

Supplementary Information

DFT calculations reveal origin of controllable synthesis of β -boronyl carbonyl compounds from Cu/Pd-cocatalyzed four-component borocarbonylation of vinylarenes

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I. Geometrical optimization calculations including the solvation effect.

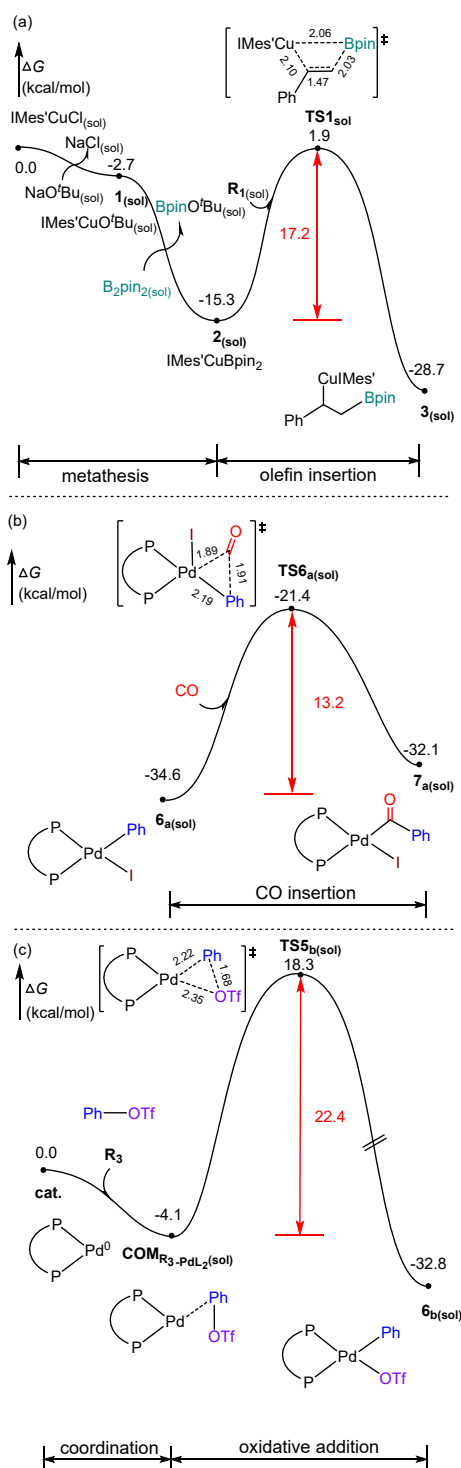


Fig. S1 Calculated Gibbs free energy profiles for the formations of the alkyl copper intermediate **3**, acyl palladium intermediate **7a**, and aryl palladium complex **6b** by performing geometrical optimization calculations including the solvation effect followed by the single-point energy calculations. Bond distances are in Å. The solvent used in the PCM solvation model is toluene.

II. Olefine insertion into Cu–B bond via 1,2-insertion mode.

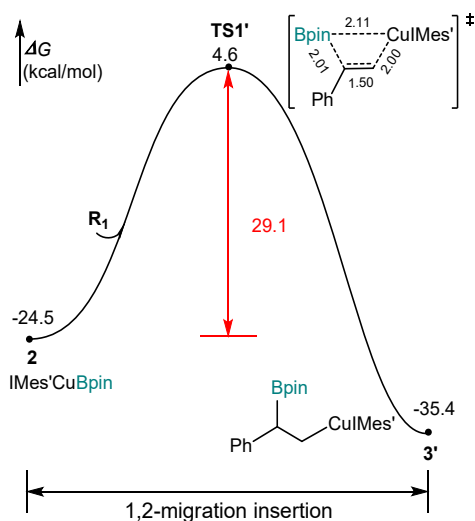


Fig. S2 Calculated Gibbs energy profile for the 1,2-insertion mode of the asymmetric olefin R_1 . Bond distances are given in Å.

III. Reaction of CO insertion into the Cu–B bond.

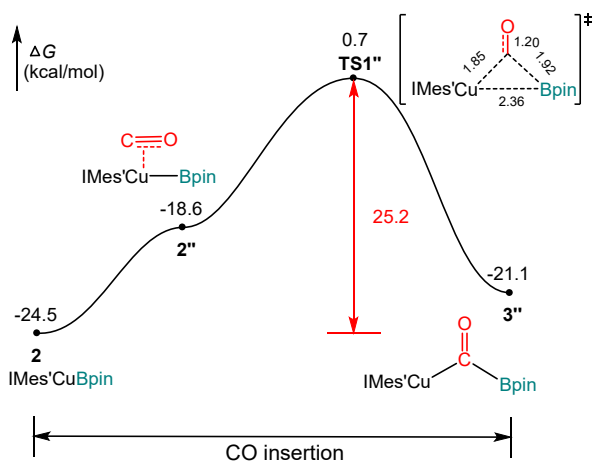


Fig. S3 Calculated Gibbs energy profile for the reaction of CO insertion into the Cu–B bond of the copper-boryl complex IMes'CuBpin **2**. Bond distances are in Å.

IV. Calculated results using the real IMes ligand for formations of alkylcopper and vinyl alkoxide copper intermediates.

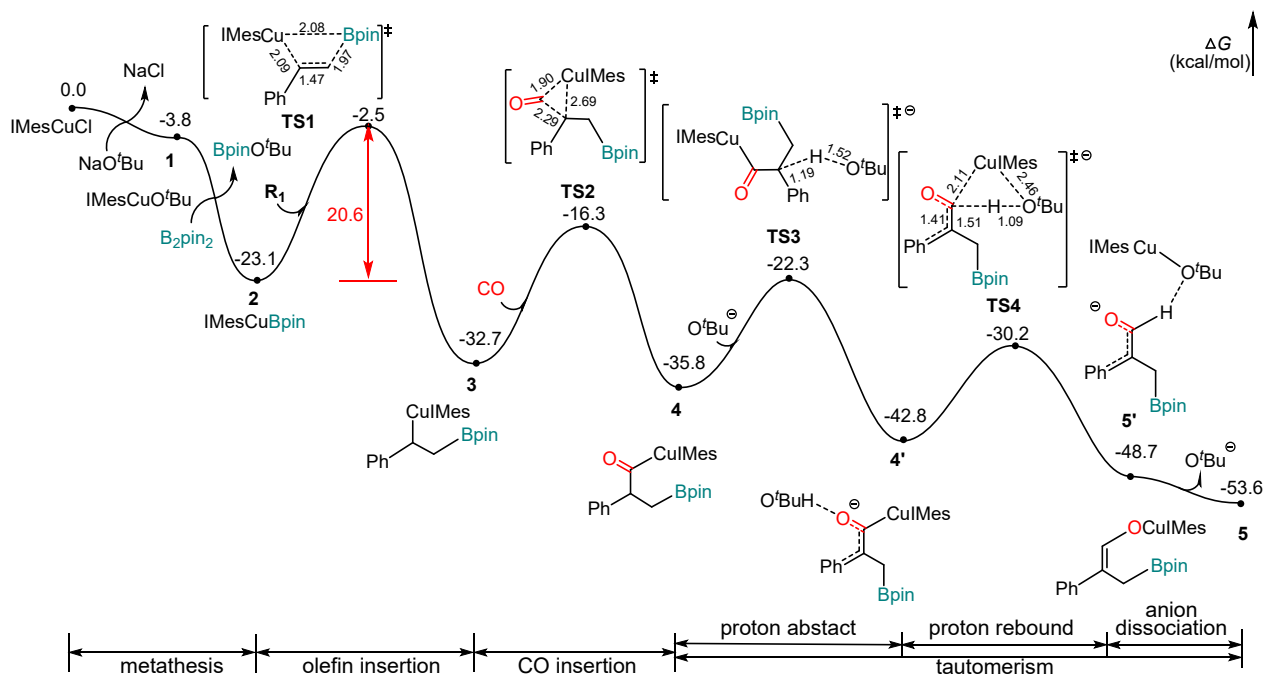


Fig. S4 Gibbs energy profile calculated using the real IMes ligand for formations of copper alkyl intermediate

3A and the copper vinyl alkoxide intermediate **5A**. Bond distances are in Å.

V. Formations of alkyl palladium intermediates and vinyl alkoxide palladium intermediates.

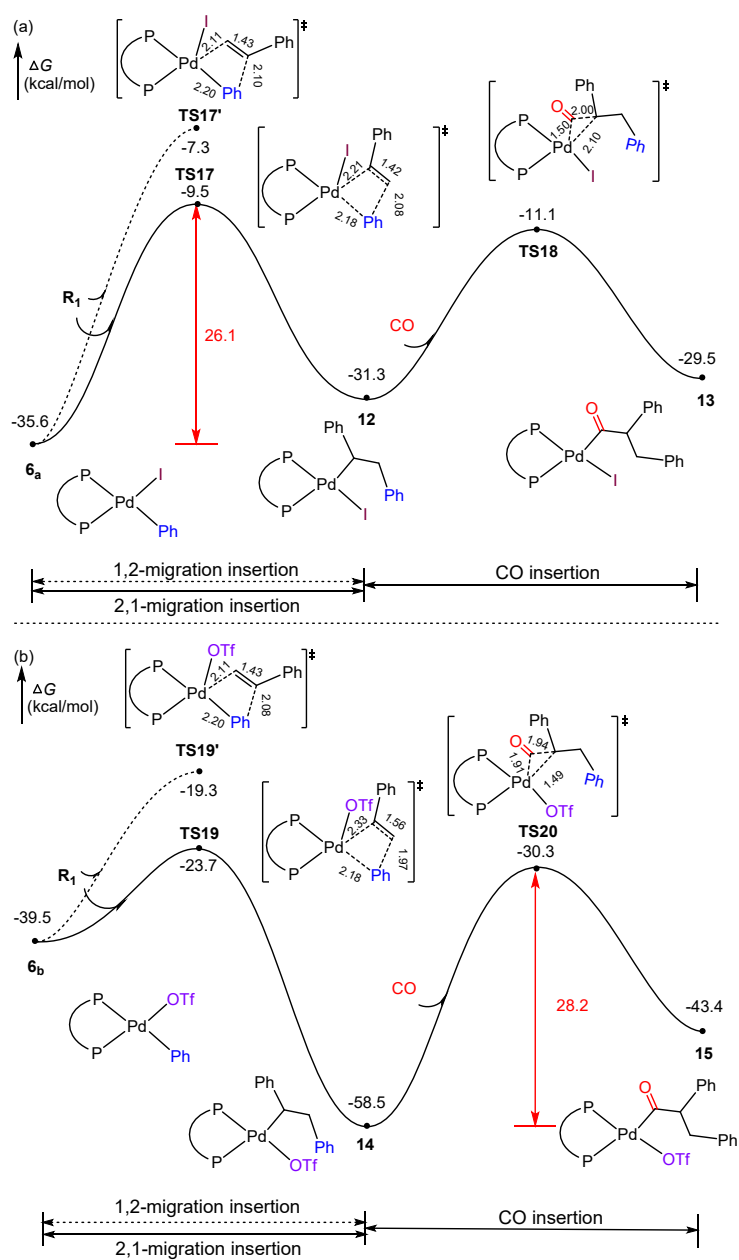


Fig. S5 Calculated Gibbs energy profiles for formations of the alkyl palladium intermediates **12** and **14** and vinyl alkoxide palladium intermediates **13** and **15**. Bond distances are in Å.

VI. Structural analysis of intermediates **6_a**/**7_a** and **6_b**/**7_b**

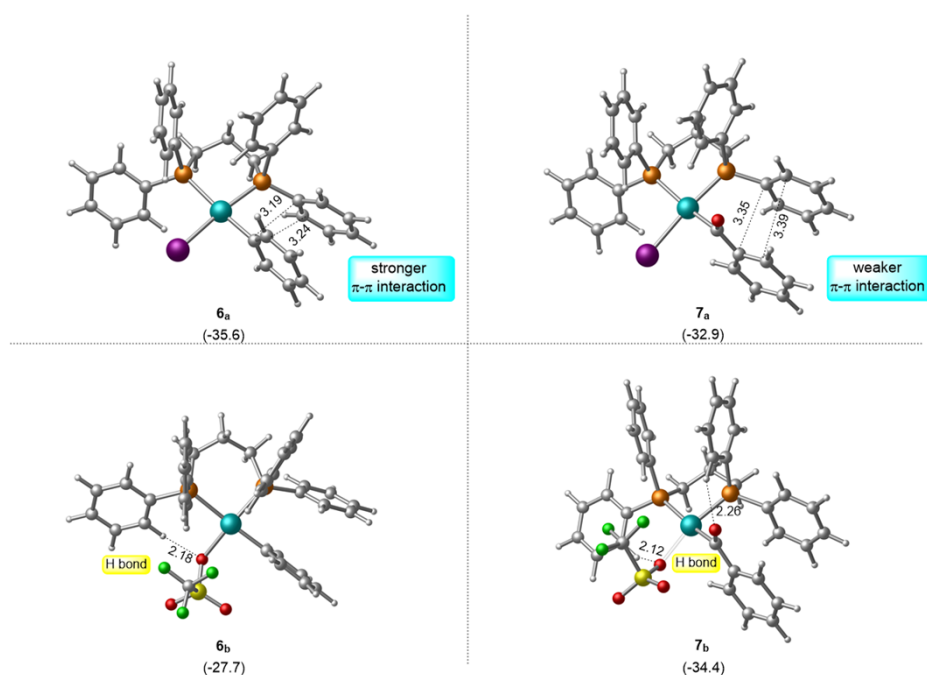


Fig. S6 Visualization of non-covalent interactions between molecules of intermediates **6_a**, **7_a** and **6_b**, **7_b** with corresponding Gibbs free energy in parentheses.

