

Electronic Supplementary Information

On the Mechanism of Copper-Catalyzed Oxytrifluoromethylation of Allylamines with CO₂: A Computational Study

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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, 2013.

2. Test for Stability of Wavefunction

In this multi-spin state system, test for the stability of the wavefunction was absolutely necessary. Before the calculation, we had tested the stability of the wavefunction with singlet, doublet, and triplet state intermediates. The test was conducted with B3-LYP/6-31(d) (SDD for Cu and I) level. All the test results confirmed that the wavefunction is stable under the perturbations considered. As:

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The wavefunction is stable under the perturbations considered.  
The wavefunction is already stable.
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3. Discussion for Competitive Mechanisms

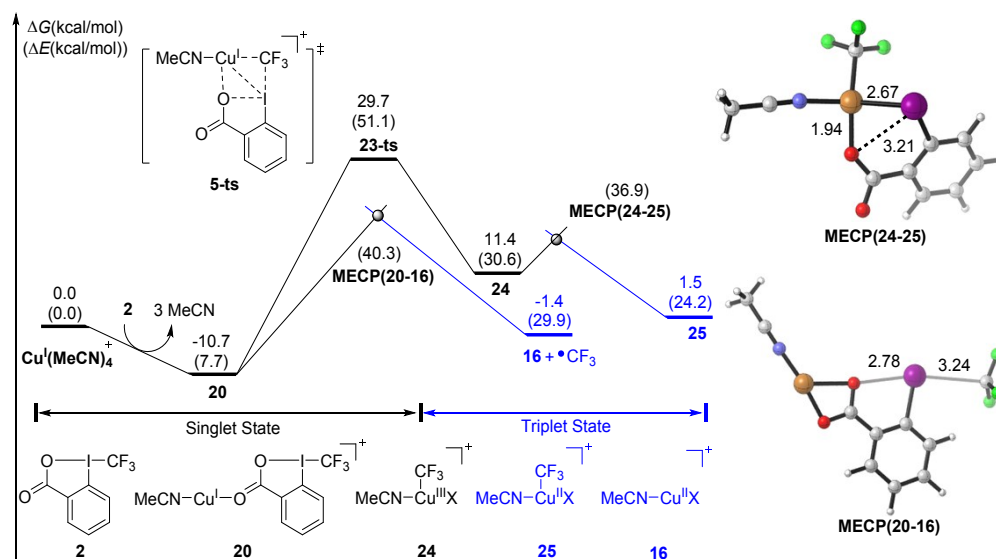


Fig. S1. Energy profiles for oxidation and free radical initiation of the cationic Cu(I) complex. The relative free energies (ΔG) and relative electronic energies (ΔE , in parentheses) in acetonitrile are given in kcal/mol. The bond distances are in angstroms. (X = 2-iodobenzoate)

Because we are using the $[\text{Cu}(\text{MeCN})_4] \text{PF}_6$ catalyst, we initially considered activation of Togni reagent II in the cationic Cu(I) complex, and the calculated energy profiles are summarized in Fig. S1. After ligand exchange, intermediate **20** forms with a free energy decrease of 10.7 kcal/mol. Subsequent oxidative addition of intermediate **20** proceeds via transition state **23-ts** with a free energy barrier of 41.4 kcal/mol to give the singlet state Cu(III) species **24**. The relative free energy of intermediate **24** is 22.1 kcal/mol higher than that of **20**. Then the triplet Cu(II) complex **25** was generated via the minimum energy crossing point (**MECP(24-25)**) with an activation energy of 6.3 kcal/mol. The calculated results indicate that the oxidization pathway is unfavorable in this system both thermodynamically and kinetically. Meanwhile, cationic Cu(I) mediated I- CF_3 bond homo-cleavage was also investigated. This cleavage walks along the singlet state potential energy surface via **MECP(20-16)** with an electronic energy (ΔE) barrier of 32.6 kcal/mol and concomitant generation of free radical $\text{CF}_3\cdot$ and Cu(II) **16**. Structural analysis of

MECP(20–16) show that the bond lengths of O–I and I–CF₃ are 2.78 and 3.24 Å, respectively, which indicates simultaneous cleavage of the O–I and I–CF₃ bonds. Although the corresponding relative electronic energy of **MECP(20–16)** is 10.8 kcal/mol lower than that of **23-ts**, homo cleavage of the I–CF₃ bond in the cationic Cu(I) complex at room temperature can be excluded.

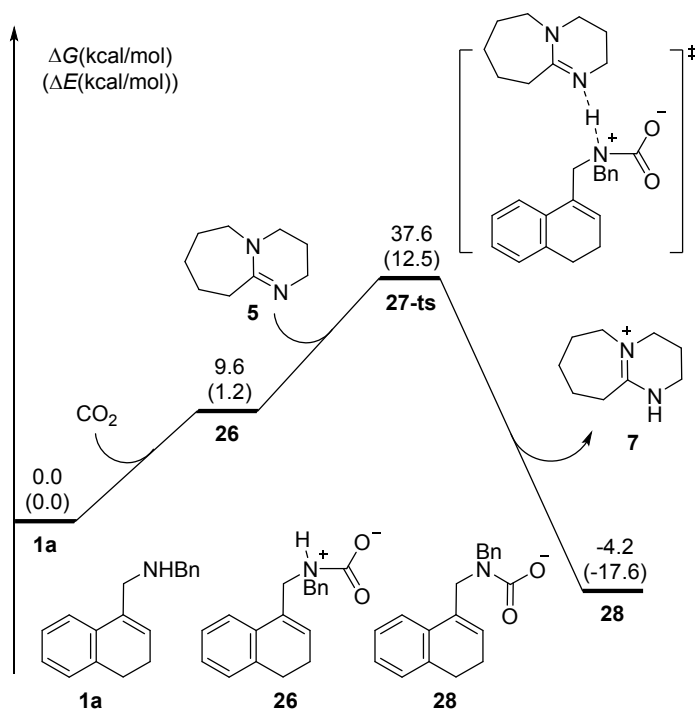


Fig. S2. Free energy profile for deprotonation of allylamines and CO₂ activation. The relative free energies (ΔG) and relative electronic energies (ΔE , in parentheses) in acetonitrile are given in kcal/mol.

As depicted in Fig. S2, we also investigated deprotonation and CO₂ activation without assistance of copper catalysts. The combination of allylamines **1a** and CO₂ leads to generation of a zwitterion intermediate **26**, which is endergonic by 9.6 kcal/mol. Subsequently, the formed zwitterion intermediate **16** undergoes deprotonation by DBU (1,8-diazabicyclo[5.4.0]undec-7-ene), thereby resulting in formation of carbamate intermediate **28**. The overall of this process is up to 37.6 kcal/mol, which indicates that the CO₂ activation by allylamines is unfavorable in this case. Comparing with the pathway in Fig. 2, these results suggest that allylamine and CO₂ exhibit enhanced reactivity in presence of copper catalysts.

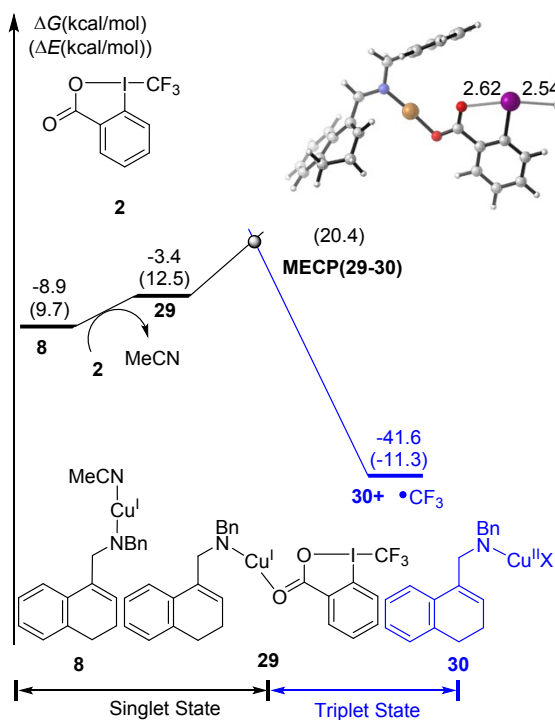


Fig. S3. Free energy profile for $\text{CF}_3\cdot$ initiation in the copper amino species. The relative free energies (ΔG) and relative electronic energies (ΔE , in parentheses) in acetonitrile are given in kcal/mol. The bond distances are in angstroms. ($X = 2$ -iodobenzoate)

As shown in Fig. S3, after ligand exchange, generation of carbonyl coordinated intermediate **29** is endergonic by 2.8 kcal/mol. Subsequently, the $\text{I}-\text{CF}_3$ bond homocleavage proceeds via **MECP(29-30)** to generate the free radical $\text{CF}_3\cdot$ and cupric amide **30** with an electronic energy barrier of 7.9 kcal/mol. The relative electronic energy of **MECP(29-30)** is 10.5 kcal/mol higher than that of **9-ts**, which indicates that the CO_2 insertion would preferentially occur in the copper amide species.

4. Benchmark for Different DFT Methods

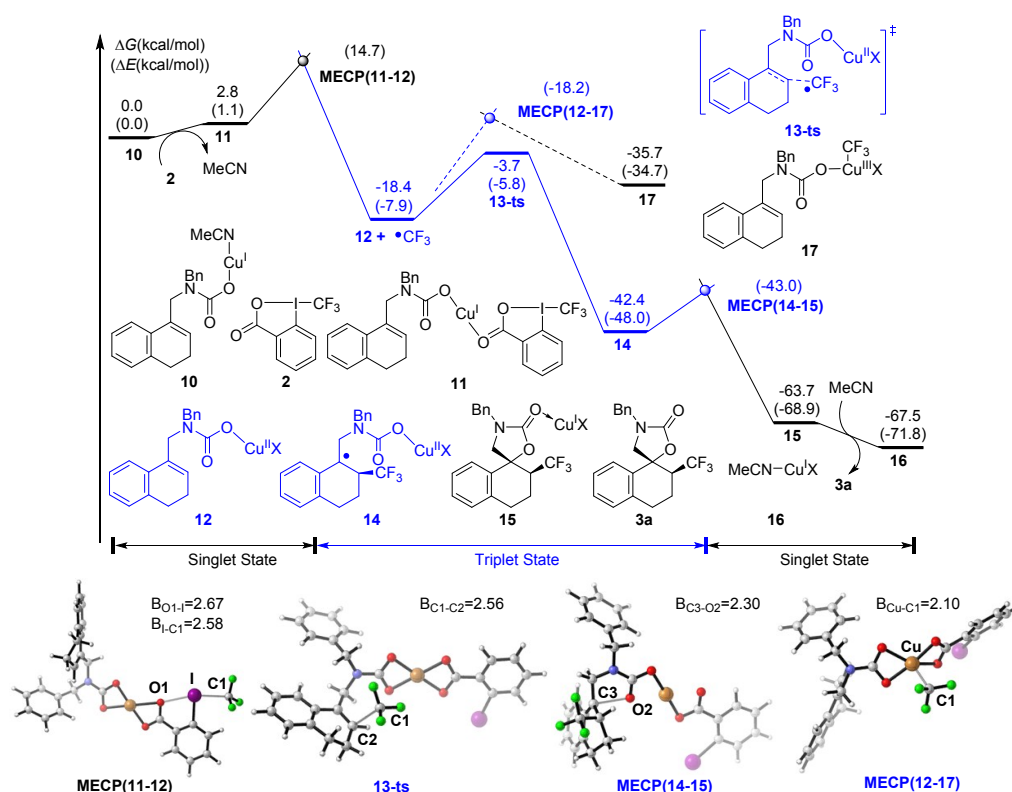


Fig. S4. B3LYP method calculated free energy profiles for the generation of 2-oxazolidone.

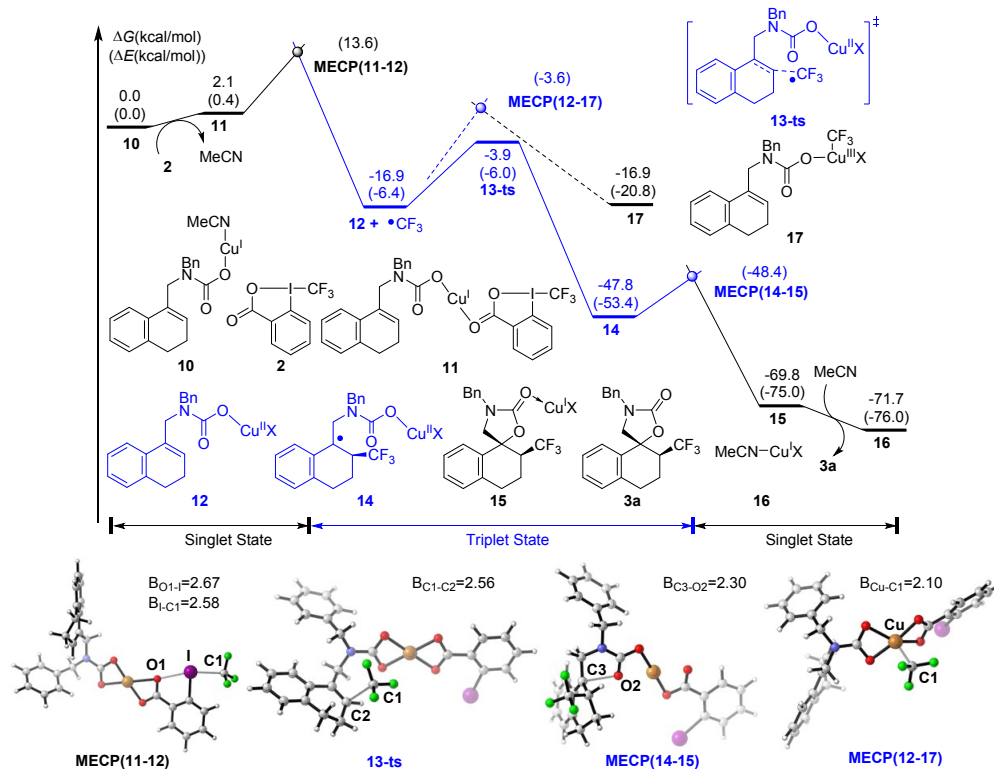


Fig. S5. B3LYP-D3 method calculated free energy profiles for the generation of 2-oxazolidone.

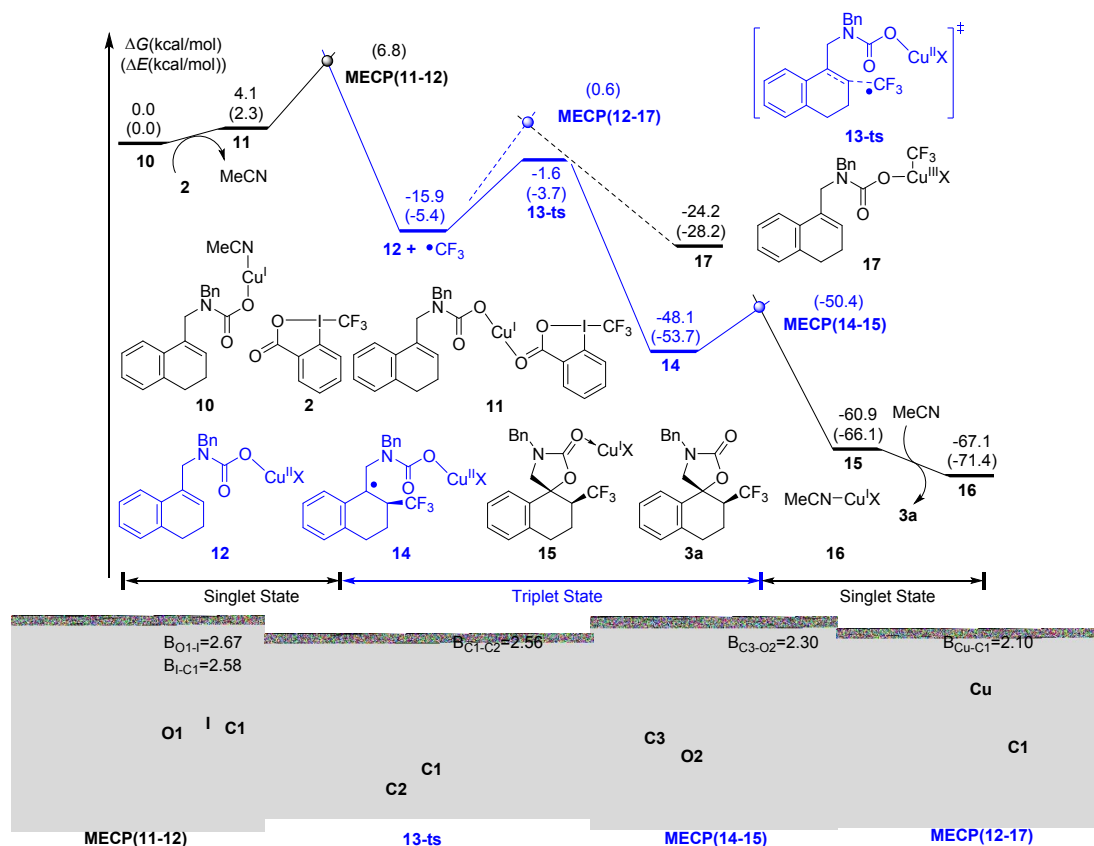


Fig. S6. B3LYP-D3 method calculated free energy profiles for the generation of 2-oxazolidone.

We have tested some other functionals, such as B3LYP-D3 and M06-L, which take the dispersion energy into consideration. As shown in the fig. S4-6, the computation results indicate that when different functionals are used to calculate the generation of 2-oxazolidone, the fluctuation tendency of free energy profiles is almost the same. All these calculated results proven that the radical addition process is more favorable than the oxidation. Therefore, the conclusion can be drawn as that the B3-LYP functional could provide great accuracy in energetic information for this work and the utilization of other functionals will not affect the overall conclusions on which is the preferred pathway. What's more, the B3-LYP results are in good agreement with the experiment.

