

Supporting Information

Mechanism of Synergistic Cu(II)/Cu(I)-Mediated Alkyne Coupling: Dinuclear 1,2-Reductive Elimination after Minimum Energy Crossing Point

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1. Complete reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

2. CYLview structures of triplet Cu dimers **26** and **27**, and singlet Cu dimer **28**.

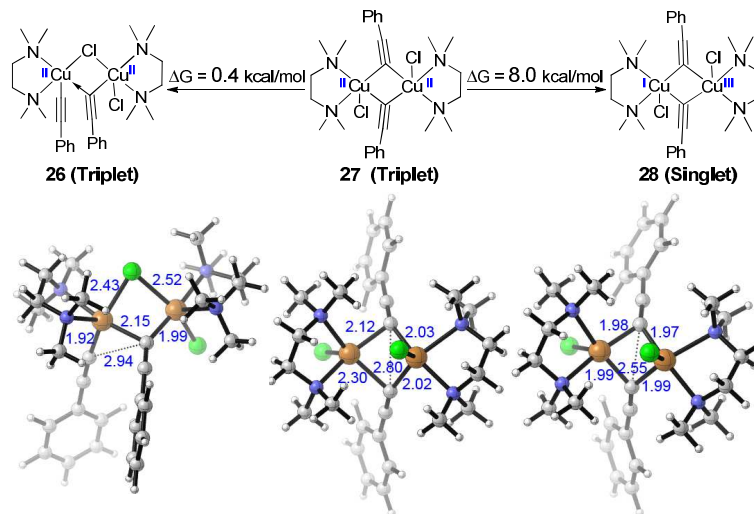


Figure S1. Optimized structures of triplet Cu dimers **26** and **27**, and singlet Cu dimer **28**.

Optimized structures in Figure S1 suggest that the terminal alkynyl carbons act as bridging bonds in the triplet dimer **27** and singlet dimer **28**, and the alkynyl groups all lie in *trans* positions. When the alkynyl groups are located in *cis* positions, a triplet dimer isomer **26**, in which chlorine and alkynyl groups are simultaneously used as bridging bonds, could be obtained, whereas the corresponding singlet dimer was not located. A comparison of the energies of these dimers indicates that the relative free energy of the singlet dimer **28** is 7.6 and 8.0 kcal/mol higher than those of triplet dimers **26** and **27**, respectively.

3. The generation of Cu(III)-acetylide **28b** from singlet Cu Dimer **28**

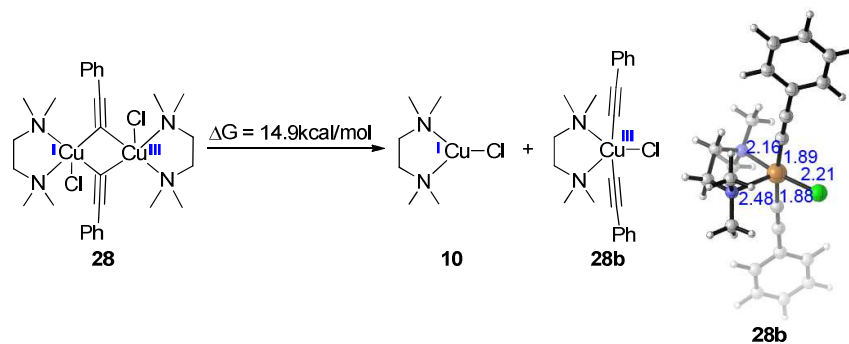


Figure S2. The generation of Cu(III)-acetylide complex **28b** from singlet Cu dimer **28**.

The 1,1-reductive elimination occurring from a Cu(III)-acetylide complex was also considered in this work. We calculated the decomposition of singlet Cu dimer **28** into a Cu(III)-acetylide complex and (TMEDA)CuCl **10**. The result shown in Figure S2 indicates that the barrier for the generation of Cu(III)-acetylide complex from complex **28** was 14.9 kcal/mol. Therefore, the formation of Cu(III)-acetylide complex is energetically unfavorable. The Cu(III) mechanism for C-C bond formation is thereby excluded.

4. The dissociation of another chloride from intermediate **29** and **32**

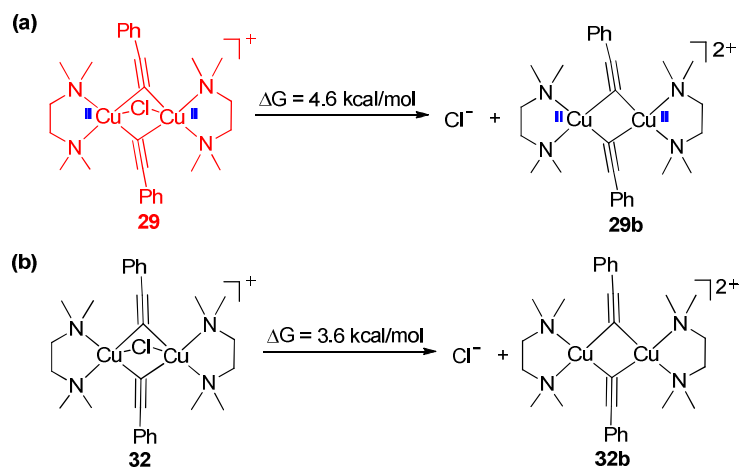


Figure S3. The dissociation of another chloride from intermediate **29** (a) and **32** (b).

As the dissociation of one chloride from intermediate **26**, **27**, and **28** are exergonic, the dissociation of another chloride is also calculated. Computational results suggest that the dissociation of chloride from triplet intermediate **29** is endergonic by 4.6 kcal/mol (Figure S3a). Corresponding process occurring on intermediate **32** is endergonic by 3.6 kcal/mol (Figure S3b). These data suggest that the formation of dicationic Cu species is energetically unfavorable. It is noteworthy that the transition states for chloride dissociation from **26**, **27**, and **28** are not located. This case might be ascribed to the fact that the generations of **29** and **32** are facile process.

5. Computational results about singlet diradical state reductive elimination

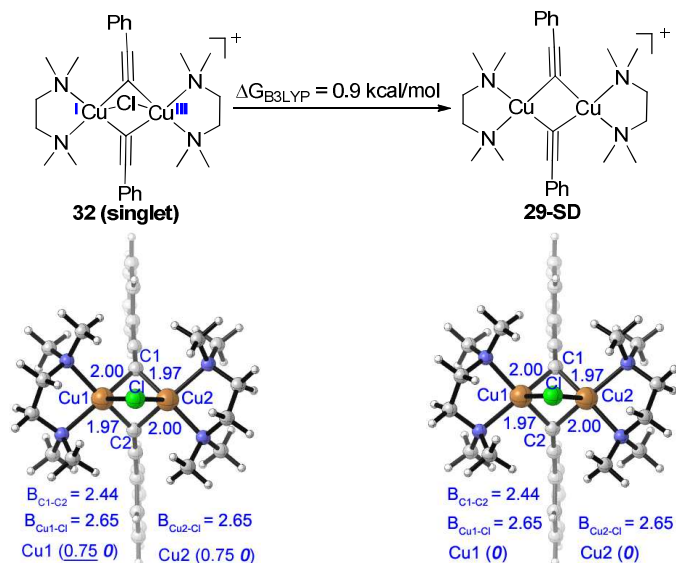


Figure S4. The energy and structural information of singlet diradical state complex **29-SD**.

In the manuscript, triplet cationic Cu complex **29** is proven to be the most stable intermediate for 1,2-reductive elimination. Actually, corresponding singlet diradical (SD) structure of **29** is also considered in calculation. The keyword “guess=mix” is used to obtain the SD state structure **29-SD**. However, computational results given in Figure S4 suggest that the relative free energy and structure of **29-SD** are almost the same as the singlet intermediate **32**. More importantly, calculated Mulliken spin densities of Cu1 and Cu2 in **29-SD** are zero, which imply that the spin state of complex **29-SD** is singlet. After many attempts, the obtained structures are always singlet and no SD state complex could be gained.

Besides, we have also optimized the SD state structure of each point in Figure 7.

Corresponding energies are added in Figure S5. The blue line stands for the energy changes on singlet diradical state potential energy surface during C–C bond formation. It is obvious that the blue line almost coincides with the black line. Moreover, Mulliken spin densities located on Cu atoms in these points are all zero. Therefore, the structures on the blue line are singlet. This result is consistent with the data given in Figure S4. All in all, the singlet diradical state intermediate cannot be located in this work.

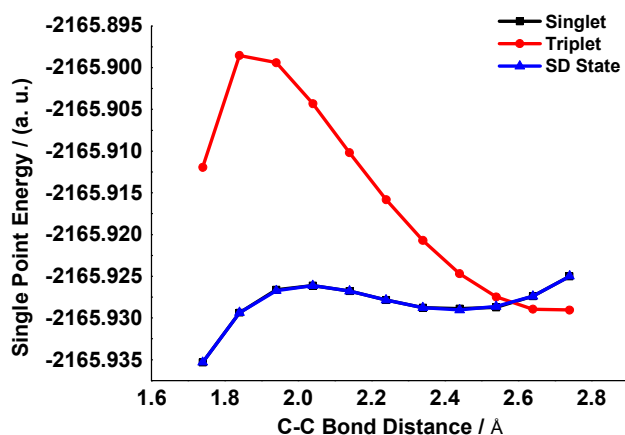


Figure S5. Triplet, singlet, and singlet diradical state potential energy curves during C–C bond formation. The distance between carbon C1 and C2 in **29** was chosen as the coordinate. The step size between each point was set to 0.1 Å.

6. Comparison between M06-L and M11-L calculated deprotonation data

data

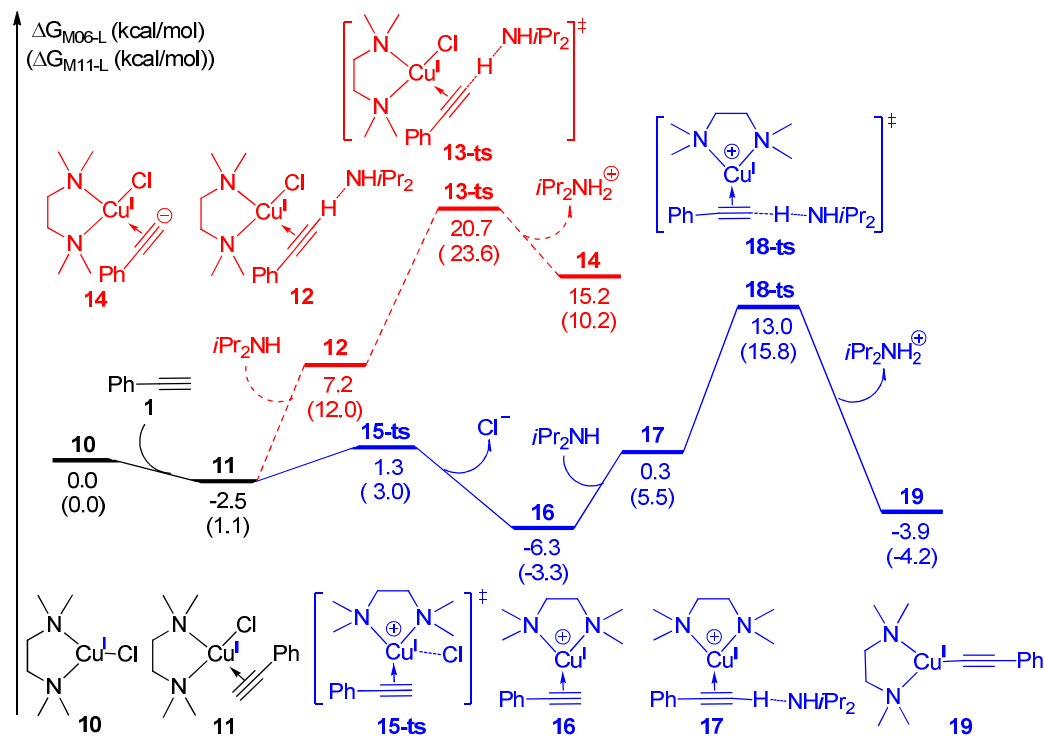


Figure S6. Comparison between M06-L and M11-L calculated deprotonation data.

In order to confirm the accuracy of M11-L/6-311+G(d)//B3LYP calculated data, DFT functional M06-L was employed to calculate Cu(I)-mediated deprotonation process. The same basis set is used in the solvation singlet point energy calculation. As shown in Figure S6, both M06-L and M11-L calculated data are given on the free energy profile. The comparison between these two sets of data indicates that M06-L results and M11-L results show a similar trend. Both data suggest the Cu(I) cationic catalyzed deprotonation is the favorable pathway. Moreover, although M06-L calculated data are generally lower than M11-L calculated data, the exact values are close.

7. The dissociation of Cl⁻ from Cu(II)-acetylide **9**

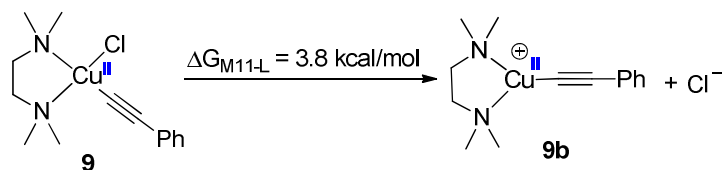


Figure S7. The dissociation of Cl⁻ from Cu(II)-acetylide **9**.

We have also calculated the dissociation of Cl⁻ from Cu(II)-acetylide **9** using the same method and basis set. As shown in Figure S7, the dissociation of Cl⁻ from **9** is endergonic by 3.8 kcal/mol, which indicates this process is unfavorable.

8. Absolute calculation energies, enthalpies, and free energies

Geometry	$E_{(\text{elec-B3LYP})}^1$	$E_{(\text{solv, M11-L})}^2$	$G_{(\text{corr-B3LYP})}^3$	$H_{(\text{corr-B3LYP})}^4$	IF ⁵
1	-308.386937	-308.399284	0.079122	0.116976	-
2	-1465.601407	-1465.868188	0.185960	0.246618	-
3	-615.607604	-615.633916	0.159874	0.216658	-
4	-2010.799841	-2011.263206	0.390028	0.486682	-
5	-1005.150596	-1005.454140	0.187912	0.244049	-
6	-1313.560285	-1313.865888	0.288798	0.363203	-
7	-1605.997702	-1606.309646	0.480965	0.582585	-
8-ts	-1605.992132	-1606.299808	0.481351	0.579279	-930.6
9	-1313.157363	-1313.420074	0.275885	0.351546	-
9b	-852.728459	-853.008410	0.278116	0.348870	-
10	-1005.389096	-1005.624753	0.186724	0.242754	-
11	-1313.786890	-1314.043166	0.286765	0.361358	-

12	-1606.218188	-1606.479736	0.479380	0.581147	-
13-ts	-1606.198823	-1606.461212	0.479425	0.578782	-119.6
14	-1313.215216	-1313.557881	0.271276	0.348279	-
15-ts	-1313.780334	-1314.039016	0.288564	0.360501	-26.1
16	-853.370385	-853.647168	0.291550	0.359701	-
17	-1145.805836	-1146.085475	0.482523	0.579077	-
18-ts	-1145.790825	-1146.070232	0.483710	0.577302	-20.7
19	-852.942228	-853.181936	0.275236	0.347651	-
20	-2318.568664	-2319.064840	0.486755	0.596367	-
21-ts	-2318.562372	-2319.062179	0.488033	0.595080	-77.4
22	-2318.974804	-2319.509806	0.502628	0.608918	-
23	-2611.403757	-2611.954801	0.694660	0.828199	-
24	-1858.789335	-1859.279888	0.496461	0.604616	-
25	-2151.216816	-2151.710745	0.686168	0.824271	-
26	-2626.320088	-2626.850228	0.577069	0.704742	-
27	-2626.320331	-2626.855343	0.581653	0.705789	-
28	-2626.313915	-2626.845874	0.584940	0.706087	-
28b	-1620.888834	-1621.167707	0.368539	0.460707	-
29	-2165.929714	-2166.471615	0.584494	0.703785	-
29b	-1705.416093	-1706.056658	0.584738	0.700807	-
29-SD	-2165.929094	-	0.588332	0.704040	-
30-ts	-2165.898198	-2166.431580	0.579738	0.700488	-395.4
31	-1550.299419	-1550.795968	0.398478	0.485850	-
32	-2165.928912	-2166.464806	0.586688	0.703868	-
32b	-1705.408161	-1706.054344	0.589816	0.700169	-
33-ts	-2165.926061	-2166.456207	0.585106	0.702063	-235.6
34	-1550.382551	-1550.851552	0.395533	0.485438	-
35-MECP	-2165.926532	-2166.470024	0.586997	0.703106	-

¹The electronic energy calculated by B3LYP in gas phase. ²The electronic energy calculated by M11-L in DMF solvent. ³The thermal correction to Gibbs free energy

calculated by B3LYP in gas phase. ⁴The thermal correction to enthalpy calculated by B3LYP in gas phase. ⁵The B3LYP calculated imaginary frequencies for the transition states.