VII. Coupling reaction between intermediates **4** and **6_a**.

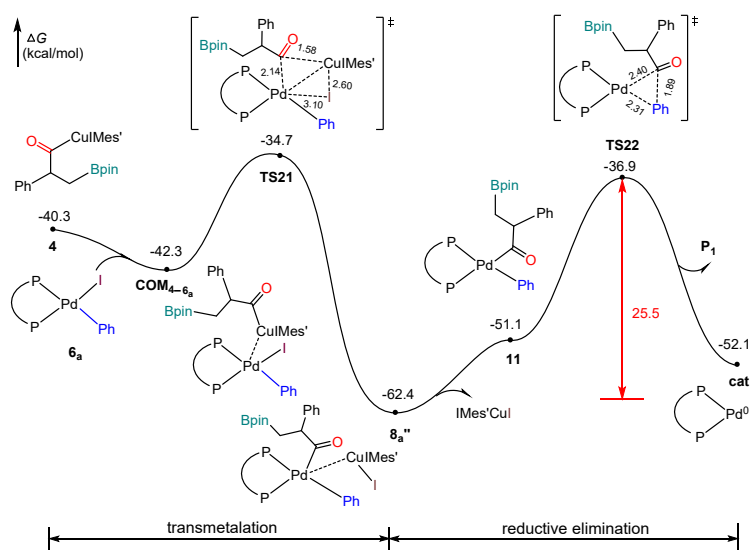


Fig. S7 Calculated Gibbs energy profile for the coupling between **4** and **6_a** to produce the β -boryl ketone **P₁**.

Bond distances are given in Å.

VIII. Coupling reaction between intermediates **5** and **7_a**.

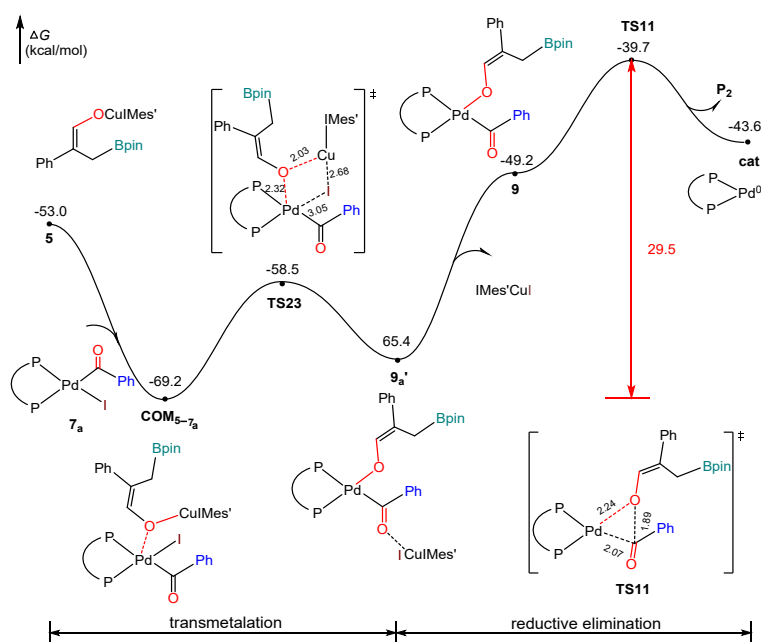


Fig. S8 Calculated Gibbs energy profile for the coupling between intermediates **5** and **7_a** to form the β -boryl ketone **P₂**. Bond distances are given in Å.

IV. Coupling reaction between intermediates **4** and **6_b**.

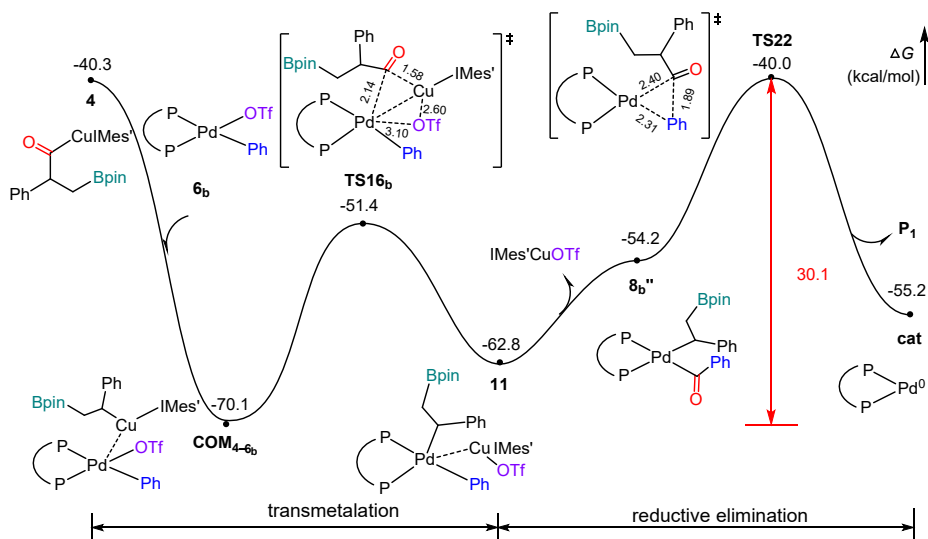


Fig. S9 Calculated Gibbs energy profile for coupling between intermediates **4** and **6_b** to form the β -boryl ketone **P₁**. Bond distances are given in Å.

X. Oxidative addition of intermediate **3**, **4**, or **5** with aryl iodide.

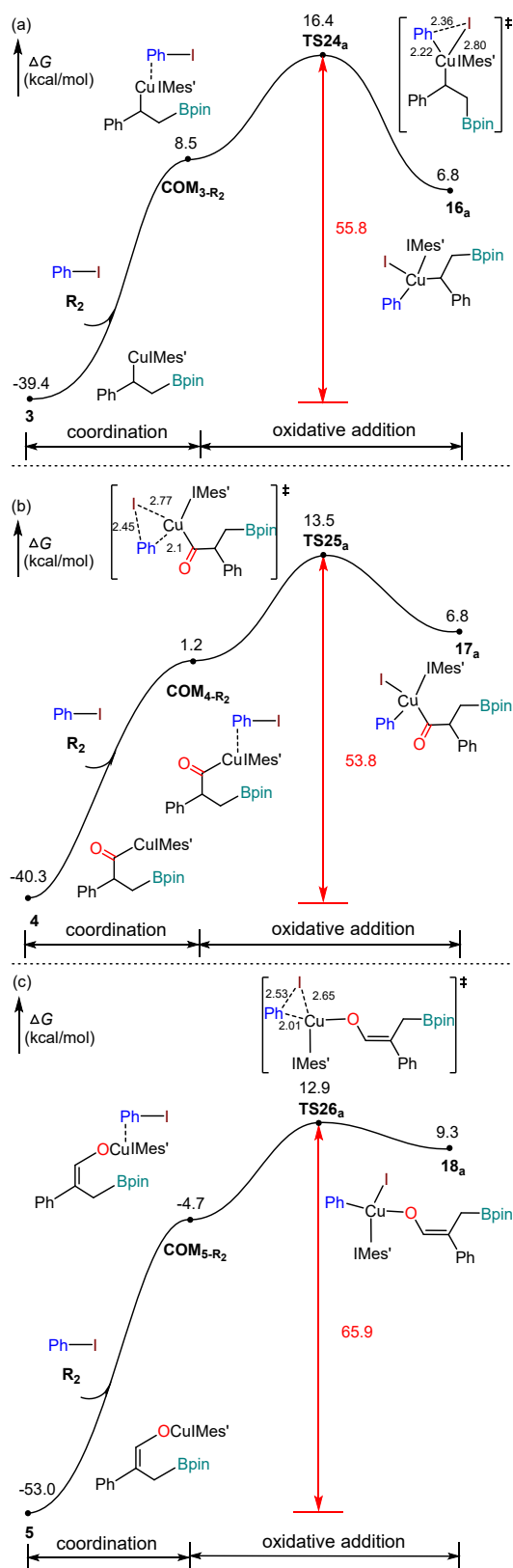


Fig. S10 Calculated Gibbs energy profile for the oxidative addition between intermediate **3**, **4**, or **5** and aryl iodide. Bond distances are given in Å.

XI. Oxidative addition of intermediate **3**, **4**, or **5** with aryl triflates.

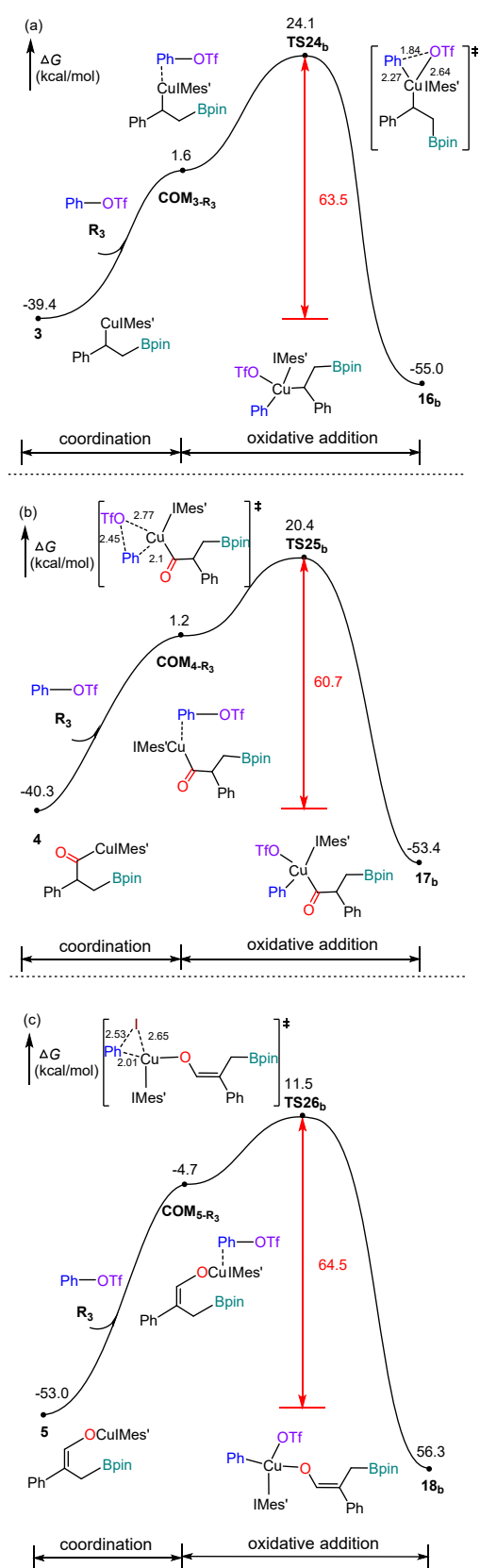


Fig. S11 Calculated Gibbs energy profile for oxidative addition between intermediates **3,4,5** and aryl triflates. Bond distances are given in Å.