5. Absolute Calculation Energies, Enthalpies, and Free Energies

Table S1 B3-LYP calculated energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3LYP})}^1$	$G_{(\text{corr-B3LYP})}^2$	$H_{(\text{corr-B3LYP})}^3$	$E_{(\text{solv,B3LYP})}^4$	IF ⁵
MeCN	-132.7514859	0.022666	0.050179	-132.8070662	-
CO₂	-188.5775705	-0.0091	0.015204	-188.6506338	-
CF₃·	-337.5473784	-0.01352	0.016564	-337.6728114	-
1a	-752.0847807	0.281075	0.343428	-752.3359381	-
2	-768.5267359	0.065327	0.120424	-768.8046292	-
4	-1082.068373	0.318185	0.4002	-1082.410712	-
5	-462.0786162	0.212259	0.258055	-462.2343475	-
6-ts	-1544.159763	0.549117	0.656049	-1544.633538	-144.59
7	-462.4977364	0.226659	0.273069	-462.7285636	-
8	-1081.618819	0.303153	0.384689	-1081.908018	-
9-ts	-1270.203564	0.312879	0.400529	-1270.558264	-133.78
10	-1270.238397	0.315803	0.404073	-1270.601965	-
11	-1906.015907	0.361228	0.474562	-1906.597775	-
MECP(11-12)	-1906.003416			-1906.576115	-
12	-1568.501258	0.355249	0.45658	-1568.93933	-
13-ts	-1906.056675	0.361798	0.473801	-1906.608815	-149.52
14	-1906.121494	0.367402	0.476396	-1906.676052	-
MECP(14-15)	-1906.096575			-1906.66805	-
MECP(14-15) iso	-1906.09267169			-1906.6612	-
15	-1906.144936	0.366748	0.478309	-1906.709349	-
16	-761.1870205	0.091993	0.157589	-761.3798936	-
MECP(12-17)	-1906.048941			-1906.600604	-
17	-1906.072445	0.364741	0.475289	-1906.626947	-
18-ts	-1270.189176	0.320035	0.401585	-1270.544793	-202.52
19	-1270.207257	0.319263	0.403961	-1270.561237	-

20	-1098.524822	0.102028	0.176736	-1098.874089	-
MECP(20-16)	-1098.474024			-1098.822083	-
21-ts	-2368.750288	0.433514	0.582091	-2369.44248	-479.80
22	-1607.64516	0.332083	0.424221	-1608.168692	-
23-ts	-1098.43747	0.097154	0.174168	-1098.804876	-139.26
24	-1098.476979	0.100787	0.175708	-1098.83763	-
MECP(24-25)	-1098.466273			-1098.827591	-
25	-1098.498154	0.095075	0.175402	-1098.847747	-
26	-940.6643801	0.285364	0.360466	-940.9845826	-
27-ts	-1402.729034	0.524315	0.617504	-1403.201012	-1221.87
28	-940.1046779	0.278966	0.346703	-940.5204787	-
29	-1717.396708	0.349998	0.454707	-1717.901066	-
MECP(29-30)	-1717.387863			-1717.888406	-
30	-1379.890889	0.340576	0.437606	-1380.266205	-

¹The electronic energy calculated by B3-LYP in gas phase. ²The thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. ³The thermal correction to enthalpy calculated by B3-LYP in gas phase. ⁴The electronic energy calculated by B3-LYP in acetonitrile solvent. ⁵The B3-LYP calculated imaginary frequencies for the transition states.

Table S2 B3-LYP-D3 and M06-L calculated energies, enthalpies, and free energies.

Geometry	$E_{(\text{solv},\text{B3LYP-D3})}^1$	$E_{(\text{solv},\text{M06-L})}^2$
2	-768.821085	-768.7022687
MeCN	-132.808127	-132.7848496
3a	-1278.19348	-1277.968608
CF₃·	-337.673348	-337.6205025
10	-1270.648101	-1270.466799
11	-1906.660438	-1906.380519
MECP(11-12)	-1906.639307	-1906.373352
12	-1568.997905	-1568.772349
13-ts	-1906.67062	-1906.390179
14	-1906.746235	-1906.469855

MECP(14-15)	-1906.738162	-1906.464592
15	-1906.78062	-1906.489574
16	-761.396859	-761.314289
MECP(12-17)	-1906.666752	-1906.383277
17	-1906.69425	-1906.429124

¹The electronic energy calculated by B3LYP-D3 in acetonitrile solvent. ²The electronic energy calculated by M06-L in acetonitrile solvent.

6. B3-LYP Geometries for All the Optimized Compounds and Transition State

MeCN				C	4.40295600	-2.03653800	-0.25988200
C	0.00000000	0.00000000	0.28061800	H	3.01081700	2.05216800	1.74237700
N	0.00000000	0.00000000	1.44087200	H	6.43151200	-1.46291400	0.20277600
C	0.00000000	0.00000000	-1.18107100	H	5.82589800	0.88810900	0.72249600
H	0.00000000	1.02660900	-1.56113000	C	3.34078400	2.03940200	0.69128300
H	0.88907000	-0.51330500	-1.56113000	C	1.32636800	0.20733300	-0.19483100
H	-0.88907000	-0.51330500	-1.56113000	H	2.31889100	-2.31859400	-0.67153200
CO2				H	4.65501800	-3.06811900	-0.49126300
C	0.00000000	0.00000000	0.00000000	C	1.08373200	1.52927300	-0.26279400
O	0.00000000	0.00000000	1.16958400	C	2.18929600	2.55107800	-0.18364100
O	0.00000000	0.00000000	-1.16958400	H	0.06601400	1.87168900	-0.42654400
CF3•				H	1.80740800	3.49878200	0.21456900
C	0.00000000	0.00000000	0.32915400	H	4.20772900	2.70710200	0.62731000
F	0.00000000	1.26437500	-0.07314500	H	2.55718300	2.77330500	-1.19928600
F	-1.09498100	-0.63218800	-0.07314500	C	0.21158500	-0.81666000	-0.29716600
F	1.09498100	-0.63218800	-0.07314500	H	0.25034800	-1.30602700	-1.28275600
1a				H	0.39721900	-1.62358200	0.43892500
C	5.39681700	-1.13921100	0.12746800	N	-1.11643300	-0.23130600	-0.15348700
C	5.05414100	0.18443700	0.41714700	H	-1.18409400	0.22467600	0.75567100
C	3.73408800	0.62433300	0.32442800	C	-2.19254100	-1.21450000	-0.27571700
C	2.72031400	-0.28132800	-0.07064900	H	-2.08269600	-2.06298700	0.42663600
C	3.07780700	-1.60878500	-0.35648600	H	-2.12260300	-1.64721200	-1.28493300

C	-3.55669400	-0.58189500	-0.08445900	C	1.40556000	1.52855200	0.33716400
C	-4.52239100	-1.19437200	0.72230300	C	1.00536400	2.35151300	1.39289800
C	-3.88127900	0.62070000	-0.72884400	C	1.33168300	3.70920800	1.38407000
C	-5.78985700	-0.62759700	0.87763500	H	1.65873700	0.94670100	-2.49177000
H	-4.27979100	-2.12322500	1.23441100	H	2.32638300	5.30049700	0.31921100
C	-5.14413800	1.19130100	-0.57190500	H	3.04875900	3.83434800	-1.54980900
H	-3.12942100	1.10607700	-1.34416000	C	2.53494000	1.13389300	-1.85449900
C	-6.10400300	0.56794400	0.23049400	C	1.06520300	0.04540900	0.29871700
H	-6.52707000	-1.11724300	1.50876600	H	0.45204700	1.92456900	2.22173500
H	-5.38131500	2.12416000	-1.07731300	H	1.01776600	4.34331000	2.20857900
H	-7.08790800	1.01347300	0.35196500	C	2.37078000	-0.73484800	-0.04606400
2				C	3.08165000	-0.21391000	-1.33374700
O	1.28186500	-2.12327100	0.00008800	H	3.02268900	-0.56143700	0.81620800
C	2.09618300	0.10820300	-0.00027000	H	3.00375200	-0.95789000	-2.13159700
C	0.82308600	0.64067200	0.00006600	H	3.28091700	1.60436100	-2.50404900
C	3.16264100	1.01765500	-0.00026400	H	4.14745400	-0.11024500	-1.11154500
C	0.52152100	1.99234600	0.00035700	C	-0.16102500	-0.26528200	-0.61970200
C	2.92021600	2.38890300	0.00006500	H	-0.71923300	0.65104400	-0.85270800
C	1.60911200	2.87376000	0.00035500	H	0.12419100	-0.74789300	-1.55788200
H	-0.49100200	2.37182400	0.00063700	N	-0.93131600	-1.16118300	0.21762200
H	3.75284000	3.08618300	0.00009200	C	-2.21775400	-1.72374100	-0.17436600
H	1.41796100	3.94303600	0.00074000	H	-2.48148000	-2.43494800	0.61347000
H	4.16616900	0.60404600	-0.00048100	H	-2.07682500	-2.28720400	-1.10439000
I	-0.70401300	-0.94648000	0.00030700	C	-3.31491700	-0.68728900	-0.34855900
C	-2.44353800	0.55593600	-0.00031100	C	-3.81459800	0.00035200	0.76808400
F	-3.55819700	-0.18930400	-0.00092400	C	-3.83752100	-0.39706100	-1.61321000
F	-2.45303100	1.34252400	-1.08639100	C	-4.81547900	0.95898000	0.61618300
F	-2.45373100	1.34202200	1.08606100	H	-3.41740700	-0.22722400	1.75419800
C	2.36077500	-1.39288000	-0.00038200	C	-4.84275400	0.56165300	-1.76684400
O	3.51205900	-1.80252500	-0.00054400	H	-3.46051700	-0.92918500	-2.48448300
3a				C	-5.33234300	1.24217800	-0.65190000
C	2.06558100	4.24562200	0.32550300	H	-5.19829300	1.48185200	1.48868700
C	2.47164400	3.42149100	-0.72546000	H	-5.24098500	0.77460400	-2.75545000
C	2.14402100	2.06325200	-0.73226000	H	-6.11496300	1.98724600	-0.76778000

O	0.61980400	-0.36646500	1.60803000	C	0.85080400	-1.24140000	-0.50733200
C	-0.54619100	-1.09055500	1.53032800	H	0.88518500	-0.96346400	-1.56545200
O	-1.09361200	-1.56308700	2.49983200	H	1.09208200	-2.31331900	-0.45824200
C	2.23934300	-2.25281600	-0.12527700	N	-0.56130400	-1.04027600	-0.06852300
F	1.72741000	-2.80707400	0.98714700	H	-0.61207000	-1.28025900	0.92551100
F	1.46877700	-2.65850200	-1.16835200	C	-1.50359600	-1.98514800	-0.77249700
F	3.46354300	-2.80191500	-0.31470900	H	-1.16718000	-3.01245000	-0.58290200
4				H	-1.40863800	-1.79422100	-1.84517200
Cu	-1.12624400	0.82041100	-0.17926500	C	-2.92272200	-1.77958800	-0.30537200
N	-1.64226700	2.59762000	-0.32752300	C	-3.36219400	-2.35458500	0.89597700
C	-1.95140800	3.70825000	-0.41574600	C	-3.81214200	-0.98973000	-1.04871700
C	-2.33948000	5.10612900	-0.52682300	C	-4.66067600	-2.12971000	1.35510700
H	-3.15381500	5.20842400	-1.25128700	H	-2.69438400	-2.99833200	1.46585000
H	-2.67650800	5.47500300	0.44728800	C	-5.11354800	-0.76863900	-0.59269300
H	-1.48404300	5.70218100	-0.86076100	H	-3.49454200	-0.57017300	-2.00155300
C	5.95823200	-0.55901000	-1.05298800	C	-5.53679200	-1.33421200	0.61203600
C	5.63557400	-0.12946600	0.23618800	H	-4.99264100	-2.58645300	2.28273300
C	4.31249800	-0.09800800	0.67600000	H	-5.79953100	-0.16973700	-1.18474600
C	3.27698900	-0.50278500	-0.20079500	H	-6.55093900	-1.16915300	0.96361200
C	3.61620600	-0.93862900	-1.49267500	5			
C	4.94410400	-0.96670500	-1.91806200	C	-2.95889100	0.00499800	0.07933500
H	3.91708200	-0.60525700	2.71693200	C	-2.10057800	-1.18760800	0.53179400
H	6.99473800	-0.57461900	-1.37686300	C	-0.92090200	-1.48150600	-0.41456000
H	6.42584100	0.18247100	0.91464500	C	-2.12688500	1.15888600	-0.50496600
C	3.96542400	0.30145600	2.09400700	C	0.37010900	-0.72098400	-0.13425800
C	1.87418200	-0.45337700	0.28366400	C	-0.84292500	1.47433600	0.27296200
H	2.84710300	-1.25621100	-2.19019900	H	-3.55151900	0.37030300	0.92860100
H	5.18152000	-1.30417600	-2.92258100	H	-2.73343200	-2.08011600	0.60631800
C	1.56720500	0.25163400	1.39217500	H	-1.22936400	-1.30977800	-1.45582000
C	2.61293200	1.01928200	2.16375200	H	-2.74247400	2.06704300	-0.52613500
H	0.54722200	0.29631900	1.77156400	H	-0.56464900	2.51220200	0.05762800
H	2.30108600	1.14189000	3.20654000	N	0.34275700	0.67795300	-0.07516100
H	4.75544900	0.92896400	2.51942800	C	1.59356500	1.35682900	0.27922300
H	2.70350400	2.03468900	1.74540800	H	1.55028400	2.37624300	-0.12427700

H	1.68803900	1.45093600	1.37540900	C	0.78534800	-2.76821600	0.18325300
C	2.79532000	0.60748700	-0.28370500	C	1.56948900	-3.58895700	1.17500700
H	2.76461700	0.64763300	-1.37976500	H	-0.30196300	-2.81831000	0.22356800
H	3.72479600	1.09174800	0.03920700	H	1.00780800	-4.48433800	1.46496400
N	1.42227000	-1.45880900	-0.03950500	H	3.56909800	-4.42936700	1.36484800
C	2.72538600	-0.84742300	0.18060200	H	1.71214300	-3.00513900	2.10056100
H	3.47712600	-1.45345300	-0.34144300	C	0.52961200	-1.09085300	-1.63288300
H	2.97495300	-0.91460800	1.25145000	H	1.06233800	-0.92984500	-2.58178700
H	-0.63013200	-2.53119800	-0.34461100	H	-0.37763400	-1.65775800	-1.90311300
H	-1.71209300	-1.01316100	1.54386500	N	0.15982300	0.21633300	-1.02878100
H	-3.68151900	-0.32477600	-0.67881900	H	-1.07925500	-0.04545100	-0.14095300
H	-1.85302600	0.95337200	-1.54649500	C	-0.26647500	1.16652400	-2.08522600
H	-1.04198500	1.43351500	1.35898900	H	-1.20799500	0.82204500	-2.54777200
6-ts				H	0.47594200	1.18658200	-2.89930600
Cu	1.44534100	0.91864700	0.17874600	C	-0.45239700	2.57282600	-1.55497400
N	2.67236200	1.58875100	1.40583600	C	-1.66944800	2.99112300	-0.99980500
C	3.49544700	1.98713300	2.11433700	C	0.60971400	3.48909700	-1.59661400
C	4.53919200	2.48657900	2.99873000	C	-1.81870000	4.28054100	-0.48437400
H	4.58946900	3.57823800	2.93651000	H	-2.51388100	2.30589400	-0.98590000
H	4.32523200	2.19700400	4.03236900	C	0.46617200	4.78016800	-1.08389600
H	5.50589600	2.06655500	2.70313600	H	1.55083900	3.19268000	-2.05583000
C	5.67187800	-1.70464600	-0.78587800	C	-0.74882900	5.17774800	-0.52126300
C	5.02259800	-2.72935200	-0.09168100	H	-2.77418600	4.59164500	-0.07003600
C	3.63027800	-2.82136600	-0.07325900	H	1.29569300	5.47988200	-1.14005400
C	2.85610900	-1.85597900	-0.76166200	H	-0.86713500	6.18484900	-0.13157400
C	3.52340100	-0.84092000	-1.47015100	C	-5.54237300	-2.24109200	-1.46105000
C	4.91727800	-0.76179300	-1.48264800	C	-4.01145800	-2.36059900	-1.42912100
H	2.76925900	-4.77168300	-0.16450900	C	-3.31149500	-1.01342400	-1.16447100
H	6.75715600	-1.65513500	-0.79299200	C	-6.08372300	-1.28937100	-0.38362900
H	5.60883400	-3.47986900	0.43383400	C	-3.12230600	-0.64164100	0.29599700
C	2.93039800	-3.98783800	0.59207800	C	-5.41852600	-1.44760900	0.98691400
C	1.37409100	-1.95092400	-0.71273500	H	-5.98482000	-3.23640500	-1.33512100
H	2.95248300	-0.10410200	-2.02755200	H	-3.65249600	-2.75608600	-2.38502300
H	5.40793700	0.02871300	-2.04405100	H	-3.85659100	-0.20098400	-1.66262100

H	-7.15571200	-1.47117600	-0.24626100	H	1.73471300	1.38618400	1.47885900
H	-6.08762300	-1.03283800	1.74483300	C	2.75612700	0.69466400	-0.31741400
N	-4.12600300	-0.74381800	1.19525300	H	2.64614900	0.80656900	-1.40150800
C	-3.88442700	-0.36963700	2.60545300	H	3.68576800	1.19071900	-0.02555900
H	-4.83244800	-0.01236200	3.01671300	N	1.45941900	-1.34578900	-0.07695800
H	-3.59732000	-1.26495200	3.17436900	C	2.80917000	-0.78030400	0.05551700
C	-2.81720800	0.71167200	2.71830500	H	3.47493800	-1.33919200	-0.60745400
H	-3.19145600	1.64875500	2.29041300	H	3.15794000	-0.92303600	1.08504300
H	-2.58983600	0.89511100	3.77281400	H	-0.64880300	-2.54381700	-0.08820800
N	-1.92714300	-0.18635200	0.61885100	H	-1.81342900	-0.88653600	1.59319200
C	-1.57392500	0.26053300	1.96615900	H	-3.65289100	-0.38469200	-0.79304100
H	-0.85268700	1.07713300	1.85841200	H	-1.77151000	0.85168500	-1.62626200
H	-1.06629600	-0.55607000	2.49675400	H	-1.18072500	1.58200900	1.29396400
H	-2.31552100	-1.02400000	-1.60656300	H	1.38708700	-2.34511700	-0.21415600
H	-3.69764600	-3.08783100	-0.66943300	8			
H	-5.86674800	-1.88133100	-2.44489900	Cu	-1.14913800	0.69404900	-0.28409600
H	-5.99843900	-0.24255800	-0.69894500	N	-1.85112600	2.38698000	-0.50012300
H	-5.28889500	-2.51103100	1.23298300	C	-2.30666600	3.43891900	-0.66469100
				C	-2.88096400	4.75956900	-0.88379900
7				H	-3.75474000	4.68233300	-1.53887900
C	-2.98682000	0.00546000	-0.01477700	H	-3.19023300	5.20066300	0.06924900
C	-2.15399400	-1.13896100	0.58134400	H	-2.14152200	5.41510100	-1.35495200
C	-0.93545000	-1.50614600	-0.28670000	C	6.02594500	-0.54357700	-1.02397600
C	-2.11924000	1.11883000	-0.62073200	C	5.68527700	0.06580500	0.18616300
C	0.30887100	-0.66454900	-0.06953800	C	4.36260000	0.11023300	0.62652600
C	-0.91156400	1.51453600	0.23222800	C	3.33368500	-0.46479600	-0.16240700
H	-3.63374000	0.42024300	0.76654100	C	3.69565200	-1.07749700	-1.37433400
H	-2.77513300	-2.03340000	0.69047200	C	5.02346300	-1.11818800	-1.80258700
H	-1.19632800	-1.46406300	-1.35237900	H	3.96784400	-0.08432300	2.72014700
H	-2.72620000	2.02150700	-0.75077100	H	7.06209500	-0.56661400	-1.35164000
H	-0.57600000	2.50743600	-0.07404300	H	6.46191000	0.51287200	0.80383100
N	0.30275200	0.65280800	0.11404300	C	4.00548900	0.71794200	1.96566700
C	1.58094600	1.35907800	0.39271700	C	1.92809000	-0.39283100	0.32045900
H	1.46469400	2.38872600	0.04983700	H	2.93303800	-1.52499400	-2.00231700