9. B3LYP geometries for all the compounds and transition states

1				C	1.39447200	-1.00941100	-1.93963900
C	2.21346200	-0.00000600	0.00011000	H	0.38470100	-1.05468700	-2.35273200
C	1.51280900	-1.20888600	0.00006500	H	1.85555200	-0.08054800	-2.28203900
C	0.11987100	-1.21340300	-0.00001900	H	1.97837300	-1.86353100	-2.31707000
C	-0.59448100	0.00000700	-0.00006400	N	-1.39037600	-0.96431500	0.45871300
C	0.11988000	1.21340700	-0.00002000	N	1.35703400	-1.01005200	-0.45848200
C	1.51282100	1.20887700	0.00006400	Cl	-1.31221000	1.94589700	-1.19001300
H	3.30003500	-0.00001300	0.00017800	Cl	1.37919900	1.90531700	1.18683600
H	2.05324900	-2.15159100	0.00009700				
H	-0.42863600	-2.15025800	-0.00005600	3			
H	-0.42861300	2.15027100	-0.00005800	C	-0.68004400	0.00006600	-0.00032500
H	2.05326500	2.15158100	0.00009500	C	-1.90130200	0.00004500	-0.00026700
C	-2.02447600	0.00000700	-0.00018600	C	-3.32420600	0.00000300	-0.00010100
C	-3.23465400	0.00000500	-0.00011100	C	-4.04045500	-0.86007700	0.85803700
H	-4.30069000	-0.00004400	0.00070700	C	-4.04070400	0.86005300	-0.85806200
				C	-5.43267900	-0.85616300	0.85428300
2				H	-3.49212400	-1.52334400	1.51969800
Cu	0.00914400	0.62879600	0.00499400	C	-5.43292700	0.85608600	-0.85395500
C	0.71785300	-2.23476800	0.07403600	H	-3.49256500	1.52334500	-1.51985600
H	1.12374600	-3.13422300	-0.41589800	C	-6.13330700	-0.00005100	0.00025300
H	0.97803400	-2.30284200	1.13421900	H	-5.97320200	-1.52344500	1.52006400
C	-0.79955000	-2.20311300	-0.09716400	H	-5.97364300	1.52335100	-1.51959600
H	-1.24084500	-3.09470800	0.37634400	H	-7.21981200	-0.00006900	0.00039300
H	-1.06263500	-2.24047600	-1.15823500	C	0.68004500	0.00001000	-0.00029700
C	-1.41834300	-0.98439600	1.93993000	C	1.90130200	-0.00000600	-0.00023700
H	-1.84532300	-0.04548400	2.29876400	C	3.32420500	0.00000500	-0.00008200
H	-2.02842300	-1.82357400	2.30927800	C	4.04067700	-0.85806300	-0.86004800
H	-0.40806700	-1.07001700	2.34529500	C	4.04048100	0.85807700	0.86004100
C	2.73289300	-0.87872800	0.06695600	C	5.43289900	-0.85412800	-0.85595200
H	3.34677500	-1.73905400	-0.24151800	H	3.49251800	-1.51980800	-1.52337100
H	3.17442400	0.04439500	-0.30922000	C	5.43270600	0.85414900	0.85625600
H	2.70532400	-0.81269200	1.15535200	H	3.49217200	1.51981800	1.52324500
C	-2.76358300	-0.77535800	-0.05611000	C	6.13330700	0.00001200	0.00023000
H	-2.73824200	-0.68767100	-1.14286600	H	5.97359500	-1.51985500	-1.52314900
H	-3.40501600	-1.62002300	0.23908500	H	5.97324900	1.51987800	1.52357400
H	-3.17143500	0.15463500	0.34076800	H	7.21981200	0.00001300	0.00035200

4

C	4.12152700	0.69319200	-0.33499000
C	4.12506200	-0.68912500	0.32766900
H	5.05950500	1.21706100	-0.07604500
H	4.11218200	0.57873000	-1.42327300
H	4.12208300	-0.57464700	1.41598900
H	5.06256500	-1.21096800	0.06305900
Cu	1.27996400	-0.00125800	0.00371800
N	2.94221800	1.49565600	0.03773600
N	2.94526600	-1.49432200	-0.03784600
C	2.70981900	-2.56008800	0.94746200
H	1.82285200	-3.12796200	0.65458900
H	3.56619900	-3.25493100	1.01689200
H	2.51799100	-2.11829100	1.92818700
C	3.07554300	-2.07526300	-1.38274600
H	3.91347200	-2.79408000	-1.43430500
H	2.14564600	-2.58423300	-1.64562100
H	3.23504100	-1.29006600	-2.12413400
C	2.69883000	2.56148400	-0.94554900
H	1.81233800	3.12726100	-0.64720200
H	3.55330900	3.25821300	-1.01945600
H	2.50214200	2.11980900	-1.92534900
C	3.07855600	2.07587600	1.38228900
H	3.91490400	2.79681600	1.42982100
H	2.14884400	2.58227200	1.65075200
H	3.24434700	1.29050700	2.12214800
Cl	0.00252500	-0.00286700	-2.01291000
C	-4.12426300	-0.69109300	-0.32826100
C	-4.12228900	0.69185700	0.33309100
H	-4.12050900	-0.57764500	-1.41668500
H	-5.06161300	-1.21334900	-0.06390400
H	-5.06041800	1.21481100	0.07286900
H	-4.11377200	0.57842000	1.42148600
Cu	-1.27994000	-0.00046500	-0.00298300
C	-2.70713200	-2.56161300	-0.94503400
H	-1.81986800	-3.12839900	-0.65095700
H	-3.56287300	-3.25725700	-1.01434000
H	-2.51492800	-2.12066500	-1.92605900
C	-3.07493200	-2.07461500	1.38440200
H	-2.14481400	-2.58257500	1.64846300
H	-3.23557200	-1.28874800	2.12483800
H	-3.91231600	-2.79405500	1.43620000
C	-3.07899500	2.07379300	-1.38458200

H	-3.91615000	2.79369900	-1.43355100
H	-2.14965200	2.58112400	-1.65256900
H	-3.24309300	1.28759000	-2.12392500
C	-2.70160800	2.56182800	0.94314100
H	-1.81529900	3.12804600	0.64509600
H	-3.55672700	3.25791400	1.01563000
H	-2.50545200	2.12120400	1.92351600
N	-2.94417800	-1.49503000	0.03898300
N	-2.94325500	1.49489100	-0.03938700
Cl	-0.00265000	0.00219500	2.01342500

5

C	-2.05980000	-0.56953800	-0.33282000
C	-1.98019700	0.80440600	0.32807600
H	-2.96318400	-1.10206000	-0.01029100
H	-2.10875500	-0.47309100	-1.42071100
H	-2.04447900	0.71512700	1.41574600
H	-2.81332700	1.43920100	0.00159200
Cu	0.68134700	-0.04244500	0.00042300
N	-0.83834400	-1.37015600	-0.00480500
N	-0.67177300	1.45546200	0.00474500
C	-0.30857300	2.48087200	1.02442700
H	0.66063500	2.91435900	0.76996300
H	-1.06455300	3.27581900	1.04660000
H	-0.24428900	2.01689600	2.01127900
C	-0.68096200	2.07980600	-1.35055100
H	-1.40249700	2.90603700	-1.37605100
H	0.31498600	2.46631100	-1.57676800
H	-0.95522100	1.34461700	-2.10987100
C	-0.59736800	-2.43328900	-1.02195100
H	0.31374400	-2.97731100	-0.76513200
H	-1.44153900	-3.13396000	-1.04405200
H	-0.47768100	-1.98244300	-2.00967900
C	-0.92544200	-1.98686900	1.35121000
H	-1.74438700	-2.71667500	1.37804400
H	0.01452400	-2.49438000	1.57782700
H	-1.10539100	-1.22260700	2.11001500
Cl	2.77571800	-0.15261300	-0.00004200

6

C	2.47828700	-1.81739400	0.94382100
C	3.51324500	-0.84642200	0.39317600
H	2.87481300	-2.84132900	0.95662700
H	2.22269600	-1.55581500	1.97411200

H	3.80535300	-1.13019800	-0.62201000	Cu	-1.01696800	0.85130000	-0.16615800
H	4.42268900	-0.86932200	1.00891200	N	-1.93972800	2.76952200	-0.39732400
Cu	0.93176900	0.27649700	-0.29246200	N	-1.57235100	1.04325200	1.86663700
N	1.22258400	-1.75849200	0.13562000	C	-2.21280600	-0.19995400	2.36646600
N	2.94802500	0.52857500	0.34130800	H	-1.48441000	-1.01057100	2.35249900
C	3.68707600	1.36648700	-0.63950300	H	-2.57595700	-0.05927500	3.39359500
H	3.23499400	2.35796800	-0.67008400	H	-3.05536600	-0.46764700	1.72367100
H	4.74351700	1.44916100	-0.35049100	C	-0.38320300	1.34654900	2.70494800
H	3.62438400	0.91551600	-1.63359000	H	-0.67824200	1.47067500	3.75578400
C	2.99636300	1.18366600	1.67589600	H	0.33127300	0.52643400	2.62499100
H	4.04006200	1.31057200	1.99336900	H	0.09991700	2.26424000	2.36289700
H	2.50621700	2.15449900	1.60919500	C	-1.07184300	3.68251500	-1.18512900
H	2.47002400	0.57967500	2.41831900	H	-0.93315400	3.26581500	-2.18272900
C	0.08245500	-2.28003800	0.93319600	H	-1.53167700	4.67761900	-1.25819000
H	-0.82838100	-2.23326400	0.33502700	H	-0.09637800	3.77415400	-0.70033200
H	0.26329100	-3.32204900	1.22925300	C	-3.24335100	2.61651600	-1.09658900
H	-0.05012200	-1.67239400	1.83198600	H	-3.72999600	3.59534000	-1.20527500
C	1.35933900	-2.56967800	-1.10363400	H	-3.06638200	2.17809300	-2.07855100
H	1.54164400	-3.62230400	-0.85030000	H	-3.90399500	1.95228200	-0.53474900
H	0.44011200	-2.49438600	-1.68565800	Cl	-0.92604700	0.48879900	-2.35340600
H	2.18960900	-2.20364400	-1.71130400	C	0.50507600	-0.61639400	0.19798500
Cl	0.43897700	2.42267000	-0.16776900	H	1.48449700	-0.07836200	0.23199000
C	-0.61807800	-0.02879800	-1.78046600	C	-0.03849300	-1.72737900	0.10940400
H	-0.11694200	0.07102200	-2.72905400	C	-0.73160700	-2.94175700	-0.09421400
C	-1.72908400	-0.06479300	-1.23194900	C	-1.12947200	-3.29775200	-1.40541000
C	-2.92901500	-0.01336200	-0.49816000	C	-1.00894000	-3.81226000	0.98565000
C	-3.36318200	1.23090200	0.02304000	C	-1.80017400	-4.49638800	-1.61882600
C	-3.71633300	-1.17494700	-0.30792600	H	-0.91566400	-2.61781100	-2.22359900
C	-4.55825000	1.29799800	0.72829400	C	-1.67110800	-5.01148000	0.75462300
H	-2.74709200	2.11106600	-0.12927100	H	-0.68342800	-3.54568600	1.98677500
C	-4.91216600	-1.08802300	0.39183300	C	-2.06871100	-5.35177800	-0.54423300
H	-3.38915000	-2.12064100	-0.72939900	H	-2.11107200	-4.76940500	-2.62245900
C	-5.33064900	0.14459900	0.91025800	H	-1.87669200	-5.68524400	1.58062000
H	-4.89412400	2.24745300	1.13301900	H	-2.58720600	-6.29002400	-0.71907500
H	-5.52437200	-1.97317300	0.53260600	N	3.34297900	0.51939700	0.25023100
H	-6.26744000	0.20602000	1.45644100	H	3.42325200	1.34254900	0.85147100
7				C	3.75095900	0.93626500	-1.11746100
C	-2.12693200	3.29061100	0.98174600	C	2.94773600	2.18153200	-1.50710700
C	-2.55290100	2.16732000	1.91552300	C	3.54114800	-0.19405000	-2.12956600
H	-2.87137900	4.09869800	0.99507000	H	4.81662300	1.21216500	-1.12635400
H	-1.17764400	3.72348400	1.31052500	H	3.07436900	2.98536400	-0.76919100
H	-3.52658600	1.77139500	1.61477400	H	3.28891400	2.56740400	-2.47319000
H	-2.65645100	2.53766200	2.94445500	H	1.88062900	1.94705400	-1.59856800
				H	4.15357500	-1.07264100	-1.90196000

H	2.48992400	-0.50177700	-2.16140200	C	-3.48415800	-0.91698200	1.30538500
H	3.82313600	0.14880300	-3.13051200	C	-3.76158200	-1.44962800	-1.06206500
C	4.13334200	-0.56468000	0.89140600	C	-4.72007400	-1.49542700	1.57245100
C	3.60020400	-0.77423900	2.31358900	H	-2.88591900	-0.48628600	2.10233400
C	5.65096000	-0.31938600	0.91221800	C	-4.99961200	-2.01777200	-0.78319500
H	3.93604700	-1.47749200	0.31652600	H	-3.38692500	-1.41748000	-2.08095300
H	2.52980600	-1.00733500	2.30890300	C	-5.47800100	-2.04339800	0.53161700
H	4.12379700	-1.60069200	2.80449200	H	-5.09749600	-1.51763000	2.59025800
H	3.75756000	0.12368500	2.92663100	H	-5.59531300	-2.43978600	-1.58689300
H	6.07590000	-0.25188500	-0.09373000	H	-6.44495700	-2.48965500	0.74496600
H	5.89198000	0.60902100	1.44636800	N	-0.23201500	2.91619500	-0.87033500
H	6.15975700	-1.14142200	1.42736300	H	-0.30878800	3.05301400	-1.88201400
8-ts				C	1.15889600	3.29600000	-0.45758800
C	3.52239600	-2.05941200	-0.51243100	C	1.39691400	4.80965500	-0.39898700
C	2.40233300	-2.96724600	-0.99754800	C	2.13227600	2.62958700	-1.43612800
H	4.42086400	-2.65209300	-0.28809700	H	1.30338400	2.86260000	0.53763200
H	3.79733100	-1.34178500	-1.29137500	H	0.79376700	5.29947000	0.37004000
H	2.16989700	-3.71930600	-0.23931200	H	2.44787800	5.00210500	-0.15887700
H	2.70955900	-3.50721400	-1.90382900	H	1.18305500	5.28623900	-1.36371700
Cu	1.06451400	-0.67575800	0.27191800	H	1.95985200	1.54962900	-1.50160000
N	3.08546800	-1.29066900	0.68047900	H	2.03073900	3.05170900	-2.44475000
N	1.16081100	-2.18359200	-1.25490700	H	3.16479200	2.79558900	-1.11332700
C	-0.01496800	-3.08708100	-1.20367800	C	-1.37651900	3.65147000	-0.23353300
H	-0.91982600	-2.51757300	-1.41284100	C	-1.45164800	3.36544600	1.26740200
H	0.08565600	-3.89109700	-1.94591900	C	-2.66899200	3.27876100	-0.96662500
H	-0.09856400	-3.52946800	-0.20768900	H	-1.20504200	4.72496900	-0.38060300
C	1.21452200	-1.53386800	-2.58853500	H	-0.55144600	3.69277100	1.79591300
H	1.26233400	-2.29089600	-3.38367500	H	-2.30178200	3.90709100	1.69454000
H	0.32160800	-0.92146200	-2.71982900	H	-1.58305400	2.29806700	1.46461700
H	2.09380600	-0.88985500	-2.66241700	H	-2.59734800	3.48946000	-2.04123600
C	3.98103300	-0.12636400	0.89393400	H	-2.91830200	2.22140100	-0.83737800
H	3.62341800	0.44198400	1.75266500	H	-3.49949800	3.87203400	-0.57191300
H	5.01180800	-0.46261400	1.07379900	9			
H	3.96593500	0.51602300	0.00980900	C	-1.94205000	1.53789500	1.38100600
C	3.10315600	-2.13557300	1.90380000	C	-2.58782100	0.21579900	1.81235200
H	4.12577700	-2.47894100	2.11292900	H	-2.51182500	2.37168900	1.82438000
H	2.72990300	-1.54596200	2.74113400	H	-0.92313200	1.59940400	1.77293500
H	2.45562600	-3.00623100	1.77946200	H	-3.58388400	0.12748600	1.36988100
Cl	0.90746600	0.43583600	2.21256400	H	-2.71922400	0.22556500	2.90722300
C	-0.62274600	0.25731600	-0.44477300	Cu	-1.18243500	-0.38359900	-0.69505400
H	-0.37779000	1.52798000	-0.67444100	N	-1.86597200	1.68792500	-0.08806900
C	-1.72690400	-0.29632100	-0.28084900	N	-1.80741400	-0.97054500	1.39791100
C	-2.98676100	-0.89125900	-0.01920400	C	-2.65566600	-2.17912500	1.40109800