XII. Calculated data.

Table S1. Calculated Energies and Imaginary Frequencies

Stationary point	Thermal correction to Gibbs free energy at B3LYP-D3/LanL2DZ /6-31G(d,p) (in a.u.) (1)	Single-point energy at B3LYP-D3/LANL2D /6-311+G(d,p) (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3)=(1)+(2)	Imaginary frequencies (cm ⁻¹)
IMes'CuCl	0.082398	-961.430538	-961.34814	
NaO'Bu	0.082177	-395.5068407	-395.4246637	
NaCl	-0.026459	-622.635064	-622.661523	
1	0.196144	-734.314553	-734.118409	
B ₂ pin ₂	0.318296	-822.857296	-822.539	
BpinO'Bu	0.257098	-644.651749	-644.394651	
2	0.246104	-912.540661	-912.294557	
R₁	0.094548	-309.759997	-309.665449	
TS1	0.37081	-1222.299319	-1221.928509	-226.03
3	0.373791	-1222.357725	-1221.983934	
CO	-0.014101	-113.3499087	-113.3640097	
TS2	0.377886	-1335.700486	-1335.3226	-189.90
4	0.380549	-1335.729917	-1335.349368	
TS3	0.485002	-1568.93866	-1568.43285	-1474.70
4'	0.491183	-1568.97467	-1568.4629	
TS4	0.493610	-1568.93607	-1568.42699	-984.64
5'	0.493610	-1569.01451	-1568.5004	
5	0.379578	-1335.78097	-1335.38377	
^t BuO ⁻	0.091141	-233.215348	-233.124207	
Cat.	0.373858	-1854.51632	-1854.12471	
R₂	0.051187	-243.118117	-243.05962	
COM_{R₂-Pd(dppp)}	0.449203	-2097.667851	-2097.218648	

TS5_a	0.452276	-2097.665252	-2097.212976	-69.88
6_a	0.455362	-2097.721417	-2097.266055	
TS6_a	0.457625	-2211.068515	-2210.61089	-319.14
7_a	0.461241	-2211.093734	-2210.632493	
R₃	0.079395	-1193.35328	-1193.27389	
COM_{R₃-Pd(dppp)}	0.473564	-3047.903655	-3047.430091	
TS5_b	0.470717	-3047.866983	-3047.396266	-409.82
6_b	0.472806	-3047.846127	-3047.373321	
TS6_b	0.501499	-3161.319327	-3160.817828	-409.82
7_b	0.500876	-3161.335983	-3160.835107	
COM_{3-7a}	0.867986	-3433.50761	-3432.639624	
TS7	0.872791	-3433.477517	-3432.604726	-29.36
8'	0.873862	-3433.486208	-3432.612346	
8	0.75801	-2920.887669	-2920.129659	
TS8	0.757728	-2920.86293	-2920.105204	-230.93
P₁	0.367388	-1066.338402	-1065.971014	
COM_{3-6a}	0.858583	-3320.11945	-3319.26087	
TS7'	0.863057	-3320.089453	-3319.226396	-56.84
10'	0.859287	-3320.096845	-3319.237558	
10	0.751403	-2807.49961	-2806.748207	
TS8'	0.749241	-2807.463098	-2806.713857	-19.87
P₃	0.359434	-952.96955	-952.610116	
COM_{3-7b}	0.921844	-4383.739454	-4382.81761	
TS9	0.892314	-4383.734329	-4382.842015	-15.63
8''	0.942142	-4383.768455	-4382.826313	
COM_{5-7b}	0.75801	-2920.887669	-2920.129659	
TS10	0.757728	-2920.862932	-2920.105204	-24.30
9'	0.893188	-4497.149145	-4496.255957	
9	0.76429	-3034.255516	-3033.491226	
TS11	0.765643	-3034.241782	-3033.476139	-109.06
P₂	0.374273	-1179.701116	-1179.326843	

COM_{4-R₂}	0.460778	-1578.86712	-1578.38602	
TS12	0.454877	-1578.83373	-1578.35771	-172.52
CuI	0.089275	-512.593975	-512.5047	
CuOTf	0.095715	-1462.834607	-1462.72582	
TS13	0.464656	-1692.23315	-1692.23315	-351.18
12	0.462451	-1692.31403	-1691.82906	
TS14	0.383367	-1449.02013	-1448.61945	-511.49
COM_{3-R₂}	0.446605	-1465.49225	-1465.0248	
TS15	0.447735	-1465.465598	-1464.99748	-141.67
TS5_c	0.472501	-4660.42414	-4659.95164	-144.71
6_c	0.474866	-4660.47017	-4659.99531	
TS6_c	0.481198	-4773.82391	-4773.34271	-311.01
7_c	0.481197	-4773.8239	-4773.34271	
R₄	0.05289	-691.958284	-2805.878882	
COM_{R₄-Pd(dppp)}	0.451232	-4660.470174	-4660.018942	
TS5_c	0.452186	-4660.424143	-4659.971957	-234.81
6_c	0.452186	-4660.470174	-4660.017988	
TS6_c	0.481198	-4773.823907	-4773.342709	-302.42
7_c	0.458917	-4773.839715	-4773.380798	
R₅	0.054554	-691.805652	-691.958285	
COM_{R₅-Pd(dppp)}	0.453332	-2546.502707	-2546.049375	
TS5_d	0.453947	-2546.480671	-2546.026724	-234.81
6_d	0.461005	-2659.915156	-2659.454151	
TS6_d	0.459835	-2659.896342	-2659.436507	-302.42
7_d	0.461178	-2659.910916	-2659.449738	
TS1'	0.369770	-1221.653953	-1222.319747	-248.37
3'	0.371260	-1221.717624	-1920.623635	
2''	0.262716	-1025.89691	-1222.348777	
TS1''	0.621406	-1954.264553	-1955.314501	-355.59
3''	0.626443	-1025.9049	-1025.63856	
1A	0.319552	-1353.93082	-1353.47415	
2A	0.492733	-1531.334095	-1532.153395	

TS1A	0.669147	-1919.480342	-1919.86578	-292.95
3A	0.669212	-1919.542901	-1919.92934	
TS2A	0.621406	-1954.264553	-1954.66852	-139.13
4A	0.650695	-1955.34296	-1954.69227	
TS3A	0.760703	-2188.56165	-2187.80094	-1359.97
4A'	0.766585	-2188.58364	-2187.81706	
TS4A	0.679917	-2188.6363	-2187.95638	-1208.23
5A'	0.766182	-2188.6247	-2187.85849	
5A	0.64719	-1955.396	-1954.74879	
TS21	0.872476	-3433.47886	-3432.57344	-46.84
8_a''	0.865591	-3433.51612	-3432.61645	
11	0.75801	-2920.881089	- 2,920.097676	
TS22	0.757728	-2920.86293	-2920.07735	-230.93
COM_{5-7a}	0.876729	-3546.90464	-3545.99368	
TS23	0.874777	-3546.88552	-3545.97651	-21.57
9_a'	0.873511	-1692.31403	-1691.82906	
COM_{4-6b}	0.889662	-4383.74348	-4382.81774	
TS10_b	0.890496	-4383.73676	-4382.81051	-28.12
8_b''	0.887513	-4383.73614	-4382.81225	
TS17	0.580535	-2406.431275	-2407.470567	-314.58
TS17'	0.585271	-2406.439311	-2407.481325	-295.38
12	0.582755	-2406.468467	-2407.507441	
TS18	0.586024	-2519.761425	-2520.842628	-328.42
13	0.584467	-2519.789172	-2520.870378	
14	0.606873	-3469.659696	-3471.12505	
TS20	0.6042	-3469.775502	-3471.098257	-305.49
15	0.608982	-3469.799824	-3471.124	
COM_{3-R₂}	0.449905	-1464.73107	-1465.49301	
TS24_a	0.451223	-1464.70186	-1465.46521	-180.25
16_a	0.455134	-1464.730624	-1465.500311	
COM_{4-R₂}	0.455733	-1578.061038	-1578.866702	
TS25_a	0.458724	-1578.030114	-1578.838118	-147.52

17_a	0.460243	-1578.154304	-1578.962591	
COM_{5-R₂}	0.459513	-1578.092742	-1578.899238	
TS26_a	0.459408	-1578.049999	-1578.857564	-97.87
18_a	0.459543	-1578.052835	-1578.861125	
COM_{3-R₃}	0.468966	-2414.733700	-2415.730626	
TS24_b	0.470248	-2414.689457	-2415.688898	-343.15
16_b	0.473256	-2414.820049	-2415.825068	
COM_{4-R₃}	0.476522	-2528.062133	-2529.103467	
TS25_b	0.477277	-2528.018141	-2529.062661	-268.57
17_b	0.478451	-2528.145948	-2529.193347	
COM_{5-R₃}	0.479198	-2528.098428	-2529.138996	
TS26_b	0.475980	-2528.030043	-2529.072403	-210.91
18_b	0.479005	-2528.052650	-2529.102008	
IMes'⁺CuCl_{sol}	0.091968	-961.217	-961.430538	
NaO⁺Bu_{sol}	0.091466	-395.3399	-395.507966	
NaCl_{sol}	-0.021897	-622.613	-622.636301	
B₂pin_{2sol}	0.102445	-507.933	-508.182186	
BpinO⁺Bu_{sol}	0.268198	-644.2201	-644.651817	
R_{1(sol)}	0.102146	-309.5809	-309.759985	
1_(sol)	0.268198	-644.2201	-644.651817	
2_(sol)	0.385234	-1221.674	-1222.31347	
TS1_(sol)	0.388284	-1221.658	-1222.29958	-201.99
3_(sol)	0.388702	-1221.717	-1222.35818	
6a_(sol)	0.483559	-2210.213	-2211.08717	
TS6_{a(sol)}	0.47866	-2210.201	-2211.06873	-322.57
7_{a(sol)}	0.48234	-2210.234	-2211.10544	
COM_{R₃-Pd(dppp)_(sol)}	0.494904	-3046.843	-3047.90331	
TS6_{b(sol)}	0.494371	-3046.804	-3047.86701	-412.33
7_{b(sol)}	0.497415	-3046.881	-3047.95323	

XIII. Cartesian coordinates of all the structures.

IMes'CuCl

C	2.92797600	0.67944500	0.00020100
C	2.92803100	-0.67929900	0.00024300
N	1.59968800	-1.07375100	0.00008000
N	1.59960100	1.07378900	0.00006700
C	0.76355100	-0.00001600	0.00009700
C	1.14837700	2.46003700	-0.00019300
H	1.51074700	2.97561800	-0.89322100
H	0.05850700	2.46206500	0.00025700
H	1.51149500	2.97614900	0.89222100
C	1.14856800	-2.46003300	0.00013400
H	0.05869900	-2.46214000	-0.00063900
H	1.51199200	-2.97608400	-0.89219100
H	1.51071100	-2.97562100	0.89325000
Cu	-1.15603400	-0.00003700	-0.00004200
Cl	-3.29502600	-0.00001200	-0.00017200
H	3.74206200	1.38667400	0.00022200
H	3.74217400	-1.38646300	0.00032600

NaO'Bu

Na	2.69158800	0.00110800	0.00136000
O	0.75860900	0.00699500	0.00819400
C	-0.61842500	0.00023300	0.00028600
C	-1.15504500	1.33926800	0.55557100
H	-0.78173800	2.16604900	-0.05912800
H	-2.25123800	1.38599400	0.57104500
H	-0.78772600	1.48527300	1.57753300
C	-1.14473500	-1.15682900	0.87975800
H	-2.24049500	-1.20692800	0.90801700
H	-0.76429700	-2.11033700	0.49646700
H	-0.77716800	-1.03384600	1.90470900
C	-1.13597300	-0.18955700	-1.44374800
H	-0.76206800	0.62350000	-2.07608000
H	-0.75511200	-1.13442700	-1.84738100
H	-2.23143200	-0.20211900	-1.50690100

NaCl

Na	0.00000000	0.00000000	-1.44229900
Cl	0.00000000	0.00000000	0.93325200

1

Cu	-0.22524900	0.18998000	-0.33987400
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C	2.27021800	2.42027800	0.01102900
C	1.65212500	0.01272700	-0.08071500
N	2.58170900	0.99812500	0.06214200
N	2.37262700	-1.13819200	0.02928700
C	3.85046300	0.47490900	0.25723400
C	3.71794200	-0.87694700	0.23776900
C	1.79010500	-2.47090400	-0.05447100
H	0.72311900	-2.35858900	-0.24791800
H	1.93347700	-3.00843900	0.88676300
H	2.25027600	-3.03451900	-0.87033700
H	2.60909800	2.91347600	0.92581400
H	1.18848600	2.52351000	-0.07657000
H	2.75057100	2.88595400	-0.85378400
C	-3.13432600	0.84751500	1.39474100
H	-3.19689300	1.90631100	1.12418000
H	-4.00258900	0.59317700	2.01524700
H	-2.22700000	0.70309300	1.99335000
C	-3.05288000	-0.00755000	0.11388700
C	-2.92086100	-1.49489800	0.50330400
H	-2.82574500	-2.10386800	-0.40191900
H	-2.01747500	-1.63902400	1.10954400
H	-3.78144600	-1.85732800	1.07915400
C	-4.33562200	0.18904000	-0.71691500
H	-4.42760800	1.24057900	-1.00575100
H	-4.27628200	-0.40797200	-1.63240400
H	-5.23693500	-0.10316700	-0.16502400
O	-1.97555500	0.40193200	-0.67513200
H	4.44976700	-1.66059400	0.35211000
H	4.72050300	1.09798700	0.38978100