H	5.26897300	-1.59737100	-2.74701000	C	4.74369400	0.90986100	-0.57934900
C	1.61404700	0.48071100	1.29746300	C	3.95915000	-0.18277100	-0.20688500
C	2.63493500	1.40133100	1.91950400	C	2.66201500	-0.33562400	-0.75412300
H	0.58891500	0.51952400	1.65433500	C	2.21511800	0.61444600	-1.68921400
H	2.32401200	1.69096600	2.93061800	C	3.01138600	1.70048100	-2.05693100
H	4.78618700	1.41693600	2.28895100	H	4.94776700	-2.05171000	0.08043800
H	2.70473300	2.33701700	1.33925600	H	4.90545300	2.69978500	-1.77456900
C	0.89259200	-1.33275600	-0.27832300	H	5.73947700	1.01464900	-0.15276100
H	1.07349500	-1.41929100	-1.36768200	C	4.50187700	-1.26189000	0.70632800
H	1.11781500	-2.34508200	0.11557300	C	1.82638800	-1.48885500	-0.33416300
N	-0.48942400	-1.00191200	0.00379300	H	1.22939900	0.50652200	-2.13019800
C	-1.35674600	-2.13257900	-0.29168400	H	2.63975000	2.41965700	-2.78266700
H	-1.04971100	-3.00666100	0.31695500	C	2.19103500	-2.21875100	0.73839800
H	-1.27951500	-2.47158000	-1.34636400	C	3.40450800	-1.89346200	1.57070900
C	-2.81161400	-1.82700100	0.00184400	H	1.56343900	-3.05084800	1.05128100
C	-3.25154700	-1.66989300	1.32522800	H	3.78742400	-2.79419400	2.06490400
C	-3.74544400	-1.67928700	-1.03139500	H	5.31193900	-0.86539600	1.32976600
C	-4.58523400	-1.37196500	1.60608800	H	3.11352300	-1.20209400	2.37966400
H	-2.53428100	-1.78227400	2.13429100	C	0.54564300	-1.81680400	-1.07647200
C	-5.08344000	-1.38113900	-0.75641800	H	0.69127300	-1.62394300	-2.15613400
H	-3.41835600	-1.80504500	-2.06159600	H	0.35693900	-2.89996600	-0.99131600
C	-5.50695500	-1.22591600	0.56442600	N	-0.62900200	-1.08904600	-0.57449100
H	-4.90930200	-1.26118800	2.63825800	C	-1.76717700	-1.36486400	-1.45789900
H	-5.79357900	-1.27594000	-1.57329800	H	-1.98360200	-2.44728900	-1.44281300
H	-6.54790500	-1.00044800	0.78286900	H	-1.51640200	-1.11826800	-2.50787700
9-ts				C	-3.01508900	-0.60227500	-1.06621600
Cu	-0.45998200	0.61253200	0.19365800	C	-3.94568200	-1.14789500	-0.17151500
N	-0.30447700	2.24478300	1.05014800	C	-3.26076200	0.67797400	-1.58479400
C	-0.19541100	3.25207100	1.60863900	C	-5.08201300	-0.42960200	0.20701100
C	-0.05539900	4.51929500	2.31320900	H	-3.77752100	-2.14625000	0.22447400
H	-0.78348400	5.24215100	1.93177100	C	-4.39664500	1.39971100	-1.21189200
H	-0.22779200	4.37270700	3.38422300	H	-2.55900500	1.10387500	-2.29947900
H	0.95315900	4.91849900	2.16621000	C	-5.30975100	0.84756000	-0.31009500
C	4.27860100	1.85656600	-1.49588600	H	-5.79324100	-0.87093000	0.90070800

H	-4.57458300	2.38620500	-1.63347800	H	0.58412400	-1.27148600	-1.74396200
H	-6.19793000	1.40398300	-0.02151700	N	-0.06792500	0.65283100	-1.30356600
C	-1.13964800	-2.15569400	1.43480600	C	0.13220400	2.02304500	-1.78807500
O	-1.06474100	-1.25849600	2.20788400	H	-0.83038200	2.35737700	-2.18255600
O	-1.30815700	-3.25745500	1.03357900	H	0.84551900	1.98196900	-2.62029100
10				C	0.62534900	3.02081900	-0.75239800
Cu	-3.31254000	-1.04189800	-0.16929800	C	1.92513300	3.53496500	-0.80700700
N	-5.06272500	-1.30995500	0.31032800	C	-0.23112200	3.45397100	0.27231300
C	-6.17640900	-1.42500500	0.60263700	C	2.37063700	4.45869400	0.14224200
C	-7.57855600	-1.56838800	0.96995400	H	2.59713900	3.21029800	-1.59902100
H	-7.66704800	-2.15857700	1.88760600	C	0.21276200	4.37347100	1.22249000
H	-8.02317100	-0.58204100	1.13633600	H	-1.24174800	3.05644400	0.30977300
H	-8.12508900	-2.07404000	0.16753800	C	1.51491600	4.87941000	1.16073300
C	4.95980100	-3.51179500	-0.24347400	H	3.38435100	4.84740300	0.08496600
C	4.46024500	-3.04156000	0.97429300	H	-0.46057200	4.70216100	2.01054900
C	3.43053700	-2.10242600	1.01818900	H	1.85784300	5.59852700	1.90039200
C	2.88028300	-1.60553100	-0.18896100	C	-1.33419400	0.26278300	-0.92064300
C	3.38709700	-2.09349400	-1.40492300	O	-1.48420600	-0.99797100	-0.61829900
C	4.41620600	-3.03644900	-1.43521200	O	-2.28071300	1.08682300	-0.87149700
H	1.95300400	-2.26381400	2.55172800	11			
H	5.76425000	-4.24257200	-0.25732700	Cu	-0.07653100	-1.05360900	-0.64707700
H	4.87499000	-3.41460200	1.90876600	C	-5.65211500	5.37183900	-0.42360700
C	2.83528300	-1.64187300	2.33115000	C	-5.36891700	4.78135700	0.81133700
C	1.80493800	-0.58623900	-0.12537900	C	-5.03188300	3.43167800	0.90678400
H	2.98273500	-1.73348400	-2.34570000	C	-4.98080300	2.63449600	-0.26347900
H	4.79137800	-3.39409500	-2.39069100	C	-5.25912000	3.24439000	-1.49820700
C	1.58117100	0.08000200	1.01986600	C	-5.59169300	4.59785400	-1.58077600
C	2.38730900	-0.17704600	2.26764400	H	-3.55634400	2.83945000	2.33216000
H	0.82422100	0.85708300	1.04680700	H	-5.91547000	6.42510600	-0.47741400
H	1.80116200	0.07500300	3.15932200	H	-5.40591500	5.38165500	1.71853200
H	3.54571300	-1.80108400	3.15104900	C	-4.65289700	2.80333100	2.23045800
H	3.26609300	0.48916400	2.28176700	C	-4.65070000	1.19379600	-0.14324800
C	1.01005000	-0.32414900	-1.39733000	H	-5.22347200	2.65989200	-2.41195800
H	1.69118700	0.02522800	-2.18503600	H	-5.80581900	5.04172600	-2.54979900

C	-4.70772800	0.59359700	1.05771400	H	7.34219300	-1.09017800	0.40419300
C	-5.09521500	1.33763800	2.31022000	H	5.32196100	-4.88137600	0.19097700
H	-4.50987700	-0.47079500	1.13119500	H	7.41115400	-3.55542000	0.45493500
H	-4.65137200	0.85944900	3.19148800	H	3.13576400	-3.70277700	-0.13013300
H	-5.06576600	3.38570600	3.06298400	I	4.92509600	1.12381100	0.03958600
H	-6.18778900	1.27902300	2.44923300	C	7.14660600	1.56741100	0.35589000
C	-4.28667700	0.44381800	-1.41821100	F	7.23837600	2.89784800	0.36034600
H	-5.13156400	0.49860300	-2.11931400	F	7.90041000	1.07427300	-0.62886400
H	-3.44530000	0.95676300	-1.89554800	F	7.59028400	1.08816400	1.51969500
N	-3.93986400	-0.96202800	-1.27318400	C	2.69015200	-1.03298000	-0.23898700
C	-4.93283200	-1.99817000	-1.56652000	O	1.66099300	-1.73823500	-0.36889000
H	-4.38671000	-2.83809200	-2.00335800	MECP(11-12)			
H	-5.61894200	-1.60360500	-2.32653600	Cu	0.07821100	-1.34248200	-0.51645600
C	-5.73910100	-2.49392900	-0.37569100	C	-5.85490300	5.26257500	-0.44970500
C	-5.12226200	-3.27169600	0.61753400	C	-5.52536200	4.70619000	0.79046500
C	-7.10150800	-2.20110300	-0.25224200	C	-5.07784500	3.38836300	0.89557100
C	-5.85609600	-3.73376800	1.71002200	C	-4.95550900	2.59240600	-0.27176100
H	-4.06478800	-3.50031400	0.51600400	C	-5.28414000	3.16798400	-1.51160700
C	-7.83912700	-2.66607100	0.84000300	C	-5.73020200	4.48858900	-1.60307800
H	-7.59162600	-1.60194700	-1.01737900	H	-3.57512700	2.90576000	2.33850300
C	-7.21697700	-3.43316000	1.82544500	H	-6.20620300	6.28981200	-0.51054800
H	-5.36669200	-4.33580700	2.47210600	H	-5.61368000	5.30750800	1.69397900
H	-8.89705000	-2.42771400	0.91986400	C	-4.66574400	2.79385200	2.22532000
H	-7.78753500	-3.79703000	2.67645000	C	-4.49716100	1.18727400	-0.14010700
C	-2.62336400	-1.35331800	-1.05316900	H	-5.20200400	2.58204500	-2.42238700
O	-2.32410400	-2.56073600	-0.98894500	H	-5.98039300	4.90630000	-2.57533500
O	-1.77480700	-0.36599100	-0.92671100	C	-4.52500200	0.58590800	1.06266900
O	2.72875200	0.23848800	-0.25910800	C	-5.00746100	1.30140300	2.29987600
C	3.99715600	-1.75055100	-0.04334800	H	-4.22869800	-0.45464300	1.15264200
C	5.19056600	-1.06195600	0.11002900	H	-4.56277600	0.85640900	3.19801700
C	4.06254800	-3.15186500	-0.01103600	H	-5.12830900	3.34695900	3.05180900
C	6.42787200	-1.65512100	0.28904000	H	-6.09822100	1.16817900	2.39865300
C	5.28357500	-3.79681200	0.16773600	C	-4.02396700	0.48856100	-1.40646200
C	6.45737900	-3.05506900	0.31621000	H	-4.83449100	0.48327000	-2.14791800

H	-3.20321400	1.07008500	-1.84089800	F	7.36332300	1.63434400	1.49916900
N	-3.57391800	-0.89221200	-1.26536300	C	2.53380400	-1.50509000	-0.17507900
C	-4.47497900	-2.00587900	-1.59316500	O	1.66737300	-2.42972900	-0.24797700
H	-3.84934500	-2.80518300	-1.99756000	12			
H	-5.14558100	-1.66584900	-2.39148900	Cu	0.99827500	-0.98049400	-0.66127100
C	-5.29659900	-2.53949000	-0.43240800	C	-5.83050200	4.71617700	-0.26983200
C	-4.67360500	-3.25396100	0.60326100	C	-5.34218800	4.20578000	0.93602700
C	-6.68099300	-2.34516300	-0.38192900	C	-4.67031000	2.98494900	0.98437800
C	-5.42389700	-3.74988400	1.66923200	C	-4.48305600	2.24060500	-0.20594900
H	-3.59917200	-3.41165000	0.56049700	C	-4.97198200	2.76965300	-1.41173500
C	-7.43502300	-2.84704200	0.68241700	C	-5.63983700	3.99500500	-1.44665300
H	-7.17487400	-1.79585100	-1.18152300	H	-3.02090400	2.77446300	2.32482200
C	-6.80704400	-3.54824600	1.71236800	H	-6.35258900	5.66910100	-0.28642600
H	-4.92963400	-4.30274600	2.46430600	H	-5.48098800	4.76900800	1.85654500
H	-8.51059100	-2.69014700	0.70435900	C	-4.07535300	2.46053900	2.27329600
H	-7.39067600	-3.93956800	2.54202100	C	-3.79168100	0.93080000	-0.13100800
C	-2.26287700	-1.15936000	-0.98271700	H	-4.84092500	2.22433200	-2.34130900
O	-1.83456900	-2.35541100	-0.91351200	H	-6.01039800	4.38000600	-2.39294100
O	-1.44719200	-0.17241300	-0.78880700	C	-3.63083300	0.32074100	1.05524500
O	2.19570200	-0.28484200	-0.25400700	C	-4.12814400	0.92986300	2.34121600
C	3.96898600	-1.88346600	-0.00131000	H	-3.16781600	-0.65978900	1.10130000
C	4.99968300	-0.95064900	0.09501400	H	-3.53228300	0.57014200	3.18794600
C	4.31261800	-3.24258200	0.06129800	H	-4.57910000	2.90813900	3.13778200
C	6.33077000	-1.31117200	0.24290500	H	-5.16106400	0.59250000	2.52822700
C	5.63787200	-3.63580900	0.21252100	C	-3.31060700	0.32779300	-1.44167600
C	6.64271200	-2.67249400	0.30139500	H	-4.16205600	0.16708000	-2.11391900
H	7.12031600	-0.57712400	0.30893800	H	-2.64568400	1.04204700	-1.93935700
H	5.88689000	-4.69105900	0.25955200	N	-2.60991800	-0.95521900	-1.35055700
H	7.68046400	-2.97014200	0.41689800	C	-3.30985700	-2.21815200	-1.65367100
H	3.51088800	-3.96845600	-0.01373800	H	-2.55675300	-2.90908800	-2.03824700
I	4.43372800	1.14985100	0.00251300	H	-4.01619800	-2.00681400	-2.46402200
C	6.84857900	1.98727600	0.31887000	C	-4.04239200	-2.84732900	-0.48282100
F	6.71362200	3.31138000	0.26533200	C	-3.32893300	-3.53712300	0.50890900
F	7.66854400	1.57983500	-0.65515500	C	-5.43473600	-2.75852200	-0.37794900

C	-3.99849900	-4.11450500	1.58788000	H	-8.74087300	-2.23083700	0.06877200
H	-2.24804100	-3.61610200	0.42700300	H	-7.02991800	-3.92443100	0.67256300
C	-6.10708900	-3.33866800	0.70017200	C	-4.33036100	-3.76461200	0.43363700
H	-5.99896100	-2.23228700	-1.14512500	C	-3.51035700	-1.30532500	-0.84245100
C	-5.38933200	-4.01631600	1.68653300	H	-5.65483000	0.37633500	-1.34989700
H	-3.43522700	-4.64815900	2.34896900	H	-8.02251900	-0.06690500	-0.94574600
H	-7.18906600	-3.26169500	0.76740900	C	-2.63203300	-2.34917600	-0.74595900
H	-5.91019600	-4.47023600	2.52540000	C	-3.10739400	-3.75715900	-0.48870300
C	-1.28504400	-0.96896000	-1.09627900	H	-1.61663900	-2.20608300	-1.10656000
O	-0.61715600	-2.07419100	-1.02249400	H	-2.30723800	-4.36874000	-0.06081400
O	-0.61961400	0.12097700	-0.92060100	H	-4.77684100	-4.76455800	0.47475000
O	2.64188500	0.09701900	-0.28846000	H	-3.36288200	-4.21496400	-1.45843400
C	4.75181100	-1.05840000	0.08937800	C	-2.97849400	0.04839500	-1.30119100
C	5.61009900	0.04117800	0.27652300	H	-2.19684500	-0.10710700	-2.04493700
C	5.29836800	-2.35360400	0.19035800	H	-3.75644400	0.65361800	-1.77195900
C	6.96354300	-0.16300900	0.55628500	N	-2.38174300	0.85827300	-0.22848900
C	6.64328900	-2.55791000	0.46892400	C	-3.25350500	1.55590900	0.72413400
C	7.47833200	-1.45562400	0.65317200	H	-2.63417500	1.81156100	1.58635200
H	7.61820700	0.68919800	0.69892900	H	-4.01977700	0.85190900	1.06563800
H	7.03637300	-3.56745600	0.54161500	C	-3.90160300	2.80338700	0.14914900
H	8.53367700	-1.59330900	0.87225200	C	-3.11147200	3.82027800	-0.40626700
H	4.62771800	-3.19240200	0.04274400	C	-5.28956100	2.97472200	0.19578400
I	5.01617700	2.10825800	0.15888800	C	-3.70046200	4.97905900	-0.90971000
C	3.29505100	-0.99350000	-0.20585700	H	-2.03111900	3.70249600	-0.43181200
O	2.63658300	-2.08059100	-0.38582900	C	-5.88179900	4.13813000	-0.30401800
13-ts				H	-5.91106500	2.19331000	0.62720900
Cu	1.25244800	0.81488400	0.26725400	C	-5.08845900	5.14128400	-0.86046400
C	-7.68826000	-2.02717200	-0.10743300	H	-3.07624900	5.76011900	-1.33576800
C	-6.72359000	-2.97957200	0.22887700	H	-6.96132900	4.25665400	-0.26016000
C	-5.36641100	-2.74682500	0.00977700	H	-5.54615300	6.04581700	-1.25200400
C	-4.94568300	-1.51969700	-0.57028200	C	-1.04276000	0.89132900	-0.08287200
C	-5.93323800	-0.57061500	-0.90137200	O	-0.47608400	1.58304800	0.84867500
C	-7.28607800	-0.81808800	-0.67350800	O	-0.25921600	0.22186800	-0.86260800
H	-3.99912000	-3.53115400	1.45559000	O	3.01718400	0.05991800	-0.30153300