H	-2.05810800	-3.03502200	1.07763400	C	-2.69048200	-2.03591100	1.32911200
H	-3.05098200	-2.38279400	2.40959700	H	-3.51337400	-2.76352500	1.36317300
H	-3.47747400	-2.05186700	0.69554900	H	-1.75161300	-2.54799000	1.55040400
C	-0.64246500	-1.18518300	2.27782200	H	-2.85978400	-1.27616100	2.09534800
H	-0.96684900	-1.38215400	3.31291800	C	-2.21804800	2.49071500	1.03088800
H	-0.06910100	-2.03874200	1.91139300	H	-1.27580800	2.97998800	0.77603500
H	0.01826400	-0.31859300	2.25887100	H	-3.01672600	3.24478100	1.06265000
C	-0.86280000	2.70527100	-0.45690400	H	-2.12017400	2.03182600	2.01774900
H	-0.82853300	2.79353200	-1.54577700	C	-2.57373100	2.07296200	-1.32896000
H	-1.11756100	3.68907500	-0.02995800	H	-3.35140000	2.84880600	-1.36199600
H	0.12196900	2.39048300	-0.10849300	H	-1.60652600	2.52658000	-1.55553000
C	-3.17407300	2.05539800	-0.66411900	H	-2.79149100	1.32288200	-2.09238600
H	-3.49925200	3.04157700	-0.29318800	C	0.77656100	-0.04415900	-0.00309000
H	-3.09107300	2.08620700	-1.75181500	C	2.02273800	-0.03600100	-0.00231300
H	-3.92702700	1.30675900	-0.41822400	C	3.42586300	-0.02523000	-0.00108300
Cl	-2.91020300	-1.09175500	-1.87134900	C	4.14522600	0.01537600	-1.22616800
C	0.69103000	-0.20229700	-0.46483400	C	4.14343600	-0.05185300	1.22544300
C	1.90824800	-0.12652000	-0.32688100	C	5.53127300	0.02951900	-1.21699000
C	3.33049900	-0.06918400	-0.19628500	H	3.59348200	0.03536000	-2.16030000
C	4.14432100	-1.07881800	-0.75041500	C	5.52949100	-0.03726400	1.21908600
C	3.95334700	0.99169300	0.49247800	H	3.59032200	-0.08322200	2.15845300
C	5.52970800	-1.02566700	-0.61731100	C	6.22511100	0.00347900	0.00175900
H	3.67332500	-1.89812900	-1.28501300	H	6.08014200	0.06097300	-2.15299500
C	5.33940800	1.03744700	0.62378700	H	6.07698700	-0.05733700	2.15620900
H	3.33642700	1.77604000	0.92160900	H	7.31112600	0.01496900	0.00287500
C	6.13398600	0.03036300	0.07018900				
H	6.14103100	-1.81205800	-1.05246800				
H	5.80159700	1.86305300	1.15899200				
H	7.21512800	0.06861600	0.17267000				
				10			
				C	-1.21054200	-1.80316800	-0.22529800
				C	-1.98261200	-0.66289700	0.44951100
				H	-1.61646500	-2.76287700	0.14403500
				H	-1.39388000	-1.78552800	-1.30453600
				H	-1.83226800	-0.70673800	1.53231300
				H	-3.06235500	-0.78829500	0.26603300
				Cu	0.50009600	0.73169600	-0.00912500
				N	0.23158100	-1.68385500	-0.00609900
				N	-1.54355700	0.68710300	0.00242000
				C	-2.07189500	1.71254500	0.93300400
				H	-1.74216900	2.70114500	0.60672200
				H	-3.17364700	1.69190100	0.96182200
				H	-1.68329500	1.53138100	1.93769200
				C	-2.04253900	0.98093900	-1.36176800
				H	-3.14408600	0.94820800	-1.39319000
				H	-1.70557500	1.97588300	-1.66039800
				H	-1.64457800	0.25896900	-2.07674300
9b							
C	-3.78774800	0.74019300	0.34422800				
C	-3.83148400	-0.62828100	-0.33344700				
H	-4.65732800	1.34124000	0.04399700				
H	-3.83351500	0.62795300	1.43118900				
H	-3.87936000	-0.51363700	-1.42007500				
H	-4.73262900	-1.17661000	-0.02578600				
Cu	-1.04948900	-0.02826600	-0.00204500				
N	-2.51739100	1.44701700	0.01762000				
N	-2.60255000	-1.41048100	-0.01648500				
C	-2.37386900	-2.46865500	-1.03356900				
H	-1.46142200	-3.01494700	-0.78594600				
H	-3.21698800	-3.17279400	-1.06072100				
H	-2.25517200	-2.01451300	-2.02037300				

C 1.02927900 -2.31994100 -1.05719600
H 2.08206200 -2.06879200 -0.90250900
H 0.92000500 -3.41951700 -1.06530500
H 0.73148600 -1.93087800 -2.03550500
C 0.65034800 -2.15892500 1.31502300
H 0.50772900 -3.24934100 1.42775600
H 1.70674300 -1.91985400 1.46190100
H 0.08424400 -1.65374000 2.10282900
Cl 2.55381600 1.32028500 -0.00189300

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C -3.39502800 0.13610900 -0.65756000
C -3.06586000 1.25319800 0.33605100
H -4.46328700 -0.12540800 -0.56801900
H -3.24464700 0.49606000 -1.68026600
H -3.13915600 0.86796800 1.35692600
H -3.82990000 2.04754600 0.23581500
Cu -0.47180400 -0.38335400 -0.05431200
N -2.55604800 -1.07191800 -0.47829000
N -1.70919800 1.78294000 0.15867300
C -1.25189600 2.48735700 1.36279600
H -0.23273400 2.85050300 1.19973100
H -1.89481500 3.35272500 1.60770200
H -1.22867200 1.79078500 2.20337900
C -1.60237200 2.65964300 -1.00815600
H -2.22436400 3.56844400 -0.90654800
H -0.55990500 2.96469300 -1.13691600
H -1.90875900 2.13657200 -1.91841000
C -2.60762200 -1.90480800 -1.69283200
H -1.96070500 -2.77627900 -1.56217400
H -3.63220100 -2.25478400 -1.90359300
H -2.25285600 -1.33376500 -2.55484100
C -3.03552200 -1.87741000 0.66487600
H -4.07413200 -2.20901600 0.49711200
H -2.38933400 -2.74854700 0.78616600
H -2.96945600 -1.30314200 1.58772000
Cl -0.24964700 -0.83222500 2.15021000
C 0.38212100 -0.18236400 -1.84378800
H -0.12510300 -0.15670000 -2.78879000
C 1.33472700 -0.17403600 -1.03927000
C 2.68880700 -0.10725200 -0.54184600
C 3.00182500 -0.25978800 0.81948300
C 3.72578900 0.11960600 -1.47085000
C 4.33047300 -0.18645000 1.23658600

H 2.19868300 -0.43767200 1.52807400
C 5.04755500 0.19185600 -1.04182900
H 3.48223200 0.23635400 -2.52292600
C 5.35387800 0.03893200 0.31397400
H 4.56456100 -0.30744400 2.29070400
H 5.83954200 0.36653300 -1.76520300
H 6.38679800 0.09495800 0.64732800

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C -1.93336900 -3.07467800 0.58196200
C -2.80125100 -2.31993400 -0.42697100
H -2.59181900 -3.69670000 1.21702700
H -1.26760700 -3.76160400 0.05215500
H -3.41797100 -1.58151800 0.09493700
H -3.49227800 -3.02971000 -0.91388600
Cu -0.35414600 -0.60605200 -0.40730800
N -1.09947000 -2.17437400 1.38795200
N -2.01064000 -1.59582200 -1.45046500
C -2.88030100 -0.63237000 -2.15294700
H -2.29059700 -0.09103000 -2.89779300
H -3.71129900 -1.14197400 -2.66989100
H -3.29412300 0.08822700 -1.44487000
C -1.45697100 -2.53730600 -2.44830000
H -2.26897200 -3.08432800 -2.95620900
H -0.87697000 -1.97817600 -3.18440600
H -0.77253100 -3.23920800 -1.97415500
C 0.06206700 -2.87876600 1.94350600
H 0.66095600 -2.17501200 2.52884300
H -0.23499400 -3.71550700 2.60206200
H 0.68615100 -3.24843600 1.12735400
C -1.86160900 -1.53465700 2.46118000
H -2.23303300 -2.26647200 3.20283200
H -1.22022600 -0.81381000 2.97699300
H -2.71906900 -0.99000700 2.05732500
Cl 1.51890100 -1.74479900 -1.11895700
C 0.39695700 1.10348600 0.34318200
H 1.48210700 1.16561800 0.42760800
C -0.80825400 1.39364600 0.31673300
C -2.09051800 2.04126700 0.40611900
C -2.80385700 2.06491800 1.62099400
C -2.63838100 2.69875200 -0.71392000
C -4.03009600 2.72128800 1.70738300
H -2.38025800 1.57611900 2.49233600
C -3.86426300 3.35395400 -0.61813400

H	-2.08822600	2.69471200	-1.65001100	H	0.47512800	-2.09670900	3.14302200
C	-4.56683500	3.36568200	0.58991100	H	0.44365000	-3.33621600	1.90676600
H	-4.56530100	2.73460800	2.65308400	C	-0.13639500	-2.95208400	-2.03191200
H	-4.27042500	3.86103000	-1.48924000	H	-0.70900600	-2.24913600	-2.64414600
H	-5.52231900	3.87776400	0.66102300	H	0.21490700	-3.77372300	-2.68400200
N	3.56502700	0.85705400	0.08185600	H	-0.80377800	-3.34762800	-1.26316400
H	3.17465600	0.04782300	-0.41026200	C	1.78826000	-1.56064500	-2.40248900
C	4.42818600	0.35519900	1.16903700	H	2.22513300	-2.26956000	-3.13160700
C	5.48682100	-0.66011000	0.69876400	H	1.16557700	-0.84212400	-2.94295300
C	3.54177600	-0.25447900	2.26243100	H	2.60135000	-1.00285300	-1.93173100
H	4.94650300	1.22267300	1.59735100	Cl	-1.83043200	-1.85236900	0.96505900
H	6.13159600	-0.24538400	-0.08402800	C	-0.49041800	1.19477500	-0.38777400
H	6.13266100	-0.96745300	1.53066900	H	-2.03080200	1.08485100	-0.24560700
H	5.00067000	-1.55778600	0.29673600	C	0.73930600	1.42372400	-0.34020200
H	2.85136500	0.49532600	2.66414900	C	2.05709000	2.00330900	-0.39861900
H	2.94903400	-1.08039000	1.85104600	C	2.79006300	2.02620100	-1.60347000
H	4.14780000	-0.64602400	3.08835800	C	2.63568900	2.60011700	0.74143500
C	4.19727000	1.76095900	-0.89645200	C	4.05270000	2.61398700	-1.66077200
C	4.38521100	3.16256000	-0.30012900	H	2.34910600	1.58754300	-2.49312400
C	3.32531800	1.82114100	-2.15602400	C	3.89838500	3.18665900	0.67850500
H	5.19251100	1.38834100	-1.19977000	H	2.07517000	2.60271800	1.67163500
H	5.01593900	3.14921300	0.59557100	C	4.61523700	3.19443000	-0.52107400
H	4.86279300	3.82819400	-1.02908100	H	4.59780500	2.62341000	-2.60138100
H	3.41431400	3.59006100	-0.02268500	H	4.32266000	3.64395700	1.56892400
H	3.18208800	0.82434300	-2.58761100	H	5.59945600	3.65254300	-0.56818700
H	2.33507900	2.22935400	-1.92074900	N	-3.15940400	0.85851000	-0.00937900
H	3.78888400	2.46289300	-2.91396300	H	-3.05333800	-0.09685300	0.38587000
				C	-3.95806000	0.77834300	-1.27394500
13-ts				C	-5.39480100	0.31107300	-1.01883200
C	1.77191400	-3.14064300	-0.55540100	C	-3.22660900	-0.14874300	-2.25137400
C	2.57332200	-2.39694800	0.51559800	H	-3.97413700	1.78924300	-1.69543300
H	2.47298400	-3.74456200	-1.16263200	H	-5.95850000	1.00497700	-0.38710800
H	1.08608400	-3.84454000	-0.07579600	H	-5.92821300	0.22719500	-1.97197600
H	3.21685100	-1.64912200	0.04206000	H	-5.40172500	-0.67587300	-0.54103900
H	3.23893400	-3.11492800	1.02819600	H	-2.21573600	0.21604500	-2.45290000
Cu	0.13810500	-0.63571700	0.31041100	H	-3.14573500	-1.16020500	-1.83927100
N	0.97364500	-2.23858000	-1.39361400	H	-3.77896900	-0.19680600	-3.19627400
N	1.72105700	-1.69349500	1.49738200	C	-3.63273400	1.79292800	1.06463600
C	2.53544300	-0.73683500	2.26637200	C	-3.56589200	3.24662700	0.58656500
H	1.89480600	-0.21136200	2.97997700	C	-2.78220200	1.56670200	2.31997600
H	3.33875400	-1.24580400	2.82853400	H	-4.67275800	1.53543000	1.29770900
H	2.98310100	-0.00085900	1.59586600	H	-4.24224300	3.44521100	-0.25139600
C	1.09972600	-2.64657000	2.43662900	H	-3.85446200	3.91310600	1.40629300
H	1.87063500	-3.21085700	2.99077700	H	-2.54669600	3.50424100	0.27864800

H	-2.80720100	0.51823800	2.63262200
H	-1.73787200	1.83580100	2.13413500
H	-3.16586200	2.18779500	3.13692500

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C	-3.24089000	0.14698300	-1.08700400
C	-3.21719000	1.25714500	-0.02782900
H	-4.30001700	-0.04357000	-1.36367400
H	-2.72969800	0.49523800	-1.98899100
H	-3.60222200	0.86528000	0.91869100
H	-3.92760500	2.05000300	-0.34886900
Cu	-0.36110100	-0.41551700	0.05524600
N	-2.58367100	-1.09557600	-0.67284100
N	-1.88859200	1.80181600	0.22156900
C	-1.77363200	2.39786300	1.54467700
H	-0.74997400	2.75762700	1.68747000
H	-2.46695500	3.25260700	1.69845700
H	-1.95700700	1.63222900	2.30330100
C	-1.43837600	2.70382700	-0.82719200
H	-2.09591800	3.59407500	-0.93305300
H	-0.42357800	3.04125300	-0.59814800
H	-1.38189200	2.17580700	-1.78152100
C	-2.36725600	-1.96328700	-1.83069700
H	-1.87765200	-2.88516500	-1.50099300
H	-3.31729200	-2.23306600	-2.33627000
H	-1.69594600	-1.45671000	-2.52879200
C	-3.31740000	-1.79946000	0.37563100
H	-4.35000600	-2.05712200	0.06020400
H	-2.78229000	-2.71790300	0.62833300
H	-3.35185700	-1.20135100	1.28736200
Cl	-0.50799200	-0.95159300	2.28204400
C	0.40875100	-0.04438400	-1.77909500
C	1.44443000	-0.07569300	-1.05283700
C	2.79795800	-0.03788000	-0.57697500
C	3.12111500	-0.27931500	0.77771700
C	3.86110600	0.24740600	-1.46565800
C	4.44392900	-0.23627500	1.21337400
H	2.31176100	-0.50044600	1.46893800
C	5.18046200	0.28860500	-1.02075800
H	3.62765900	0.43442600	-2.51035100
C	5.48465300	0.04735100	0.32277600
H	4.66431800	-0.42723400	2.26218800
H	5.97817600	0.51039900	-1.72831600
H	6.51566600	0.07969600	0.66926900

15-ts

C	-2.69158700	-1.66979700	0.23507300
C	-1.98233700	-1.67959600	-1.12066800
H	-3.72529800	-2.03133900	0.10026600
H	-2.20316700	-2.37425500	0.91554800
H	-2.45513500	-0.95714700	-1.79147700
H	-2.09049600	-2.67979900	-1.57658600
Cu	-0.68367900	0.54905500	0.14145400
N	-2.67829400	-0.33545500	0.87034000
N	-0.55327600	-1.30547600	-1.02093100
C	-0.01642200	-1.02943700	-2.36997400
H	1.04458600	-0.77928300	-2.28607300
H	-0.12230900	-1.90847200	-3.02804300
H	-0.54058900	-0.16979400	-2.79191600
C	0.24492200	-2.36971300	-0.38784800
H	0.19695600	-3.30902400	-0.96554100
H	1.28708600	-2.04848700	-0.32566600
H	-0.10665900	-2.56671400	0.62759400
C	-2.78655500	-0.45043700	2.33094000
H	-2.75305600	0.54842900	2.77510000
H	-3.72808300	-0.93519100	2.64306100
H	-1.94566800	-1.03010500	2.72317400
C	-3.77067500	0.51050700	0.35536200
H	-4.75594900	0.06890700	0.58659500
H	-3.70235200	1.50110800	0.80994700
H	-3.66346400	0.65164400	-0.72013000
Cl	-1.35292100	2.07577800	-1.50503000
C	0.16677300	1.52761000	1.70198900
H	-0.41344700	2.18507600	2.31936900
C	1.17625700	1.00137600	1.22055800
C	2.43598400	0.50739400	0.74783300
C	2.93833100	0.94603100	-0.49518800
C	3.19259200	-0.39874400	1.51644500
C	4.17248500	0.48694900	-0.94874500
H	2.34730700	1.63909300	-1.08644000
C	4.42435200	-0.85397500	1.04979600
H	2.80898100	-0.73208700	2.47613700
C	4.91782600	-0.41329900	-0.18106500
H	4.55431600	0.83329300	-1.90513600
H	5.00233900	-1.55074200	1.65074000
H	5.87974200	-0.76864000	-0.54008100