B₂pin₂

B	-0.84861600	-0.00018300	0.00081300
C	-2.99315800	0.52942300	0.57875400
O	-1.61053200	0.49181800	1.03336400
C	-2.99278400	-0.52949900	-0.57885300
O	-1.60978400	-0.49209200	-1.03236100
B	0.84861500	-0.00017100	0.00084200
O	1.60966400	0.49261600	-1.03200800
O	1.61063000	-0.49279200	1.03300300
C	2.99267200	0.52993300	-0.57854500
C	2.99324500	-0.52980000	0.57839600
C	-3.90255200	0.19890600	1.75615600
H	-3.82040300	0.98176800	2.51488100
H	-4.94744800	0.14543600	1.43331100
H	-3.62978700	-0.75045000	2.21889000
C	-3.25329300	1.95806600	0.09103300
H	-4.29648400	2.09945300	-0.20591800
H	-3.02647900	2.65409500	0.90257400

H	-2.61131600	2.20595600	-0.75831200
C	-3.90120300	-0.19881500	-1.75695700
H	-3.81859400	-0.98166500	-2.51564300
H	-4.94633300	-0.14519200	-1.43490100
H	-3.62793700	0.75051700	-2.21944600
C	-3.25352100	-1.95811100	-0.09136500
H	-4.29699700	-2.09937800	0.20464600
H	-3.02605200	-2.65415900	-0.90270600
H	-2.61234600	-2.20609200	0.75856200
C	3.25368400	-1.95807300	0.08974400
H	4.29690900	-2.09905800	-0.20725400
H	3.02696000	-2.65468600	0.90081000
H	2.61178700	-2.20552700	-0.75979200
C	3.90258900	-0.19984700	1.75599500
H	3.82063200	-0.98321000	2.51422400
H	4.94745900	-0.14595700	1.43314100
H	3.62964200	0.74916700	2.21931300
C	3.90112900	0.20013600	-1.75686000
H	3.81845600	0.98347300	-2.51503800
H	4.94625700	0.14641800	-1.43481300
H	3.62797800	-0.74893500	-2.21994500
C	3.25319900	1.95826500	-0.09012500
H	4.29665500	2.09950900	0.20594900
H	3.02558500	2.65480400	-0.90100400
H	2.61199500	2.20558000	0.75997500

BpinO'Bu

C	1.58670200	0.80787600	0.07122000
C	1.97633800	-0.70962800	-0.05929100
O	0.16234200	0.73158000	0.34168200
B	-0.27648000	-0.47301000	-0.18313200
O	0.75638100	-1.29873700	-0.57126800
C	2.25966800	-1.36779000	1.29487500
H	1.46233300	-1.14876300	2.01042600
H	2.30503700	-2.45093800	1.15710100
H	3.21010300	-1.03032100	1.71802500
C	3.10825900	-0.99983300	-1.03737400
H	4.02975800	-0.49908300	-0.72323700
H	3.29932000	-2.07590300	-1.06870400
H	2.85675600	-0.67208500	-2.04698300
C	2.26105900	1.55329200	1.21597400
H	1.91260800	2.58964700	1.23662900
H	2.02941200	1.09863800	2.18024000
H	3.34769200	1.56264700	1.08364900
C	1.75143200	1.58038000	-1.24097400
H	1.27963600	1.04733200	-2.07087800
H	1.26754100	2.55563600	-1.14217300
H	2.80540900	1.74019000	-1.48514100

O	-1.56379900	-0.85873700	-0.32376700
C	-2.71078300	-0.03718300	0.00451100
C	-3.91962700	-0.90402300	-0.35032100
H	-3.90139800	-1.83293400	0.22654700
H	-4.85171900	-0.37437800	-0.13185200
H	-3.90324500	-1.16057200	-1.41328900
C	-2.69607700	0.28402700	1.50291100
H	-3.59789800	0.83795300	1.78190400
H	-2.66936100	-0.64265000	2.08433000
H	-1.82303700	0.88680600	1.76147000
C	-2.69109500	1.23919500	-0.84297300
H	-2.65763400	0.98338200	-1.90645600
H	-3.59421100	1.82970200	-0.66012500
H	-1.81934400	1.85001300	-0.60033800

2

Cu	-0.83642600	-0.00012300	0.00016200
B	1.16616400	-0.00000700	0.00016100
C	-3.20464800	-2.42737500	0.35853200
O	1.97065700	0.50636700	1.02204800
O	1.97043000	-0.50642100	-1.02187200
C	-2.82145200	-0.00006000	0.00001400
N	-3.66231600	-1.05958600	0.15441400
N	-3.66198400	1.05972400	-0.15448300
C	-4.99263900	-0.67191600	0.09804700
C	-4.99242700	0.67240100	-0.09858600
C	3.34461400	-0.53968700	-0.56577300
C	-3.20391400	2.42742300	-0.35829600
H	-5.80753600	-1.37085500	0.20081300
H	-5.80710800	1.37155600	-0.20158600
H	-3.53867900	2.80095600	-1.32997400
H	-3.58643600	3.07796900	0.43278300
H	-2.11410800	2.42347100	-0.32806800
H	-3.58710700	-3.07791400	-0.43258200
H	-2.11483500	-2.42369300	0.32860900
H	-3.53978400	-2.80071900	1.33015500
C	3.34471900	0.53967100	0.56564200
C	3.60586200	1.95799200	0.04275600
H	3.37455000	2.67295000	0.83697400
H	4.64902600	2.09877400	-0.25791000
H	2.96053300	2.17900200	-0.81123600
C	4.26595900	0.24164100	1.74435800
H	5.31074300	0.18471900	1.41905600
H	4.18446400	1.04116300	2.48648300
H	3.99976500	-0.69787700	2.23104100
C	4.26561000	-0.24172300	-1.74470200
H	5.31044900	-0.18466500	-1.41959700
H	4.18406000	-1.04134500	-2.48671200

H	3.99923800	0.69770500	-2.23145100
C	3.60588500	-1.95795800	-0.04285200
H	2.96076500	-2.17889900	0.81131700
H	3.37439800	-2.67298300	-0.83695700
H	4.64912400	-2.09870000	0.25758600

R₁

C	-0.40724600	-1.28237200	0.00001000
C	0.51466200	-0.22295800	-0.00012400
C	0.01276300	1.09078500	-0.00018100
C	-1.35719900	1.33038700	-0.00005800
C	-2.26192700	0.26440100	0.00010500
C	-1.78062500	-1.04431000	0.00013200
H	-0.03637300	-2.30408800	0.00004000
H	0.70011100	1.93062700	-0.00037100
H	-1.72375000	2.35277000	-0.00011300
H	-3.33080800	0.45501700	0.00017900
H	-2.47345100	-1.88060600	0.00024500
C	1.95223900	-0.53224500	-0.00022200
H	2.18510500	-1.59653900	-0.00071600
C	2.97015900	0.33638900	0.00028700
H	2.82406600	1.41230800	0.00088900
H	3.99813800	-0.00995400	0.00015100

TS1

Cu	0.48654100	0.25865700	-0.84209500
B	-1.36072300	-0.55435200	-0.39794600
C	1.37432900	-1.39475400	-1.77427000
C	-1.03658000	3.25852000	-0.90744300
O	-1.65683600	-1.17029600	0.80687800
O	-2.50538200	-0.07013300	-1.01540500
C	0.95764400	1.97399900	-0.16913800
N	0.23402000	3.12841800	-0.20840100
N	2.06348200	2.29380300	0.55687100
C	0.87849500	4.14871900	0.47532300
C	2.02926300	3.61697600	0.96624200
C	-3.03190600	-0.84426000	1.14163400
C	-3.65575100	-0.57042300	-0.26923000
C	3.11634000	1.33318900	0.87981600
H	0.47175500	5.14452900	0.54750400
H	2.81366000	4.05756400	1.56039400
H	2.77396800	0.62229600	1.63419800
H	3.98769100	1.87542900	1.24953700
H	3.38393600	0.77009800	-0.01382800
H	-1.50025300	2.27228800	-0.97380700
H	-0.88719200	3.65493500	-1.91634600
H	-1.69058000	3.93342400	-0.35007100
C	2.33798800	-1.74208400	-0.75690800

C	1.95338500	-2.04766900	0.57879300
C	2.90730000	-2.29085300	1.56730400
C	4.27228600	-2.24938100	1.28099900
C	3.73266200	-1.73204900	-1.02922100
C	4.67039600	-1.97362200	-0.03657700
H	0.90094900	-2.08745900	0.84271500
H	5.72838900	-1.95394200	-0.28782000
H	1.72580500	-1.23622300	-2.78734700
H	2.57273100	-2.51904400	2.57679300
H	5.00965500	-2.44218600	2.05389400
H	4.06158300	-1.51478000	-2.04288000
C	-2.98916100	0.40344200	2.03064300
H	-3.98466600	0.68176700	2.38905800
H	-2.35336400	0.19684900	2.89520400
H	-2.55826500	1.25096600	1.49088100
C	-3.64034300	-2.01709700	1.90038900
H	-3.12667900	-2.14162100	2.85755500
H	-4.70165200	-1.83934100	2.10382800
H	-3.54183600	-2.94865400	1.34113300
C	-4.75248200	0.48573300	-0.29824500
H	-5.10734100	0.62166500	-1.32368100
H	-5.60378000	0.17756400	0.31782200
H	-4.38981600	1.44832500	0.06610800
C	-4.11752900	-1.84604200	-0.97772900
H	-5.01974600	-2.26108200	-0.51881100
H	-4.33687500	-1.61207700	-2.02268400
H	-3.33449100	-2.60866600	-0.95647800
C	-0.06853500	-1.57137900	-1.55188300
H	-0.66064300	-1.52318000	-2.46425900
H	-0.35061900	-2.42664000	-0.93219300

3

Cu	0.66235200	0.62695900	-1.25708000
B	-1.10478200	-1.80253500	-0.91492300
C	1.20680700	-1.18095200	-1.86627700
C	-1.48986800	3.32416500	-1.41841600
O	-1.35199100	-2.45801000	0.27464000
O	-1.93799300	-0.70465300	-1.07158500
C	0.34422100	2.20322000	-0.18035300
N	-0.58502100	3.19162500	-0.28492800
N	0.97448100	2.46386900	0.99883600
C	-0.53910700	4.05075400	0.80295900
C	0.44552200	3.58556200	1.61718400
C	-2.18176400	-1.59375600	1.08885900
C	-2.90930400	-0.72553700	0.00405900
C	2.01098500	1.60550800	1.57206100
H	-1.19169100	4.90396000	0.89786400
H	0.80825000	3.94989200	2.56508500

H	2.50777000	1.05598300	0.77291700
H	1.57228600	0.88412100	2.26548400
H	2.74053100	2.22397800	2.09841300
H	-1.49774700	2.37519000	-1.95467600
H	-1.15698400	4.12232300	-2.08801000
H	-2.49841100	3.54535300	-1.06187800
C	2.20964500	-1.38594100	-0.79027400
C	1.92982400	-2.04869700	0.42767000
C	2.86569600	-2.09844200	1.46207000
C	4.12363700	-1.50917900	1.32790300
C	3.50695900	-0.82531400	-0.91538600
C	4.43792200	-0.88140800	0.11539800
H	0.96390200	-2.51729900	0.57078200
H	5.41977800	-0.43568900	-0.02671800
H	1.71259800	-1.11859100	-2.83462300
H	2.60639700	-2.61390900	2.38446500
H	4.84914300	-1.55330600	2.13458100
H	3.76351700	-0.32046400	-1.84454100
C	-1.23288400	-0.77171900	1.96997900
H	-1.78249800	-0.13685000	2.67138100
H	-0.59797200	-1.45439600	2.53971500
H	-0.58230900	-0.14129600	1.35801200
C	-3.09600700	-2.45503100	1.95094400
H	-2.49543500	-3.03314300	2.65846800
H	-3.78967900	-1.83056500	2.52347900
H	-3.67288900	-3.15686300	1.34661200
C	-3.20943600	0.70761500	0.42852800
H	-3.70040500	1.23754400	-0.39290600
H	-3.88426500	0.72200500	1.29059100
H	-2.29728300	1.24543900	0.68770900
C	-4.17203200	-1.39183800	-0.54991800
H	-4.98645400	-1.38778400	0.18041900
H	-4.49925500	-0.84471700	-1.43793300
H	-3.97011500	-2.42524700	-0.84304300
C	0.01972100	-2.17899100	-1.93378500
H	-0.40579000	-2.11225300	-2.94258600
H	0.35114900	-3.21981700	-1.79016400
CO			
C	0.00000000	0.00000000	-0.65011400
O	0.00000000	0.00000000	0.48758500
TS2			
Cu	0.83813900	-0.45686400	1.12463100
B	-2.24146000	0.46805900	0.68774000
C	-0.41959800	1.90426300	1.79514900
C	3.18469900	-2.83233400	1.21047800
O	-3.45961500	0.26849200	0.08992900

