	0	3.992052	-3.084739	0.564187
119	1	0	7.342872	-0.172869	1.867191
120	6	0	6.118591	-0.393293	3.641408
121	1	0	4.664619	-0.647859	5.199497
122	1	0	4.497866	-2.915334	-4.377260
123	6	0	4.790491	-4.073832	-2.594243
124	1	0	4.962911	-4.992034	-0.639537
125	1	0	6.953078	-0.260701	4.327720
126	1	0	5.212178	-4.929020	-3.119365

Filename: IM4BINAP2

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.876452 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.20249 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.167916 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.303433 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.267841	2.420660	0.350612
2	1	0	-2.630929	2.147420	1.355025
3	6	0	-1.663385	3.764474	0.447096
4	6	0	-1.506844	4.694346	-0.607690
5	6	0	-1.119148	4.166890	1.693486
6	6	0	-0.893045	5.929439	-0.416466
7	1	0	-1.856752	4.450053	-1.607140
8	6	0	-0.484187	5.385404	1.877389
9	1	0	-1.211216	3.478261	2.538346
10	6	0	-0.369654	6.294183	0.821224
11	1	0	-0.811228	6.611851	-1.263582
12	1	0	-0.086030	5.638182	2.860299
13	1	0	0.113144	7.259317	0.964132
14	29	0	-0.602959	1.278098	0.259829
15	15	0	1.635567	1.418005	-0.391219
16	15	0	-0.419813	-1.013757	0.885864
17	6	0	1.787807	-0.031635	-1.501061
18	6	0	2.858500	1.272059	0.963251
19	6	0	2.346735	2.807799	-1.339967
20	6	0	-1.418953	-1.417473	2.363529
21	6	0	-1.002427	-2.055052	-0.493946
22	6	0	1.236501	-1.698321	1.302171
23	6	0	2.005568	-1.342692	-1.072999
24	6	0	1.421956	0.207779	-2.856152
25	6	0	2.388281	1.274058	2.280416
26	6	0	4.239100	1.233590	0.732278
27	6	0	3.339170	2.677768	-2.320725
28	6	0	1.905570	4.085691	-0.978087
29	6	0	-1.819962	-0.341762	3.163663
30	6	0	-1.751084	-2.717326	2.763390
31	6	0	-1.569217	-1.401952	-1.596210
32	6	0	-0.834778	-3.443772	-0.538761
33	6	0	1.541638	-2.024995	2.650335
34	6	0	2.269413	-1.681552	0.356625
35	6	0	1.966916	-2.413790	-2.026080
36	6	0	1.339379	-0.811497	-3.766849
37	1	0	1.202420	1.227571	-3.170275
38	1	0	1.310416	1.306016	2.461100

39	6	0	3.279347	1.220472	3.349136
40	6	0	5.128123	1.171316	1.798742
41	1	0	4.617947	1.245553	-0.290003
42	1	0	3.688352	1.687009	-2.613884
43	6	0	3.871935	3.808588	-2.932055
44	6	0	2.447297	5.214645	-1.585723
45	1	0	1.130588	4.196369	-0.218687
46	1	0	-1.587777	0.674339	2.837006
47	6	0	-2.521227	-0.558106	4.347388
48	6	0	-2.464680	-2.934845	3.938471
49	1	0	-1.450603	-3.567340	2.150865
50	1	0	-1.692104	-0.316043	-1.565667
51	6	0	-1.964074	-2.124587	-2.717683
52	6	0	-1.249941	-4.168212	-1.652155
53	1	0	-0.335804	-3.957536	0.283890
54	1	0	0.745366	-2.026607	3.391508
55	6	0	2.820254	-2.324231	3.043861
56	6	0	3.604973	-1.996958	0.751321
57	6	0	2.241381	-3.757747	-1.665267
58	6	0	1.626583	-2.143014	-3.388500
59	1	0	1.053969	-0.605540	-4.798544
60	1	0	2.900708	1.215623	4.369909
61	6	0	4.649193	1.164790	3.108367
62	1	0	6.198946	1.120914	1.608079
63	1	0	4.638777	3.698130	-3.697278
64	6	0	3.427895	5.078263	-2.564672
65	1	0	2.087081	6.199709	-1.292725
66	1	0	-2.825820	0.289145	4.959088
67	6	0	-2.844418	-1.855750	4.736024
68	1	0	-2.721173	-3.950398	4.235683
69	1	0	-2.382734	-1.601346	-3.576844
70	6	0	-1.813966	-3.510170	-2.743280
71	1	0	-1.103581	-5.246807	-1.681177
72	1	0	3.030928	-2.566528	4.085902
73	6	0	3.887321	-2.307236	2.119050
74	6	0	4.689779	-1.966815	-0.163113
75	1	0	2.494423	-3.986134	-0.631899
76	6	0	2.192380	-4.770497	-2.595854
77	6	0	1.570393	-3.206962	-4.318253
78	1	0	5.347883	1.116358	3.942186
79	1	0	3.846198	5.960546	-3.046439
80	1	0	-3.398495	-2.028196	5.657131
81	1	0	-2.116945	-4.076451	-3.622577
82	6	0	5.220914	-2.564507	2.513470
83	6	0	5.976477	-2.221307	0.251322
84	1	0	4.493553	-1.724511	-1.206229
85	1	0	2.413542	-5.792442	-2.292139
86	6	0	1.850613	-4.497707	-3.935213
87	1	0	1.302170	-2.979490	-5.350120
88	1	0	5.416696	-2.792289	3.561492
89	6	0	6.249470	-2.522184	1.601775
90	1	0	6.792005	-2.187336	-0.469197