C	5.01420400	0.64705800	0.96234400	H	1.55680600	-1.93522600	0.11315700
C	6.00848300	0.05346900	0.16337000	H	2.29893300	-4.29808900	-0.30151500
C	5.40650100	1.24712900	2.17559100	H	4.71441900	-4.84144500	0.30882400
C	7.34261300	0.06239000	0.57745600	H	2.80561400	-3.65657700	1.25967400
C	6.73159200	1.25308200	2.59104100	C	2.89926400	0.09209300	1.02664900
C	7.70284800	0.65612000	1.78712100	H	2.13869400	-0.22004500	1.75019300
H	8.10320500	-0.39433100	-0.04553300	H	3.63401900	0.68664500	1.57279200
H	7.00406200	1.71971100	3.53284500	N	2.22039700	0.98900200	0.07849100
H	8.74542400	0.65027300	2.09326000	C	3.04134600	1.81146400	-0.81843300
H	4.63228300	1.70579300	2.78008300	H	2.39386800	2.13004700	-1.63785200
I	5.66139800	-0.88216600	-1.74599400	H	3.82090800	1.16873900	-1.24291000
C	3.55845000	0.70044200	0.65735200	C	3.66459900	3.01217600	-0.13053000
O	2.78505800	1.40999200	1.39495500	C	2.85294400	3.96619600	0.50032200
C	-1.47261900	-2.07941400	1.52045200	C	5.05104800	3.20066200	-0.13627400
F	-1.62514800	-3.22185100	2.20063500	C	3.41984100	5.08050300	1.11660600
F	-2.00600500	-1.06980700	2.20923900	H	1.77392500	3.83356900	0.49670800
F	-0.16914500	-1.85600600	1.31971300	C	5.62141300	4.31982000	0.47745200
14				H	5.68911100	2.46953000	-0.62833900
Cu	-1.42631400	0.84982100	-0.31769900	C	4.80663500	5.26046600	1.10712600
C	7.64467300	-2.14134200	0.91901700	H	2.77962500	5.81366800	1.60013700
C	6.72422300	-3.10192500	0.49324100	H	6.69997400	4.45290500	0.46349800
C	5.37684800	-2.80023600	0.30912200	H	5.24677400	6.13084700	1.58632000
C	4.90466700	-1.46988300	0.57047000	C	0.88117800	0.96023800	-0.04883100
C	5.86601600	-0.51133000	1.01256100	O	0.25464700	1.74416100	-0.86026100
C	7.20237400	-0.83802000	1.17635000	O	0.15097200	0.14064600	0.63799800
H	4.53857900	-4.02786600	-1.23410700	O	-3.12978600	-0.05107600	0.21559100
H	8.68954900	-2.40647500	1.05269800	C	-5.20425600	0.60202600	-0.87667500
H	7.06124100	-4.11930200	0.30474300	C	-6.14122400	-0.09683300	-0.09362700
C	4.42857500	-3.88767900	-0.15097800	C	-5.66658300	1.27664700	-2.02413600
C	3.52292000	-1.13556900	0.40303600	C	-7.48841300	-0.11930100	-0.46149700
H	5.55911800	0.51210200	1.19803900	C	-7.00494700	1.25090500	-2.39427500
H	7.90504400	-0.07658100	1.50405100	C	-7.91822900	0.54703300	-1.60912300
C	2.57763100	-2.13801100	-0.23080100	H	-8.20490300	-0.65675700	0.14910100
C	2.96566900	-3.57515800	0.17808000	H	-7.33235800	1.77538200	-3.28682000

H	-8.96971800	0.51437800	-1.88107600	C	3.67661400	2.33877800	-1.19534000
H	-4.93656600	1.81731900	-2.61583700	H	3.01265600	2.89143300	-1.86369500
I	-5.68310500	-1.14148000	1.73377100	H	4.54784100	2.01447500	-1.77597400
C	-3.74144400	0.69024500	-0.62115500	C	4.11758400	3.21125800	-0.03203500
O	-3.03270800	1.53065700	-1.28215100	C	3.16563700	3.91137400	0.72627700
C	2.49921300	-1.99658100	-1.75611400	C	5.47082500	3.32768700	0.30505700
F	1.73905300	-2.97408800	-2.29962600	C	3.56453200	4.70421100	1.80156200
F	3.71060200	-2.05154900	-2.35650600	H	2.11397500	3.83698200	0.46220600
F	1.93938900	-0.81912600	-2.12969600	C	5.87207000	4.12570700	1.38005900
MECP(14-15)				H	6.21940600	2.79714600	-0.28079700
Cu	-0.82872600	1.29751800	-0.61950500	C	4.91897000	4.81392300	2.13115900
C	2.26729300	-3.57498000	3.45011200	H	2.81824400	5.24352700	2.37888800
C	1.91392200	-4.06339700	2.19153800	H	6.92720000	4.20853200	1.62727100
C	2.10575000	-3.31272900	1.03248300	H	5.22817500	5.43689600	2.96626800
C	2.67677000	-2.00071300	1.12788700	C	1.58290700	1.14549900	-0.69676000
C	3.01438500	-1.52298800	2.42797600	O	0.88381100	2.11981200	-1.13641000
C	2.82105200	-2.29378700	3.56181700	O	0.98840100	0.12430400	-0.18111700
H	2.51723100	-4.58910000	-0.63334200	O	-2.51888400	0.44977200	-0.04262500
H	2.10399900	-4.18265100	4.33578700	C	-4.70699900	1.45125400	-0.35702100
H	1.47213600	-5.05371100	2.10498200	C	-5.53547700	0.39538000	0.05581400
C	1.72108100	-3.90764600	-0.30325200	C	-5.31901300	2.68309400	-0.65977200
C	2.86961900	-1.19977600	-0.04829800	C	-6.91667600	0.57369100	0.16645300
H	3.43107700	-0.53040100	2.55052000	C	-6.69046000	2.86942100	-0.54658100
H	3.09293100	-1.89642100	4.53570800	C	-7.49309100	1.80834200	-0.12878700
C	2.61618100	-1.80805700	-1.41736900	H	-7.54406400	-0.25196400	0.48204400
C	1.47482100	-2.83813500	-1.36825700	H	-7.12891700	3.83414000	-0.78402000
H	2.34046100	-1.00789400	-2.11129700	H	-8.56838800	1.93222600	-0.03365000
H	1.34451000	-3.29594500	-2.35293000	H	-4.67149400	3.48782000	-0.98771700
H	0.82321000	-4.52453300	-0.18139000	I	-4.84971100	-1.60062500	0.51456400
H	0.56087100	-2.28448300	-1.13410800	C	-3.21541000	1.41790500	-0.50396400
C	3.63510900	0.10445600	-0.01689800	O	-2.63034600	2.38460200	-1.07660300
H	3.79946500	0.45589700	1.00483600	C	3.89681100	-2.39623600	-2.02861500
H	4.62596700	-0.03729200	-0.46745500	F	3.63484700	-3.02881700	-3.19174300
N	2.94188700	1.13460700	-0.78797600	F	4.51667300	-3.28284200	-1.21708300

F	4.80351700	-1.42511300	-2.31006100	H	-6.64796400	-1.65964200	-0.51746700
MECP(14-15) iso				C	-5.46814900	-4.15662200	1.46847600
Cu	0.46771100	-0.98787200	-1.21873800	H	-3.43926400	-4.89352900	1.44857500
C	-2.10799100	4.87817500	-2.56980100	H	-7.39896100	-3.21867500	1.25556000
C	-1.46040100	4.87369000	-1.33436600	H	-5.79534600	-4.84189300	2.24582800
C	-1.62340900	3.82821400	-0.42652600	C	-1.88722700	-0.57808300	-1.18819300
C	-2.48450800	2.73933100	-0.75681600	O	-1.35728100	-1.54569400	-1.83056900
C	-3.11684700	2.75528200	-2.03018100	O	-1.10566400	0.26168600	-0.59160600
C	-2.93565700	3.80446500	-2.91743100	O	2.21193400	-0.31059400	-0.51140200
H	0.10980600	4.29087100	0.74855900	C	4.27121300	-1.57587900	-0.71461000
H	-1.95895800	5.70413600	-3.25951100	C	5.13984100	-0.75082700	0.02044500
H	-0.80443700	5.69922000	-1.06821800	C	4.81251600	-2.73302600	-1.30833600
C	-0.89098100	3.86946700	0.89680500	C	6.49392200	-1.07304100	0.14270700
C	-2.69247600	1.64951800	0.16457600	C	6.15743300	-3.05957900	-1.18885200
H	-3.74281700	1.92190600	-2.32810800	C	7.00321000	-2.22198800	-0.46131500
H	-3.43283300	3.78770000	-3.88289800	H	7.15186500	-0.42747600	0.71296400
C	-2.18017000	1.83809900	1.58256700	H	6.54198100	-3.96079400	-1.65742100
C	-0.78568000	2.49635100	1.56075600	H	8.05942900	-2.45644700	-0.35605000
H	-0.09548900	1.85143000	1.01036400	H	4.13115300	-3.36535400	-1.86607600
H	-1.41223100	4.56055700	1.57877800	I	4.56066500	1.05230800	1.06097400
H	-0.41068300	2.60291100	2.58126900	C	2.80582500	-1.35721300	-0.93583200
C	-3.73285300	0.59002900	-0.15111000	O	2.13505000	-2.23602900	-1.56337300
H	-4.06050100	0.07359200	0.75223700	H	-2.86415500	2.54383800	2.08831700
H	-4.62546900	1.05978800	-0.58661700	C	-2.21920000	0.61397900	2.50292400
N	-3.22945500	-0.39336700	-1.11675200	F	-1.60708400	0.89108900	3.67503200
C	-4.14712600	-1.42419400	-1.61614800	F	-3.49952900	0.27694100	2.81950400
H	-3.60850300	-1.95386400	-2.40533300	F	-1.63561200	-0.48521900	1.99426900
H	-5.00584400	-0.91781300	-2.07342300	15			
C	-4.61953500	-2.38860600	-0.54116100	Cu	-1.14688000	1.28200800	-1.17679300
C	-3.72173100	-3.30876500	0.02199200	C	2.61136100	-0.77508400	4.17401900
C	-5.94233500	-2.36668800	-0.08574300	C	2.20117300	-1.97206200	3.59590600
C	-4.14363200	-4.18464100	1.02113600	C	2.18605100	-2.14715000	2.20545300
H	-2.69425400	-3.33657300	-0.33139000	C	2.61121300	-1.08707200	1.38292400
C	-6.36763700	-3.24655200	0.91327700	C	3.01068700	0.12296400	1.97475000

C	3.01399900	0.28262200	3.35658000	O	1.30927200	-0.51990700	-0.57335000
H	2.52672300	-4.21868800	1.76481000	O	-2.97008600	1.14057900	-0.88164900
H	2.60674000	-0.66306700	5.25457700	C	-4.75535700	1.39249600	0.67247900
H	1.87392000	-2.79306900	4.22963600	C	-5.64206600	0.38642300	0.26876800
C	1.72818700	-3.47492800	1.63688600	C	-5.26667100	2.41205700	1.49548000
C	2.56459100	-1.19426000	-0.13822700	C	-6.98527700	0.40300000	0.65238300
H	3.31392500	0.96236100	1.35596600	C	-6.60550100	2.45405100	1.86855900
H	3.32437700	1.22857600	3.79029300	C	-7.47035600	1.44559500	1.44197300
C	2.41321900	-2.64523700	-0.65994500	H	-7.65073700	-0.39404200	0.33899600
C	1.33926500	-3.38097700	0.15993700	H	-6.97044900	3.26389000	2.49439200
H	2.08679300	-2.57952800	-1.70361200	H	-8.51913300	1.45727500	1.72705900
H	1.16923800	-4.37562800	-0.26011800	H	-4.56720200	3.16911900	1.83431600
H	0.87501200	-3.84448700	2.21690400	I	-5.03592200	-1.34728300	-0.88075500
H	0.40554900	-2.81940000	0.05421100	C	-3.28384700	1.50728800	0.32229700
C	3.65962700	-0.36267600	-0.87739300	O	-2.50477200	1.97233200	1.16139400
H	4.46804300	-0.06631100	-0.20514900	C	3.74076500	-3.41306800	-0.69789300
H	4.09429800	-0.90684500	-1.71989200	F	3.54260700	-4.74483100	-0.74669900
N	2.91485700	0.79313200	-1.35690900	F	4.52414400	-3.15824700	0.37410100
C	3.52774800	1.93235200	-2.04068900	F	4.47035000	-3.09293800	-1.79845900
H	2.70366200	2.50347000	-2.47597000	16			
H	4.14363500	1.54867200	-2.86354600	Cu	2.49145400	0.07306900	-0.25335400
C	4.36196800	2.79595200	-1.11389000	O	0.64493400	0.06609500	-0.50297400
C	3.73641500	3.57604800	-0.12966000	C	-1.30913300	1.33523500	0.03885600
C	5.75594700	2.82713500	-1.22383200	C	-2.30625400	0.35171800	-0.02895000
C	4.49620500	4.36785500	0.73060700	C	-1.72282800	2.68005300	0.04361600
H	2.65182000	3.56883700	-0.04537400	C	-3.65765100	0.69804100	-0.10543000
C	6.51832500	3.62291700	-0.36445000	C	-3.06287200	3.03761100	-0.05000900
H	6.24942900	2.23273900	-1.98995900	C	-4.03537500	2.04048800	-0.12838400
C	5.88952000	4.39235800	0.61456300	H	-4.41468200	-0.07717400	-0.14449300
H	4.00103900	4.97275600	1.48510400	H	-3.34699300	4.08623100	-0.05506800
H	7.60027200	3.64040800	-0.46201000	H	-5.08895700	2.29802300	-0.19789800
H	6.48028500	5.01295400	1.28256900	H	-0.94701500	3.43353800	0.12743000
C	1.59004200	0.63012900	-1.19674000	I	-1.91721100	-1.77437100	0.08653100
O	0.71244400	1.42544600	-1.57182100	C	0.18519900	1.11565400	0.10532900

O	0.89639300	1.95032200	0.68444900	H	-4.06094200	2.76049600	1.64112700
C	6.90805500	-0.09423100	0.25448200	C	-3.37719200	3.16171400	-0.36024600
H	7.18363500	-0.93453300	0.89947900	C	-2.29563500	3.52602700	-1.17579800
H	7.24272800	0.83789100	0.72062200	C	-4.67601200	3.25458600	-0.87268600
H	7.40657600	-0.20854600	-0.71320000	C	-2.51356500	3.96321300	-2.48270500
C	5.46387100	-0.06324000	0.06953700	H	-1.28548100	3.46067100	-0.78013500
N	4.31657700	-0.03601200	-0.07454800	C	-4.89590400	3.69640000	-2.17905300
MECP(12-17)				H	-5.52210600	2.97761600	-0.24730400
Cu	0.92199800	0.46454400	1.50986400	C	-3.81409900	4.04969400	-2.98707900
C	-6.85088200	-3.73834500	0.11959600	H	-1.66813300	4.24082800	-3.10665000
C	-5.99104200	-3.58940600	-0.97180100	H	-5.90986200	3.76300700	-2.56468200
C	-5.03845800	-2.57232600	-1.00778300	H	-3.98289700	4.39240600	-4.00439100
C	-4.94077700	-1.66324900	0.07440600	C	-1.35197400	1.03727900	1.29236300
C	-5.80178000	-1.83372700	1.17090100	O	-0.46941400	1.96789200	1.24154300
C	-6.74918200	-2.85912400	1.19533800	O	-0.91338000	-0.17291700	1.46455500
H	-3.12642200	-2.96299800	-1.87820600	O	2.39008800	-0.61532600	0.31287800
H	-7.59034700	-4.53468500	0.12637800	C	4.57319000	0.43968600	0.18638800
H	-6.05769700	-4.27869600	-1.81071200	C	5.13855100	-0.22500100	-0.91608700
C	-4.05946100	-2.44681000	-2.15450800	C	5.40811900	1.25861700	0.97114100
C	-3.94982400	-0.56168500	-0.00465500	C	6.49425600	-0.07248000	-1.21383200
H	-5.74768200	-1.15856700	2.01922200	C	6.76151500	1.39756900	0.68841200
H	-7.40773600	-2.96409200	2.05327000	C	7.30506800	0.72871200	-0.40881200
C	-3.39096500	-0.24260900	-1.18461800	H	6.91859300	-0.57798400	-2.07436100
C	-3.72870500	-0.98082500	-2.45421600	H	7.38639400	2.02383600	1.31814900
H	-2.70660200	0.59663300	-1.25216000	H	8.36046800	0.82776100	-0.64742400
H	-2.89579900	-0.91923800	-3.16357100	H	4.96152300	1.77524700	1.81341800
H	-4.44694500	-2.95255300	-3.04609200	I	4.02724800	-1.46946600	-2.27870700
H	-4.58539200	-0.48866200	-2.94396100	C	1.36488100	-0.65014700	3.23960000
C	-3.63439100	0.18320700	1.28365800	F	0.80663800	-1.85194600	3.14868400
H	-4.55233100	0.61588200	1.69970800	F	0.80873900	0.03975700	4.24586200
H	-3.25732600	-0.52709000	2.02747000	F	2.67320300	-0.77786000	3.45834500
N	-2.67259700	1.28462600	1.18170100	C	3.15013100	0.33969500	0.61890000
C	-3.13679300	2.68142500	1.05885900	O	2.67938700	1.27778200	1.37641000
H	-2.38228500	3.30614800	1.54121100				

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Cu	-0.60525100	1.71321700	0.80581500	C	2.20504900	-5.12342300	0.09620900
C	7.85728000	1.65267000	-1.22751500	H	0.18288400	-4.59133500	-0.43947200
C	6.92781000	1.22311000	-2.17871300	H	4.21872000	-5.39401900	0.82088600
C	5.69056100	0.70556900	-1.79727400	H	2.21652000	-6.02309300	-0.51322700
C	5.36794400	0.60539400	-0.42199800	C	1.18731100	0.42529500	1.46143600
C	6.30844300	1.04744300	0.52286500	O	-0.00282300	0.04395400	1.74759600
C	7.54247700	1.56613800	0.12704100	O	1.27518900	1.57654500	0.84571400
H	3.97452400	1.15543600	-2.98770200	O	-2.16397900	0.46169100	-0.81876800
H	8.81684500	2.05169500	-1.54507100	C	-4.39912200	0.88054400	-0.00391200
H	7.16599800	1.29547000	-3.23781700	C	-5.11053000	-0.26117100	-0.40312600
C	4.65087400	0.30239500	-2.82036600	C	-5.13198800	2.02252500	0.36865000
C	4.05955900	0.02539000	-0.03428900	C	-6.50578100	-0.25527300	-0.43628100
H	6.08981300	0.98359900	1.58457400	C	-6.52184900	2.04022300	0.32142800
H	8.25385100	1.89789800	0.87858300	C	-7.20999400	0.89685800	-0.08328400
C	3.34106500	-0.67672500	-0.92665700	H	-7.04403700	-1.14762600	-0.73572400
C	3.81502700	-0.89023700	-2.34130100	H	-7.06272200	2.93891400	0.60287900
H	2.40860500	-1.14471100	-0.62788900	H	-8.29586100	0.89072800	-0.12176300
H	2.95917400	-1.04214300	-3.00851600	H	-4.58092600	2.90058400	0.68675400
H	5.12580200	0.08486600	-3.78384700	I	-4.17100200	-2.13410300	-0.91262300
H	4.41035400	-1.81694700	-2.38930900	C	-0.69649800	3.47893500	0.01114600
C	3.60911900	0.24623400	1.40105600	F	0.47737100	3.77477400	-0.54740200
H	4.31893400	-0.21802900	2.09566200	F	-0.93279300	4.33418800	1.01736600
H	3.61644600	1.32046200	1.61766800	F	-1.65232400	3.60036700	-0.90881400
N	2.28734000	-0.28131300	1.75798000	C	-2.90152500	0.98915900	0.00819000
C	2.15168900	-1.54267900	2.51703900	O	-2.44155800	1.75114700	0.98660000
H	1.21138600	-1.47473700	3.06824900	8			
H	2.96788000	-1.56370300	3.24696900	Cu	-1.14913800	0.69404900	-0.28409600
C	2.17341300	-2.80086900	1.67086500	N	-1.85112600	2.38698000	-0.50012300
C	1.04422000	-3.16613800	0.92223400	C	-2.30666600	3.43891900	-0.66469100
C	3.31077700	-3.61426800	1.62761700	C	-2.88096400	4.75956900	-0.88379900
C	1.06287800	-4.31861000	0.13686800	H	-3.75474000	4.68233300	-1.53887900
H	0.15455100	-2.54252200	0.95664800	H	-3.19023300	5.20066300	0.06924900
C	3.32873400	-4.77085300	0.84469000	H	-2.14152200	5.41510100	-1.35495200
H	4.18869100	-3.34392100	2.21079300	C	6.02594500	-0.54357700	-1.02397600