O	-1.30988700	-0.47658500	0.25965500
C	2.09364800	-1.10166700	-0.21232200
N	3.00946300	-2.09747500	-0.03457600
N	2.28426100	-0.70839600	-1.49860700
C	3.75209100	-2.31574300	-1.18384300
C	3.29342200	-1.43313300	-2.10999200
C	-3.29720800	-0.73745400	-0.94539000
C	-2.02894000	-1.51958300	-0.45674200
C	1.55371900	0.38461600	-2.12713100
H	4.52538700	-3.06506600	-1.24176800
H	3.59357500	-1.25876700	-3.13093800
H	0.72376200	0.66566200	-1.48333500
H	1.17491500	0.06470300	-3.10131900
H	2.19409000	1.25923900	-2.24663200
H	4.21008800	-2.72139300	1.57311900
H	2.96558100	-3.89351500	1.06163500
H	2.49309500	-2.41479700	1.94347800
C	0.17467400	2.50645400	0.61219300
C	-0.54081500	2.72002900	-0.59701200
C	0.05079900	3.32902100	-1.70448400
C	1.38124000	3.74873800	-1.66792400
C	1.52610700	2.95155300	0.62150900
C	2.11035600	3.55150500	-0.48333000
H	-1.59443900	2.46482400	-0.64859800
H	3.14468200	3.88262100	-0.42504100
H	-0.09580900	2.39193300	2.71324000
H	-0.54498900	3.49353800	-2.59979000
H	1.83602000	4.23511900	-2.52548000
H	2.10457200	2.81887800	1.53294100
C	-3.06420400	0.01649100	-2.25879200
H	-3.00520600	-0.66677900	-3.11085800
H	-3.89960400	0.70183500	-2.42219900
H	-2.14506300	0.60706300	-2.21539900
C	-4.56984300	-1.57057100	-1.02350600
H	-5.39938600	-0.94363000	-1.36087700
H	-4.45053900	-2.39166500	-1.73783400
H	-4.83470900	-1.98708200	-0.05062300
C	-1.14144400	-2.06744700	-1.56507800
H	-0.26365800	-2.55146700	-1.12979500
H	-1.68649900	-2.80923000	-2.15732300
H	-0.79774700	-1.27503700	-2.22923900
C	-2.34335400	-2.61258000	0.56741900
H	-2.83559900	-3.47120600	0.10238600
H	-1.40626200	-2.94846600	1.02013700
H	-2.98583400	-2.22987600	1.36446400
C	-1.90231600	1.57139300	1.74317000
H	-2.20751000	1.17551000	2.72329300
H	-2.55061700	2.44824400	1.57512200

C	0.25761500	0.03735200	2.85240400
O	-0.08562100	0.18099900	3.96114800

4

Cu	1.17282700	-0.07292400	1.21227300
B	-2.21163200	0.70220300	0.52724700
C	-0.41507200	2.44760000	1.44166200
C	2.66413000	-3.14551600	1.71394400
O	-3.48890200	0.19279800	0.47849100
O	-1.31252500	-0.09938700	-0.15326300
C	1.99724800	-1.41632700	0.06078400
N	2.56279200	-2.61763800	0.36018800
N	2.09470700	-1.33471300	-1.29346500
C	3.00444200	-3.27176000	-0.78041100
C	2.71066700	-2.45527500	-1.82735900
C	-3.48918100	-0.91901500	-0.45238900
C	-1.98457300	-1.35739500	-0.43907300
C	1.64369000	-0.17441800	-2.05862900
H	3.47536000	-4.24134700	-0.74947900
H	2.88253400	-2.57334400	-2.88537400
H	0.80471100	0.28447000	-1.53798100
H	1.32188200	-0.50114700	-3.04941300
H	2.44422100	0.56050100	-2.15404100
H	3.70861600	-3.34870200	1.96449200
H	2.08224000	-4.06656300	1.80945500
H	2.26734700	-2.39356200	2.39641200
C	0.31216700	2.74932000	0.15374100
C	-0.31275900	2.83148600	-1.09766700
C	0.41387500	3.12130000	-2.25509800
C	1.79230600	3.32795100	-2.18813800
C	1.70378000	2.95140600	0.20062500
C	2.43537500	3.23997100	-0.95086400
H	-1.38417900	2.68234900	-1.17558800
H	3.50764500	3.40191900	-0.88131100
H	-0.36852300	3.34098300	2.07914400
H	-0.10153200	3.19347800	-3.20916800
H	2.35726000	3.56196900	-3.08603000
H	2.20926600	2.89552500	1.16001200
C	-3.93654900	-0.36354600	-1.80842200
H	-4.03578100	-1.15459200	-2.55728100
H	-4.90746900	0.12321300	-1.68737600
H	-3.22664100	0.38089700	-2.17972700
C	-4.47156800	-1.97292200	0.04287600
H	-5.48795800	-1.57132800	0.01204400
H	-4.43789300	-2.86356400	-0.59312700
H	-4.25531800	-2.26695600	1.07089800
C	-1.46418900	-1.91272800	-1.75886700
H	-0.42122000	-2.21776000	-1.64568200

H	-2.04341900	-2.79207800	-2.05852700
H	-1.52165200	-1.16922000	-2.55545500
C	-1.64637100	-2.31421200	0.70831300
H	-2.06622800	-3.30956600	0.53596600
H	-0.55951300	-2.39696900	0.78298900
H	-2.02102500	-1.93313500	1.66143200
C	-1.89044800	2.03778600	1.28779000
H	-2.30554400	1.92616300	2.29778500
H	-2.48110400	2.84464700	0.83123700
C	0.30123100	1.29975800	2.27591100
O	0.15122700	1.36323800	3.49128400

TS3

Cu	-1.60735600	-0.66805500	0.49036000
B	1.90230200	-1.09136800	-1.18828900
C	0.73246200	0.78306900	-0.20489000
C	-4.01370800	-2.48892400	2.04856300
O	3.26561200	-0.84926100	-1.24991900
O	1.62801600	-2.29395700	-0.56102700
C	-3.43407400	-1.19148400	0.01952900
N	-4.31835700	-1.94604900	0.73526600
N	-4.11848400	-0.88090400	-1.11602300
C	-5.52341400	-2.09988100	0.06541000
C	-5.39140000	-1.42726400	-1.10901700
C	3.87408600	-1.65788500	-0.21743700
C	2.86611300	-2.86475400	-0.09826200
C	-3.54233400	-0.10282100	-2.21296200
H	-2.81055000	0.60871900	-1.79581400
H	-4.34616400	0.44387600	-2.71324700
H	-3.05874400	-0.77186100	-2.93172400
H	-4.17058600	-3.57215300	2.05900200
H	-4.64233000	-2.02462300	2.81523300
H	-2.96513500	-2.26835900	2.25687700
C	1.80641300	1.77512800	0.00444500
C	2.67251500	2.20384500	-1.02939600
C	3.60127900	3.22627600	-0.84381000
C	3.72114600	3.87134800	0.38843500
C	1.95428500	2.44158500	1.24933500
C	2.88362800	3.46105400	1.43075400
H	2.63242500	1.71242300	-1.99359200
H	2.95888600	3.93988900	2.40594000
H	4.24338200	3.51660300	-1.67419600
H	4.44813300	4.66683900	0.53490000
H	1.34603300	2.11148000	2.07988200
C	3.93622000	-0.79386600	1.04877900
H	4.46536200	-1.31276900	1.85611700
H	4.47306100	0.12807500	0.81138800
H	2.94039400	-0.50869500	1.40141600

C	5.28198000	-2.03734300	-0.66734900
H	5.88904400	-1.13130300	-0.75175700
H	5.75937400	-2.70067200	0.06256600
H	5.27621400	-2.53342900	-1.64048200
C	2.64304900	-3.36501600	1.32733600
H	1.93767300	-4.20229600	1.31374600
H	3.57975200	-3.71347200	1.77789100
H	2.21452200	-2.57216200	1.94196800
C	3.19959100	-4.02962900	-1.03684500
H	4.09836100	-4.56868300	-0.71865200
H	2.35824100	-4.72878700	-1.04142500
H	3.34893800	-3.67175300	-2.05940600
C	0.78645200	-0.05962500	-1.51827000
H	-0.18079100	-0.56264200	-1.63974700
H	0.94175100	0.57647700	-2.39395400
C	0.18424000	-0.02948600	0.94632700
O	0.72345500	-0.02595000	2.07417300
C	-2.00476600	2.66252000	1.40440400
H	-0.98073700	2.45489700	1.72263900
H	-2.37355500	3.53248200	1.96459100
H	-2.61506300	1.79102600	1.66630400
C	-2.06016900	2.89765100	-0.12038400
C	-3.52001400	3.16518500	-0.53323300
H	-3.57923100	3.31948000	-1.61665200
H	-4.14178300	2.29920800	-0.27724200
H	-3.93665000	4.04939800	-0.03274400
C	-1.18704800	4.11793600	-0.48203300
H	-0.14922800	3.93398200	-0.18938000
H	-1.21049400	4.27683300	-1.56576600
H	-1.53073900	5.03582100	0.01405900
O	-1.61370500	1.77128800	-0.82367200
H	-0.45026100	1.44536900	-0.48621200
H	-6.08304500	-1.28882200	-1.92517200
H	-6.35297100	-2.65395000	0.47592100

TS4

Cu	1.75298100	0.54716500	-0.00873900
B	-1.63736100	-0.14741100	-1.51407600
C	0.09240500	-1.83396600	-0.62689200
C	-0.13632200	-0.07947300	2.47406600
O	-1.70163200	0.61774300	-0.35976100
O	-2.74212800	0.08190200	-2.32448400
C	0.97184100	1.77455900	1.23425900
N	0.16746800	1.33731700	2.24409500
N	0.86222200	3.13618800	1.29245700
C	-0.43151400	2.39336500	2.90535000
C	0.00478100	3.53659000	2.30929700
C	-2.79433500	1.54423600	-0.48863300

C	-3.70138000	0.84437300	-1.56205900
C	1.55709800	4.02629000	0.38236800
H	-1.10458900	2.24470500	3.73503900
H	-0.20766700	4.57281400	2.51989500
H	2.18152700	3.40895200	-0.26478200
H	2.18673900	4.73124200	0.93507200
H	0.84401900	4.58517100	-0.23277200
H	-0.98551600	-0.37301600	1.85602700
H	-0.35961800	-0.22270500	3.53418600
H	0.72075800	-0.69081600	2.17795500
C	-0.80682500	-2.69063600	0.11099100
C	-2.15995400	-2.89055600	-0.29666500
C	-3.06162800	-3.63902100	0.45678400
C	-2.67009200	-4.24640000	1.65244600
C	-0.42585100	-3.35252200	1.31874400
C	-1.33616200	-4.09402600	2.05998000
H	-2.50439400	-2.46511100	-1.23364400
H	-0.99931100	-4.57153100	2.97994900
H	-4.08338500	-3.75570300	0.09621100
H	-3.37378200	-4.83051400	2.24081400
H	0.60477600	-3.23635500	1.63123000
C	-2.19480500	2.87209400	-0.97045900
H	-2.94956000	3.66252600	-1.03874800
H	-1.42639300	3.17978200	-0.25729400
H	-1.72055000	2.75059500	-1.94815600
C	-3.44875000	1.73078000	0.87710200
H	-2.75068600	2.23375900	1.55108800
H	-4.35189700	2.34628500	0.79598800
H	-3.71571000	0.76887600	1.31751000
C	-4.43356500	1.79510600	-2.50342200
H	-5.02009000	1.21804500	-3.22449800
H	-5.11958900	2.44429100	-1.94778900
H	-3.73301600	2.41961200	-3.06026500
C	-4.68549800	-0.15965200	-0.94830700
H	-5.48935300	0.34199400	-0.39967000
H	-5.13125700	-0.74743200	-1.75590200
H	-4.17015300	-0.85078900	-0.27696500
C	-0.46547400	-1.12086400	-1.85160000
H	0.35698600	-0.51895300	-2.26835100
H	-0.78111900	-1.80685200	-2.65571200
C	1.41058900	-1.50223300	-0.24268500
O	2.01399200	-1.95186800	0.81709600
C	5.65920500	0.29674200	-1.87024000
H	5.49702200	1.36841300	-1.70684000
H	6.68618200	0.05144000	-1.56760900
H	5.55439300	0.09761400	-2.94206800
C	4.62283800	-0.51243000	-1.07879300
C	4.80709600	-2.02022200	-1.32786700