91	1	0	1.809325	-5.307141	-4.661917
92	1	0	7.272142	-2.719323	1.918219
93	6	0	-3.363467	2.073468	-0.643994
94	6	0	-4.147605	3.128768	-1.408880
95	6	0	-3.185959	2.265340	-2.150859
96	1	0	-3.885863	4.168543	-1.234854
97	1	0	-5.209274	2.955096	-1.569936
98	1	0	-3.594368	1.513803	-2.829502
99	1	0	-2.235937	2.683073	-2.484991
100	5	0	-4.189603	0.798512	-0.352817
101	8	0	-3.742012	-0.324236	0.313473
102	8	0	-5.480394	0.651431	-0.821313
103	6	0	-5.833825	-0.740249	-0.680970
104	6	0	-4.875247	-1.222656	0.454091
105	6	0	-5.545495	-1.400172	-2.022930
106	1	0	-6.093195	-0.869465	-2.809442
107	1	0	-4.475623	-1.352230	-2.259310
108	1	0	-5.849517	-2.453865	-2.038954
109	6	0	-7.309658	-0.840043	-0.348537
110	1	0	-7.909051	-0.473601	-1.189280
111	1	0	-7.598391	-1.881913	-0.158386
112	1	0	-7.566605	-0.243806	0.531804
113	6	0	-5.437665	-0.996484	1.849805
114	1	0	-5.780713	0.037468	1.975837
115	1	0	-6.278572	-1.667762	2.063248
116	1	0	-4.651083	-1.185003	2.589127
117	6	0	-4.408748	-2.656828	0.297920
118	1	0	-3.864025	-2.813172	-0.638583
119	1	0	-3.744264	-2.930676	1.124705
120	1	0	-5.268336	-3.340312	0.317398

Filename: IM5BINAP2

SCF Energy (M06L/LANL2DZ-6-31g(d))

-3372.885487 A.U.

SCF Energy (M06/SDD-6-311+G(d,p)) in solution

-3373.206187 A.U.

Enthalpy at 298K (M06/SDD-6-311+G(d,p))

-3372.171421 A.U.

Gibbs Free Energy at 298K and 1 mol/L with Truhlar's quasiharmonic approximation (M06/SDD-6-311+G(d,p))

-3372.307409 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.001190	-1.505603	-1.582254
2	1	0	-3.710107	-2.323285	-2.253763
3	6	0	-3.501554	-0.278844	-1.848844
4	6	0	-4.916459	-1.904202	-0.519044
5	6	0	-1.462316	0.874131	-2.803527
6	6	0	-2.646062	-0.061189	-3.078519
7	5	0	-3.635792	0.982891	-0.938721
8	6	0	-5.727880	-0.988118	0.171147
9	6	0	-5.049684	-3.262505	-0.189624
10	1	0	-0.702433	0.757517	-3.595879
11	1	0	-1.811422	1.917063	-2.889433
12	1	0	-3.295590	0.325576	-3.888389
13	1	0	-2.298419	-1.045163	-3.434662
14	8	0	-4.227891	2.161476	-1.326040
15	8	0	-3.095383	1.063536	0.335028
16	6	0	-6.586576	-1.401456	1.180643
17	1	0	-5.713587	0.059575	-0.127226
18	6	0	-5.920842	-3.682771	0.808112
19	1	0	-4.441215	-3.992573	-0.724534
20	6	0	-3.837548	3.178564	-0.363655
21	6	0	-3.506207	2.333836	0.906547
22	6	0	-6.686420	-2.753587	1.509055
23	1	0	-7.202925	-0.666508	1.698317
24	1	0	-5.996465	-4.743583	1.046363
25	6	0	-4.982883	4.156288	-0.198857
26	6	0	-2.608756	3.869156	-0.930942
27	6	0	-2.365191	2.871645	1.747755
28	6	0	-4.719911	2.061638	1.784399
29	1	0	-7.371425	-3.080597	2.289807
30	1	0	-4.752383	4.897720	0.577043
31	1	0	-5.151032	4.695048	-1.137543
32	1	0	-5.916099	3.652550	0.070342
33	1	0	-2.834078	4.258175	-1.930214
34	1	0	-2.272605	4.703757	-0.302191
35	1	0	-1.779829	3.157273	-1.030643
36	1	0	-2.587255	3.883052	2.111705
37	1	0	-2.209212	2.229998	2.623965
38	1	0	-1.427354	2.905159	1.181119