C	5.68527700	0.06580500	0.18616300	H	-5.79357900	-1.27594000	-1.57329800
C	4.36260000	0.11023300	0.62652600	H	-6.54790500	-1.00044800	0.78286900
C	3.33368500	-0.46479600	-0.16240700	9-ts			
C	3.69565200	-1.07749700	-1.37433400	Cu	-0.45998200	0.61253200	0.19365800
C	5.02346300	-1.11818800	-1.80258700	N	-0.30447700	2.24478300	1.05014800
H	3.96784400	-0.08432300	2.72014700	C	-0.19541100	3.25207100	1.60863900
H	7.06209500	-0.56661400	-1.35164000	C	-0.05539900	4.51929500	2.31320900
H	6.46191000	0.51287200	0.80383100	H	-0.78348400	5.24215100	1.93177100
C	4.00548900	0.71794200	1.96566700	H	-0.22779200	4.37270700	3.38422300
C	1.92809000	-0.39283100	0.32045900	H	0.95315900	4.91849900	2.16621000
H	2.93303800	-1.52499400	-2.00231700	C	4.27860100	1.85656600	-1.49588600
H	5.26897300	-1.59737100	-2.74701000	C	4.74369400	0.90986100	-0.57934900
C	1.61404700	0.48071100	1.29746300	C	3.95915000	-0.18277100	-0.20688500
C	2.63493500	1.40133100	1.91950400	C	2.66201500	-0.33562400	-0.75412300
H	0.58891500	0.51952400	1.65433500	C	2.21511800	0.61444600	-1.68921400
H	2.32401200	1.69096600	2.93061800	C	3.01138600	1.70048100	-2.05693100
H	4.78618700	1.41693600	2.28895100	H	4.94776700	-2.05171000	0.08043800
H	2.70473300	2.33701700	1.33925600	H	4.90545300	2.69978500	-1.77456900
C	0.89259200	-1.33275600	-0.27832300	H	5.73947700	1.01464900	-0.15276100
H	1.07349500	-1.41929100	-1.36768200	C	4.50187700	-1.26189000	0.70632800
H	1.11781500	-2.34508200	0.11557300	C	1.82638800	-1.48885500	-0.33416300
N	-0.48942400	-1.00191200	0.00379300	H	1.22939900	0.50652200	-2.13019800
C	-1.35674600	-2.13257900	-0.29168400	H	2.63975000	2.41965700	-2.78266700
H	-1.04971100	-3.00666100	0.31695500	C	2.19103500	-2.21875100	0.73839800
H	-1.27951500	-2.47158000	-1.34636400	C	3.40450800	-1.89346200	1.57070900
C	-2.81161400	-1.82700100	0.00184400	H	1.56343900	-3.05084800	1.05128100
C	-3.25154700	-1.66989300	1.32522800	H	3.78742400	-2.79419400	2.06490400
C	-3.74544400	-1.67928700	-1.03139500	H	5.31193900	-0.86539600	1.32976600
C	-4.58523400	-1.37196500	1.60608800	H	3.11352300	-1.20209400	2.37966400
H	-2.53428100	-1.78227400	2.13429100	C	0.54564300	-1.81680400	-1.07647200
C	-5.08344000	-1.38113900	-0.75641800	H	0.69127300	-1.62394300	-2.15613400
H	-3.41835600	-1.80504500	-2.06159600	H	0.35693900	-2.89996600	-0.99131600
C	-5.50695500	-1.22591600	0.56442600	N	-0.62900200	-1.08904600	-0.57449100
H	-4.90930200	-1.26118800	2.63825800	C	-1.76717700	-1.36486400	-1.45789900

H	-1.98360200	-2.44728900	-1.44281300	C	1.80493800	-0.58623900	-0.12537900
H	-1.51640200	-1.11826800	-2.50787700	H	2.98273500	-1.73348400	-2.34570000
C	-3.01508900	-0.60227500	-1.06621600	H	4.79137800	-3.39409500	-2.39069100
C	-3.94568200	-1.14789500	-0.17151500	C	1.58117100	0.08000200	1.01986600
C	-3.26076200	0.67797400	-1.58479400	C	2.38730900	-0.17704600	2.26764400
C	-5.08201300	-0.42960200	0.20701100	H	0.82422100	0.85708300	1.04680700
H	-3.77752100	-2.14625000	0.22447400	H	1.80116200	0.07500300	3.15932200
C	-4.39664500	1.39971100	-1.21189200	H	3.54571300	-1.80108400	3.15104900
H	-2.55900500	1.10387500	-2.29947900	H	3.26609300	0.48916400	2.28176700
C	-5.30975100	0.84756000	-0.31009500	C	1.01005000	-0.32414900	-1.39733000
H	-5.79324100	-0.87093000	0.90070800	H	1.69118700	0.02522800	-2.18503600
H	-4.57458300	2.38620500	-1.63347800	H	0.58412400	-1.27148600	-1.74396200
H	-6.19793000	1.40398300	-0.02151700	N	-0.06792500	0.65283100	-1.30356600
C	-1.13964800	-2.15569400	1.43480600	C	0.13220400	2.02304500	-1.78807500
O	-1.06474100	-1.25849600	2.20788400	H	-0.83038200	2.35737700	-2.18255600
O	-1.30815700	-3.25745500	1.03357900	H	0.84551900	1.98196900	-2.62029100
10				C	0.62534900	3.02081900	-0.75239800
Cu	-3.31254000	-1.04189800	-0.16929800	C	1.92513300	3.53496500	-0.80700700
N	-5.06272500	-1.30995500	0.31032800	C	-0.23112200	3.45397100	0.27231300
C	-6.17640900	-1.42500500	0.60263700	C	2.37063700	4.45869400	0.14224200
C	-7.57855600	-1.56838800	0.96995400	H	2.59713900	3.21029800	-1.59902100
H	-7.66704800	-2.15857700	1.88760600	C	0.21276200	4.37347100	1.22249000
H	-8.02317100	-0.58204100	1.13633600	H	-1.24174800	3.05644400	0.30977300
H	-8.12508900	-2.07404000	0.16753800	C	1.51491600	4.87941000	1.16073300
C	4.95980100	-3.51179500	-0.24347400	H	3.38435100	4.84740300	0.08496600
C	4.46024500	-3.04156000	0.97429300	H	-0.46057200	4.70216100	2.01054900
C	3.43053700	-2.10242600	1.01818900	H	1.85784300	5.59852700	1.90039200
C	2.88028300	-1.60553100	-0.18896100	C	-1.33419400	0.26278300	-0.92064300
C	3.38709700	-2.09349400	-1.40492300	O	-1.48420600	-0.99797100	-0.61829900
C	4.41620600	-3.03644900	-1.43521200	O	-2.28071300	1.08682300	-0.87149700
H	1.95300400	-2.26381400	2.55172800	11			
H	5.76425000	-4.24257200	-0.25732700	Cu	-0.07653100	-1.05360900	-0.64707700
H	4.87499000	-3.41460200	1.90876600	C	-5.65211500	5.37183900	-0.42360700
C	2.83528300	-1.64187300	2.33115000	C	-5.36891700	4.78135700	0.81133700

C	-5.03188300	3.43167800	0.90678400	H	-7.78753500	-3.79703000	2.67645000
C	-4.98080300	2.63449600	-0.26347900	C	-2.62336400	-1.35331800	-1.05316900
C	-5.25912000	3.24439000	-1.49820700	O	-2.32410400	-2.56073600	-0.98894500
C	-5.59169300	4.59785400	-1.58077600	O	-1.77480700	-0.36599100	-0.92671100
H	-3.55634400	2.83945000	2.33216000	O	2.72875200	0.23848800	-0.25910800
H	-5.91547000	6.42510600	-0.47741400	C	3.99715600	-1.75055100	-0.04334800
H	-5.40591500	5.38165500	1.71853200	C	5.19056600	-1.06195600	0.11002900
C	-4.65289700	2.80333100	2.23045800	C	4.06254800	-3.15186500	-0.01103600
C	-4.65070000	1.19379600	-0.14324800	C	6.42787200	-1.65512100	0.28904000
H	-5.22347200	2.65989200	-2.41195800	C	5.28357500	-3.79681200	0.16773600
H	-5.80581900	5.04172600	-2.54979900	C	6.45737900	-3.05506900	0.31621000
C	-4.70772800	0.59359700	1.05771400	H	7.34219300	-1.09017800	0.40419300
C	-5.09521500	1.33763800	2.31022000	H	5.32196100	-4.88137600	0.19097700
H	-4.50987700	-0.47079500	1.13119500	H	7.41115400	-3.55542000	0.45493500
H	-4.65137200	0.85944900	3.19148800	H	3.13576400	-3.70277700	-0.13013300
H	-5.06576600	3.38570600	3.06298400	I	4.92509600	1.12381100	0.03958600
H	-6.18778900	1.27902300	2.44923300	C	7.14660600	1.56741100	0.35589000
C	-4.28667700	0.44381800	-1.41821100	F	7.23837600	2.89784800	0.36034600
H	-5.13156400	0.49860300	-2.11931400	F	7.90041000	1.07427300	-0.62886400
H	-3.44530000	0.95676300	-1.89554800	F	7.59028400	1.08816400	1.51969500
N	-3.93986400	-0.96202800	-1.27318400	C	2.69015200	-1.03298000	-0.23898700
C	-4.93283200	-1.99817000	-1.56652000	O	1.66099300	-1.73823500	-0.36889000
H	-4.38671000	-2.83809200	-2.00335800	MECP(11-12)			
H	-5.61894200	-1.60360500	-2.32653600	Cu	0.07821100	-1.34248200	-0.51645600
C	-5.73910100	-2.49392900	-0.37569100	C	-5.85490300	5.26257500	-0.44970500
C	-5.12226200	-3.27169600	0.61753400	C	-5.52536200	4.70619000	0.79046500
C	-7.10150800	-2.20110300	-0.25224200	C	-5.07784500	3.38836300	0.89557100
C	-5.85609600	-3.73376800	1.71002200	C	-4.95550900	2.59240600	-0.27176100
H	-4.06478800	-3.50031400	0.51600400	C	-5.28414000	3.16798400	-1.51160700
C	-7.83912700	-2.66607100	0.84000300	C	-5.73020200	4.48858900	-1.60307800
H	-7.59162600	-1.60194700	-1.01737900	H	-3.57512700	2.90576000	2.33850300
C	-7.21697700	-3.43316000	1.82544500	H	-6.20620300	6.28981200	-0.51054800
H	-5.36669200	-4.33580700	2.47210600	H	-5.61368000	5.30750800	1.69397900
H	-8.89705000	-2.42771400	0.91986400	C	-4.66574400	2.79385200	2.22532000

C	-4.49716100	1.18727400	-0.14010700	C	6.33077000	-1.31117200	0.24290500
H	-5.20200400	2.58204500	-2.42238700	C	5.63787200	-3.63580900	0.21252100
H	-5.98039300	4.90630000	-2.57533500	C	6.64271200	-2.67249400	0.30139500
C	-4.52500200	0.58590800	1.06266900	H	7.12031600	-0.57712400	0.30893800
C	-5.00746100	1.30140300	2.29987600	H	5.88689000	-4.69105900	0.25955200
H	-4.22869800	-0.45464300	1.15264200	H	7.68046400	-2.97014200	0.41689800
H	-4.56277600	0.85640900	3.19801700	H	3.51088800	-3.96845600	-0.01373800
H	-5.12830900	3.34695900	3.05180900	I	4.43372800	1.14985100	0.00251300
H	-6.09822100	1.16817900	2.39865300	C	6.84857900	1.98727600	0.31887000
C	-4.02396700	0.48856100	-1.40646200	F	6.71362200	3.31138000	0.26533200
H	-4.83449100	0.48327000	-2.14791800	F	7.66854400	1.57983500	-0.65515500
H	-3.20321400	1.07008500	-1.84089800	F	7.36332300	1.63434400	1.49916900
N	-3.57391800	-0.89221200	-1.26536300	C	2.53380400	-1.50509000	-0.17507900
C	-4.47497900	-2.00587900	-1.59316500	O	1.66737300	-2.42972900	-0.24797700
H	-3.84934500	-2.80518300	-1.99756000	12			
H	-5.14558100	-1.66584900	-2.39148900	Cu	0.99827500	-0.98049400	-0.66127100
C	-5.29659900	-2.53949000	-0.43240800	C	-5.83050200	4.71617700	-0.26983200
C	-4.67360500	-3.25396100	0.60326100	C	-5.34218800	4.20578000	0.93602700
C	-6.68099300	-2.34516300	-0.38192900	C	-4.67031000	2.98494900	0.98437800
C	-5.42389700	-3.74988400	1.66923200	C	-4.48305600	2.24060500	-0.20594900
H	-3.59917200	-3.41165000	0.56049700	C	-4.97198200	2.76965300	-1.41173500
C	-7.43502300	-2.84704200	0.68241700	C	-5.63983700	3.99500500	-1.44665300
H	-7.17487400	-1.79585100	-1.18152300	H	-3.02090400	2.77446300	2.32482200
C	-6.80704400	-3.54824600	1.71236800	H	-6.35258900	5.66910100	-0.28642600
H	-4.92963400	-4.30274600	2.46430600	H	-5.48098800	4.76900800	1.85654500
H	-8.51059100	-2.69014700	0.70435900	C	-4.07535300	2.46053900	2.27329600
H	-7.39067600	-3.93956800	2.54202100	C	-3.79168100	0.93080000	-0.13100800
C	-2.26287700	-1.15936000	-0.98271700	H	-4.84092500	2.22433200	-2.34130900
O	-1.83456900	-2.35541100	-0.91351200	H	-6.01039800	4.38000600	-2.39294100
O	-1.44719200	-0.17241300	-0.78880700	C	-3.63083300	0.32074100	1.05524500
O	2.19570200	-0.28484200	-0.25400700	C	-4.12814400	0.92986300	2.34121600
C	3.96898600	-1.88346600	-0.00131000	H	-3.16781600	-0.65978900	1.10130000
C	4.99968300	-0.95064900	0.09501400	H	-3.53228300	0.57014200	3.18794600
C	4.31261800	-3.24258200	0.06129800	H	-4.57910000	2.90813900	3.13778200

H	-5.16106400	0.59250000	2.52822700	C	3.29505100	-0.99350000	-0.20585700
C	-3.31060700	0.32779300	-1.44167600	O	2.63658300	-2.08059100	-0.38582900
H	-4.16205600	0.16708000	-2.11391900	13-ts			
H	-2.64568400	1.04204700	-1.93935700	Cu	1.25244800	0.81488400	0.26725400
N	-2.60991800	-0.95521900	-1.35055700	C	-7.68826000	-2.02717200	-0.10743300
C	-3.30985700	-2.21815200	-1.65367100	C	-6.72359000	-2.97957200	0.22887700
H	-2.55675300	-2.90908800	-2.03824700	C	-5.36641100	-2.74682500	0.00977700
H	-4.01619800	-2.00681400	-2.46402200	C	-4.94568300	-1.51969700	-0.57028200
C	-4.04239200	-2.84732900	-0.48282100	C	-5.93323800	-0.57061500	-0.90137200
C	-3.32893300	-3.53712300	0.50890900	C	-7.28607800	-0.81808800	-0.67350800
C	-5.43473600	-2.75852200	-0.37794900	H	-3.99912000	-3.53115400	1.45559000
C	-3.99849900	-4.11450500	1.58788000	H	-8.74087300	-2.23083700	0.06877200
H	-2.24804100	-3.61610200	0.42700300	H	-7.02991800	-3.92443100	0.67256300
C	-6.10708900	-3.33866800	0.70017200	C	-4.33036100	-3.76461200	0.43363700
H	-5.99896100	-2.23228700	-1.14512500	C	-3.51035700	-1.30532500	-0.84245100
C	-5.38933200	-4.01631600	1.68653300	H	-5.65483000	0.37633500	-1.34989700
H	-3.43522700	-4.64815900	2.34896900	H	-8.02251900	-0.06690500	-0.94574600
H	-7.18906600	-3.26169500	0.76740900	C	-2.63203300	-2.34917600	-0.74595900
H	-5.91019600	-4.47023600	2.52540000	C	-3.10739400	-3.75715900	-0.48870300
C	-1.28504400	-0.96896000	-1.09627900	H	-1.61663900	-2.20608300	-1.10656000
O	-0.61715600	-2.07419100	-1.02249400	H	-2.30723800	-4.36874000	-0.06081400
O	-0.61961400	0.12097700	-0.92060100	H	-4.77684100	-4.76455800	0.47475000
O	2.64188500	0.09701900	-0.28846000	H	-3.36288200	-4.21496400	-1.45843400
C	4.75181100	-1.05840000	0.08937800	C	-2.97849400	0.04839500	-1.30119100
C	5.61009900	0.04117800	0.27652300	H	-2.19684500	-0.10710700	-2.04493700
C	5.29836800	-2.35360400	0.19035800	H	-3.75644400	0.65361800	-1.77195900
C	6.96354300	-0.16300900	0.55628500	N	-2.38174300	0.85827300	-0.22848900
C	6.64328900	-2.55791000	0.46892400	C	-3.25350500	1.55590900	0.72413400
C	7.47833200	-1.45562400	0.65317200	H	-2.63417500	1.81156100	1.58635200
H	7.61820700	0.68919800	0.69892900	H	-4.01977700	0.85190900	1.06563800
H	7.03637300	-3.56745600	0.54161500	C	-3.90160300	2.80338700	0.14914900
H	8.53367700	-1.59330900	0.87225200	C	-3.11147200	3.82027800	-0.40626700
H	4.62771800	-3.19240200	0.04274400	C	-5.28956100	2.97472200	0.19578400
I	5.01617700	2.10825800	0.15888800	C	-3.70046200	4.97905900	-0.90971000