H	4.06695100	-2.56848300	-0.73858000
H	4.65364100	-2.24650600	-2.38855100
H	5.81175800	-2.35799600	-1.04043500
C	4.76476200	-0.23326000	0.42978100
H	4.64129800	0.84018700	0.62249000
H	3.98143800	-0.78989100	0.95765400
H	5.74812200	-0.54005000	0.81167700
O	3.33850800	-0.11808800	-1.53897400
H	2.48386400	-0.80960800	-1.15850200

4'

Cu	-1.29406700	0.21432200	-1.02713100
B	1.63438600	-1.70516700	-0.73573000
C	1.65047700	0.54447800	-1.41084400
C	-2.47528300	-2.98783000	-0.95864500
O	2.78248200	-1.96270900	0.00311000
O	0.50212400	-2.16422100	-0.05035400
C	-3.08125900	-0.57596600	-0.96016800
N	-3.43617300	-1.89384100	-0.93141100
N	-4.27654700	0.08034500	-0.94085000
C	-4.81311400	-2.05391600	-0.90094700
C	-5.34382100	-0.80237300	-0.90830500
C	2.36110000	-2.09309200	1.37654200
C	0.92623600	-2.71005600	1.21504600
C	-4.39968000	1.53539400	-0.99779200
H	-3.50125800	1.99308600	-0.56202600
H	-5.27888400	1.83799100	-0.42194500
H	-4.52129900	1.86220800	-2.03566600
H	-2.48381800	-3.47983300	-1.93703300
H	-2.73150200	-3.72228200	-0.18839900
H	-1.47933500	-2.58858700	-0.75867800
C	2.97804700	1.11468900	-1.22034700
C	4.16631100	0.39014500	-1.51792500
C	5.43533800	0.93473500	-1.34085800
C	5.60173900	2.23374100	-0.85584600
C	3.17849600	2.43535400	-0.72158400
C	4.45022900	2.96899200	-0.55001100
H	4.09638700	-0.63259200	-1.86609200
H	4.54520600	3.98549400	-0.16900300
H	6.30800500	0.32831200	-1.58164500
H	6.59369500	2.65821500	-0.71755400
H	2.29635200	3.01122600	-0.47898100
C	2.34000200	-0.68038600	1.97438200
H	2.05468800	-0.69003800	3.03137900
H	3.33796400	-0.24654600	1.87684200
H	1.65732900	-0.03396600	1.41698100
C	3.36316800	-2.97265900	2.11612200
H	4.33173700	-2.46604300	2.14817000

H	3.03743300	-3.15379600	3.14667100
H	3.50023800	-3.93397900	1.61634900
C	-0.07706700	-2.29250200	2.28517300
H	-1.04835800	-2.75729100	2.08556200
H	0.25452000	-2.61323400	3.27923400
H	-0.21671100	-1.21203100	2.28836400
C	0.94688200	-4.23580100	1.06335300
H	1.19706700	-4.73655900	2.00438800
H	-0.04368500	-4.57569200	0.74546500
H	1.67190500	-4.53515900	0.30190300
C	1.55332200	-0.86437100	-2.03576700
H	0.57657200	-0.97366800	-2.51694300
H	2.32826400	-1.04796200	-2.78662300
C	0.43672300	1.12081200	-0.98233800
O	0.38342600	2.29504000	-0.40238100
C	-1.47308700	1.30762000	2.22455700
H	-0.51985000	1.02476900	1.77256000
H	-1.39274400	1.22727900	3.31647400
H	-2.23506200	0.60256700	1.87508100
C	-1.83037200	2.73717800	1.77363400
C	-3.20336600	3.13642700	2.33017700
H	-3.47601000	4.13336800	1.96809100
H	-3.97001700	2.42934900	1.99336100
H	-3.20658300	3.14849600	3.42688400
C	-0.74757600	3.71463600	2.26920500
H	0.21109200	3.44216800	1.81966900
H	-0.99607400	4.73446700	1.95571800
H	-0.65144300	3.69765200	3.36251800
O	-1.91489500	2.79924800	0.36528100
H	-0.93279400	2.60953300	-0.01990300
H	-6.36931400	-0.46879700	-0.88186900
H	-5.28443900	-3.02354300	-0.86415100

5'

Cu	-2.05965800	0.60052800	0.35190000
B	0.85604600	-1.03012800	-0.96768500
C	2.39935100	1.03064000	-1.13655400
C	0.81713400	1.92301600	1.79737400
O	0.40789400	-0.92569500	0.33944300
O	0.86415700	-2.33924100	-1.39701300
C	-1.22853300	2.32335500	0.40985000
N	-0.08007000	2.75146000	0.99417600
N	-1.70018300	3.42903800	-0.23795200
C	0.17894500	4.07918300	0.70279900
C	-0.84535100	4.51235700	-0.07583300
C	0.41378500	-2.26021700	0.91936200
C	0.28903800	-3.16949800	-0.35692000
C	-2.89869600	3.44835100	-1.05356200

H	1.12579000	4.52783200	0.95069800
H	-1.02249600	5.46390600	-0.55050600
H	-3.37836000	2.47251000	-0.97245700
H	-2.64787500	3.63756900	-2.10241700
H	-3.59002400	4.22226500	-0.70390700
H	0.67954800	0.88279100	1.51077000
H	0.59888200	2.06508200	2.86169800
H	1.83942100	2.22691600	1.56594800
C	3.59602400	0.39718500	-0.62338500
C	3.90712100	-0.95935500	-0.92123800
C	5.04541700	-1.58553500	-0.41668000
C	5.94149300	-0.89752700	0.40370900
C	4.54061800	1.08421000	0.19437000
C	5.67076700	0.44735600	0.69050300
H	3.25216800	-1.53086900	-1.56889300
H	6.35995700	1.01185200	1.31770400
H	5.23400200	-2.62666100	-0.67555700
H	6.82666900	-1.38827400	0.80085600
H	4.34478600	2.12855900	0.40274700
C	-0.74102700	-2.38663600	1.90636900
H	-0.79658100	-3.41357800	2.28701600
H	-0.55865600	-1.72597600	2.76088700
H	-1.69461500	-2.10883000	1.45180800
C	1.75611300	-2.40606900	1.64551300
H	1.83205500	-1.61699800	2.39891500
H	1.83081100	-3.37336500	2.15325100
H	2.60170900	-2.28865100	0.96445400
C	-1.16205900	-3.45067200	-0.75418800
H	-1.17033300	-3.86109700	-1.76906800
H	-1.61909100	-4.18472400	-0.08161800
H	-1.76783000	-2.54043200	-0.71856400
C	1.09283100	-4.46468100	-0.29253200
H	0.75019000	-5.09317000	0.53671100
H	0.95790800	-5.02462200	-1.22294000
H	2.15806600	-4.26388800	-0.16583900
C	1.35749100	0.17328000	-1.84556300
H	0.49368000	0.81368600	-2.07813900
H	1.70395200	-0.23075100	-2.81220100
C	2.13224000	2.39631600	-0.99757700
O	2.75007400	3.29313900	-0.34313900
C	-5.24231500	-0.09514300	0.73270100
H	-4.92209700	0.93914800	0.56003000
H	-6.31278300	-0.17348600	0.50003500
H	-5.09606300	-0.31525400	1.79536400
C	-4.37902800	-1.05477100	-0.11463400
C	-4.83814700	-2.50478900	0.14687300
H	-4.24132600	-3.19685600	-0.45495500
H	-4.67882000	-2.75211600	1.20150900

H	-5.89802300	-2.65767400	-0.09335000
C	-4.56767300	-0.72575300	-1.61105000
H	-4.24484700	0.30355600	-1.80634500
H	-3.93918500	-1.38982800	-2.21261200
H	-5.60970700	-0.83170800	-1.94095500
O	-3.03482200	-0.96234400	0.23596300
H	1.19908300	2.71049300	-1.53060200

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Cu	-1.35532700	-1.67330200	-0.17663900
B	0.70520000	0.72591200	0.83434200
C	2.12248500	-1.20986800	0.35338200
C	-2.70359700	-0.30643300	2.52666900
O	-0.54065100	0.72036000	0.22741300
O	1.34994200	1.92813300	0.65044600
C	-3.11065100	-1.01894900	0.17889300
N	-3.52337000	-0.41542800	1.32716900
N	-4.15501200	-0.84625600	-0.67820000
C	-4.78978300	0.13245200	1.18647300
C	-5.19106400	-0.14139900	-0.08220600
C	-0.76315500	2.02078800	-0.37721600
C	0.69832700	2.59123000	-0.46544600
C	-4.16066100	-1.32159700	-2.05457500
H	-5.00653500	-1.99351200	-2.22143200
H	-3.22862100	-1.86028300	-2.22550900
H	-4.22248600	-0.47849400	-2.74823300
H	-1.83784200	-0.95526900	2.40339500
H	-3.27884900	-0.62170200	3.40044100
H	-2.35709000	0.72066200	2.65907700
C	3.56764900	-0.94185600	0.24251100
C	4.45807400	-1.90561500	-0.28027900
C	5.81961900	-1.64775400	-0.40793300
C	6.35427100	-0.42661200	0.00960100
C	4.13031300	0.27924200	0.67106000
C	5.49709200	0.52865700	0.55642100
H	4.07504600	-2.88118700	-0.56085100
H	5.89293700	1.48419200	0.89191900
H	6.47217100	-2.41658300	-0.81399000
H	7.41891900	-0.23045600	-0.07792300
H	3.48477000	1.05531500	1.06382200
C	-1.66582500	2.80833700	0.57610000
H	-1.91585400	3.79365500	0.17284200
H	-2.59701000	2.25394500	0.72316500
H	-1.18246500	2.94373000	1.54755500
C	-1.46070300	1.81084000	-1.71648400
H	-2.45686500	1.39306900	-1.54555600
H	-1.57386100	2.75949600	-2.25118300
H	-0.90424000	1.11417000	-2.34468100

C	0.81601700	4.09728300	-0.27722500
H	1.86816400	4.38934800	-0.32691800
H	0.27730100	4.63009400	-1.06758700
H	0.42201400	4.41222600	0.69043600
C	1.44055200	2.13921600	-1.72716300
H	1.04838800	2.62580100	-2.62479600
H	2.49731200	2.39571400	-1.62194200
H	1.37683800	1.05438300	-1.85040100
C	1.32827600	-0.54914700	1.48148400
H	0.55525400	-1.24346300	1.83324100
H	1.99013900	-0.32058600	2.32189100
C	1.51027800	-2.02098000	-0.56536900
O	0.26304200	-2.41293600	-0.63006200
H	2.14324400	-2.42875700	-1.36319900
H	-6.10792800	0.09105100	-0.59988500
H	-5.28942800	0.64996300	1.98978500

^tBuO⁻

C	-4.95041200	-1.45280000	-1.16252700
H	-5.03500500	-2.14783300	-0.32117400
H	-5.65956600	-1.75485900	-1.94190900
H	-3.94123800	-1.52054300	-1.57883700
C	-5.21368500	-0.01355000	-0.67800700
C	-5.00687500	0.98733200	-1.82941700
H	-5.14680800	2.00878600	-1.46130000
H	-3.98936500	0.88529900	-2.21881800
H	-5.71250900	0.81139800	-2.64999600
C	-6.66249000	0.09770500	-0.13936300
H	-6.80998700	-0.60174200	0.68815700
H	-6.84976200	1.11139900	0.22537100
H	-7.38101400	-0.13268000	-0.93350300
O	-4.41217000	0.30140100	0.41830300

Cat.