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C	2.17980400	1.91390400	-0.29557700	H	-1.81942700	-3.35676200	-1.62720400
C	3.15147300	0.95594800	0.39346500	H	-2.77594200	-3.03064700	1.27115600
H	2.38070800	2.94485100	0.02867800	H	-3.81156400	-3.31421200	-0.12739500
H	2.32629200	1.88495900	-1.37908500	Cu	-0.89372500	-0.80228900	-0.02602400
H	3.05632300	1.03796700	1.48027700	N	-0.40343000	-2.85250400	-0.16568800
H	4.18545700	1.23112300	0.13960600	N	-2.91283900	-1.37325600	-0.00721000
Cu	0.77032800	-0.53926000	-0.02601300	C	-3.69614600	-0.72978000	1.07633600
N	0.76013500	1.54440700	-0.02323500	H	-3.70406700	0.35145800	0.92425900
N	2.87446400	-0.45996600	0.02325600	H	-4.73233900	-1.09758100	1.08775500
C	3.47172800	-1.37870700	1.02287000	H	-3.23318600	-0.94450600	2.04295100
H	3.25310000	-2.41126900	0.74131500	C	-3.53029500	-1.03323700	-1.31399400
H	4.56232400	-1.25173100	1.07671600	H	-4.57263300	-1.38155800	-1.35702900
H	3.04194400	-1.18487500	2.00880500	H	-3.51203400	0.05074000	-1.44815900
C	3.42392500	-0.78087200	-1.31813700	H	-2.97207700	-1.49334500	-2.13272300
H	4.51817300	-0.67379200	-1.32955000	C	0.63050100	-3.12779600	-1.19084100
H	3.16682500	-1.81055800	-1.57690200	H	1.56043700	-2.63098700	-0.90550600
H	2.99796600	-0.12040300	-2.07657900	H	0.81755200	-4.20724800	-1.28828000
C	-0.12644800	2.13672200	-1.05693700	H	0.30729400	-2.73474100	-2.15806700
H	-1.16015000	1.84758200	-0.85683200	C	0.07050400	-3.35249900	1.14770800
H	-0.05490500	3.23357300	-1.05509300	H	0.25568800	-4.43631200	1.11231000
H	0.15848900	1.76431600	-2.04427600	H	0.99864500	-2.84178400	1.41324100
C	0.33115000	2.03295600	1.31314400	H	-0.66794000	-3.14772700	1.92612100
H	0.38084100	3.13010200	1.36130900	C	0.59548200	0.49957000	-0.01594000
H	-0.69767400	1.71555000	1.49767000	H	1.67434900	0.27405600	-0.03964200
H	0.96904100	1.61726200	2.09656500	C	-0.42703100	1.21233400	0.01609600
C	-0.08337600	-2.30350200	-0.02637100	C	-1.42442200	2.25169500	0.04024500
H	0.37654100	-3.27585300	-0.02386200	C	-1.89571100	2.75824400	1.26751500
C	-1.06023200	-1.52902800	-0.01971400	C	-1.92144800	2.78213000	-1.16714700
C	-2.32829600	-0.85292100	-0.00419600	C	-2.84538400	3.77764300	1.28071100
C	-2.98504200	-0.55049900	-1.21407700	H	-1.50354100	2.35838400	2.19785500
C	-2.93262300	-0.51388700	1.22365400	C	-2.87097500	3.80128100	-1.14100200
C	-4.22793600	0.07750200	-1.18907900	H	-1.54614800	2.40268600	-2.11300100
H	-2.52406600	-0.82391300	-2.15838200	C	-3.33583900	4.29861800	0.07985000
C	-4.17589700	0.11354500	1.23401200	H	-3.19848200	4.17065200	2.22942900
H	-2.43268800	-0.76294500	2.15496100	H	-3.24358000	4.21278500	-2.07430400
C	-4.82350700	0.41122600	0.03114300	H	-4.07396700	5.09488700	0.09546400
H	-4.73623600	0.30024700	-2.12229900	N	3.71651800	0.11305700	-0.07857000
H	-4.64401600	0.36360000	2.18122600	C	4.24017600	0.22099900	1.30553100
H	-5.79435800	0.89735100	0.04473100	H	5.34122200	0.18255400	1.31033300
				C	4.22257500	1.09329800	-1.07402600
				H	3.86916600	2.07972400	-0.75025000
17				C	3.81109100	1.53794600	1.96003300
C	-1.69535900	-3.48481700	-0.54770900	H	2.71849400	1.63213700	1.97189300
C	-2.86953900	-2.84866800	0.19664700	H	4.16811900	1.57449000	2.99461200
H	-1.67522900	-4.56715400	-0.35183300				

H	4.22211800	2.41039000	1.44248600	C	-0.59959900	2.35416900	0.00663900
C	5.75407500	1.14030500	-1.20003600	C	-0.86218600	3.02057800	1.21997900
H	6.15331400	0.16010200	-1.49215200	C	-0.95972100	2.97882000	-1.20418200
H	6.05070700	1.86250500	-1.96855400	C	-1.46571300	4.27718900	1.21799900
H	6.23997400	1.43944200	-0.26625000	H	-0.58327200	2.54683000	2.15672100
H	3.96951000	-0.81568900	-0.42345000	C	-1.56231500	4.23577800	-1.19797600
C	3.73623100	-0.98342500	2.10800800	H	-0.75247400	2.47367700	-2.14328000
H	4.03820800	-1.92975400	1.64051900	C	-1.81792800	4.88780300	0.01131000
H	4.14920800	-0.97171400	3.12187000	H	-1.65790500	4.78283600	2.16007300
H	2.64164900	-0.96935400	2.18726600	H	-1.82933800	4.70914700	-2.13857100
C	3.57462400	0.78082300	-2.42781300	H	-2.28623000	5.86769600	0.01334600
H	3.88242800	-0.20954800	-2.79032400	N	3.49339200	-0.54772600	-0.06737400
H	2.48144200	0.79703900	-2.36028300	C	4.06047900	-0.45721800	1.33034100
H	3.88024300	1.51391200	-3.18117500	H	5.13550300	-0.65191100	1.25736100
18-ts							
C	-2.70438100	-3.02069200	-0.52058300	C	4.05613500	0.36357600	-1.13219600
C	-3.55777700	-2.05014900	0.29690300	H	3.74643000	1.37150400	-0.83960800
H	-3.03951900	-4.05307100	-0.33599600	C	3.82793400	0.93723000	1.91429700
H	-2.83867900	-2.82738000	-1.58903700	H	2.76253600	1.18858400	1.91606600
H	-3.46475700	-2.27762300	1.36308800	H	4.18728800	0.95678700	2.94772100
H	-4.61867100	-2.17923600	0.03346700	H	4.36917100	1.71380900	1.36535900
Cu	-0.99801100	-0.73387700	-0.01052000	C	5.58114200	0.29049100	-1.21848400
N	-1.25967000	-2.86716900	-0.21546700	H	5.92066400	-0.73080900	-1.43135400
N	-3.12865700	-0.64210800	0.09854200	H	5.92487200	0.92874700	-2.03846000
C	-3.60151300	0.20099100	1.22081700	H	6.07463000	0.63756300	-0.30629500
H	-3.25897400	1.22719500	1.07239300	H	3.60284700	-1.51415000	-0.39045300
H	-4.70009600	0.19640100	1.28889500	C	3.41327400	-1.55779000	2.17549700
H	-3.18714800	-0.17233900	2.16113300	H	3.58043800	-2.55150300	1.74119700
C	-3.66064100	-0.09577400	-1.17193400	H	3.85463300	-1.55994800	3.17661600
H	-4.76150100	-0.08679100	-1.16781100	H	2.33509700	-1.39479600	2.27518200
H	-3.29659200	0.92563400	-1.30328800	C	3.38347200	0.00407700	-2.45982900
H	-3.31792400	-0.69466400	-2.01913400	H	3.66459100	-1.00651300	-2.78435000
C	-0.43757800	-3.42400800	-1.30928300	H	2.29414900	0.06015600	-2.37959700
H	0.61880700	-3.26975800	-1.07704700	H	3.70824100	0.70154000	-3.23770300
H	-0.61869000	-4.50163600	-1.44457600	19			
H	-0.66562500	-2.90601400	-2.24444500	C	-3.90757300	-0.13754700	-0.41174400
C	-0.90478900	-3.54053200	1.05245300	C	-3.62232200	1.22270700	0.23369400
H	-1.08419200	-4.62547200	0.99201000	H	-4.94619900	-0.43932000	-0.19699200
H	0.15209700	-3.36671200	1.26778800	H	-3.81446000	-0.05635100	-1.49894000
H	-1.49081900	-3.13409900	1.87969300	H	-3.76090900	1.15371300	1.31748600
C	0.83426000	0.07872300	0.00136400	H	-4.37328300	1.94740800	-0.13100800
H	2.33866900	-0.35470300	-0.00858500	Cu	-1.02785700	-0.46639500	-0.01505400
C	0.04221700	1.05882200	0.00131400	N	-2.96279700	-1.19647300	0.03026600
				N	-2.24995900	1.66303300	-0.02353400

C	-1.73839500	2.57019000	1.00594400	H	-1.62084500	2.24433400	-2.94967300
H	-0.68006500	2.76543200	0.81344600	H	-2.66223100	2.26534800	-1.51950600
H	-2.27982600	3.53333400	1.03066800	C	1.55540700	2.75988100	2.16003700
H	-1.81840600	2.09671300	1.98908900	H	2.30698400	3.00749000	1.40537300
C	-2.08246500	2.24820100	-1.35590100	H	1.61506000	3.49141600	2.98497700
H	-2.64636500	3.19250500	-1.46813600	H	1.77050100	1.76259100	2.55053700
H	-1.02152300	2.44493600	-1.53048500	C	0.23957100	3.85359000	-2.07467800
H	-2.42073600	1.55105300	-2.12800300	H	1.13266000	4.06169000	-1.48474500
C	-3.07025600	-2.36676800	-0.87138200	H	0.53494500	3.20452500	-2.90164300
H	-2.36574600	-3.13665200	-0.54980000	H	-0.15462800	4.80026800	-2.48166500
H	-4.09045800	-2.78435700	-0.86098600	N	0.21876500	2.74749000	1.54215600
H	-2.81498000	-2.06917400	-1.89114200	N	-0.77675100	3.16638300	-1.25742100
C	-3.26304500	-1.63166600	1.41370400	Cl	2.18200900	1.19244100	-1.11244900
H	-4.28650100	-2.03514300	1.48663800	Cu	1.65872400	-0.69958800	0.17138300
H	-2.55069700	-2.40523200	1.70841600	C	3.07659400	-3.21869200	-0.27581200
H	-3.16039500	-0.79503900	2.10697500	H	3.92849700	-3.87088800	-0.53489400
C	0.80867100	-0.36842300	-0.02827200	H	2.59451500	-3.64776100	0.60728200
C	2.03589400	-0.27254800	-0.02020500	C	2.09081500	-3.18768800	-1.44502200
C	3.45868500	-0.16613600	-0.00633500	H	1.82196300	-4.22354000	-1.71424300
C	4.20308000	-0.18929400	-1.20566200	H	2.57193500	-2.74914900	-2.32477500
C	4.16562700	-0.03479200	1.20871400	C	-0.07613100	-3.16080100	-0.32774200
C	5.59199600	-0.08489400	-1.18716000	H	-0.92491800	-2.51892900	-0.08872000
H	3.67234700	-0.29159900	-2.14773000	H	-0.42643500	-4.05419600	-0.87291400
C	5.55456300	0.06881400	1.22041400	H	0.38224000	-3.46591400	0.61458700
H	3.60545500	-0.01667700	2.13907700	C	4.22069000	-1.91317500	1.41401400
C	6.27687700	0.04474200	0.02419000	H	5.09179900	-2.58889700	1.39225000
H	6.14402300	-0.10574800	-2.12397800	H	4.55916900	-0.90794900	1.67758100
H	6.07711400	0.16872500	2.16897400	H	3.50879300	-2.23970500	2.17265200
H	7.36075200	0.12549000	0.03587900	C	0.23300400	-1.94028800	-2.38359700
				H	0.91573500	-1.29445500	-2.94348300
20				H	-0.06209400	-2.79245400	-3.01985800
Cu	0.01839100	1.30153800	-0.27369900	H	-0.65687600	-1.36427900	-2.12177200
C	-1.19201200	3.99000400	-0.10030300	C	4.49221300	-1.32810100	-0.90231400
H	-1.45117400	5.01134500	-0.42958400	H	4.01029000	-1.23664100	-1.87642700
H	-2.10169700	3.53988400	0.30777700	H	4.80575300	-0.32872400	-0.59508300
C	-0.11814100	4.06904900	0.98742800	H	5.38145500	-1.97377600	-0.99693300
H	-0.46573000	4.75738200	1.77793400	N	0.88621000	-2.39151100	-1.14210000
H	0.79660300	4.50470700	0.57348500	N	3.55295500	-1.86837700	0.09856800
C	-0.77818000	2.30485800	2.53528400	C	-1.55590000	0.25665900	-0.12797100
H	-0.51600400	1.29960400	2.87033600	C	-2.62171800	-0.34928800	-0.03929600
H	-0.80646500	2.99043700	3.40065400	C	-3.83814700	-1.08801300	0.10419000
H	-1.77123000	2.25643900	2.08393500	C	-4.80558800	-1.11046500	-0.92211500
C	-1.94545800	2.84912500	-2.09872000	C	-4.09745500	-1.82070700	1.28234800
H	-2.42434100	3.76716400	-2.47836700	C	-5.98529900	-1.83678500	-0.77428600

H	-4.61680600	-0.55192300	-1.83463700	H	1.68610500	-0.38536400	2.82577300
C	-5.27934400	-2.54470900	1.42340900	H	3.46798800	-0.58905300	2.88149900
H	-3.35796200	-1.81038800	2.07752700	H	2.69032400	0.29798700	1.53724700
C	-6.22892300	-2.55715600	0.39798600	C	1.63956200	-1.17618000	-2.62098700
H	-6.71797700	-1.84109900	-1.57765700	H	2.39357900	-1.39882600	-3.39153800
H	-5.46021800	-3.10286600	2.33869400	H	0.65616600	-1.51485400	-2.94964400
H	-7.14970100	-3.12330200	0.51113100	H	1.59773000	-0.10349300	-2.43559300
Cl	1.08257100	-0.98514900	2.32901100	C	2.32920100	-2.93652600	2.41043900
21-ts				H	2.18957600	-3.86847600	1.85597200
Cu	-1.51922000	-0.42370600	-0.43164100	H	3.23503400	-3.01893700	3.03138700
C	-4.04196400	2.19097700	0.54024800	H	1.45712700	-2.78183100	3.04680800
H	-4.57352800	2.67853700	1.38671100	C	2.02637700	-3.33606000	-1.63525500
H	-4.62272900	2.43665600	-0.35574200	H	2.16570800	-3.90266700	-0.71262900
C	-4.13234200	0.68514800	0.80274900	H	1.07377700	-3.63495000	-2.07112400
H	-5.20213000	0.47257200	0.97477100	H	2.85141700	-3.56637200	-2.32715700
H	-3.60398200	0.41585400	1.72165800	N	2.43748800	-1.80464400	1.46634800
C	-4.15590600	0.13724900	-1.59593000	N	1.97724900	-1.87901200	-1.36065500
H	-3.85164000	-0.62896900	-2.31340700	C	0.06772800	0.64967600	-0.35793400
H	-5.25690600	0.20879700	-1.59879600	C	0.91785500	1.54491300	-0.36530500
H	-3.72981600	1.09330100	-1.90551100	C	1.88485200	2.59664000	-0.36270400
C	-2.73121400	4.07068400	-0.19178700	C	2.30110300	3.19615500	0.84756100
H	-3.22530300	4.81055500	0.47091300	C	2.45556400	3.06638400	-1.56654900
H	-1.70711700	4.41058600	-0.37586500	C	3.25296900	4.21364800	0.85014400
H	-3.26396800	4.06523400	-1.14933000	H	1.86061500	2.85481100	1.77989500
C	-4.14012000	-1.59320300	0.08295700	C	3.40419900	4.08629200	-1.55633700
H	-3.75008600	-1.88016600	1.06231600	H	2.13581400	2.62560300	-2.50636700
H	-5.24235100	-1.60224800	0.11052900	C	3.81037400	4.66337300	-0.34974600
H	-3.77829100	-2.31431000	-0.64937700	H	3.55753600	4.66122500	1.79284800
C	-1.92717400	2.69579800	1.60473100	H	3.82773900	4.43452800	-2.49501600
H	-1.79836200	1.66893200	1.95455900	H	4.55057900	5.45881000	-0.34536300
H	-0.92865400	3.09625900	1.41317400	Cl	-1.26714300	-2.66661500	-1.36983200
H	-2.40040700	3.29400100	2.41078500	22			
N	-3.64207700	-0.23751100	-0.26235100	C	4.18306600	-2.08388900	-0.74670400
N	-2.70109700	2.72655700	0.36883100	C	4.95929700	-0.77292200	-0.79798500
Cl	-0.75665400	-1.56668600	2.06033000	H	4.44271100	-2.71615700	-1.60759800
Cu	0.60847400	-1.50831900	0.23327900	H	4.44491600	-2.64385800	0.15611000
C	3.26740200	-1.37810200	-0.83151400	H	4.74053100	-0.23764800	-1.72657100
H	4.08654400	-1.60537000	-1.53282700	H	6.03967300	-0.97803700	-0.79387600
H	3.18434000	-0.28993500	-0.75567600	Cu	2.45435100	-0.24466500	0.63112400
C	3.57503700	-1.99068400	0.53161700	N	2.71152300	-1.84331500	-0.71412200
H	4.49330000	-1.54522000	0.94112300	N	4.57519100	0.09945300	0.33811400
H	3.76513700	-3.06194200	0.42843900	C	4.84549800	1.52343000	0.03424000
C	2.58389400	-0.54187500	2.22583200	H	4.50425600	2.13229200	0.87290700