H	-2.03111900	3.70249600	-0.43181200	C	5.86601600	-0.51133000	1.01256100
C	-5.88179900	4.13813000	-0.30401800	C	7.20237400	-0.83802000	1.17635000
H	-5.91106500	2.19331000	0.62720900	H	4.53857900	-4.02786600	-1.23410700
C	-5.08845900	5.14128400	-0.86046400	H	8.68954900	-2.40647500	1.05269800
H	-3.07624900	5.76011900	-1.33576800	H	7.06124100	-4.11930200	0.30474300
H	-6.96132900	4.25665400	-0.26016000	C	4.42857500	-3.88767900	-0.15097800
H	-5.54615300	6.04581700	-1.25200400	C	3.52292000	-1.13556900	0.40303600
C	-1.04276000	0.89132900	-0.08287200	H	5.55911800	0.51210200	1.19803900
O	-0.47608400	1.58304800	0.84867500	H	7.90504400	-0.07658100	1.50405100
O	-0.25921600	0.22186800	-0.86260800	C	2.57763100	-2.13801100	-0.23080100
O	3.01718400	0.05991800	-0.30153300	C	2.96566900	-3.57515800	0.17808000
C	5.01420400	0.64705800	0.96234400	H	1.55680600	-1.93522600	0.11315700
C	6.00848300	0.05346900	0.16337000	H	2.29893300	-4.29808900	-0.30151500
C	5.40650100	1.24712900	2.17559100	H	4.71441900	-4.84144500	0.30882400
C	7.34261300	0.06239000	0.57745600	H	2.80561400	-3.65657700	1.25967400
C	6.73159200	1.25308200	2.59104100	C	2.89926400	0.09209300	1.02664900
C	7.70284800	0.65612000	1.78712100	H	2.13869400	-0.22004500	1.75019300
H	8.10320500	-0.39433100	-0.04553300	H	3.63401900	0.68664500	1.57279200
H	7.00406200	1.71971100	3.53284500	N	2.22039700	0.98900200	0.07849100
H	8.74542400	0.65027300	2.09326000	C	3.04134600	1.81146400	-0.81843300
H	4.63228300	1.70579300	2.78008300	H	2.39386800	2.13004700	-1.63785200
I	5.66139800	-0.88216600	-1.74599400	H	3.82090800	1.16873900	-1.24291000
C	3.55845000	0.70044200	0.65735200	C	3.66459900	3.01217600	-0.13053000
O	2.78505800	1.40999200	1.39495500	C	2.85294400	3.96619600	0.50032200
C	-1.47261900	-2.07941400	1.52045200	C	5.05104800	3.20066200	-0.13627400
F	-1.62514800	-3.22185100	2.20063500	C	3.41984100	5.08050300	1.11660600
F	-2.00600500	-1.06980700	2.20923900	H	1.77392500	3.83356900	0.49670800
F	-0.16914500	-1.85600600	1.31971300	C	5.62141300	4.31982000	0.47745200
14				H	5.68911100	2.46953000	-0.62833900
Cu	-1.42631400	0.84982100	-0.31769900	C	4.80663500	5.26046600	1.10712600
C	7.64467300	-2.14134200	0.91901700	H	2.77962500	5.81366800	1.60013700
C	6.72422300	-3.10192500	0.49324100	H	6.69997400	4.45290500	0.46349800
C	5.37684800	-2.80023600	0.30912200	H	5.24677400	6.13084700	1.58632000
C	4.90466700	-1.46988300	0.57047000	C	0.88117800	0.96023800	-0.04883100

O	0.25464700	1.74416100	-0.86026100	H	3.09293100	-1.89642100	4.53570800
O	0.15097200	0.14064600	0.63799800	C	2.61618100	-1.80805700	-1.41736900
O	-3.12978600	-0.05107600	0.21559100	C	1.47482100	-2.83813500	-1.36825700
C	-5.20425600	0.60202600	-0.87667500	H	2.34046100	-1.00789400	-2.11129700
C	-6.14122400	-0.09683300	-0.09362700	H	1.34451000	-3.29594500	-2.35293000
C	-5.66658300	1.27664700	-2.02413600	H	0.82321000	-4.52453300	-0.18139000
C	-7.48841300	-0.11930100	-0.46149700	H	0.56087100	-2.28448300	-1.13410800
C	-7.00494700	1.25090500	-2.39427500	C	3.63510900	0.10445600	-0.01689800
C	-7.91822900	0.54703300	-1.60912300	H	3.79946500	0.45589700	1.00483600
H	-8.20490300	-0.65675700	0.14910100	H	4.62596700	-0.03729200	-0.46745500
H	-7.33235800	1.77538200	-3.28682000	N	2.94188700	1.13460700	-0.78797600
H	-8.96971800	0.51437800	-1.88107600	C	3.67661400	2.33877800	-1.19534000
H	-4.93656600	1.81731900	-2.61583700	H	3.01265600	2.89143300	-1.86369500
I	-5.68310500	-1.14148000	1.73377100	H	4.54784100	2.01447500	-1.77597400
C	-3.74144400	0.69024500	-0.62115500	C	4.11758400	3.21125800	-0.03203500
O	-3.03270800	1.53065700	-1.28215100	C	3.16563700	3.91137400	0.72627700
C	2.49921300	-1.99658100	-1.75611400	C	5.47082500	3.32768700	0.30505700
F	1.73905300	-2.97408800	-2.29962600	C	3.56453200	4.70421100	1.80156200
F	3.71060200	-2.05154900	-2.35650600	H	2.11397500	3.83698200	0.46220600
F	1.93938900	-0.81912600	-2.12969600	C	5.87207000	4.12570700	1.38005900
MECP(14-15)				H	6.21940600	2.79714600	-0.28079700
Cu	-0.82872600	1.29751800	-0.61950500	C	4.91897000	4.81392300	2.13115900
C	2.26729300	-3.57498000	3.45011200	H	2.81824400	5.24352700	2.37888800
C	1.91392200	-4.06339700	2.19153800	H	6.92720000	4.20853200	1.62727100
C	2.10575000	-3.31272900	1.03248300	H	5.22817500	5.43689600	2.96626800
C	2.67677000	-2.00071300	1.12788700	C	1.58290700	1.14549900	-0.69676000
C	3.01438500	-1.52298800	2.42797600	O	0.88381100	2.11981200	-1.13641000
C	2.82105200	-2.29378700	3.56181700	O	0.98840100	0.12430400	-0.18111700
H	2.51723100	-4.58910000	-0.63334200	O	-2.51888400	0.44977200	-0.04262500
H	2.10399900	-4.18265100	4.33578700	C	-4.70699900	1.45125400	-0.35702100
H	1.47213600	-5.05371100	2.10498200	C	-5.53547700	0.39538000	0.05581400
C	1.72108100	-3.90764600	-0.30325200	C	-5.31901300	2.68309400	-0.65977200
C	2.86961900	-1.19977600	-0.04829800	C	-6.91667600	0.57369100	0.16645300
H	3.43107700	-0.53040100	2.55052000	C	-6.69046000	2.86942100	-0.54658100

C	-7.49309100	1.80834200	-0.12878700	H	-4.62546900	1.05978800	-0.58661700
H	-7.54406400	-0.25196400	0.48204400	N	-3.22945500	-0.39336700	-1.11675200
H	-7.12891700	3.83414000	-0.78402000	C	-4.14712600	-1.42419400	-1.61614800
H	-8.56838800	1.93222600	-0.03365000	H	-3.60850300	-1.95386400	-2.40533300
H	-4.67149400	3.48782000	-0.98771700	H	-5.00584400	-0.91781300	-2.07342300
I	-4.84971100	-1.60062500	0.51456400	C	-4.61953500	-2.38860600	-0.54116100
C	-3.21541000	1.41790500	-0.50396400	C	-3.72173100	-3.30876500	0.02199200
O	-2.63034600	2.38460200	-1.07660300	C	-5.94233500	-2.36668800	-0.08574300
C	3.89681100	-2.39623600	-2.02861500	C	-4.14363200	-4.18464100	1.02113600
F	3.63484700	-3.02881700	-3.19174300	H	-2.69425400	-3.33657300	-0.33139000
F	4.51667300	-3.28284200	-1.21708300	C	-6.36763700	-3.24655200	0.91327700
F	4.80351700	-1.42511300	-2.31006100	H	-6.64796400	-1.65964200	-0.51746700
MECP(14-15) iso				C	-5.46814900	-4.15662200	1.46847600
Cu	0.46771100	-0.98787200	-1.21873800	H	-3.43926400	-4.89352900	1.44857500
C	-2.10799100	4.87817500	-2.56980100	H	-7.39896100	-3.21867500	1.25556000
C	-1.46040100	4.87369000	-1.33436600	H	-5.79534600	-4.84189300	2.24582800
C	-1.62340900	3.82821400	-0.42652600	C	-1.88722700	-0.57808300	-1.18819300
C	-2.48450800	2.73933100	-0.75681600	O	-1.35728100	-1.54569400	-1.83056900
C	-3.11684700	2.75528200	-2.03018100	O	-1.10566400	0.26168600	-0.59160600
C	-2.93565700	3.80446500	-2.91743100	O	2.21193400	-0.31059400	-0.51140200
H	0.10980600	4.29087100	0.74855900	C	4.27121300	-1.57587900	-0.71461000
H	-1.95895800	5.70413600	-3.25951100	C	5.13984100	-0.75082700	0.02044500
H	-0.80443700	5.69922000	-1.06821800	C	4.81251600	-2.73302600	-1.30833600
C	-0.89098100	3.86946700	0.89680500	C	6.49392200	-1.07304100	0.14270700
C	-2.69247600	1.64951800	0.16457600	C	6.15743300	-3.05957900	-1.18885200
H	-3.74281700	1.92190600	-2.32810800	C	7.00321000	-2.22198800	-0.46131500
H	-3.43283300	3.78770000	-3.88289800	H	7.15186500	-0.42747600	0.71296400
C	-2.18017000	1.83809900	1.58256700	H	6.54198100	-3.96079400	-1.65742100
C	-0.78568000	2.49635100	1.56075600	H	8.05942900	-2.45644700	-0.35605000
H	-0.09548900	1.85143000	1.01036400	H	4.13115300	-3.36535400	-1.86607600
H	-1.41223100	4.56055700	1.57877800	I	4.56066500	1.05230800	1.06097400
H	-0.41068300	2.60291100	2.58126900	C	2.80582500	-1.35721300	-0.93583200
C	-3.73285300	0.59002900	-0.15111000	O	2.13505000	-2.23602900	-1.56337300
H	-4.06050100	0.07359200	0.75223700	H	-2.86415500	2.54383800	2.08831700

C	-2.21920000	0.61397900	2.50292400	C	5.75594700	2.82713500	-1.22383200
F	-1.60708400	0.89108900	3.67503200	C	4.49620500	4.36785500	0.73060700
F	-3.49952900	0.27694100	2.81950400	H	2.65182000	3.56883700	-0.04537400
F	-1.63561200	-0.48521900	1.99426900	C	6.51832500	3.62291700	-0.36445000
15				H	6.24942900	2.23273900	-1.98995900
Cu	-1.14688000	1.28200800	-1.17679300	C	5.88952000	4.39235800	0.61456300
C	2.61136100	-0.77508400	4.17401900	H	4.00103900	4.97275600	1.48510400
C	2.20117300	-1.97206200	3.59590600	H	7.60027200	3.64040800	-0.46201000
C	2.18605100	-2.14715000	2.20545300	H	6.48028500	5.01295400	1.28256900
C	2.61121300	-1.08707200	1.38292400	C	1.59004200	0.63012900	-1.19674000
C	3.01068700	0.12296400	1.97475000	O	0.71244400	1.42544600	-1.57182100
C	3.01399900	0.28262200	3.35658000	O	1.30927200	-0.51990700	-0.57335000
H	2.52672300	-4.21868800	1.76481000	O	-2.97008600	1.14057900	-0.88164900
H	2.60674000	-0.66306700	5.25457700	C	-4.75535700	1.39249600	0.67247900
H	1.87392000	-2.79306900	4.22963600	C	-5.64206600	0.38642300	0.26876800
C	1.72818700	-3.47492800	1.63688600	C	-5.26667100	2.41205700	1.49548000
C	2.56459100	-1.19426000	-0.13822700	C	-6.98527700	0.40300000	0.65238300
H	3.31392500	0.96236100	1.35596600	C	-6.60550100	2.45405100	1.86855900
H	3.32437700	1.22857600	3.79029300	C	-7.47035600	1.44559500	1.44197300
C	2.41321900	-2.64523700	-0.65994500	H	-7.65073700	-0.39404200	0.33899600
C	1.33926500	-3.38097700	0.15993700	H	-6.97044900	3.26389000	2.49439200
H	2.08679300	-2.57952800	-1.70361200	H	-8.51913300	1.45727500	1.72705900
H	1.16923800	-4.37562800	-0.26011800	H	-4.56720200	3.16911900	1.83431600
H	0.87501200	-3.84448700	2.21690400	I	-5.03592200	-1.34728300	-0.88075500
H	0.40554900	-2.81940000	0.05421100	C	-3.28384700	1.50728800	0.32229700
C	3.65962700	-0.36267600	-0.87739300	O	-2.50477200	1.97233200	1.16139400
H	4.46804300	-0.06631100	-0.20514900	C	3.74076500	-3.41306800	-0.69789300
H	4.09429800	-0.90684500	-1.71989200	F	3.54260700	-4.74483100	-0.74669900
N	2.91485700	0.79313200	-1.35690900	F	4.52414400	-3.15824700	0.37410100
C	3.52774800	1.93235200	-2.04068900	F	4.47035000	-3.09293800	-1.79845900
H	2.70366200	2.50347000	-2.47597000	16			
H	4.14363500	1.54867200	-2.86354600	Cu	2.49145400	0.07306900	-0.25335400
C	4.36196800	2.79595200	-1.11389000	O	0.64493400	0.06609500	-0.50297400
C	3.73641500	3.57604800	-0.12966000	C	-1.30913300	1.33523500	0.03885600

C	-2.30625400	0.35171800	-0.02895000	C	-3.72870500	-0.98082500	-2.45421600
C	-1.72282800	2.68005300	0.04361600	H	-2.70660200	0.59663300	-1.25216000
C	-3.65765100	0.69804100	-0.10543000	H	-2.89579900	-0.91923800	-3.16357100
C	-3.06287200	3.03761100	-0.05000900	H	-4.44694500	-2.95255300	-3.04609200
C	-4.03537500	2.04048800	-0.12838400	H	-4.58539200	-0.48866200	-2.94396100
H	-4.41468200	-0.07717400	-0.14449300	C	-3.63439100	0.18320700	1.28365800
H	-3.34699300	4.08623100	-0.05506800	H	-4.55233100	0.61588200	1.69970800
H	-5.08895700	2.29802300	-0.19789800	H	-3.25732600	-0.52709000	2.02747000
H	-0.94701500	3.43353800	0.12743000	N	-2.67259700	1.28462600	1.18170100
I	-1.91721100	-1.77437100	0.08653100	C	-3.13679300	2.68142500	1.05885900
C	0.18519900	1.11565400	0.10532900	H	-2.38228500	3.30614800	1.54121100
O	0.89639300	1.95032200	0.68444900	H	-4.06094200	2.76049600	1.64112700
C	6.90805500	-0.09423100	0.25448200	C	-3.37719200	3.16171400	-0.36024600
H	7.18363500	-0.93453300	0.89947900	C	-2.29563500	3.52602700	-1.17579800
H	7.24272800	0.83789100	0.72062200	C	-4.67601200	3.25458600	-0.87268600
H	7.40657600	-0.20854600	-0.71320000	C	-2.51356500	3.96321300	-2.48270500
C	5.46387100	-0.06324000	0.06953700	H	-1.28548100	3.46067100	-0.78013500
N	4.31657700	-0.03601200	-0.07454800	C	-4.89590400	3.69640000	-2.17905300
MECP(12-17)				H	-5.52210600	2.97761600	-0.24730400
Cu	0.92199800	0.46454400	1.50986400	C	-3.81409900	4.04969400	-2.98707900
C	-6.85088200	-3.73834500	0.11959600	H	-1.66813300	4.24082800	-3.10665000
C	-5.99104200	-3.58940600	-0.97180100	H	-5.90986200	3.76300700	-2.56468200
C	-5.03845800	-2.57232600	-1.00778300	H	-3.98289700	4.39240600	-4.00439100
C	-4.94077700	-1.66324900	0.07440600	C	-1.35197400	1.03727900	1.29236300
C	-5.80178000	-1.83372700	1.17090100	O	-0.46941400	1.96789200	1.24154300
C	-6.74918200	-2.85912400	1.19533800	O	-0.91338000	-0.17291700	1.46455500
H	-3.12642200	-2.96299800	-1.87820600	O	2.39008800	-0.61532600	0.31287800
H	-7.59034700	-4.53468500	0.12637800	C	4.57319000	0.43968600	0.18638800
H	-6.05769700	-4.27869600	-1.81071200	C	5.13855100	-0.22500100	-0.91608700
C	-4.05946100	-2.44681000	-2.15450800	C	5.40811900	1.25861700	0.97114100
C	-3.94982400	-0.56168500	-0.00465500	C	6.49425600	-0.07248000	-1.21383200
H	-5.74768200	-1.15856700	2.01922200	C	6.76151500	1.39756900	0.68841200
H	-7.40773600	-2.96409200	2.05327000	C	7.30506800	0.72871200	-0.40881200
C	-3.39096500	-0.24260900	-1.18461800	H	6.91859300	-0.57798400	-2.07436100

H	7.38639400	2.02383600	1.31814900	N	2.28734000	-0.28131300	1.75798000
H	8.36046800	0.82776100	-0.64742400	C	2.15168900	-1.54267900	2.51703900
H	4.96152300	1.77524700	1.81341800	H	1.21138600	-1.47473700	3.06824900
I	4.02724800	-1.46946600	-2.27870700	H	2.96788000	-1.56370300	3.24696900
C	1.36488100	-0.65014700	3.23960000	C	2.17341300	-2.80086900	1.67086500
F	0.80663800	-1.85194600	3.14868400	C	1.04422000	-3.16613800	0.92223400
F	0.80873900	0.03975700	4.24586200	C	3.31077700	-3.61426800	1.62761700
F	2.67320300	-0.77786000	3.45834500	C	1.06287800	-4.31861000	0.13686800
C	3.15013100	0.33969500	0.61890000	H	0.15455100	-2.54252200	0.95664800
O	2.67938700	1.27778200	1.37641000	C	3.32873400	-4.77085300	0.84469000
17				H	4.18869100	-3.34392100	2.21079300
Cu	-0.60525100	1.71321700	0.80581500	C	2.20504900	-5.12342300	0.09620900
C	7.85728000	1.65267000	-1.22751500	H	0.18288400	-4.59133500	-0.43947200
C	6.92781000	1.22311000	-2.17871300	H	4.21872000	-5.39401900	0.82088600
C	5.69056100	0.70556900	-1.79727400	H	2.21652000	-6.02309300	-0.51322700
C	5.36794400	0.60539400	-0.42199800	C	1.18731100	0.42529500	1.46143600
C	6.30844300	1.04744300	0.52286500	O	-0.00282300	0.04395400	1.74759600
C	7.54247700	1.56613800	0.12704100	O	1.27518900	1.57654500	0.84571400
H	3.97452400	1.15543600	-2.98770200	O	-2.16397900	0.46169100	-0.81876800
H	8.81684500	2.05169500	-1.54507100	C	-4.39912200	0.88054400	-0.00391200
H	7.16599800	1.29547000	-3.23781700	C	-5.11053000	-0.26117100	-0.40312600
C	4.65087400	0.30239500	-2.82036600	C	-5.13198800	2.02252500	0.36865000
C	4.05955900	0.02539000	-0.03428900	C	-6.50578100	-0.25527300	-0.43628100
H	6.08981300	0.98359900	1.58457400	C	-6.52184900	2.04022300	0.32142800
H	8.25385100	1.89789800	0.87858300	C	-7.20999400	0.89685800	-0.08328400
C	3.34106500	-0.67672500	-0.92665700	H	-7.04403700	-1.14762600	-0.73572400
C	3.81502700	-0.89023700	-2.34130100	H	-7.06272200	2.93891400	0.60287900
H	2.40860500	-1.14471100	-0.62788900	H	-8.29586100	0.89072800	-0.12176300
H	2.95917400	-1.04214300	-3.00851600	H	-4.58092600	2.90058400	0.68675400
H	5.12580200	0.08486600	-3.78384700	I	-4.17100200	-2.13410300	-0.91262300
H	4.41035400	-1.81694700	-2.38930900	C	-0.69649800	3.47893500	0.01114600
C	3.60911900	0.24623400	1.40105600	F	0.47737100	3.77477400	-0.54740200
H	4.31893400	-0.21802900	2.09566200	F	-0.93279300	4.33418800	1.01736600
H	3.61644600	1.32046200	1.61766800	F	-1.65232400	3.60036700	-0.90881400