C	1.84578900	-0.51089000	0.02337600
C	1.29622600	-0.71441800	1.79962600
H	1.26355800	-1.79691000	1.96569400
H	2.08601200	-0.33120600	2.45675600
C	-0.05372700	-0.07687300	2.18556000
H	-0.06782500	-0.01266300	3.28050600
H	-0.09923200	0.95701600	1.82830400
C	-1.33801300	-0.82308700	1.77002500
H	-2.15678900	-0.52007600	2.43307000
H	-1.19587300	-1.90163200	1.89614900
P	-1.89022800	-0.52019000	0.00089300
Pd	-0.00096900	-1.08225800	-1.16984500
C	3.53295000	-1.25013100	0.14341700
C	4.62244900	-0.58308700	0.72163000

C	3.71107800	-2.55170900	-0.34321700
C	5.86368300	-1.21122800	0.81654800
H	4.50243400	0.43265300	1.08579800
C	4.95017600	-3.18445600	-0.23852600
H	2.87119200	-3.05855700	-0.81171200
C	6.02869200	-2.51395800	0.34030900
H	6.70357300	-0.68405200	1.26014600
H	5.07605800	-4.19457900	-0.61728100
H	6.99659500	-3.00106300	0.41373400
C	2.19723400	1.29322800	-0.10551400
C	2.31006300	2.15478700	0.99405400
C	2.29294000	1.83781300	-1.39612100
C	2.50745800	3.52459700	0.80899700
H	2.23475300	1.76667100	2.00382800
C	2.50416400	3.20218100	-1.58291700
H	2.17735000	1.18119600	-2.25419500
C	2.60621400	4.05178600	-0.47814300
H	2.58075300	4.17905800	1.67260400
H	2.57714700	3.60477300	-2.58894100
H	2.75727200	5.11760300	-0.62115900
C	-3.62441500	-1.14082400	0.04324800
C	-4.02065700	-2.19635900	0.87697400
C	-4.56118600	-0.61239500	-0.86096300
C	-5.32011400	-2.70332100	0.81577900
H	-3.31763800	-2.63121800	1.57965400
C	-5.85857200	-1.11451800	-0.91722700
H	-4.27141600	0.20539600	-1.51466400
C	-6.24389800	-2.16375100	-0.07831600
H	-5.60954100	-3.51920200	1.47201200
H	-6.57139700	-0.68685000	-1.61643800
H	-7.25492600	-2.55708200	-0.12401000
C	-2.13921800	1.30539000	0.07375200
C	-3.13804900	1.89536100	0.86310400
C	-1.22560100	2.13098400	-0.59401900
C	-3.21422100	3.28202100	0.98304800
H	-3.85965500	1.26803100	1.37764600
C	-1.29178900	3.51872300	-0.46284900
H	-0.45328700	1.67249000	-1.20275100
C	-2.28724300	4.09593400	0.32548500
H	-3.99327800	3.72917000	1.59398400
H	-0.56004300	4.13920600	-0.97064300
H	-2.34438900	5.17577600	0.42829400

R₂(Ph-I)

C	1.24874500	-1.21564200	0.00000500
C	0.56386800	0.00063000	0.00000600
C	1.24950800	1.21617600	0.00000500
C	2.64568600	1.20678700	-0.00000100

C	3.34524100	-0.00046300	-0.00000600
C	2.64484000	-1.20737800	-0.00000100
H	0.70488000	-2.15317000	0.00001200
H	0.70643500	2.15418100	0.00001100
H	3.18341200	2.15012900	-0.00000100
H	4.43065200	-0.00075400	-0.00001500
H	3.18187400	-2.15110000	-0.00000200
I	-1.55461500	0.00000100	-0.00000100

R₃(Ph-OTf)

S	-1.26824700	-0.89950400	-0.09329100
O	-2.31727500	-1.44116000	-0.93237000
O	-0.84833100	-1.50595100	1.15855600
C	-1.70854200	0.87909300	0.27887600
F	-2.90708800	0.90233500	0.85454200
F	-1.73779200	1.58075900	-0.85416100
F	-0.80204800	1.40298000	1.10257800
O	0.00942600	-0.66826500	-1.09341400
C	1.26174600	-0.30566700	-0.55043200
C	2.03526400	-1.25198500	0.11216100
C	1.70102200	0.99524500	-0.77049400
C	3.29520500	-0.87037300	0.57387000
H	1.65095500	-2.25286100	0.26502400
C	2.96596900	1.35898100	-0.30956400
H	1.05756500	1.69505900	-1.29120700
C	3.76120000	0.42902100	0.36325300
H	3.91323200	-1.59320300	1.09650200
H	3.32685600	2.36892600	-0.47528900
H	4.74395200	0.71658900	0.72280000

COM_{R₂}-Pd(dppp)

P	-2.04933300	0.08708700	-0.43273300
C	-1.91828600	0.09367900	-2.27298800
H	-1.76507300	-0.95986700	-2.52864600
H	-2.88524200	0.39813300	-2.68763600
C	-0.78331500	0.94774600	-2.86623500
H	-0.93012100	0.96604200	-3.95226700
H	-0.86145200	1.98792500	-2.53264500
C	0.63724300	0.42699400	-2.60652300
H	1.34543200	0.93129000	-3.27135200
H	0.68936900	-0.64826100	-2.79929800
P	1.24958800	0.66401200	-0.87877000
C	-3.53183800	-0.93522400	-0.10016700
C	-4.81724900	-0.37468300	-0.15366000
C	-3.38062800	-2.29503200	0.20506000
C	-5.93684800	-1.16678300	0.09411100
H	-4.94243800	0.68049900	-0.37397800

C	-4.50620800	-3.08192600	0.44938200
H	-2.38925800	-2.73736900	0.22284200
C	-5.78275900	-2.52128700	0.39698500
H	-6.92818800	-0.72508300	0.05572200
H	-4.37990400	-4.13491900	0.68124300
H	-6.65608900	-3.13616000	0.59341700
C	-2.59941300	1.77030900	0.04177200
C	-2.95087900	2.76271800	-0.88066000
C	-2.64052300	2.07486100	1.41232100
C	-3.31085700	4.03980400	-0.44435300
H	-2.94446700	2.55147500	-1.94360700
C	-3.01472300	3.34253900	1.84801500
H	-2.36411500	1.31406000	2.13660700
C	-3.34154900	4.33352600	0.91758200
H	-3.56820400	4.80295800	-1.17246700
H	-3.04430900	3.56078200	2.91126600
H	-3.62077100	5.32700000	1.25487600
C	3.01228000	0.22298800	-0.97883200
C	3.39770800	-0.95554500	-1.63388900
C	3.97261500	0.99382000	-0.31042300
C	4.73591100	-1.34532600	-1.62809300
H	2.65368600	-1.59165400	-2.10072200
C	5.30648500	0.59308700	-0.30387000
H	3.67518300	1.88987500	0.22160700
C	5.69110900	-0.57452100	-0.96456100
H	5.02671300	-2.26191500	-2.13201500
H	6.04283000	1.18874700	0.22666300
H	6.73104800	-0.88717800	-0.95446200
C	1.21176000	2.47696600	-0.65638000
C	1.84033100	3.33675000	-1.57085300
C	0.49355400	3.02096900	0.41357400
C	1.73602800	4.71745400	-1.41887800
H	2.41845300	2.92699500	-2.39352900
C	0.38434400	4.40376700	0.56214000
H	0.00807000	2.35191200	1.11409300
C	1.00315700	5.25223100	-0.35498700
H	2.22460400	5.37734200	-2.12942500
H	-0.19287500	4.81040000	1.38579900
H	0.91869600	6.32910100	-0.24347800
Pd	-0.01811700	-0.50023400	0.71640200
C	2.63395600	-1.66162400	1.60104600
C	1.76539400	-0.58393900	1.77783800
C	2.12449600	0.47155300	2.61928100
C	3.36766400	0.46253200	3.26197600
C	4.24534700	-0.60420000	3.07151300
C	3.87352600	-1.66632300	2.24473900
H	2.35275200	-2.47500100	0.93987600
H	3.64631600	1.29192500	3.90710900

H	5.21351300	-0.60874600	3.56408600
H	4.55267000	-2.50018800	2.09027300
I	0.16386000	-3.04711200	-1.06800100
H	1.45511800	1.31379100	2.76606900
C	-0.81461800	-1.27850900	2.31359800
O	-1.24453300	-1.78611500	3.24407900

TS5_a

P	0	2.07311500	-0.32873000	0.73071900
C	0	2.01050200	0.16587700	2.52195900
H	0	1.65672100	-0.73178200	3.04218000
H	0	3.03088700	0.34499900	2.87953500
C	0	1.11388300	1.36560000	2.87805400
H	0	1.33156100	1.63224600	3.91937500
H	0	1.39625600	2.23791200	2.27941700
C	0	-0.40613200	1.14648000	2.76912300
H	0	-0.92750700	1.94734600	3.30348900
H	0	-0.69374700	0.20471600	3.24917000
P	0	-1.04344400	1.05783700	1.01944400
C	0	3.29778700	-1.69214600	0.78911000
C	0	4.66769600	-1.46859400	0.98546400
C	0	2.82446100	-3.00415300	0.65312200
C	0	5.55012500	-2.54549000	1.05264200
H	0	5.04341300	-0.45286800	1.06940100
C	0	3.70883700	-4.08092100	0.72900100
H	0	1.76394900	-3.17174000	0.48117400
C	0	5.07105300	-3.85221600	0.92796800
H	0	6.61149600	-2.36690300	1.19833900
H	0	3.33472400	-5.09489300	0.62463800
H	0	5.76081100	-4.68944200	0.97898300
C	0	2.95884600	1.03897700	-0.10941200
C	0	3.64360400	2.06374100	0.55553900
C	0	2.88668100	1.06881800	-1.51178300
C	0	4.23783500	3.10158100	-0.16530800
H	0	3.71140400	2.06596000	1.63822700
C	0	3.49745500	2.09266100	-2.23065000
H	0	2.32415400	0.29683200	-2.03013300
C	0	4.16796700	3.11712600	-1.55779000
H	0	4.75424800	3.89729700	0.36331300
H	0	3.43541400	2.10152900	-3.31485500
H	0	4.62919100	3.92584900	-2.11663900
C	0	-2.85404300	1.17529000	1.23605900
C	0	-3.51202400	0.08034800	1.82025800
C	0	-3.61478800	2.24671200	0.74561100
C	0	-4.89975600	0.07302200	1.93836800
H	0	-2.94063500	-0.78215100	2.14749400
C	0	-5.00560400	2.23037000	0.85747600
H	0	-3.12147700	3.09016900	0.27538200

C	0	-5.65046700	1.14792900	1.45719900
H	0	-5.39524000	-0.78236800	2.38707200
H	0	-5.58499700	3.06482600	0.47306900
H	0	-6.73316900	1.13585700	1.53892400
C	0	-0.54475000	2.68636400	0.33776700
C	0	-0.62617600	3.87469100	1.08091900
C	0	-0.01428800	2.73047400	-0.95852600
C	0	-0.17108500	5.07752300	0.54365100
H	0	-1.04805900	3.86258900	2.08140200
C	0	0.44059000	3.93463100	-1.49600700
H	0	0.05152500	1.81237400	-1.53321800
C	0	0.36837400	5.10724100	-0.74486400
H	0	-0.23369400	5.98980100	1.12964400
H	0	0.86494200	3.95001500	-2.49457200
H	0	0.73128800	6.04307700	-1.15951000
Pd	0	-0.04475600	-0.69352900	-0.26422900
C	0	-2.37219600	-0.18548500	-2.04012100
C	0	-1.41680600	-1.12478700	-1.58749500
C	0	-0.40967900	-1.61493800	-2.46175900
C	0	-0.25094400	-0.98567200	-3.71836200
C	0	-1.11860900	0.01713500	-4.11783200
C	0	-2.19208700	0.39723200	-3.28168700
H	0	0.13491100	-2.52267100	-2.23405200
H	0	0.52276300	-1.34325600	-4.39291000
H	0	-1.00500300	0.48141100	-5.09262100
H	0	-2.87797200	1.17512000	-3.60639800
I	0	-2.32177500	-2.99606000	-0.13557100
H	0	-3.17792700	0.12251700	-1.38410700

6a

P	-1.32772800	4.01063100	2.73723700
C	0.47749500	3.62072200	2.86496100
H	0.87215600	3.80972000	1.85540400
H	0.94687500	4.37208600	3.51533000
C	0.85101300	2.20807300	3.31132400
H	1.93158700	2.19489700	3.50484500
H	0.37590500	1.96245500	4.27258800
C	0.55083000	1.10784700	2.29562500
H	1.11393800	0.19885500	2.54560200
H	0.87809500	1.42295200	1.29500300
P	-1.23460700	0.63393200	2.17138500
C	-1.21501800	5.74212700	2.15793400
C	-1.07677300	6.81212700	3.04498200
C	-1.18907200	5.98073200	0.78150800
C	-0.91409000	8.10520600	2.55806300
H	-1.09961500	6.63602400	4.11975600
C	-1.01732200	7.27248300	0.29766400
H	-1.32355100	5.15000200	0.08919600