39	1	0	-4.482727	1.261321	2.495499
40	1	0	-5.011637	2.953999	2.351475
41	1	0	-5.584216	1.736862	1.195468
42	29	0	-0.645664	0.543937	-0.993156
43	15	0	1.097537	1.869341	-0.130802
44	15	0	-0.057341	-1.474867	0.051176
45	6	0	2.324275	0.871267	-1.090135
46	6	0	1.876488	2.099116	1.510164
47	6	0	1.108890	3.555791	-0.851702
48	6	0	-1.330426	-2.328238	1.046626
49	6	0	0.525074	-2.699262	-1.173264
50	6	0	1.364424	-1.372477	1.221830
51	6	0	2.798151	-0.354677	-0.606094
52	6	0	2.644621	1.262111	-2.416500
53	6	0	1.152237	1.737355	2.650763
54	6	0	3.180362	2.589932	1.661353
55	6	0	0.546225	3.727596	-2.128607
56	6	0	1.484687	4.698364	-0.133072
57	6	0	-2.129809	-1.518564	1.865548
58	6	0	-1.514523	-3.715019	1.079844
59	6	0	0.327621	-2.413670	-2.529040
60	6	0	1.206101	-3.869597	-0.813138
61	6	0	1.217199	-1.775745	2.574413
62	6	0	2.571369	-0.807747	0.800769
63	6	0	3.611989	-1.182242	-1.448692
64	6	0	3.405014	0.470802	-3.236783
65	1	0	2.291680	2.220116	-2.788028
66	1	0	0.150454	1.320712	2.533580
67	6	0	1.715676	1.864519	3.917458
68	6	0	3.742030	2.720742	2.926744
69	1	0	3.761030	2.856762	0.777101
70	1	0	0.173619	2.855331	-2.666726
71	6	0	0.415042	4.993641	-2.686645
72	6	0	1.331820	5.967835	-0.687265
73	1	0	1.891236	4.602925	0.871495
74	1	0	-2.027606	-0.435862	1.805306
75	6	0	-3.067681	-2.084876	2.721918
76	6	0	-2.453427	-4.278806	1.939788
77	1	0	-0.924310	-4.359857	0.431028
78	1	0	-0.169850	-1.480816	-2.803047
79	6	0	0.791467	-3.290207	-3.506643
80	6	0	1.658465	-4.748916	-1.791141
81	1	0	1.400092	-4.079093	0.240183
82	1	0	0.274961	-2.211186	2.900300
83	6	0	2.238531	-1.629989	3.478005
84	6	0	3.658158	-0.682460	1.725278
85	6	0	4.148234	-2.417897	-1.004051
86	6	0	3.907559	-0.769263	-2.785393
87	1	0	3.642342	0.800210	-4.248422
88	1	0	1.147180	1.562769	4.795825
89	6	0	3.010579	2.357520	4.056203
90	1	0	4.762220	3.086738	3.031484

91	1	0	-0.020588	5.099406	-3.679008
92	6	0	0.807991	6.120790	-1.967315
93	1	0	1.627385	6.842522	-0.109816
94	1	0	-3.694463	-1.443240	3.339737
95	6	0	-3.223483	-3.467756	2.768938
96	1	0	-2.589684	-5.359497	1.954308
97	1	0	0.643754	-3.052920	-4.558886
98	6	0	1.453106	-4.458976	-3.138830
99	1	0	2.193636	-5.652535	-1.502266
100	1	0	2.105095	-1.945366	4.513351
101	6	0	3.481706	-1.086469	3.086151
102	6	0	4.919060	-0.150797	1.348924
103	1	0	3.927428	-2.756028	0.006368
104	6	0	4.927838	-3.195485	-1.828541
105	6	0	4.705039	-1.594274	-3.612348
106	1	0	3.458269	2.445801	5.044861
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108	1	0	-3.967565	-3.910684	3.428992
109	1	0	1.824039	-5.139726	-3.903490
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111	6	0	5.941930	-0.028128	2.260423
112	1	0	5.072237	0.167905	0.319822
113	1	0	5.321599	-4.142000	-1.461318
114	6	0	5.209818	-2.785105	-3.146598
115	1	0	4.915098	-1.260556	-4.628552
116	1	0	4.391271	-1.244469	5.036425
117	6	0	5.758603	-0.419504	3.602246
118	1	0	6.900136	0.380271	1.943251
119	1	0	5.825636	-3.410031	-3.790976
120	1	0	6.574130	-0.314221	4.315679

NMR Spectra

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