H	5.91894700	1.69474400	-0.13180600	H	-4.18821400	-2.95823300	-0.08432000
H	4.29519400	1.82017100	-0.86315300	H	-4.33031800	-2.33592400	1.56787600
C	5.29863000	-0.27894900	1.57649400	C	-5.04405300	-0.78381200	-1.34297800
H	6.37954000	-0.11621300	1.45728600	H	-4.54717400	-1.51960000	-1.97668100
H	4.92364400	0.32556900	2.40338000	H	-6.12773000	-0.97139300	-1.34129900
H	5.12511500	-1.33162700	1.81349700	H	-4.85793500	0.21413200	-1.74984900
C	2.01595600	-3.07965100	-0.26933700	N	-2.80612500	0.86087900	1.63483800
H	0.93660300	-2.92223400	-0.30600900	N	-4.48859800	-0.87733100	0.02647000
H	2.27206400	-3.91958300	-0.92960100	H	0.20500600	-1.17764500	1.46369800
H	2.31849800	-3.32655600	0.75210700	Cl	-1.84548200	-2.10879100	-1.38072000
C	2.20247000	-1.47405000	-2.06179100	Cl	2.22960500	1.15642200	2.34234200
H	2.42953600	-2.27118800	-2.78329600				
H	1.12202600	-1.33941400	-2.00916200	23			
H	2.66140400	-0.54415500	-2.40386600	C	-4.15354500	0.77742100	-1.90304500
C	0.41745200	-0.45719400	0.68488700	C	-5.18121500	0.23692500	-0.91651600
C	-0.29923400	0.20656000	-0.14165900	H	-4.55095300	0.73845200	-2.92771600
C	-0.27004100	1.30370800	-1.09582500	H	-3.93152400	1.82517400	-1.68034700
C	-0.83670400	1.18932600	-2.38287400	H	-5.43231400	-0.79947000	-1.15820300
C	0.34048200	2.52256700	-0.71808600	H	-6.11263900	0.81662500	-0.99710500
C	-0.78076700	2.26344600	-3.26984000	Cu	-2.47232500	-0.14294000	0.24272800
H	-1.30012000	0.25295300	-2.67709300	N	-2.86707100	0.02314600	-1.82961300
C	0.39114900	3.58690100	-1.61595800	N	-4.64086800	0.27550600	0.46075300
H	0.78355800	2.60929700	0.27008700	C	-5.28649000	-0.74067700	1.32097500
C	-0.17157800	3.46299600	-2.89075500	H	-4.82311400	-0.71165700	2.30838800
H	-1.21222500	2.16210800	-4.26152900	H	-6.36595800	-0.55110300	1.41661300
H	0.86833800	4.51660300	-1.31903500	H	-5.13874900	-1.73607800	0.89236800
H	-0.13489300	4.29779500	-3.58462700	C	-4.82260500	1.61361000	1.06912400
C	-4.16372500	0.43428900	2.08928000	H	-5.89201600	1.83984700	1.19433000
C	-5.08770600	0.14527000	0.91358300	H	-4.32592500	1.63119300	2.04002200
H	-4.03694800	-0.46425200	2.69993400	H	-4.37239600	2.38359500	0.43781600
H	-4.60022100	1.20782000	2.73686500	C	-1.82281800	0.78146400	-2.56743500
H	-6.07189300	-0.17588100	1.28555800	H	-0.87775300	0.23833700	-2.54267500
H	-5.25178500	1.05256000	0.32530500	H	-2.12896100	0.93101200	-3.61233100
Cu	-2.33006700	-0.46255400	0.05048400	H	-1.68062400	1.75653900	-2.09598600
C	-1.86980600	0.77692200	2.78741900	C	-3.01791200	-1.31241600	-2.46319900
H	-0.87574400	1.11060900	2.49010800	H	-3.33941100	-1.20365200	-3.50864100
H	-2.23027000	1.40363200	3.61475300	H	-2.06326100	-1.83580400	-2.43575100
H	-1.80611600	-0.25825600	3.13326500	H	-3.75334200	-1.91417600	-1.92622300
C	-2.84320300	2.26737400	1.15473500	C	0.35575400	-0.03580700	-0.09315000
H	-1.84316900	2.57365900	0.84919800	C	-0.49709700	-0.97962000	-0.00358100
H	-3.50903500	2.36346100	0.29494200	C	-0.67677900	-2.42282300	-0.09020600
H	-3.19515300	2.93344200	1.95488400	C	-0.12304900	-3.12077100	-1.18825900
C	-4.71714400	-2.24539300	0.54948500	C	-1.38674900	-3.14404300	0.89271400
H	-5.79108600	-2.48273400	0.55832700	C	-0.26959700	-4.50355500	-1.28449300

H	0.43157500	-2.56877700	-1.94188800	H	3.24794300	2.43629500	0.03680600
C	-1.52731700	-4.52716300	0.78237500	C	2.22480800	5.39702200	-1.48171200
H	-1.80603100	-2.61251100	1.74134400	H	1.48015300	6.17357500	-1.27569400
C	-0.97388300	-5.21021400	-0.30407600	H	3.20832700	5.88006300	-1.49780200
H	0.16521400	-5.03056300	-2.12925000	H	2.03428900	5.00059400	-2.48804000
H	-2.06851600	-5.07302500	1.54995600	C	0.02430000	4.28071900	1.93995200
H	-1.08967300	-6.28699500	-0.38691300	H	1.04182000	4.52934400	2.26066500
C	4.03978700	-0.56433900	2.12976300	H	-0.66037200	4.93928600	2.48620500
C	4.72701500	-1.58571900	1.23045300	H	-0.18554400	3.24525400	2.23249400
H	4.41680800	0.44130900	1.92078300	C	-1.56474100	4.04711700	-0.00159800
H	4.25624700	-0.78067400	3.18596300	H	-2.31759200	4.62971800	0.53977900
H	5.81350800	-1.55940100	1.39850600	H	-1.72037400	4.21654300	-1.07549700
H	4.39179900	-2.59611800	1.48055400	H	-1.73470700	2.98518000	0.21964900
Cu	2.34326400	-0.58580000	-0.18627400				
C	1.98476700	0.66942800	2.53954600	24			
H	0.89939600	0.65146500	2.42938100	C	5.19449200	0.11054600	-0.85151500
H	2.23463700	0.69237700	3.60938600	C	5.30626600	0.21490500	0.67227900
H	2.37960400	1.56622600	2.05747400	H	6.00330100	0.69074500	-1.32187100
C	1.91962900	-1.74056400	2.50355600	H	5.32215000	-0.93005600	-1.16423800
H	0.84192500	-1.67095800	2.35801900	H	5.22982500	1.26241800	0.98000800
H	2.28180700	-2.65448100	2.02873600	H	6.30692400	-0.13161700	0.97965800
H	2.13310800	-1.78758100	3.58063700	Cu	2.46059700	-0.19790400	-0.05775700
C	5.27616300	-0.28030900	-0.76456500	N	3.86991800	0.56581700	-1.35981300
H	6.32173000	-0.62108800	-0.78618700	N	4.23498700	-0.53723000	1.35132200
H	4.94200000	-0.05440900	-1.77809200	C	3.99500600	-0.03019000	2.71245800
H	5.21566800	0.63432900	-0.16999900	H	3.14966000	-0.56713900	3.15064200
C	4.52660600	-2.56257000	-1.00032400	H	4.87434400	-0.16096200	3.36444700
H	4.23797100	-2.34185300	-2.02905900	H	3.74211800	1.03318000	2.67196700
H	5.55923500	-2.94070300	-0.98142000	C	4.52337900	-1.98096900	1.40137400
H	3.85872800	-3.33359800	-0.60601600	H	5.42066100	-2.19624400	2.00518800
N	2.56634100	-0.54326800	1.90457000	H	3.66882000	-2.50310800	1.83923300
N	4.39811200	-1.32879400	-0.19211600	H	4.67957900	-2.37640600	0.39422900
H	0.37549100	1.05123800	-0.10729400	C	3.67237200	0.07513600	-2.74471700
Cl	2.18345200	-0.38291500	-2.39885000	H	2.70047600	0.41196600	-3.11225300
Cl	-2.06193400	0.03884600	2.42816500	H	4.45753600	0.45434000	-3.41689300
N	0.83982900	3.64335100	-0.31047600	H	3.69252100	-1.01735200	-2.75539000
H	0.49152800	3.49381800	-1.25865600	C	3.78757400	2.04713300	-1.36273100
C	-0.15307800	4.45672000	0.42722200	H	4.56479200	2.48244400	-2.00977500
H	-0.03439200	5.52795900	0.19084100	H	2.80592800	2.35274500	-1.73149100
C	2.17980700	4.26691100	-0.43906500	H	3.91086800	2.43779700	-0.35090400
H	2.42141200	4.69224800	0.54264500	C	-1.69170500	0.36131000	-2.19889500
C	3.21948800	3.18884300	-0.76009600	C	-1.83499700	1.26625500	-1.35950800
H	2.97955100	2.67024100	-1.69599800	C	-1.99927100	2.48598300	-0.61511700
H	4.21972500	3.62632600	-0.86009200	C	-2.99178300	3.40926500	-0.99967200

C	-1.16278700	2.77764000	0.48106900	Cu	3.53592200	0.71167000	-0.00023200
C	-3.13673000	4.60583400	-0.30081800	N	4.57845700	2.15766800	1.05960700
H	-3.63306200	3.18460500	-1.84652500	N	5.60257800	0.16824000	-0.85861100
C	-1.31750200	3.97909700	1.16950900	C	5.87923900	-1.27530300	-0.79621400
H	-0.40739800	2.05526700	0.77645800	H	5.14375700	-1.80698700	-1.40565700
C	-2.30179200	4.89363900	0.78230000	H	6.88919000	-1.52085900	-1.16478800
H	-3.90083100	5.31555800	-0.60386100	H	5.78587600	-1.62537000	0.23569200
H	-0.66867100	4.20331000	2.01139500	C	5.66890300	0.62912100	-2.25526400
H	-2.41804000	5.82816400	1.32333000	H	6.66439200	0.45283900	-2.69656200
C	-3.21076600	-2.23451400	1.54146900	H	4.92036300	0.09445500	-2.84567000
C	-3.50370300	-2.99388000	0.24805200	H	5.44642100	1.69759400	-2.31885700
H	-2.25109200	-2.55597900	1.95558700	C	3.87219500	3.46011100	1.03047600
H	-3.98556000	-2.46917800	2.28809200	H	2.89522800	3.35178500	1.50692400
H	-3.56741700	-4.07179600	0.46003700	H	4.44481300	4.23614600	1.56210700
H	-4.47495400	-2.69107200	-0.15354600	H	3.72246000	3.77464700	-0.00518100
Cu	-2.05119900	-0.64422400	-0.51896700	C	4.72486400	1.72454700	2.46978100
C	-2.48541700	-0.11980400	2.48596700	H	5.30603400	2.45896100	3.04934400
H	-2.43004600	0.95700000	2.31243100	H	3.73443800	1.62040300	2.91850000
H	-3.06769600	-0.30403700	3.40161000	H	5.22764500	0.75688900	2.52128500
H	-1.47176100	-0.50381000	2.60917700	C	-2.60809600	-0.08657100	0.62837600
C	-4.46863000	-0.17443000	1.12027300	C	-2.07666400	-0.96575600	1.33449300
H	-4.36182900	0.89651400	0.93351400	C	-1.58601000	-1.81106600	2.39331600
H	-4.96871400	-0.62294700	0.25899200	C	-2.49324900	-2.52635100	3.19893600
H	-5.09878700	-0.32087700	2.01082200	C	-0.20307900	-1.90758100	2.64442900
C	-1.27549000	-3.56457800	-0.57921600	C	-2.02131800	-3.31911600	4.24275400
H	-1.53002200	-4.63217300	-0.66418900	H	-3.55874000	-2.44690600	3.00516200
H	-0.52153000	-3.31245300	-1.32750000	C	0.25475600	-2.70295400	3.69294200
H	-0.84248400	-3.36716700	0.40129200	H	0.49238500	-1.36241400	2.01202000
C	-3.03030800	-3.01410500	-2.13673600	C	-0.64906600	-3.40882500	4.49231700
H	-2.26582100	-2.81988300	-2.89311800	H	-2.72535100	-3.86491800	4.86407600
H	-3.34530800	-4.06512700	-2.22108200	H	1.32139600	-2.77293300	3.88671600
H	-3.89010700	-2.36850600	-2.33355800	H	-0.28567400	-4.02711600	5.30807100
N	-3.12449700	-0.76769900	1.31638900	C	-0.56178100	-2.85385700	-2.69282400
N	-2.47708300	-2.72394800	-0.79495400	C	-1.61978800	-2.05430700	-3.45197000
H	-1.45440100	-0.06802100	-3.15407600	H	0.36274100	-2.27571600	-2.60789500
Cl	0.48358600	-0.79603700	0.66303400	H	-0.33043100	-3.77740000	-3.24626100
				H	-1.24602700	-1.80816200	-4.45664400
				H	-2.52285300	-2.65603800	-3.58834300
25				Cu	-1.82581800	-1.35211300	-0.67201700
C	5.90796800	2.28962900	0.40389100	C	0.15172300	-3.66729900	-0.51966500
C	6.50673900	0.93401900	0.01786100	H	-0.17280100	-3.87607500	0.50170600
H	6.60795200	2.82926300	1.06079200	H	0.55375300	-4.59108300	-0.96291800
H	5.76958400	2.90367800	-0.49086300	H	0.93010700	-2.90265800	-0.49385200
H	6.68674700	0.33851700	0.91812000	C	-2.06434400	-4.20816700	-1.29950100
H	7.49020700	1.09991100	-0.45304400				

H	-2.34485500	-4.42261800	-0.26568900	H	5.37573300	2.72495200	0.11873300
H	-2.95394600	-3.86196700	-1.83015700	Cu	2.07653600	0.44080800	0.73164800
H	-1.70954400	-5.13711000	-1.77114300	N	3.97275400	0.06687600	1.79389500
C	-1.04516400	0.28171500	-2.99403500	N	3.50948600	1.88727100	-0.49902100
H	-1.03815100	0.52587800	-4.06748300	C	3.58903900	1.52856300	-1.92074500
H	-1.34693900	1.16756500	-2.43034100	H	2.58586200	1.57687300	-2.35130600
H	-0.03930500	0.00800800	-2.67068600	H	4.25385000	2.20607000	-2.48464200
C	-3.36532300	-0.38879300	-3.10365700	H	3.95044400	0.50178500	-2.02411800
H	-3.63678100	0.50632600	-2.54024400	C	2.94689700	3.23944100	-0.34504100
H	-3.42111900	-0.16209800	-4.17914000	H	3.58626300	3.99387800	-0.83588000
H	-4.08526600	-1.17768500	-2.87013700	H	1.95060500	3.26704700	-0.79098600
N	-1.00415400	-3.17181300	-1.30751700	H	2.83601900	3.48081900	0.71325500
N	-2.00283400	-0.81836600	-2.71637300	C	3.75340600	-0.20790000	3.23373500
H	-3.12987000	0.85384900	0.42502500	H	3.20837800	-1.14995200	3.33553300
Cl	1.75332000	-0.37860100	-0.61015300	H	4.71745200	-0.29331300	3.75944400
N	-4.03785000	2.76132200	0.67378800	H	3.15371400	0.59009100	3.66892500
H	-3.91608800	2.66784800	1.68180200	C	4.78802500	-1.03779100	1.24128900
C	-3.12951700	3.85563300	0.24369200	H	5.78757600	-1.04137000	1.70466000
H	-2.12394800	3.49936300	0.50875900	H	4.29215700	-1.98625200	1.44639700
C	-5.49334900	2.92861600	0.40891800	H	4.88930300	-0.95000500	0.16038500
H	-5.71582300	3.98318800	0.19090700	Cl	1.29757200	1.80910400	2.42706600
C	-3.15644000	4.05643900	-1.27455400	C	0.42615500	0.66885200	-0.35378900
H	-4.11841000	4.45414300	-1.61689400	C	-0.26765000	1.46875300	-1.00307600
H	-2.38281500	4.77248800	-1.57159500	C	-1.17113700	2.38394000	-1.60884500
H	-2.96957800	3.11330100	-1.80003300	C	-0.95883200	2.87544100	-2.91604100
C	-3.35782400	5.18420300	0.98804900	C	-2.30614500	2.82245600	-0.88917300
H	-3.29263300	5.04359800	2.07379100	C	-1.85012800	3.78281500	-3.48158200
H	-2.59931700	5.92229100	0.70245300	H	-0.08763600	2.54011400	-3.47172100
H	-4.33858900	5.61707400	0.76078600	C	-3.19561400	3.72333000	-1.46719400
C	-5.93032100	2.08959200	-0.79996600	H	-2.47198800	2.43460500	0.11000900
H	-6.99167300	2.25290000	-1.02093600	C	-2.97001800	4.20773000	-2.75977900
H	-5.35845600	2.34710700	-1.69671400	H	-1.67453500	4.15909700	-4.48584900
H	-5.78523300	1.02160800	-0.59543800	H	-4.06739300	4.05081800	-0.90761900
C	-6.29131100	2.53350400	1.65694700	H	-3.66558300	4.91462000	-3.20432400
H	-6.06943600	1.49769100	1.94538000	C	-1.90258300	-0.91425800	0.48355400
H	-6.05318600	3.18491900	2.50630100	C	-2.94214400	-0.52062600	1.00380600
H	-7.36795600	2.60447700	1.47185900	C	-4.12027000	-0.03570400	1.65218900
				C	-5.40847600	-0.37403100	1.18833000
				C	-4.01593500	0.80651600	2.78044200
				C	-6.54683800	0.11223500	1.82786700
				H	-5.50166000	-1.02001900	0.31981300
				C	-5.15878800	1.28774600	3.41547000
				H	-3.02787600	1.07239600	3.14439100
				C	-6.42907000	0.94443700	2.94422200
26							
C	4.67698100	1.36668900	1.63798100				
C	4.81936300	1.77471900	0.17139300				
H	5.67753700	1.30845800	2.09831200				
H	4.09365100	2.11190300	2.18431400				
H	5.42050300	1.03540000	-0.36544000				