C	-2.90152500	0.98915900	0.00819000	H	2.51619100	2.04419400	-0.96363600
O	-2.44155800	1.75114700	0.98660000	H	2.31776900	0.94309900	-2.34050000
18-ts				C	3.49091700	0.13385800	-0.72385300
Cu	-2.10146300	1.72729000	-0.55327500	C	4.17166700	-0.75030300	-1.56785900
N	-1.95050500	3.45778600	0.21838600	C	3.87019300	0.20751000	0.62602000
C	-1.28231100	4.12254700	0.89310200	C	5.21200300	-1.54729800	-1.08187000
C	-0.39354000	4.88378700	1.75469300	H	3.88908700	-0.81303600	-2.61719200
H	0.45287400	4.21935000	1.96680100	C	4.90607500	-0.58859500	1.11342000
H	-0.04334200	5.78674900	1.24543100	H	3.34776100	0.89849300	1.28237800
H	-0.90417200	5.16226800	2.68154900	C	5.58065000	-1.46850200	0.26119300
C	-1.96751100	-4.19409700	1.73990700	H	5.73116300	-2.22791700	-1.75196400
C	-2.73629600	-3.83449800	0.63482200	H	5.19291200	-0.51909400	2.15979200
C	-2.45911000	-2.67119600	-0.09244600	H	6.38953000	-2.08611400	0.64293600
C	-1.37008200	-1.85887600	0.29846900	C	0.56501300	1.23968200	0.46045500
C	-0.60620700	-2.22839800	1.41908100	O	1.10989000	2.24241700	0.94893800
C	-0.90101200	-3.38285400	2.13682900	O	-0.51274800	0.65020500	0.89877700
H	-2.83403900	-2.63739300	-2.21448200	19			
H	-2.20534800	-5.09739900	2.29578800	Cu	-2.82881000	0.27538100	-0.54413300
H	-3.57286200	-4.45955200	0.33067500	N	-3.85709300	1.80337300	-0.10820300
C	-3.30088100	-2.27397300	-1.28528900	C	-4.36656000	2.75043100	0.31861800
C	-1.00440600	-0.69517900	-0.56014400	C	-4.99241600	3.94302100	0.87346300
H	0.20008300	-1.57943400	1.74099300	H	-4.38446200	4.32416500	1.70025900
H	-0.30543600	-3.64598100	3.00660700	H	-5.07558000	4.71730500	0.10445100
C	-2.02648700	-0.09754600	-1.36626600	H	-5.99244900	3.70240200	1.24751800
C	-3.42088500	-0.74668700	-1.33504400	C	1.98304000	-4.66291700	0.64767800
H	-1.67858700	0.15774700	-2.37329000	C	0.69136300	-4.76988000	0.14172900
H	-3.98457300	-0.42742400	-2.21847600	C	-0.08602500	-3.63425300	-0.13383200
H	-4.28709500	-2.75023500	-1.22146800	C	0.46337900	-2.36033800	0.09720400
H	-4.00376700	-0.42564800	-0.46138600	C	1.75954300	-2.26440800	0.63086000
C	0.45540700	-0.63594100	-1.03331000	C	2.51939800	-3.39788600	0.90186500
H	1.02651700	-1.45692000	-0.57821200	H	-1.48046600	-3.91993400	-1.74627900
H	0.48079500	-0.78817500	-2.12068700	H	2.56338100	-5.55826500	0.85602600
N	1.03881700	0.65450100	-0.71995800	H	0.26112200	-5.75337500	-0.03696900
C	2.35374300	1.00056600	-1.24480600	C	-1.49965700	-3.79731100	-0.65121700

C	-0.32249400	-1.07936900	-0.19589800	C	6.31839200	-1.06212200	-0.00030900
H	2.17754700	-1.28469900	0.84784100	C	7.60072900	-1.74967600	-0.00109600
H	3.52042200	-3.29586700	1.31262900	H	8.40152000	-1.03894500	-0.22926500
C	-1.71208700	-1.28612800	-0.81771200	H	7.78372100	-2.19346800	0.98278400
C	-2.36882000	-2.58112400	-0.30686200	H	7.59628400	-2.54102000	-0.75751800
H	-1.54904200	-1.41602700	-1.90108500	O	0.81800800	-0.46320800	0.00020000
H	-3.36425500	-2.70552900	-0.75066100	C	-0.23281700	1.65967700	0.00002600
H	-1.92891900	-4.72464600	-0.24810100	C	-1.51834100	1.12882500	-0.00014100
H	-2.51333500	-2.53526500	0.78140100	C	-0.12503200	3.05918300	-0.00007100
C	0.50488900	-0.04182600	-1.01711000	C	-2.67868300	1.88125400	-0.00041000
H	1.55234800	-0.34110000	-1.14705000	C	-1.26491100	3.85923500	-0.00033200
H	0.06399400	0.10943900	-2.00928600	C	-2.53183400	3.27508800	-0.00050500
N	0.39123200	1.15793100	-0.21196800	H	-3.66773900	1.44490800	-0.00055100
C	1.06066100	2.40922300	-0.52657700	H	-1.16598900	4.93988700	-0.00040700
H	0.64935600	3.14955000	0.16623200	H	-3.42420400	3.89355300	-0.00071900
H	0.78617600	2.70713700	-1.54644100	H	0.86951400	3.49120700	0.00005900
C	2.57417000	2.34543700	-0.39383600	I	-1.58676900	-1.07560100	0.00004100
C	3.40396900	2.43377400	-1.51615700	C	-3.86873100	-1.23510800	-0.00002900
C	3.15853000	2.18222600	0.87200900	F	-4.11295400	-2.53734600	0.00016500
C	4.79360100	2.36103600	-1.38425600	F	-4.37934400	-0.66915500	-1.08518000
H	2.96059100	2.56244500	-2.50172500	F	-4.37942900	-0.66881000	1.08489900
C	4.54445700	2.10679700	1.00518800	C	0.98286800	0.78420000	0.00024700
H	2.51700800	2.12076200	1.74766400	O	2.11553000	1.36683200	0.00045600
C	5.36605200	2.19605100	-0.12302000	MECP(20-16)			
H	5.42528400	2.43077300	-2.26609300	Cu	3.58943100	0.47224800	0.03732800
H	4.98569800	1.98368500	1.99090900	O	1.40517400	-0.05579800	0.01110600
H	6.44621800	2.13889500	-0.01712700	C	-0.04896800	1.87210900	0.00464200
C	-0.10480300	0.89928000	1.04306500	C	-1.25276800	1.15448800	-0.02791900
O	-0.21715100	1.69572600	1.95877600	C	-0.10458000	3.27694400	0.01055500
O	-0.47600900	-0.40048100	1.12194000	C	-2.48366200	1.79589500	-0.05771400
20				C	-1.32903100	3.93483500	-0.01697300
Cu	3.68611300	0.36789600	0.00046600	C	-2.51308400	3.19533700	-0.05192600
N	5.29939900	-0.51611600	0.00020800	H	-3.41005100	1.23590800	-0.08964600
				H	-1.36075600	5.01913900	-0.01311800

H	-3.47418600	3.70089300	-0.07588700	H	-2.53987200	-4.69401800	-2.81322100
H	0.82918100	3.82920600	0.03577900	C	-2.34953200	-1.46511700	2.03400400
I	-1.20928800	-0.99987200	-0.03096100	C	-1.48665000	-2.40958200	2.83194200
C	-4.42247300	-1.45489600	0.04492600	H	-2.62851200	-0.51146400	2.47589900
F	-4.65521200	-2.75001200	0.00402900	H	-1.65645800	-2.23608600	3.90043400
F	-4.86513700	-0.82940600	-1.03452700	H	-0.41836700	-2.19524400	2.67133300
F	-4.88014200	-0.89403900	1.15047600	C	-3.92738300	-0.90897400	0.14969700
C	1.26596100	1.21660900	0.02377300	H	-3.53755800	-0.55142700	-0.80741300
O	2.34767700	1.90471000	0.04933900	H	-4.80571800	-1.52408600	-0.08818300
C	6.86371400	-2.58567700	-0.04676000	N	-4.36302900	0.23619900	0.92473000
H	7.59742000	-2.33174900	-0.81886200	C	-5.54569100	0.07360600	1.78714000
H	6.42172700	-3.56120700	-0.27422300	H	-5.58619900	0.96277200	2.41827100
H	7.36344600	-2.63269700	0.92651500	H	-5.37707900	-0.79638800	2.43357700
C	5.81731300	-1.57677000	-0.01285900	C	-6.84261200	-0.09935500	1.01811800
N	4.97986500	-0.78069900	0.01229200	C	-7.37399900	0.97150100	0.28206500
21-ts				C	-7.52476600	-1.32140100	1.02456200
Cu	-2.69396300	3.46201000	-0.32966400	C	-8.56024300	0.81502600	-0.43294700
N	-2.39198700	5.24742500	-0.65660800	H	-6.85379500	1.92570600	0.28586200
C	-2.28057300	6.38503900	-0.83449700	C	-8.71530300	-1.47915800	0.30889500
C	-2.14573900	7.81761000	-1.05781000	H	-7.13008100	-2.15416900	1.60391200
H	-2.67628200	8.36681000	-0.27345500	C	-9.23361400	-0.41094400	-0.42260900
H	-1.08870100	8.10130100	-1.04127300	H	-8.96670200	1.65250400	-0.99382800
H	-2.57195200	8.08364400	-2.03036300	H	-9.23553400	-2.43300000	0.32693600
C	-1.74917500	-5.50911200	-0.97749400	H	-10.16022400	-0.52853200	-0.97768500
C	-1.53738700	-5.28959900	0.38620600	C	-3.88873600	1.50581000	0.65137700
C	-1.92533500	-4.09335300	0.98920300	O	-4.40228400	2.51939600	1.16573300
C	-2.53717100	-3.08599000	0.20113200	O	-2.86332700	1.57233300	-0.16510700
C	-2.75410600	-3.32306000	-1.16858600	O	6.26350500	-1.11589800	0.08028700
C	-2.36255300	-4.52524800	-1.75515600	C	4.26473700	-1.42510100	-1.14055200
H	-1.44324500	-6.44915400	-1.42766800	C	2.96376200	-1.06715900	-1.50621400
H	-1.07318300	-6.06408400	0.99173900	C	4.67500800	-2.73122700	-1.46359700
C	-1.78877000	-3.87468300	2.48053900	C	2.10845600	-1.93845300	-2.17940400
C	-2.90385000	-1.80510700	0.83861900	C	3.83945200	-3.62006000	-2.13423400
H	-3.23039700	-2.56615900	-1.78407100	C	2.55332700	-3.22306600	-2.49785000

H	1.11201900	-1.62533400	-2.47239500	H	-0.99571800	-2.45070000	4.54239000
H	4.19458500	-4.61702500	-2.37728200	H	-3.22671000	-2.23927200	3.51633800
H	1.89170800	-3.90067500	-3.02971400	C	-3.87938800	-1.35241900	1.05991600
H	5.67853800	-3.02179000	-1.17547400	C	-1.42795900	-0.54315000	-0.37858700
I	2.10908000	0.87578000	-1.02389000	H	0.86175500	-0.91468400	1.00027600
C	-0.43216000	-0.37008600	0.22764200	H	1.05395100	-1.80188400	3.28824500
F	-1.03889700	-0.35767800	-0.88436100	C	-2.75705700	-0.58689000	-1.09391700
F	0.23847800	-1.40564500	0.54565100	C	-3.94681500	-0.40454100	-0.13733300
F	-0.49548800	0.61360000	1.02549600	H	-4.87937300	-0.54442400	-0.69070900
C	5.26711500	-0.49688100	-0.48054200	H	-3.92939300	0.63343200	0.20905100
O	5.11726000	0.72543500	-0.52299900	C	-0.23768200	-0.07482200	-1.19584700
H	-1.02234000	-4.53564600	2.89820500	H	0.45774200	-0.91881300	-1.29263100
H	-2.73751700	-4.15902800	2.95948600	H	-0.58675200	0.17574500	-2.20413900
Cu	7.53725400	0.03687300	0.77667300	N	0.50890900	1.04015000	-0.63678800
N	8.88547600	1.06924100	1.48174600	C	-0.02200800	2.37773700	-0.92069500
C	9.73996100	1.72273400	1.90580000	H	-0.13791600	2.51007300	-2.00745000
C	10.81675800	2.54576300	2.43743700	H	0.75171400	3.07497200	-0.59019100
H	11.39633200	1.97334300	3.16859200	C	-1.33753000	2.67218600	-0.23135700
H	11.47844700	2.86151600	1.62458200	C	-2.43659000	3.14125600	-0.96587500
H	10.40076100	3.43289100	2.92534500	C	-1.45893500	2.55780300	1.16414300
22				C	-3.62733900	3.49385300	-0.32573300
Cu	4.19838400	-0.23623700	-0.23034800	H	-2.35023400	3.25638800	-2.04430900
N	6.03248000	-0.26910300	-0.09180900	C	-2.64649900	2.90733400	1.80610500
C	7.18613900	-0.23996100	-0.01976200	H	-0.60810800	2.21029000	1.74428400
C	8.63847000	-0.19967800	0.07018000	C	-3.73460000	3.37815800	1.06315300
H	8.96068900	0.78842500	0.41390700	H	-4.46439200	3.86847000	-0.90808000
H	8.98929900	-0.95772100	0.77761700	H	-2.71946700	2.83141200	2.88763400
H	9.07684800	-0.39714700	-0.91323900	H	-4.65506600	3.66381500	1.56442200
C	-1.08213700	-2.05823000	3.53268000	C	1.89587200	0.91267400	-0.42850100
C	-2.34820000	-1.93818500	2.95299100	O	2.60192500	1.90770000	-0.25100400
C	-2.50318100	-1.43692200	1.66587300	O	2.32691400	-0.32618900	-0.40033800
C	-1.32299000	-1.03162000	0.93506900	C	-2.85570800	-1.88498400	-1.92596700
C	-0.03393500	-1.17325000	1.55598700	F	-2.77307500	-2.98860200	-1.15322400
C	0.07736400	-1.68449000	2.83035000	F	-1.85792300	-1.95215400	-2.83091900

F	-4.02065600	-1.92383200	-2.58576500	C	-3.10433000	2.41181300	0.50150000
H	-4.59759600	-1.04460100	1.82752100	C	-3.92915700	3.59003900	0.71178200
H	-4.17325000	-2.36750900	0.76029700	H	-3.47512700	4.44674100	0.20291000
H	-2.77243900	0.21534800	-1.83830100	H	-4.93122800	3.41555900	0.30665200
23-ts				H	-4.00403300	3.80183100	1.78335100
Cu	-1.15295800	0.68284200	-0.09957700	O	-0.03557000	1.43642100	-0.87386200
N	-3.03367200	1.06525500	0.15219000	C	2.29081400	1.17540500	-0.13032700
C	-4.07309800	1.56363500	0.24760100	C	2.32472100	-0.16887700	0.22673300
C	-5.37804600	2.19515600	0.36714400	C	3.42017500	1.93387700	0.22610300
H	-5.28212400	3.26882900	0.17435200	C	3.37215900	-0.77652000	0.90852900
H	-6.07106500	1.75934800	-0.35967900	C	4.49833100	1.36538500	0.90224000
H	-5.77210100	2.04539400	1.37748400	C	4.47608500	0.01449000	1.24635500
O	0.05022900	2.10847300	-0.23131800	H	3.34805100	-1.82616300	1.18148600
C	2.30846700	1.22630900	0.17825100	H	5.35373300	1.98019700	1.16307900
C	2.20227800	-0.15608900	0.04529100	H	5.30577000	-0.43690500	1.78150000
C	3.52334600	1.66765500	0.73571400	H	3.41833000	2.98334800	-0.04963800
C	3.16874100	-1.08350100	0.43580200	I	0.72938800	-1.53739500	-0.37422800
C	4.52013800	0.78311900	1.14708100	C	-2.51307200	-1.29884600	0.27800000
C	4.34774500	-0.59359400	0.99968700	F	-2.19143500	-2.53062300	-0.12704300
H	3.02239400	-2.15035100	0.30914000	F	-3.64183100	-0.93494700	-0.32601800
H	5.43476000	1.17368100	1.58212600	F	-2.66211900	-1.28253100	1.59999300
H	5.11684800	-1.29139700	1.31571900	C	1.19404900	1.91087000	-0.86084700
H	3.65386100	2.74064200	0.82386700	O	1.44197600	2.96346900	-1.42283300
I	0.49564600	-1.09700000	-0.97530900	MECP(24-25)			
C	-1.59153500	-1.93284000	0.73470500	Cu	0.92199800	0.46454400	1.50986400
F	-2.72898000	-1.99764700	0.09650900	C	-6.85088200	-3.73834500	0.11959600
F	-1.63504900	-1.24424900	1.84875800	C	-5.99104200	-3.58940600	-0.97180100
F	-1.04880400	-3.10626300	0.89959300	C	-5.03845800	-2.57232600	-1.00778300
C	1.33196900	2.34172100	-0.21277000	C	-4.94077700	-1.66324900	0.07440600
O	1.80666100	3.44148700	-0.44168400	C	-5.80178000	-1.83372700	1.17090100
24				C	-6.74918200	-2.85912400	1.19533800
Cu	-1.15519900	0.11607400	-0.16793600	H	-3.12642200	-2.96299800	-1.87820600
N	-2.44910400	1.47701800	0.33223400	H	-7.59034700	-4.53468500	0.12637800
				H	-6.05769700	-4.27869600	-1.81071200

C	-4.05946100	-2.44681000	-2.15450800	C	5.40811900	1.25861700	0.97114100
C	-3.94982400	-0.56168500	-0.00465500	C	6.49425600	-0.07248000	-1.21383200
H	-5.74768200	-1.15856700	2.01922200	C	6.76151500	1.39756900	0.68841200
H	-7.40773600	-2.96409200	2.05327000	C	7.30506800	0.72871200	-0.40881200
C	-3.39096500	-0.24260900	-1.18461800	H	6.91859300	-0.57798400	-2.07436100
C	-3.72870500	-0.98082500	-2.45421600	H	7.38639400	2.02383600	1.31814900
H	-2.70660200	0.59663300	-1.25216000	H	8.36046800	0.82776100	-0.64742400
H	-2.89579900	-0.91923800	-3.16357100	H	4.96152300	1.77524700	1.81341800
H	-4.44694500	-2.95255300	-3.04609200	I	4.02724800	-1.46946600	-2.27870700
H	-4.58539200	-0.48866200	-2.94396100	C	1.36488100	-0.65014700	3.23960000
C	-3.63439100	0.18320700	1.28365800	F	0.80663800	-1.85194600	3.14868400
H	-4.55233100	0.61588200	1.69970800	F	0.80873900	0.03975700	4.24586200
H	-3.25732600	-0.52709000	2.02747000	F	2.67320300	-0.77786000	3.45834500
N	-2.67259700	1.28462600	1.18170100	C	3.15013100	0.33969500	0.61890000
C	-3.13679300	2.68142500	1.05885900	O	2.67938700	1.27778200	1.37641000
H	-2.38228500	3.30614800	1.54121100	25			
H	-4.06094200	2.76049600	1.64112700	Cu	-2.28809400	0.52027700	-0.27791000
C	-3.37719200	3.16171400	-0.36024600	N	-3.96683600	0.06720900	-1.12069000
C	-2.29563500	3.52602700	-1.17579800	C	-5.00745700	-0.21459200	-1.53732300
C	-4.67601200	3.25458600	-0.87268600	C	-6.31723100	-0.56898000	-2.06021300
C	-2.51356500	3.96321300	-2.48270500	H	-6.26759800	-0.66826600	-3.14931100
H	-1.28548100	3.46067100	-0.78013500	H	-6.64195700	-1.51955300	-1.62464800
C	-4.89590400	3.69640000	-2.17905300	H	-7.03988500	0.21163300	-1.80109300
H	-5.52210600	2.97761600	-0.24730400	O	0.31497800	-0.64364300	-0.21419000
C	-3.81409900	4.04969400	-2.98707900	C	1.81153500	1.22753200	-0.24212300
H	-1.66813300	4.24082800	-3.10665000	C	2.95686400	0.42752500	-0.18688000
H	-5.90986200	3.76300700	-2.56468200	C	1.97239600	2.62160700	-0.26552300
H	-3.98289700	4.39240600	-4.00439100	C	4.23727700	0.95646100	-0.15406600
C	-1.35197400	1.03727900	1.29236300	C	3.24761200	3.17829700	-0.23244700
O	-0.46941400	1.96789200	1.24154300	C	4.37170500	2.35057200	-0.17757000
O	-0.91338000	-0.17291700	1.46455500	H	5.11564300	0.32211700	-0.11029700
O	2.39008800	-0.61532600	0.31287800	H	3.36696500	4.25658100	-0.24798800
C	4.57319000	0.43968600	0.18638800	H	5.36728100	2.78314600	-0.15110500
C	5.13855100	-0.22500100	-0.91608700	H	1.08551100	3.24542000	-0.30576600

I	2.65955300	-1.70452100	-0.15182400	C	-2.36188200	1.07079400	-0.75900800
C	-2.54855000	0.00031700	1.66551800	C	-3.39384400	0.76164100	0.13903400
F	-2.87168300	-1.30277600	1.73459200	C	-2.01588100	2.41345400	-0.94876600
F	-3.56230400	0.72541100	2.17090500	C	-4.06440300	1.77454300	0.82394600
F	-1.45003300	0.21546100	2.40313900	H	-3.66114800	-0.27798800	0.30154000
C	0.46488200	0.62607700	-0.27439000	C	-2.68848300	3.43077200	-0.26671100
O	-0.56469300	1.36592700	-0.36662700	H	-1.21107400	2.66513200	-1.63633800
26				C	-3.71560900	3.11327000	0.62217700
C	4.49147800	0.92531200	1.95999000	H	-4.86306100	1.51935000	1.51602000
C	4.60626300	0.86521100	0.56856100	H	-2.40456600	4.46786900	-0.42616400
C	3.56886700	0.36740500	-0.21928000	H	-4.23967700	3.90142200	1.15659600
C	2.37738000	-0.08758500	0.39559100	C	-2.79246400	-3.33253500	0.75034900
C	2.27416500	-0.01750600	1.79459900	O	-3.83142300	-2.81199400	0.88140600
C	3.31993300	0.48281200	2.57179700	O	-1.77441200	-3.89919400	0.63855700
H	3.18975200	1.26970000	-2.12073400	H	-1.00585100	-1.94997900	-1.25673900
H	5.31167200	1.31390800	2.55772600	27-ts			
H	5.51726400	1.21302900	0.08573900	C	-5.58038600	-2.72698000	-0.54974400
C	3.65948800	0.35295100	-1.73010900	C	-5.92656600	-1.42501100	-0.17886100
C	1.28908600	-0.63692800	-0.45046500	C	-4.97235800	-0.54604500	0.33189100
H	1.37436000	-0.36671700	2.29087100	C	-3.62879200	-0.97448700	0.47661100
H	3.21675700	0.52244300	3.65290800	C	-3.29340900	-2.28696200	0.10601900
C	1.55800900	-1.00094800	-1.71757600	C	-4.26196000	-3.15373700	-0.40390900
C	2.93019500	-0.85677300	-2.32708800	H	-5.09284600	1.54632100	-0.12897300
H	0.77955600	-1.44930700	-2.33134200	H	-6.33731900	-3.39910100	-0.94599000
H	2.85748900	-0.75190500	-3.41606300	H	-6.95505200	-1.08584600	-0.28608800
H	4.70710000	0.37567100	-2.05163700	C	-5.33531200	0.87395900	0.70978800
H	3.51293700	-1.77522800	-2.14579000	C	-2.63820300	-0.03310500	1.06101700
C	-0.08334400	-0.83754400	0.19108200	H	-2.27257000	-2.63945200	0.21031000
H	-0.01222900	-1.65397300	0.92335400	H	-3.97691000	-4.16323400	-0.68752300
H	-0.34649800	0.05919800	0.76463400	C	-3.08159200	1.03520300	1.75702300
N	-1.21655400	-1.13655600	-0.68380800	C	-4.54753600	1.33278600	1.94232200
C	-1.65550400	-0.02378500	-1.53999800	H	-2.36179400	1.69565300	2.23848600
H	-2.35198500	-0.45112500	-2.27411300	H	-4.70289100	2.40412400	2.11779100
H	-0.82894100	0.42652800	-2.11227500	H	-6.41467700	0.96125100	0.87956000

H	-4.92164300	0.81542000	2.84161600	C	4.26158500	1.01933800	1.88716200
C	-1.14191800	-0.28520500	0.98731500	H	4.89401500	0.74430500	2.73723800
H	-0.66154900	0.45882500	1.63258200	H	4.77524200	1.83034500	1.35022700
H	-0.88522900	-1.27245700	1.38035000	C	2.89638800	1.48337900	2.37496500
N	-0.47933200	-0.24631700	-0.35497700	H	2.48162800	0.74659300	3.07318500
C	-1.04564700	0.71417500	-1.34537500	H	3.00024200	2.43216500	2.91209100
H	-2.12405000	0.80075800	-1.18620000	N	1.96199800	0.40394000	0.37278900
H	-0.88037600	0.24142800	-2.31455300	C	1.97895900	1.63094500	1.17047100
C	-0.41114800	2.09158300	-1.33161300	H	0.95415900	1.85546300	1.47241200
C	-0.95417600	3.14410700	-0.58110800	H	2.30164900	2.46552800	0.53428600
C	0.73147400	2.34611800	-2.10549400	H	2.10918200	-1.27755300	-1.37679300
C	-0.36567100	4.41127400	-0.58985600	H	4.67471200	-1.13922500	-1.78561700
H	-1.85199400	2.96714000	0.00595000	H	4.60831800	-3.96178200	-0.61476600
C	1.32378600	3.60997900	-2.11724800	H	4.41872000	-2.76322000	1.44143800
H	1.14952400	1.54248400	-2.70715000	H	6.01349100	-0.55240600	0.06346900
C	0.77791800	4.64757400	-1.35574700	H	0.81632900	0.07974300	-0.06339300
H	-0.80589000	5.21617700	-0.00621000				
H	2.20319600	3.78974800	-2.73103400	28			
H	1.23265000	5.63485700	-1.37014700	C	-4.53454000	-1.89020700	1.09080100
C	-0.19740900	-1.68823600	-0.97707700	C	-4.57539000	-1.18215600	-0.11448600
O	-0.00743600	-1.65666300	-2.19568500	C	-3.52429300	-0.34931900	-0.49707900
O	-0.10083100	-2.56915200	-0.11179600	C	-2.39148400	-0.21058500	0.34317300
C	5.03669500	-2.95245100	-0.64175700	C	-2.36409700	-0.92870900	1.55071500
C	4.11622100	-2.01735700	-1.43440100	C	-3.42281700	-1.75969300	1.92235400
C	2.87223900	-1.56550800	-0.65333400	H	-2.96836500	-0.21246400	-2.55733800
C	5.25077100	-2.45810800	0.79592900	H	-5.36467700	-2.53310600	1.37509100
C	3.01415800	-0.38209400	0.29152300	H	-5.43984900	-1.27886900	-0.77006800
C	5.40842800	-0.93587100	0.89773200	C	-3.52970100	0.38521300	-1.82054600
H	6.00319400	-3.03688000	-1.15564600	C	-1.29212200	0.69918100	-0.05500200
H	3.76778200	-2.52730300	-2.33889100	H	-1.51005500	-0.82370200	2.21169100
H	2.42827500	-2.40421400	-0.10236800	H	-3.37743400	-2.30056100	2.86502900
H	6.15071600	-2.92108600	1.21875100	C	-1.52099600	1.62651300	-1.00310100
H	5.96521400	-0.70524800	1.80984500	C	-2.85054600	1.75614500	-1.70303500
N	4.15211200	-0.16167800	1.01020700	H	-0.72291000	2.32927400	-1.22906200

H	-2.72189000	2.19424400	-2.70134500	H	-9.73026700	-1.38462300	-1.37396300
H	-4.55426600	0.47834900	-2.20363200	H	-8.90966800	-1.94319300	0.90374500
H	-3.50483600	2.45060100	-1.14770500	C	-6.53265300	-1.27103400	2.05593700
C	0.04284300	0.61428900	0.67842900	C	-4.80769600	0.14261400	0.24314500
H	-0.06172600	1.04430100	1.68374000	H	-6.02584400	0.61436700	-2.19884800
H	0.30322900	-0.45397200	0.79929500	H	-8.26619700	-0.08241900	-2.91852300
N	1.11753500	1.35689900	0.07218600	C	-4.28810900	-0.45167800	1.33473900
C	1.80682700	0.75711600	-1.05478800	C	-5.02234700	-1.52578400	2.09807900
H	2.46030600	1.54076100	-1.44715900	H	-3.30046200	-0.15159000	1.67173800
H	1.07777900	0.48178100	-1.83293400	H	-4.67610700	-1.56264700	3.13821200
C	2.65415700	-0.46749900	-0.72181000	H	-7.08902900	-2.11356300	2.48426700
C	3.76582200	-0.33471300	0.12917700	H	-4.79824300	-2.51516600	1.66472900
C	2.35790700	-1.73373200	-1.23993000	C	-4.06011600	1.22792100	-0.51565900
C	4.55301800	-1.44207900	0.44202000	H	-4.16743900	1.03574400	-1.60273600
H	3.98259700	0.65514100	0.52474900	H	-4.61900500	2.17251700	-0.35225600
C	3.14546100	-2.84682100	-0.92568200	N	-2.67438400	1.41577500	-0.13508800
H	1.49811200	-1.84931300	-1.89868600	C	-2.17913700	2.68097800	-0.65117800
C	4.24784400	-2.70350200	-0.08314400	H	-2.86629800	3.49408200	-0.33636300
H	5.41284600	-1.32319500	1.09892600	H	-2.16792900	2.73654300	-1.76093100
H	2.89405300	-3.82343500	-1.33607000	C	-0.79094100	3.03801800	-0.14886100
H	4.86420500	-3.56569700	0.16496400	C	-0.49610000	2.99447700	1.22289200
C	1.83717300	2.35610800	0.89568400	C	0.21202300	3.46044000	-1.02914400
O	2.92520700	2.74922900	0.40491100	C	0.76156700	3.36409700	1.69798100
O	1.25975900	2.67805500	1.9566780	H	-1.26957600	2.66118600	1.90874000
29				C	1.47435900	3.83738300	-0.55999000
Cu	-1.51263900	-0.02578900	-0.23540100	H	-0.00115400	3.49894800	-2.09547600
C	-8.74009300	-1.06598100	-1.05823700	C	1.75446600	3.79074400	0.80808400
C	-8.27462400	-1.38222300	0.22052700	H	0.96607100	3.33420300	2.76598100
C	-7.00694000	-0.98672800	0.64721000	H	2.23116100	4.18232500	-1.26186300
C	-6.16093800	-0.25719600	-0.22648000	H	2.72555500	4.10980600	1.18193300
C	-6.64825900	0.05763800	-1.50672500	O	1.36434600	0.07930500	-0.14696100
C	-7.92082900	-0.33958300	-1.92019400	C	2.01654300	-2.19401200	-0.18372700
H	-6.75374000	-0.39414100	2.68591200	C	3.36592700	-1.87206800	-0.13138500
				C	1.68347000	-3.55560700	-0.24250900

C	4.39230800	-2.80030900	-0.13559000	H	-4.15738600	-2.39462500	1.75019100
C	2.68236900	-4.52540000	-0.24429600	C	-4.26951500	1.50972900	-0.25566000
C	4.02707900	-4.15140900	-0.19062300	H	-4.60210300	1.52817400	-1.30850800
H	5.43625600	-2.52235000	-0.09670400	H	-4.80268100	2.36128700	0.21215800
H	2.41419500	-5.57646700	-0.28850900	N	-2.83988800	1.73394400	-0.19545200
H	4.80829800	-4.90586300	-0.18992800	C	-2.49876400	3.11277900	-0.49207900
H	0.63154500	-3.81720400	-0.28613900	H	-3.09899600	3.78725200	0.14962500
I	3.71199800	0.30981800	-0.05247300	H	-2.78133100	3.37798300	-1.53170500
C	5.98691800	0.07560300	0.03137100	C	-1.03264500	3.43702700	-0.29452400
F	6.46659700	1.32132800	0.09025500	C	-0.49972900	3.54527400	0.99817400
F	6.47799900	-0.53072900	-1.05510900	C	-0.18645800	3.65837400	-1.38769800
F	6.38849300	-0.59964400	1.11336700	C	0.84263800	3.86833600	1.19294600
C	0.96129700	-1.12823800	-0.18424100	H	-1.14738900	3.37745100	1.85487200
O	-0.24633100	-1.47280200	-0.22967300	C	1.15954800	3.98231400	-1.19885400
MECP(29-30)				H	-0.58885300	3.58388900	-2.39539900
Cu	-1.61835400	0.35643200	-0.22558500	C	1.67643100	4.09099200	0.09345700
C	-8.26652400	-1.83282800	-1.01329900	H	1.23698100	3.95458700	2.20243500
C	-7.76893700	-2.05881300	0.27223400	H	1.79947900	4.15837000	-2.05985500
C	-6.64120500	-1.38478700	0.74000700	H	2.71912500	4.36103700	0.24393000
C	-5.97529800	-0.45300800	-0.09756100	O	1.19069900	0.25508400	0.14625900
C	-6.49016900	-0.23908300	-1.38713500	C	1.74162800	-1.99928400	-0.36873100
C	-7.62147700	-0.91760300	-1.84240100	C	3.11241100	-1.83237900	-0.18711100
H	-6.55887800	-0.81170000	2.80043300	C	1.29221400	-3.28881000	-0.69490800
H	-9.14486000	-2.37006800	-1.36135100	C	4.03087300	-2.86745000	-0.29453500
H	-8.26612400	-2.77213700	0.92692800	C	2.18535500	-4.34862400	-0.82119200
C	-6.13522400	-1.59440100	2.15063600	C	3.55065500	-4.13994900	-0.61863300
C	-4.76081100	0.23536400	0.41723200	H	5.08809500	-2.71521100	-0.12718000
H	-6.00184900	0.45834700	-2.05946900	H	1.81823000	-5.33919400	-1.07229600
H	-7.99196400	-0.72943200	-2.84664600	H	4.25417600	-4.96272100	-0.70863100
C	-4.13168200	-0.26107700	1.50130900	H	0.22599600	-3.42645400	-0.83806900
C	-4.60736500	-1.50169600	2.21411500	I	3.80031300	0.18066800	0.29690300
H	-3.24264000	0.24043500	1.87459600	C	6.26807700	-0.36555400	0.08425000
H	-4.27186200	-1.49591900	3.25785100	F	6.87891000	0.79502700	0.33520100
H	-6.48985100	-2.55423300	2.54446800	F	6.58376800	-0.78138700	-1.14434800

F	6.67617400	-1.28172900	0.97269400	C	0.44514700	3.81577700	2.49115700
C	0.75780600	-0.87282200	-0.18987800	H	-1.11165900	2.32780800	2.56159700
O	-0.47083500	-1.14833100	-0.38713400	C	0.56200800	5.12544500	0.46346800
30				H	-0.90301000	4.65453800	-1.04581200
Cu	-0.08420900	0.97508900	-0.76476700	C	1.04913700	4.82470700	1.73745900
C	-7.27166400	-2.26038300	-1.21619500	H	0.81763100	3.57913300	3.48405600
C	-6.81204300	-2.27357700	0.10348700	H	1.02472800	5.91235100	-0.12600800
C	-5.61946400	-1.64387500	0.45804100	H	1.89350100	5.37592200	2.14231500
C	-4.85709200	-0.98006400	-0.53349300	O	1.45720500	-0.08502700	0.05375100
C	-5.33172500	-0.97193800	-1.85511800	C	3.61251100	-0.11455400	-1.05801400
C	-6.52743000	-1.60605400	-2.19628600	C	4.26253600	-1.13618800	-0.34491200
H	-5.48966900	-0.66282800	2.35401500	C	4.37534000	0.63975000	-1.97045500
H	-8.20201500	-2.75937700	-1.47369700	C	5.62437300	-1.38162100	-0.53682200
H	-7.39084400	-2.78081300	0.87255700	C	5.73193900	0.40603200	-2.15902500
C	-5.14104700	-1.60123900	1.89360800	C	6.35891100	-0.60897300	-1.43630300
C	-3.57864700	-0.33727500	-0.14491000	H	6.11257300	-2.17737100	0.01465900
H	-4.76005800	-0.47947600	-2.63597400	H	6.29449300	1.00929900	-2.86551900
H	-6.87076900	-1.59064900	-3.22719900	H	7.41854700	-0.80948000	-1.56994900
C	-2.99374500	-0.65629700	1.02433400	H	3.86211000	1.41815700	-2.52370000
C	-3.61065700	-1.64507200	1.98079700	I	3.29200500	-2.47188700	1.04566900
H	-2.02770800	-0.22792500	1.27743100	C	2.17252800	0.27222400	-0.93255700
H	-3.28545700	-1.43884900	3.00720800	O	1.64924100	1.01150900	-1.83482300
H	-5.58890600	-2.41790900	2.47118800				
H	-3.24667300	-2.65798200	1.74250800				
C	-2.93640500	0.62528400	-1.14442100				
H	-2.56377000	0.05131900	-2.00279000				
H	-3.71839600	1.29609100	-1.53640700				
N	-1.83751900	1.42557000	-0.61991500				
C	-2.28654100	2.60923200	0.11408500				
H	-2.97468100	2.29591900	0.91478500				
H	-2.87585700	3.24434900	-0.56833100				
C	-1.13569900	3.40053700	0.69179200				
C	-0.64127800	3.11064900	1.97097400				
C	-0.52386600	4.41736900	-0.05422100				