H	-7.53091800	-0.16005900	1.45382600	C	-2.40147500	-2.45486500	2.22643500
H	-5.05700700	1.93477300	4.28327300	H	-3.11271000	-2.66337600	3.04263000
H	-7.31853500	1.32166500	3.44210700	H	-2.95088500	-2.32393700	1.29289600
C	-1.05993800	-3.46488600	-2.46989000	H	-1.72970000	-3.30078600	2.08731600
C	-0.29037000	-4.20226300	-1.37188900	C	2.33785900	-2.46224000	2.03441000
H	-2.13246200	-3.51102600	-2.26227300	H	2.98152700	-1.97683800	1.30112700
H	-0.90529700	-3.99312000	-3.42681700	H	2.94314200	-2.77099600	2.90066700
H	-0.54970000	-5.27499700	-1.41143600	H	1.86704100	-3.32666700	1.56615700
H	0.78546900	-4.11566500	-1.54836400	C	1.93838300	-0.29049500	3.01445800
Cu	-0.20983500	-1.38576900	-0.28256100	H	2.50795100	-0.54498500	3.92189700
C	-1.78711000	-1.22963100	-3.07957700	H	2.61489800	0.10656400	2.25810800
H	-1.46596200	-0.18788400	-3.14929700	H	1.20337200	0.48482200	3.23476500
H	-2.12619600	-1.56113600	-4.07715200	Cl	-0.12720600	-3.14386800	-0.15459600
H	-2.62254000	-1.27538000	-2.37680900	C	-1.30154300	0.27825900	-0.28454800
C	0.50219400	-1.87812600	-3.44205400	C	-2.21132500	-0.33163800	-0.86344900
H	0.82380200	-0.83409100	-3.41057200	C	-3.25458500	-1.04680700	-1.52128000
H	1.33120100	-2.48775400	-3.07891600	C	-4.58819400	-0.58758900	-1.45738700
H	0.27872000	-2.15624800	-4.48787900	C	-2.96470100	-2.21855300	-2.25384600
C	-1.93771500	-3.96020700	0.41351300	C	-5.60057900	-1.27177100	-2.12489200
H	-2.11083900	-5.04957700	0.42270300	H	-4.81421400	0.30884400	-0.88683200
H	-2.09043100	-3.55711800	1.41497800	C	-3.98908300	-2.90323900	-2.90226500
H	-2.66508800	-3.47846800	-0.23740300	H	-1.94403600	-2.58592000	-2.26595300
C	0.37016800	-4.25551600	0.95885800	C	-5.30413100	-2.43133400	-2.84722300
H	0.19463500	-3.80070700	1.93759100	H	-6.62256800	-0.90557100	-2.07601700
H	0.21192600	-5.34383300	1.04184800	H	-3.75999700	-3.81054100	-3.45448200
H	1.39975700	-4.05863200	0.66150900	H	-6.09701200	-2.96806400	-3.36143100
N	-0.67314200	-2.04726400	-2.57813400	C	1.49992900	0.29241000	-0.21255400
N	-0.55920100	-3.66130500	-0.02159400	C	2.40052300	-0.35205900	-0.76103500
Cl	2.17670400	-1.79323800	-0.42627700	C	3.41442500	-1.13706300	-1.39086500
27							
C	0.43028500	-2.16148100	3.48614500	C	4.74615000	-0.67713800	-1.46359000
C	-0.83759100	-1.36169800	3.74813400	C	3.09046700	-2.38935000	-1.95664100
H	0.99429800	-2.28760400	4.42390300	C	5.72242200	-1.43983300	-2.10001000
H	0.18435400	-3.15761200	3.10990400	H	5.00203200	0.28141200	-1.02047500
H	-0.58896200	-0.35714800	4.10007900	C	4.07838000	-3.14836800	-2.57966400
H	-1.42475300	-1.85172500	4.54247300	H	2.07052300	-2.75243000	-1.86959000
Cu	-0.05984300	-0.97003500	0.90184600	C	5.39227700	-2.67715500	-2.65985900
N	1.28953100	-1.50845700	2.46648400	H	6.74347900	-1.07126000	-2.15505300
N	-1.64379600	-1.21865300	2.51683100	H	3.82042300	-4.11430500	-3.00579700
C	-2.59705000	-0.09927500	2.67463500	H	6.15650400	-3.27278900	-3.15221000
H	-3.20473500	-0.02311900	1.77246200	C	-0.42841600	4.51048600	-1.30605000
H	-3.25759000	-0.28042600	3.53850900	C	0.75630500	4.55997500	-0.34860400
H	-2.05005900	0.83590700	2.80711200	H	-0.07461300	4.50192300	-2.34091100
				H	-1.02967200	5.42449800	-1.19064500
				H	1.38100900	5.43819000	-0.58431100

H	0.40797800	4.64852500	0.68332400
Cu	0.09347100	1.72947000	-0.06308200
C	-1.81462100	2.82750400	-2.37324300
H	-2.43906900	1.95155300	-2.19820100
H	-2.41909500	3.60875000	-2.86241600
H	-1.00049800	2.53667000	-3.04309700
C	-2.37522300	3.59334700	-0.15700900
H	-2.92577800	2.66979500	0.03116100
H	-1.97745900	3.94123600	0.79658200
H	-3.05630100	4.34689600	-0.58628900
C	2.20408000	3.14965300	-1.74002000
H	2.83980900	4.01664400	-1.98161500
H	2.81344500	2.24598000	-1.71902500
H	1.45662000	3.02747400	-2.52586900
C	2.60709600	3.34263200	0.62426300
H	3.16267800	2.40398400	0.58313800
H	3.29822900	4.18470100	0.45953600
H	2.13015900	3.42979100	1.60106300
N	-1.26560100	3.30362200	-1.08905500
N	1.56144600	3.31917200	-0.42076700
Cl	-0.24729000	2.55473000	2.30519200

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C	0.49125200	-2.38390200	3.41128400
C	-0.80646800	-1.64696500	3.71226600
H	1.02974200	-2.59055000	4.35063400
H	0.28082400	-3.34175800	2.92928000
H	-0.59645200	-0.66761200	4.15023700
H	-1.39418000	-2.21714500	4.45004500
Cu	-0.03989700	-0.93972700	0.97574300
N	1.35601200	-1.60850800	2.48864700
N	-1.60224100	-1.42619600	2.48094900
C	-2.59257900	-0.35224400	2.71844500
H	-3.19752700	-0.22763300	1.81954500
H	-3.25150100	-0.62368400	3.55879900
H	-2.07771900	0.58612300	2.92963100
C	-2.32758500	-2.65411000	2.08691700
H	-3.04962800	-2.92958600	2.87276200
H	-2.85929000	-2.46547100	1.15341000
H	-1.63451200	-3.47179400	1.89960700
C	2.41242900	-2.48841300	1.94381000
H	3.04969200	-1.90594700	1.27702100
H	3.02445300	-2.89793400	2.76284600
H	1.94863700	-3.28904800	1.36650600

C	1.98644300	-0.45992300	3.17747700
H	2.57040200	-0.80749500	4.04488500
H	2.65424300	0.03905900	2.47373100
H	1.24000100	0.26983100	3.49196200
Cl	-0.07076200	-3.17392500	-0.24166700
C	-1.23629100	0.13276200	-0.18674000
C	-2.20407100	-0.24330900	-0.84615500
C	-3.28464800	-0.77679300	-1.61023900
C	-4.52806900	-0.11864300	-1.70206800
C	-3.10175400	-2.00339100	-2.28652300
C	-5.55757100	-0.66497000	-2.46543100
H	-4.67721500	0.81792600	-1.17183500
C	-4.14232500	-2.54169700	-3.03941100
H	-2.15109600	-2.51854500	-2.18097100
C	-5.36789600	-1.87556400	-3.13705500
H	-6.51090900	-0.14742500	-2.53263300
H	-3.99583000	-3.48856300	-3.55215800
H	-6.17365300	-2.30031700	-3.72982500
C	1.30869200	0.02635700	-0.13232200
C	2.25600700	-0.36930700	-0.81042700
C	3.29719200	-0.94903000	-1.59583500
C	4.58189600	-0.37489000	-1.67879800
C	3.02898000	-2.14194700	-2.30315400
C	5.56847200	-0.96884000	-2.46309000
H	4.79934300	0.53337200	-1.12326000
C	4.02582600	-2.72768400	-3.07917200
H	2.04688900	-2.59553100	-2.20300100
C	5.29352500	-2.14408600	-3.16703100
H	6.55478500	-0.51603000	-2.52170700
H	3.81251300	-3.64796900	-3.61631000
H	6.06562300	-2.60601000	-3.77654800
C	-0.34840400	4.42477700	-0.99089900
C	0.84497600	4.36333600	-0.04465200
H	-0.00431600	4.48820000	-2.02693800
H	-0.91747800	5.34543400	-0.79611900
H	1.50240900	5.22963900	-0.22861800
H	0.50909300	4.39613600	0.99451300
Cu	0.07919700	1.57398400	0.07914100
C	-1.76373600	2.84786000	-2.17791000
H	-2.38796200	1.96100800	-2.06945700
H	-2.36742700	3.66008600	-2.61430800
H	-0.94531800	2.60656100	-2.86202500
C	-2.33956500	3.49383400	0.07132000
H	-2.91716800	2.57541600	0.19431300

H	-1.94751500	3.77391600	1.04932800
H	-2.99505600	4.28915500	-0.32026400
C	2.22683100	2.99508800	-1.54080000
H	2.91716600	3.83496400	-1.71820300
H	2.77884300	2.05679400	-1.60209300
H	1.46906500	2.98674500	-2.32589300
C	2.65935900	3.01941500	0.82503200
H	3.17983100	2.06538300	0.71892100
H	3.38114600	3.84280500	0.70505200
H	2.19541700	3.06529700	1.81101600
N	-1.22412500	3.23253200	-0.86114400
N	1.60398900	3.09933400	-0.20680900
Cl	-0.24212200	2.28288200	2.47296000

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C	-1.87189500	-0.33991100	0.14138800
C	-3.08996400	-0.45805600	0.13955000
C	-4.50953600	-0.63023000	0.15422800
C	-5.37979000	0.47657800	0.21760000
C	-5.06848900	-1.92376000	0.10180400
C	-6.76092200	0.29462300	0.22635600
H	-4.95981700	1.47776600	0.25843400
C	-6.45022900	-2.09840600	0.11179100
H	-4.40335600	-2.78021100	0.05053400
C	-7.30223600	-0.99232500	0.17406500
H	-7.41731600	1.15977200	0.27423600
H	-6.86430800	-3.10243500	0.06959000
H	-8.37984000	-1.13217300	0.18138100
C	1.89266300	-0.35068200	0.12230600
C	3.10913900	-0.47922800	0.10961000
C	4.52948800	-0.63497900	0.13764600
C	5.10459000	-1.87144500	0.49699100
C	5.38666900	0.43512500	-0.19011300
C	6.48835800	-2.02646100	0.52650400
H	4.45061500	-2.70139100	0.74619100
C	6.76978400	0.27231200	-0.16039800
H	4.95446100	1.39147700	-0.47091200
C	7.32696500	-0.95753400	0.19890100
H	6.91471700	-2.98687600	0.80432400
H	7.41535900	1.10788300	-0.41860200
H	8.40617200	-1.08245900	0.22196200
C	0.12963900	2.75555500	-0.65722300
C	-0.57800200	2.53914000	0.68630700
H	1.19794800	2.91865600	-0.49109200

H	-0.26523500	3.68420500	-1.10515300
H	-0.51470600	3.46276400	1.28207700
H	-1.63271500	2.30919800	0.52377600
Cu	0.01519400	-0.23680900	0.08769500
C	1.09349800	1.48983500	-2.50516000
H	0.95508800	0.58426500	-3.10141300
H	1.15307000	2.35790400	-3.18467200
H	2.02988300	1.38668200	-1.95439000
C	-1.29686000	1.66019000	-2.29857300
H	-1.41679100	0.73473300	-2.86659000
H	-2.13826200	1.72992300	-1.60858000
H	-1.32098100	2.51731500	-2.99449800
C	1.32213400	1.78177200	2.02977200
H	1.21328200	2.65961700	2.68352100
H	1.71675400	0.94392000	2.60417000
H	2.02785400	1.99402900	1.23114800
C	-0.89463500	1.09414700	2.62797200
H	-0.47221100	0.24836000	3.17533300
H	-0.96011900	1.96072700	3.30177500
H	-1.88246100	0.82121000	2.26244700
N	-0.02660800	1.61159700	-1.56160200
N	-0.00703600	1.41595300	1.48048500
Cl	0.01679900	-2.12987200	-1.04695800

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C	1.26510000	-4.20620700	-0.80117500
C	2.18517300	-3.32545600	-1.63604800
H	1.00769000	-5.11437400	-1.36286100
H	1.77226200	-4.53351700	0.10988500
H	1.71303700	-3.06911500	-2.58831700
H	3.12241300	-3.85936500	-1.85281600
Cu	0.56907200	-1.33245000	-0.42620700
N	0.03423800	-3.46528700	-0.41284200
N	2.47410900	-2.04180400	-0.93815400
C	3.23105500	-1.15159800	-1.85484000
H	3.41687600	-0.20246300	-1.35148700
H	4.18871600	-1.61773300	-2.12623600
H	2.63427900	-0.96613100	-2.74776900
C	3.28124500	-2.25788600	0.28896200
H	4.21292900	-2.79013900	0.04900700
H	3.52650300	-1.29032000	0.72734200
H	2.72328800	-2.83628900	1.02761600
C	-0.46181000	-3.92842300	0.90304800
H	-1.36099100	-3.36968300	1.16345700

H	-0.69488300	-5.00282700	0.87651400	H	1.89041600	2.30961200	-2.26785900
H	0.29450800	-3.74704100	1.67137600	H	0.67673400	2.06691500	-3.52539100
C	-1.03043900	-3.64200100	-1.43043300	H	1.33806300	3.70990200	-3.23683300
H	-1.33248000	-4.69826600	-1.48430000	C	-3.27570900	2.19305300	-0.62760600
H	-1.88938000	-3.03000700	-1.15154700	H	-4.20664900	2.58885700	-1.05844400
H	-0.67861900	-3.30425700	-2.40567600	H	-3.52232600	1.48056200	0.15972500
C	1.13140100	0.80205400	0.05989600	H	-2.71505400	3.01608300	-0.18043300
C	2.03593200	1.02142500	0.87550500	C	-3.23198800	0.32369800	-2.15372200
C	3.07745100	1.26309400	1.81889400	H	-3.41525800	-0.34675800	-1.31376500
C	4.35374200	1.69431600	1.39313800	H	-4.19072200	0.64460500	-2.58484800
C	2.84454100	1.08159300	3.20066100	H	-2.63841700	-0.20235500	-2.90121300
C	5.36174300	1.93489000	2.32249400	N	-0.02876600	3.01126600	-1.76029900
H	4.53786900	1.84311700	0.33313400	N	-2.47192900	1.50402500	-1.66869600
C	3.85911500	1.32202300	4.12204300	Cl	-0.00321200	-0.60015000	-2.88054100
H	1.86366400	0.75352900	3.53095700				
C	5.11796400	1.74875100	3.68659500	29b			
H	6.33834100	2.26938800	1.98497800	C	0.29946600	-4.25374000	-1.27914400
H	3.67036400	1.17955000	5.18208100	C	1.18868300	-3.59632900	-2.32370200
H	5.90660400	1.93757600	4.40909500	H	-0.18351400	-5.14740900	-1.69601600
C	-1.12885200	-0.71462200	0.37450500	H	0.89257300	-4.58190500	-0.42152500
C	-2.03593800	-0.59090700	1.20762700	H	0.60292100	-3.31244700	-3.20293900
C	-3.08134600	-0.43534800	2.16471400	H	1.96395900	-4.29611600	-2.66323100
C	-4.35492900	-1.00557200	1.94367400	Cu	0.26314400	-1.39606500	-0.69778900
C	-2.85485500	0.28592900	3.35839200	N	-0.72521600	-3.28764700	-0.78676900
C	-5.36634600	-0.85713900	2.88836900	N	1.81119300	-2.35729300	-1.77093000
H	-4.53396900	-1.56803600	1.03197000	C	2.30299900	-1.49858300	-2.87934500
C	-3.87282300	0.43123600	4.29580500	H	2.74366100	-0.59300500	-2.46024100
H	-1.87603600	0.72213700	3.53306600	H	3.05867800	-2.02852800	-3.47419100
C	-5.12883100	-0.13901000	4.06423300	H	1.47026700	-1.22388200	-3.53262600
H	-6.34072700	-1.30254500	2.71028500	C	2.95672400	-2.69987200	-0.88532500
H	-3.68879200	0.98724400	5.21046700	H	3.72196700	-3.24796300	-1.45049500
H	-5.92010600	-0.02526500	4.79944700	H	3.39137900	-1.78332700	-0.48781700
C	-1.25876500	3.53996000	-2.40919400	H	2.62530300	-3.31729400	-0.04822400
C	-2.18397600	2.40255500	-2.82083300	C	-1.21472700	-3.70617900	0.55290700
H	-1.76143000	4.20496400	-1.70246800	H	-1.97983900	-3.00879400	0.89452700
H	-1.00128300	4.14771100	-3.28725500	H	-1.64404900	-4.71582400	0.50720900
H	-3.12135800	2.80862600	-3.22930200	H	-0.38732800	-3.70500300	1.26727900
H	-1.71533400	1.78675700	-3.59327500	C	-1.87517300	-3.22209300	-1.72650400
Cu	-0.56661900	1.05294700	-0.92074800	H	-2.38124900	-4.19515100	-1.77962300
C	0.47273300	3.95994600	-0.74027200	H	-2.57753700	-2.46519800	-1.37737000
H	1.37117600	3.54833800	-0.28019900	H	-1.53520800	-2.94890900	-2.72802100
H	0.70860300	4.93320000	-1.19467300	C	1.33303000	0.30047200	-0.13443600
H	-0.28149300	4.10393500	0.03794000	C	2.24309800	0.30517500	0.71762200
C	1.03288500	2.76375400	-2.76619200	C	3.29572800	0.31802100	1.66451500

C	4.61787900	0.63690800	1.26531300	H	-3.05794200	2.02362400	-3.47674100
C	3.03550900	0.02015300	3.02535400	H	-1.46912200	1.21970100	-3.53386700
C	5.64320000	0.65531000	2.20259200	N	0.72471300	3.28689600	-0.78965800
H	4.82084400	0.86914600	0.22408500	N	-1.81116400	2.35474600	-1.77343200
C	4.07000600	0.03976500	3.95213200				
H	2.02224800	-0.22059300	3.33189700	29-SD			
C	5.37185800	0.35692300	3.54371700	C	-0.31291900	4.00051800	-1.69005900
H	6.65448300	0.90175600	1.89466400	C	0.95519200	4.05356400	-0.85007200
H	3.86875400	-0.18894600	4.99400100	H	-0.84254800	4.96054400	-1.62731400
H	6.17663300	0.37247700	4.27254700	H	-0.06707900	3.84536700	-2.74361000
C	-1.33283800	-0.30084500	-0.13397400	H	0.71438500	4.27641000	0.19290400
C	-2.24265900	-0.30428500	0.71835700	H	1.61912400	4.84773100	-1.22412900
C	-3.29533900	-0.31578600	1.66524400	Cu	0.09621100	1.39102800	-0.39738700
C	-4.61755200	-0.63481400	1.26630200	N	-1.20600900	2.88812600	-1.25228700
C	-3.03515700	-0.01658800	3.02581400	N	1.65741000	2.74254400	-0.86018900
C	-5.64295400	-0.65200300	2.20353100	C	2.74868600	2.76219400	0.14298900
H	-4.82050800	-0.86814900	0.22531000	H	3.24990200	1.79315500	0.13694100
C	-4.06973600	-0.03500500	3.95254500	H	3.47700500	3.54823100	-0.10299100
H	-2.02185200	0.22417300	3.33222500	H	2.32364500	2.93683400	1.13178200
C	-5.37163900	-0.35227500	3.54436300	C	2.23310300	2.42783400	-2.18864800
H	-6.65426700	-0.89858100	1.89581000	H	2.96215500	3.19491800	-2.48755100
H	-3.86851800	0.19470500	4.99420000	H	2.73444200	1.46020500	-2.13541100
H	-6.17646300	-0.36690700	4.27315500	H	1.45260500	2.36608500	-2.94920500
C	-0.30021700	4.25218600	-1.28306800	C	-1.98152400	2.38066900	-2.40736700
C	-1.18898000	3.59348800	-2.32721900	H	-2.64262100	1.57971500	-2.07701600
H	-0.89360200	4.58088800	-0.42585100	H	-2.58526900	3.18462900	-2.85206400
H	0.18249200	5.14565600	-1.70067400	H	-1.30306600	1.98168600	-3.16591000
H	-1.96440600	4.29268900	-2.66761200	C	-2.14695000	3.35855000	-0.20498100
H	-0.60283100	3.30904100	-3.20601300	H	-2.80900400	4.13598700	-0.61297900
Cu	-0.26298000	1.39514400	-0.69909700	H	-2.74562000	2.51306100	0.13720000
C	1.21364500	3.70656100	0.54988200	H	-1.59398400	3.74560700	0.65057300
H	1.97883800	3.00964900	0.89229400	C	1.21550200	-0.23207800	-0.08098100
H	1.64270400	4.71628800	0.50360100	C	2.11659800	-0.81682700	-0.68485000
H	0.38601900	3.70569500	1.26398900	C	3.17549700	-1.48898200	-1.36434200
C	1.87496100	3.22114100	-1.72903300	C	4.52303700	-1.26621700	-1.00635700
H	2.57747500	2.46469500	-1.37926200	C	2.88665900	-2.39360300	-2.40921300
H	1.53537800	2.94726300	-2.73049500	C	5.54736000	-1.93022500	-1.67595800
H	2.38072700	4.19433900	-1.78257700	H	4.75388400	-0.57360000	-0.20200600
C	-2.95720800	2.69769000	-0.88864000	C	3.91820400	-3.05130300	-3.07296800
H	-3.72259900	3.24461800	-1.45473900	H	1.85180100	-2.56866200	-2.68700600
H	-3.39143000	1.78135200	-0.49015200	C	5.24877900	-2.82264900	-2.70937300
H	-2.62643900	3.31633400	-0.05219000	H	6.58038600	-1.75201300	-1.39194600
C	-2.30218600	1.49465600	-2.88111800	H	3.68550700	-3.74506300	-3.87555000
H	-2.74256100	0.58931500	-2.46119500	H	6.05030800	-3.33875400	-3.22955400

C	-1.21699700	-0.07317200	-0.23609900	H	-2.96013500	4.02439800	-0.60512600
C	-2.11616100	-0.66055100	-0.84032300	H	-2.49668500	2.37435200	-3.15314900
C	-3.17256000	-1.32156600	-1.53443700	H	-4.06756100	2.87750400	-2.51065100
C	-4.52136000	-0.97536200	-1.30104200	Cu	-1.08260100	1.22506800	-0.68505000
C	-2.87994300	-2.33597500	-2.47187800	N	-1.00739000	3.39301900	-1.04024000
C	-5.54320800	-1.62672600	-1.98666300	N	-3.04788800	1.35104200	-1.41695700
H	-4.75520600	-0.19428600	-0.58325900	C	-3.44570100	0.20377000	-2.26680700
C	-3.90902000	-2.98175800	-3.15098900	H	-3.42154500	-0.70927200	-1.66797200
H	-1.84411900	-2.60466700	-2.65520000	H	-4.46132300	0.34815700	-2.66308200
C	-5.24089300	-2.63007700	-2.91150300	H	-2.73512400	0.09428700	-3.08640300
H	-6.57723300	-1.35191500	-1.80002100	C	-3.99090300	1.45749900	-0.27586700
H	-3.67337100	-3.76108000	-3.86982000	H	-5.01490700	1.64675800	-0.63129000
H	-6.04049500	-3.13619600	-3.44430500	H	-3.97932200	0.52419900	0.29047400
C	0.30770800	-1.81798500	3.94316400	H	-3.69597300	2.26607800	0.39564000
C	-0.95626600	-0.97395500	4.02408100	C	-0.61334600	4.17222000	0.15159700
H	0.05608500	-2.86487900	3.75584700	H	0.37657300	3.84883600	0.47859000
H	0.83862400	-1.78758800	4.90403600	H	-0.58800500	5.25013900	-0.06821700
H	-1.62129300	-1.36995000	4.80660900	H	-1.32098900	3.99030800	0.96440800
H	-0.71038800	0.06024400	4.27959200	C	-0.01583800	3.60498000	-2.11879000
Cu	-0.09815000	-0.43950400	1.37666600	H	0.04965100	4.67211800	-2.38100100
C	1.96878100	-2.49316700	2.29738600	H	0.96078400	3.25671000	-1.77746900
H	2.62807000	-2.14129500	1.50416200	H	-0.28518600	3.02762900	-3.00449900
H	2.57349100	-2.96577300	3.08452300	C	-0.34972600	-0.86899100	0.55322000
H	1.28491900	-3.23579100	1.87813800	C	-1.36415800	-1.21607600	1.20597200
C	2.14980400	-0.32422400	3.34458200	C	-2.45496300	-1.55621000	2.03659700
H	2.75170000	0.03719300	2.50947200	C	-3.68156600	-2.01612300	1.49399900
H	1.60311400	0.52420000	3.75562300	C	-2.33495900	-1.46232100	3.44654300
H	2.80833100	-0.75915900	4.11034600	C	-4.74248000	-2.35231600	2.32790800
C	-2.24244200	-2.25407700	2.35801800	H	-3.77633100	-2.12162100	0.41702100
H	-2.97298900	-2.57285400	3.11561800	C	-3.40172100	-1.80456000	4.26939600
H	-2.74362500	-2.16793700	1.39266400	H	-1.39760000	-1.11813000	3.87225300
H	-1.46631200	-3.01674000	2.27211500	C	-4.60887200	-2.24727300	3.71667200
C	-2.74648700	0.06775500	2.76684200	H	-5.67488100	-2.70625400	1.89729000
H	-3.24850800	0.09480500	1.79860500	H	-3.29507200	-1.72691500	5.34758700
H	-3.47513500	-0.19999800	3.54539500	H	-5.43843300	-2.51422900	4.36456900
H	-2.31685800	1.04848400	2.97263600	C	0.34961900	0.86925100	0.55471200
N	1.20142400	-1.35042100	2.84354100	C	1.36440700	1.21511100	1.20746200
N	-1.65969900	-0.93917800	2.71401100	C	2.45570700	1.55376400	2.03804700
Cl	0.00532500	2.08869300	2.15727400	C	3.68199900	2.01453200	1.49554500
30-ts				C	2.33650700	1.45738600	3.44786900
C	-2.37485100	3.75385700	-1.48823200	C	4.74342300	2.34919700	2.32942100
C	-3.04086400	2.59656500	-2.23064300	H	3.77613900	2.12191500	0.41870400
H	-2.35356100	4.64135300	-2.13787000	C	3.40377200	1.79808600	4.27071500
				H	1.39936400	1.11254100	3.87351900

C	4.61062500	2.24170500	3.71807100	H	2.48210600	-2.14651000	1.70829800
H	5.67559400	2.70384400	1.89888900	C	2.98055000	-1.92583600	-1.61862600
H	3.29774700	1.71854400	5.34883000	H	3.87021300	-2.56812200	-1.69585700
H	5.44057800	2.50747100	4.36595700	H	2.09546600	-2.51046800	-1.87903400
C	2.37391900	-3.75213700	-1.49299200	H	3.07085900	-1.10709100	-2.33546100
C	3.03998700	-2.59417700	-2.23431300	C	2.29111000	2.57399500	-1.11505800
H	2.95941000	-4.02380600	-0.61037500	H	1.34413100	3.04671600	-0.84503600
H	2.35220400	-4.63888600	-2.14363100	H	3.07889000	3.34161100	-1.12407700
H	4.06658300	-2.87499900	-2.51481100	H	2.19552100	2.14501800	-2.11542800
H	2.49567200	-2.37087700	-3.15647700	C	2.63813200	2.08252400	1.22773500
Cu	1.08226300	-1.22378900	-0.68716400	H	3.39248600	2.88057100	1.29065500
C	0.61283300	-4.17184700	0.14694700	H	1.65599300	2.49005400	1.47435400
H	-0.37685400	-3.84849200	0.47468200	H	2.86740800	1.30989600	1.96282700
H	0.58702800	-5.24951400	-0.07405700	C	-4.00031300	-0.48130400	-0.53467300
H	1.32085700	-3.99109700	0.95968200	C	-3.85774600	0.84590700	0.20770800
C	0.01473500	-3.60206000	-2.12263900	H	-4.03086100	-0.31017500	-1.61471700
H	-0.96173000	-3.25409700	-1.78055900	H	-4.94974600	-0.96238000	-0.25824300
H	0.28382800	-3.02369000	-3.00776400	H	-4.71230500	1.49829900	-0.02534600
H	-0.05094700	-4.66888400	-2.38607900	H	-3.86614100	0.67598000	1.28801700
C	3.99039700	-1.45747700	-0.27831700	Cu	-1.16758300	-0.08339400	-0.15343200
H	5.01433300	-1.64671200	-0.63394000	C	-2.69875300	-2.39090300	-1.32340300
H	3.97912900	-0.52477000	0.28900000	H	-1.84643500	-3.03422300	-1.09311900
H	3.69518600	-2.26666300	0.39233100	H	-3.60005500	-3.01494400	-1.41148700
C	3.44560200	-0.20148300	-2.26796800	H	-2.51349400	-1.89070800	-2.27729400
H	3.42221500	0.71087100	-1.66806500	C	-3.02088700	-2.07326500	1.05345100
H	4.46100200	-0.34602500	-2.66474700	H	-2.12762300	-2.66219200	1.26797400
H	2.73480500	-0.09062300	-3.08718700	H	-3.13812200	-1.34619900	1.85819400
N	1.00667700	-3.39146600	-1.04417700	H	-3.89986800	-2.73365800	1.02750200
N	3.04741400	-1.34951500	-1.41930800	C	-2.64518400	2.19077700	-1.44721600
Cl	0.00000400	0.00174400	-2.60004500	H	-3.39673900	2.99407100	-1.43917500
				H	-1.66800200	2.61669900	-1.68411900
				H	-2.90118300	1.47400600	-2.22991600
31				C	-2.22134000	2.50861300	0.91522500
C	3.88477900	0.84235100	-0.48257400	H	-1.28987900	3.00599600	0.63538400
C	3.98142400	-0.54599300	0.14709500	H	-3.00927900	3.26828600	1.02323200
H	4.73773800	1.45699400	-0.15922000	H	-2.06767700	1.99818800	1.86823300
H	3.93901500	0.76784000	-1.57243700	N	-2.85228900	-1.38341300	-0.24936200
H	3.97922700	-0.46802800	1.23787500	N	-2.57569900	1.52044500	-0.12926300
H	4.93108600	-1.01976700	-0.14259200	Cl	0.00021100	-0.37093400	1.99105100
Cu	1.16429200	-0.08448200	-0.15025300				
N	2.59944300	1.50680600	-0.13830600				
N	2.82846700	-1.40090400	-0.24169800	32			
C	2.67812600	-2.53066200	0.70578000	C	0.28398600	4.31189400	-0.54359200
H	1.82730100	-3.14377300	0.40058600	C	-0.97606200	3.92533900	-1.30352900
H	3.58295600	-3.15546300	0.71614700	H	0.81278000	5.11191600	-1.07865800

H	0.02765200	4.70829900	0.44219600	C	5.24607900	-0.80093000	3.83156700
H	-0.72755300	3.59411200	-2.31516600	H	6.57730300	-0.23017000	2.23242400
H	-1.64611600	4.79493000	-1.38445800	H	3.68313200	-1.32145800	5.22469100
Cu	-0.10632900	1.40174600	-0.35322700	H	6.04742500	-0.97212700	4.54425200
N	1.18332000	3.13578500	-0.35247600	C	-0.28762500	-3.55045700	-2.50718100
N	-1.67365000	2.79338900	-0.63742900	C	0.97464100	-2.85384300	-2.99600700
C	-2.76053500	2.30176600	-1.51733100	H	-0.03323100	-4.36164300	-1.82013100
H	-3.25726300	1.46256100	-1.02860100	H	-0.81473800	-4.00746400	-3.35523400
H	-3.49374500	3.10080700	-1.69903200	H	1.64431300	-3.58478500	-3.47435300
H	-2.33255800	1.96095900	-2.46060100	H	0.72725700	-2.08647500	-3.73458000
C	-2.25437400	3.18528800	0.66829700	Cu	0.10364600	-1.07092900	-0.97333300
H	-2.98251800	3.99939300	0.54126400	C	-1.95414200	-3.31914200	-0.74930600
H	-2.75785000	2.32116600	1.10493300	H	-2.61971700	-2.62127200	-0.24181300
H	-1.47657000	3.51185100	1.36080700	H	-2.55252300	-4.12628000	-1.19557800
C	1.94244900	3.28398600	0.91056700	H	-1.27050200	-3.74773400	-0.01170100
H	2.60860200	2.43081100	1.03764200	C	-2.13456100	-1.96501900	-2.74166800
H	2.53968900	4.20696100	0.89790300	H	-2.74159600	-1.23792300	-2.20036100
H	1.25264700	3.31706400	1.75797600	H	-1.58768200	-1.43212000	-3.51909100
C	2.13885800	3.02103500	-1.48258900	H	-2.78805400	-2.72699600	-3.19075500
H	2.79171400	3.90523600	-1.51741100	C	2.25385700	-3.12484300	-0.90751400
H	2.74581000	2.12558200	-1.34128200	H	2.98345100	-3.78224600	-1.40223700
H	1.59823400	2.91444800	-2.42239900	H	2.75594700	-2.56435000	-0.11744400
C	-1.21550700	-0.16829300	0.18407100	H	1.47685200	-3.73881100	-0.44842500
C	-2.11567500	-0.37328500	1.00040400	C	2.75870800	-1.31792100	-2.42086100
C	-3.17112300	-0.61657100	1.92854900	H	3.25396700	-0.80680000	-1.59402900
C	-4.52059200	-0.59703600	1.51400100	H	3.49240500	-1.93782900	-2.95568500
C	-2.87628900	-0.88538200	3.28303300	H	2.33003400	-0.57424700	-3.09322000
C	-5.54087300	-0.83879900	2.42996500	N	-1.18680800	-2.59929900	-1.79169700
H	-4.75612000	-0.39501400	0.47305200	N	1.67194700	-2.16679600	-1.87618600
C	-3.90377200	-1.12488500	4.19085800	Cl	0.00053100	0.72869400	-2.91316800
H	-1.83971800	-0.90273300	3.60542900				
C	-5.23644800	-1.10225200	3.76841800	32b			
H	-6.57554300	-0.82238900	2.10020100	C	-0.32813400	-4.03133800	-1.71861700
H	-3.66646000	-1.33092000	5.23048400	C	0.93881900	-3.53430000	-2.39514100
H	-6.03512500	-1.29028600	4.47990500	H	-0.86784900	-4.72062200	-2.38126400
C	1.21355300	0.06313400	0.24225800	H	-0.08698000	-4.58631600	-0.80857500
C	2.11477400	-0.13783800	1.05832200	H	0.70366500	-3.05004000	-3.34765800
C	3.17322100	-0.35964900	1.98868300	H	1.60738100	-4.37669100	-2.61799300
C	4.52063500	-0.16425300	1.61382600	Cu	0.10260000	-1.33229100	-0.71887300
C	2.88464300	-0.77994200	3.30537200	N	-1.20595100	-2.88594700	-1.33488100
C	5.54453300	-0.38397900	2.53128500	N	1.63473300	-2.53091700	-1.53675300
H	4.75169500	0.16121000	0.60352400	C	2.62317900	-1.78066700	-2.35290100
C	3.91586800	-0.99776900	4.21441100	H	3.12276600	-1.04484500	-1.72228300
H	1.85003600	-0.93038800	3.59829200	H	3.37284400	-2.46343000	-2.77383100

H	2.11362200	-1.26795700	-3.17301700	H	-0.69996300	3.12543500	-3.27714700
C	2.34872200	-3.19547900	-0.41171100	Cu	-0.10317000	1.35325000	-0.68826100
H	3.11110800	-3.88441900	-0.79820000	C	2.14574600	3.32785400	-0.19160000
H	2.83197900	-2.43756000	0.20611900	H	2.80433700	2.49609900	0.05698400
H	1.64930900	-3.75676400	0.21116500	H	2.75353400	4.18078700	-0.52075100
C	-2.14512800	-3.31819300	-0.26744700	H	1.58393900	3.61317000	0.70103000
H	-2.80317100	-2.49155900	-0.00134900	C	1.99132700	2.46876000	-2.44905200
H	-2.75352600	-4.16342900	-0.61487300	H	2.59916000	1.60831100	-2.16516300
H	-1.58384400	-3.62325300	0.61890700	H	1.32527100	2.17934800	-3.26569600
C	-1.98946100	-2.40873200	-2.50521000	H	2.65018700	3.27304400	-2.80234700
H	-2.65210300	-3.20263300	-2.87445500	C	-2.35613600	3.20612900	-0.34532700
H	-2.59316000	-1.55150400	-2.20339200	H	-3.12188000	3.89691300	-0.72179800
H	-1.32263800	-2.10573800	-3.31627000	H	-2.83592500	2.43368000	0.25701900
C	1.22523100	0.10818000	0.03037300	H	-1.66266200	3.76103900	0.28977400
C	2.12358000	0.09889000	0.88107900	C	-2.61805200	1.83082600	-2.31561400
C	3.17299000	0.09777600	1.84016600	H	-3.11753800	1.08078800	-1.70190100
C	4.52636300	0.13338800	1.43288800	H	-3.36819000	2.51981400	-2.72544600
C	2.86452300	0.06564000	3.21937200	H	-2.10421300	1.33638400	-3.14432300
C	5.54042700	0.13656100	2.38520200	N	1.20702200	2.91830200	-1.26824500
H	4.77076500	0.16147900	0.37477000	N	-1.63480800	2.56700000	-1.48035900
C	3.88836200	0.06833500	4.16072000				
H	1.82594100	0.03944000	3.53426200	33-ts			
C	5.22431400	0.10392500	3.74735200	C	-0.30992300	-1.18482700	4.23230200
H	6.57825200	0.16511800	2.06811900	C	0.98085600	-1.86688800	3.78979600
H	3.64741100	0.04367100	5.21888400	H	-0.80973300	-1.79778400	4.99543800
H	6.01927200	0.10698000	4.48678700	H	-0.08786800	-0.22117400	4.69842700
C	-1.22597000	-0.10440900	0.02803100	H	0.76316800	-2.85018000	3.36353000
C	-2.12413100	-0.11641800	0.87892600	H	1.63937500	-2.01545800	4.65945600
C	-3.17328100	-0.14166800	1.83790400	Cu	0.09261900	-0.64948800	1.37892200
C	-4.52680900	-0.16685600	1.43053300	N	-1.22246200	-0.94108200	3.08020600
C	-2.86410000	-0.14730500	3.21731600	N	1.67299500	-1.07961900	2.73726000
C	-5.54037300	-0.19702900	2.38296200	C	2.74811200	-1.89264600	2.12471300
H	-4.77186900	-0.16536000	0.37220600	H	3.22692700	-1.30626600	1.33712400
C	-3.88737800	-0.17636100	4.15880000	H	3.50263600	-2.16870400	2.87596700
H	-1.82536100	-0.12929800	3.53222900	H	2.31400000	-2.78859200	1.67961500
C	-5.22356200	-0.20154500	3.74535700	C	2.26116600	0.16716700	3.27642200
H	-6.57835200	-0.21764500	2.06571700	H	3.01280900	-0.05591900	4.04817600
H	-3.64584600	-0.18043000	5.21711900	H	2.73852700	0.71519800	2.46198800
H	-6.01813900	-0.22539000	4.48484400	H	1.48994500	0.80721300	3.70946300
C	0.32765800	4.07149700	-1.62531300	C	-2.07630700	0.23698700	3.34606200
C	-0.93768300	3.58914200	-2.31516800	H	-2.73588600	0.40479700	2.49350000
H	0.08457300	4.60301600	-0.70186500	H	-2.68801600	0.08539900	4.24747500
H	0.86723200	4.77796200	-2.26976900	H	-1.45452600	1.12568500	3.48217000
H	-1.60604100	4.43591800	-2.52130400	C	-2.08746700	-2.12180300	2.84229400

H	-2.74188700	-2.29747300	3.70910200	C	-2.26928200	-0.42631100	-3.26109500
H	-2.69950300	-1.94287400	1.95643200	H	-3.02065500	-0.78827600	-3.97854700
H	-1.47822400	-3.00457700	2.65038000	H	-2.74943500	0.25678300	-2.55778200
C	1.00739900	0.29340800	-0.11707200	H	-1.50291900	0.12996400	-3.80431500
C	1.90732900	1.13676800	-0.20763400	C	-2.74540300	-2.24846000	-1.75914200
C	2.94837500	2.10059400	-0.31991800	H	-3.22449200	-1.53382000	-1.08613800
C	4.30616500	1.71139800	-0.29299300	H	-3.50001400	-2.65443100	-2.44880200
C	2.63315100	3.47031900	-0.46260900	H	-2.30869400	-3.05110400	-1.16399300
C	5.31319500	2.66581300	-0.40463500	N	1.21856700	-1.46182100	-2.87138900
H	4.55703800	0.66007700	-0.18559900	N	-1.67352500	-1.55286400	-2.50750600
C	3.64795400	4.41600600	-0.57300800	Cl	-0.00025300	-2.97305900	0.26179000
H	1.59125500	3.77476100	-0.48555200				
C	4.98810300	4.01818800	-0.54437600	34			
H	6.35376000	2.35555200	-0.38306900	C	-4.61764800	0.91543600	0.40774900
H	3.39498100	5.46652900	-0.68225600	C	-4.83752800	-0.42156800	-0.30578300
H	5.77661400	4.75982200	-0.63123600	H	-5.45121500	1.59690500	0.18047600
C	-1.01205600	0.30960600	0.05621500	H	-4.61250700	0.76402500	1.49120100
C	-1.90885700	1.15945200	0.00238200	H	-4.89266200	-0.26267300	-1.38717400
C	-2.94574700	2.13279100	-0.04908600	H	-5.81180900	-0.83330300	0.00334200
C	-4.30533600	1.74926900	-0.03568300	Cu	-1.95932600	0.00419100	0.00242900
C	-2.62418100	3.50698700	-0.11262300	N	-3.31811300	1.55175600	0.04262300
C	-5.30797200	2.71348400	-0.08571900	N	-3.73815100	-1.37307500	-0.04144000
H	-4.56110000	0.69491000	0.01617900	C	-3.65554500	-2.40204000	-1.09520500
C	-3.63462800	4.46243800	-0.16182900	H	-2.80129400	-3.05356500	-0.89451800
H	-1.58082900	3.80711400	-0.12199000	H	-4.56761400	-3.01835200	-1.13973800
C	-4.97663500	4.07008800	-0.14880200	H	-3.50440600	-1.92533800	-2.06772200
H	-6.35001600	2.40767800	-0.07471400	C	-3.88571800	-2.02383700	1.27502700
H	-3.37681400	5.51634600	-0.21022900	H	-4.79960800	-2.63794800	1.32123600
H	-5.76174900	4.81938300	-0.18708000	H	-3.02011100	-2.66495000	1.45961900
C	0.31004800	-1.91685200	-3.96113800	H	-3.92872000	-1.27621400	2.07137100
C	-0.97850000	-2.51298100	-3.40354900	C	-2.97190300	2.59043300	1.04336300
H	0.08514300	-1.05637700	-4.59698000	H	-2.02172200	3.05440500	0.76899300
H	0.81507200	-2.65668900	-4.59782400	H	-3.74691900	3.37035500	1.09044000
H	-1.63634300	-2.81571400	-4.23282400	H	-2.86729400	2.13302000	2.03004800
H	-0.75845800	-3.40453300	-2.80966900	C	-3.40170100	2.18645900	-1.29664800
Cu	-0.09736600	-0.87704200	-1.25313200	H	-4.17016000	2.97421400	-1.30942100
C	2.06357500	-0.34416700	-3.34627600	H	-2.43510000	2.62924700	-1.54724600
H	2.72157000	-0.01985800	-2.53888100	H	-3.64588600	1.44294400	-2.05773900
H	2.67709800	-0.65107000	-4.20597800	Cl	-0.00005300	-1.02827000	-0.00159200
H	1.43466100	0.50026400	-3.63990900	C	4.61776300	0.91613100	-0.40610100
C	2.09352400	-2.57344300	-2.42582000	C	4.83735100	-0.42079700	0.30766000
H	2.70593300	-2.23267000	-1.58906200	H	4.61384700	0.76473400	-1.48955700
H	1.49175800	-3.41129000	-2.07487700	H	5.45086900	1.59786100	-0.17791200
H	2.74787200	-2.89785600	-3.24851200	H	5.81205800	-0.83229100	-0.00043900

H	4.89132600	-0.26187300	1.38911000
Cu	1.95945700	0.00368300	-0.00329400
C	2.97179600	2.59019500	-1.04360000
H	2.02118500	3.05382400	-0.77013900
H	3.74649400	3.37046500	-1.09021700
H	2.86819500	2.13252400	-2.03027100
C	3.39977100	2.18703300	1.29684700
H	2.43262700	2.62906000	1.54668800
H	3.64411000	1.44393500	2.05828500
H	4.16753700	2.97547100	1.30998400
C	3.88761000	-2.02331800	-1.27410000
H	4.80201000	-2.63671900	-1.31958500
H	3.02263500	-2.66510100	-1.45932400
H	3.93059500	-1.27564400	-2.07040200
C	3.65549700	-2.40176100	1.09591900
H	2.80171400	-3.05366100	0.89446500
H	4.56782600	-3.01763300	1.14116800
H	3.50333100	-1.92516000	2.06832200
N	3.31764300	1.55192500	-0.04231300
N	3.73852200	-1.37267500	0.04228000

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C	-0.30926000	-3.94795100	-1.82140200
C	0.94176700	-3.34166700	-2.43889700
H	-0.84883400	-4.53963800	-2.57320400
H	-0.04176400	-4.63448800	-1.01405900
H	0.68265700	-2.71417700	-3.29591800
H	1.61083800	-4.14129600	-2.79156600
Cu	0.09871300	-1.23024800	-0.73261200
N	-1.19759800	-2.89074900	-1.25841300
N	1.64867100	-2.47014900	-1.46276200
C	2.72784000	-1.73232000	-2.16393600
H	3.23855900	-1.08949000	-1.44671000
H	3.44880800	-2.43966100	-2.59840300
H	2.28794800	-1.11304800	-2.94612700
C	2.24444400	-3.25083600	-0.35211000
H	2.95314500	-3.99714400	-0.73932700
H	2.77304800	-2.56919700	0.31549900
H	1.47229000	-3.76268300	0.22520400
C	-1.94788800	-3.42835000	-0.09992600
H	-2.61940500	-2.66158800	0.28494000
H	-2.53774800	-4.30804000	-0.39503500
H	-1.25278300	-3.71408900	0.69390800
C	-2.15941800	-2.41602000	-2.28484800

H	-2.82729300	-3.23624800	-2.58535300
H	-2.74715300	-1.59950500	-1.86355000
H	-1.62392000	-2.02977700	-3.15197900
C	1.31501400	0.12604700	0.23460000
C	2.23347500	0.03944700	1.05702900
C	3.31588700	-0.04094300	1.98162700
C	4.65098200	0.11566300	1.54529500
C	3.06824700	-0.26979100	3.35339400
C	5.70164600	0.04715900	2.45580300
H	4.84991200	0.29402500	0.49239000
C	4.12551400	-0.33876500	4.25551200
H	2.04381700	-0.38989200	3.69264300
C	5.44198400	-0.17983600	3.81051100
H	6.72432000	0.17107700	2.11124600
H	3.92553800	-0.51476700	5.30833000
H	6.26334000	-0.23143800	4.51907600
C	-1.30835400	-0.15027600	0.21938900
C	-2.23575500	-0.18870700	1.03571600
C	-3.32973000	-0.25184300	1.94784400
C	-4.65973100	-0.32484100	1.47590100
C	-3.09839000	-0.25427300	3.34159500
C	-5.72176000	-0.39919300	2.37254000
H	-4.84575300	-0.32630800	0.40563000
C	-4.16701700	-0.32752700	4.22988500
H	-2.07822800	-0.19968300	3.70819100
C	-5.47822000	-0.40097500	3.74931000
H	-6.74067800	-0.45694700	2.00038700
H	-3.97976800	-0.32945500	5.29967300
H	-6.30847000	-0.46100900	4.44693400
C	0.33509900	4.17103100	-1.26377500
C	-0.93244500	3.66451200	-1.93641700
H	0.08836600	4.75246600	-0.37180600
H	0.87319500	4.84635800	-1.94236200
H	-1.59602400	4.51041100	-2.17201500
H	-0.69142700	3.15144600	-2.87160500
Cu	-0.09201700	1.33021000	-0.54984800
C	1.97752500	3.40757400	0.36212400
H	2.63811300	2.58620100	0.63682800
H	2.57867400	4.31068400	0.18414400
H	1.28956700	3.59422700	1.19097500
C	2.16664300	2.69659500	-1.94041100
H	2.75694600	1.83335300	-1.62980100
H	1.62139800	2.42277600	-2.84373500
H	2.83487700	3.54633700	-2.14240300

C	-2.19861600	3.30471500	0.14640600
H	-2.91296600	4.09808000	-0.11736600
H	-2.71225700	2.53897500	0.72915600
H	-1.40787400	3.73156300	0.76600100
C	-2.74058800	2.05780900	-1.84721000
H	-3.25126300	1.33324300	-1.21228900
H	-3.45594500	2.82773500	-2.17022500
H	-2.32375900	1.54153200	-2.71227900
N	1.21563600	3.03990500	-0.85375100
N	-1.63792000	2.67902900	-1.07446800
Cl	-0.01771300	0.21443000	-2.95530800