C	-0.88270700	8.33580100	1.18611100
H	-0.81318500	8.93499200	3.25387000
H	-1.00308800	7.45059300	-0.77484100
H	-0.75906700	9.34774600	0.80727000
C	-1.89968400	4.14444600	4.47180500
C	-1.04545900	4.05957000	5.57451600
C	-3.27390900	4.31308100	4.68810500
C	-1.55466200	4.12552100	6.86866900
H	0.02763000	3.94142600	5.43829200
C	-3.77833000	4.38917100	5.98099200
H	-3.94836500	4.37937500	3.83222400
C	-2.92018700	4.28854600	7.07416100
H	-0.87879100	4.05252500	7.71755000
H	-4.84631100	4.52475200	6.13441300
H	-3.31689300	4.34101900	8.08544700
C	-1.17744100	-0.87134100	1.14591900
C	-0.38442500	-0.89595800	-0.00532800
C	-1.99840700	-1.96480600	1.43409600
C	-0.39628900	-2.00585600	-0.84244200
H	0.23781900	-0.04081400	-0.26574700
C	-2.00968800	-3.07217300	0.59368000
H	-2.64579900	-1.94408600	2.30902300
C	-1.20691600	-3.09656800	-0.54269300
H	0.22646100	-2.01583400	-1.73386300
H	-2.65597300	-3.91546800	0.82514100
H	-1.21842000	-3.96317200	-1.19940700
C	-1.61439100	0.06542300	3.86605900
C	-0.87846000	-0.95726700	4.47774900
C	-2.60063500	0.72976700	4.59890700
C	-1.12599000	-1.29969800	5.80123100
H	-0.11451300	-1.49480500	3.91638500
C	-2.83908800	0.39437300	5.92872000
H	-3.17269000	1.52901100	4.12578400
C	-2.10239800	-0.62032800	6.52880000
H	-0.55367700	-2.09677300	6.26985100
H	-3.59641400	0.93624200	6.49134800
H	-2.28681600	-0.88582500	7.56718100
Pd	-2.65927000	2.36154400	1.53941800
C	-3.56584700	0.53315600	-0.66141300
C	-3.79464300	0.89389200	0.66663200
C	-4.78904600	0.23424200	1.38899800
C	-5.54586700	-0.77288400	0.78828800
C	-5.31775700	-1.12569700	-0.53824100
C	-4.32736000	-0.46711500	-1.26274300
H	-2.78707400	1.03450400	-1.23743300
H	-6.32209700	-1.27801100	1.36151700
H	-5.91014300	-1.90891200	-1.00696800
H	-4.14120200	-0.73461000	-2.30195000

I	-4.58521400	4.09697100	0.79218400
H	-4.98827700	0.50781600	2.42572500
TS6_a			
P	-2.03840600	0.07645700	-0.38253000
C	-1.93382500	0.11379300	-2.23042100
H	-1.74750400	-0.93189000	-2.49774600
H	-2.92350900	0.37977900	-2.61802600
C	-0.85786400	1.01609900	-2.86600100
H	-1.06009900	1.03747300	-3.94312800
H	-0.96444400	2.04889600	-2.51792400
C	0.60161900	0.56219900	-2.68405100
H	1.25314800	1.12218000	-3.36228600
H	0.69967700	-0.50326400	-2.91242500
P	1.20074500	0.77192800	-0.94952300
C	-3.48334600	-0.99758800	-0.06197200
C	-4.78981500	-0.49883100	-0.17517400
C	-3.27827900	-2.33928000	0.28560900
C	-5.87942300	-1.33682500	0.05353200
H	-4.95448200	0.54457800	-0.42569400
C	-4.37384200	-3.17322500	0.50948300
H	-2.26810600	-2.72834300	0.35813300
C	-5.67217300	-2.67506600	0.39590400
H	-6.88865800	-0.94458000	-0.02999400
H	-4.20767600	-4.21263500	0.77475100
H	-6.52238800	-3.32610700	0.57684500
C	-2.62114400	1.73224000	0.13819500
C	-3.01936400	2.73461700	-0.75374500
C	-2.63845600	2.00212900	1.51632000
C	-3.40371500	3.99087300	-0.27901000
H	-3.03066000	2.54714400	-1.82134000
C	-3.03896200	3.24780900	1.98973200
H	-2.32212300	1.22959400	2.21208300
C	-3.41300400	4.25075200	1.09005800
H	-3.69681400	4.76417300	-0.98252500
H	-3.05199900	3.44087600	3.05826500
H	-3.71166500	5.22796500	1.45705400
C	2.98676900	0.40510500	-0.97862700
C	3.43194300	-0.80423800	-1.53496400
C	3.90489400	1.25522100	-0.34754000
C	4.78323200	-1.13985800	-1.47863100
H	2.71930700	-1.49725200	-1.97014200
C	5.25428000	0.90835100	-0.28875800
H	3.56630500	2.18229400	0.10147900
C	5.69700900	-0.28582500	-0.85794600
H	5.11853100	-2.07702900	-1.91252500
H	5.95821800	1.57230400	0.20415500
H	6.74862300	-0.55340200	-0.81257100

C	1.08791200	2.57673800	-0.67379800
C	1.59289800	3.50457900	-1.59786700
C	0.43834700	3.04041800	0.47591100
C	1.43360400	4.87122300	-1.37805700
H	2.11668000	3.15869300	-2.48389600
C	0.27552300	4.40846300	0.69460300
H	0.04571300	2.31757300	1.18178000
C	0.76974400	5.32392500	-0.23392200
H	1.82457900	5.58396000	-2.09801900
H	-0.25026200	4.75238800	1.57906400
H	0.64001100	6.38952500	-0.06962700
Pd	-0.01290200	-0.55852100	0.59668900
C	2.51648400	-1.84281900	1.72359500
C	1.54441700	-0.90781700	2.09367400
C	1.88290500	0.20337100	2.87609400
C	3.20822800	0.39258300	3.26718400
C	4.18423400	-0.53142800	2.88653700
C	3.83785500	-1.64941100	2.12468800
H	2.23963400	-2.68202900	1.09334800
H	3.47908900	1.25959400	3.86278600
H	5.21797200	-0.37764000	3.18138200
H	4.60110500	-2.35746500	1.81794300
I	0.26937100	-3.01893500	-1.18025700
H	1.11790000	0.91413600	3.17275400
C	-0.26609200	-1.46996000	2.24914100
O	-0.67999200	-2.08020400	3.15176400
7 _a			
P	-1.26254600	0.76832200	-1.20882700
C	-0.60740000	1.57244900	-2.75041700
H	-0.60867900	0.77198000	-3.49880200
H	-1.35241900	2.30462100	-3.08053600
C	0.77905500	2.23343200	-2.69207800
H	0.93382700	2.73237300	-3.65645400
H	0.78585600	3.02448900	-1.93774300
C	1.97479300	1.30297800	-2.44937000
H	2.90656000	1.84351200	-2.64589600
H	1.95281200	0.45476800	-3.14308700
P	2.05771100	0.54971400	-0.74909000
C	-2.94136400	0.29357800	-1.76196600
C	-4.09904100	0.92311200	-1.28893700
C	-3.05543100	-0.77282500	-2.66702700
C	-5.35475600	0.49172000	-1.71698300
H	-4.02204500	1.73708300	-0.57739900
C	-4.31099300	-1.19577000	-3.09677700
H	-2.16743500	-1.30158800	-2.99688200
C	-5.46354100	-0.56629400	-2.61974300
H	-6.24774800	0.98030300	-1.33891400

H	-4.38945900	-2.02902700	-3.78791800
H	-6.44214700	-0.90481600	-2.94643200
C	-1.54309100	2.11870500	-0.00833900
C	-1.40023000	3.47632600	-0.32016600
C	-1.91391800	1.75327600	1.29535600
C	-1.59642500	4.44874700	0.66161600
H	-1.13767200	3.78738100	-1.32421500
C	-2.13757600	2.72678400	2.26438300
H	-2.02447900	0.70669100	1.55013800
C	-1.96615500	4.07743000	1.95379700
H	-1.46383900	5.49703100	0.41222000
H	-2.43295400	2.42489700	3.26466000
H	-2.12064000	4.83685400	2.71431000
C	3.74427800	-0.15380200	-0.76611800
C	3.91237300	-1.42407600	-1.33643600
C	4.85679900	0.52918500	-0.26004500
C	5.18311300	-1.98823200	-1.42601400
H	3.04534000	-1.98056500	-1.67733700
C	6.12548000	-0.04578700	-0.33976700
H	4.73324100	1.50131500	0.20499700
C	6.29105500	-1.30067200	-0.92713000
H	5.30361200	-2.97424100	-1.86391200
H	6.98330700	0.48587100	0.06139600
H	7.27912100	-1.74750100	-0.98487000
C	2.11232100	1.99681400	0.36672000
C	2.67548900	3.23076200	0.00777400
C	1.49989400	1.86441400	1.62123700
C	2.61726100	4.31430000	0.88352100
H	3.15780700	3.35080500	-0.95742100
C	1.44671100	2.94723500	2.49697600
H	1.05699600	0.91142000	1.89393000
C	1.99926900	4.17392900	2.12758700
H	3.05133600	5.26688000	0.59451400
H	0.95891800	2.83622300	3.45980100
H	1.94669700	5.02033600	2.80579400
Pd	0.12757900	-0.86966500	-0.29899000
C	-1.94971500	-1.58786600	2.32872000
C	-2.39768200	-1.89460700	1.03742000
C	-3.77034100	-1.87898800	0.75148300
C	-4.68392400	-1.52654900	1.74309100
C	-4.23727300	-1.22602700	3.03154900
C	-2.87148900	-1.27446600	3.32633300
H	-0.88494500	-1.61210400	2.53458000
H	-5.74385000	-1.48734600	1.50977400
H	-4.95101300	-0.95876600	3.80548700
H	-2.52372200	-1.06004100	4.33265300
I	1.49922600	-2.67595700	1.17698600
H	-4.10139200	-2.11636300	-0.25307500

C	-1.45593400	-2.12693300	-0.10295100
O	-1.68822000	-2.91454800	-0.99188800

CuI

C	-3.95301000	0.67939600	-0.00011100
C	-3.95302200	-0.67936300	-0.00007000
H	-4.76717900	1.38641900	-0.00017000
H	-4.76720500	-1.38637000	-0.00005800
N	-2.62424900	-1.07345600	0.00009000
N	-2.62422800	1.07346300	0.00001900
C	-1.78933700	-0.00000400	0.00012200
C	-2.17211100	2.45939300	-0.00001500
H	-2.53466300	2.97532900	0.89266400
H	-1.08214300	2.46100700	0.00018100
H	-2.53434000	2.97517800	-0.89291100
C	-2.17216400	-2.45939600	-0.00004900
H	-1.08219600	-2.46103200	0.00105500
H	-2.53548000	-2.97560900	0.89215600
H	-2.53365300	-2.97488900	-0.89341700
Cu	0.14400300	-0.00000200	0.00006500
I	2.61581100	-0.00000300	-0.00002700

CuOTf

C	-3.55500200	1.07463500	0.06140300
C	-3.98852200	-0.20862700	0.24200700
N	-2.86055400	-1.01999700	0.11773600
N	-2.18182400	0.99591000	-0.16613100
C	-1.74452400	-0.28860400	-0.13310400
C	-1.31954800	2.14962400	-0.40708600
H	-1.33341800	2.81583300	0.45967100
H	-0.29918500	1.80562800	-0.58079100
H	-1.66673800	2.69861000	-1.28619800
C	-2.87145700	-2.46936100	0.23902700
H	-1.85115900	-2.82703600	0.10253900
H	-3.22903100	-2.76956500	1.22769300
H	-3.51402400	-2.91448400	-0.52554100
Cu	0.05775900	-0.83041200	-0.39787700
S	2.71929700	0.03876200	-0.77037000
O	3.94888400	-0.11832800	-1.53820300
O	1.85619600	1.21183900	-1.03001200
C	3.23180400	0.24006300	1.00198500
F	3.94321700	1.36072600	1.15644100
F	3.96263800	-0.80063400	1.40858900
F	2.13407000	0.32203400	1.78147100
O	1.89141600	-1.24616200	-0.67447900
C	-4.29274100	2.36897100	0.07845900
H	-4.21176700	2.89290200	-0.88044600
H	-5.35260800	2.19909200	0.27707400

H	-3.91060200	3.04203800	0.85402600
C	-5.34652100	-0.75632500	0.51794900
H	-5.67505400	-1.44480300	-0.26899500
H	-5.37972400	-1.30165900	1.46810500
H	-6.07604800	0.05364500	0.57516900

R₃

S	-1.26824700	-0.89950400	-0.09329100
O	-2.31727500	-1.44116000	-0.93237000
O	-0.84833100	-1.50595100	1.15855600
C	-1.70854200	0.87909300	0.27887600
F	-2.90708800	0.90233500	0.85454200
F	-1.73779200	1.58075900	-0.85416100
F	-0.80204800	1.40298000	1.10257800
O	0.00942600	-0.66826500	-1.09341400
C	1.26174600	-0.30566700	-0.55043200
C	2.03526400	-1.25198500	0.11216100
C	1.70102200	0.99524500	-0.77049400
C	3.29520500	-0.87037300	0.57387000
H	1.65095500	-2.25286100	0.26502400
C	2.96596900	1.35898100	-0.30956400
H	1.05756500	1.69505900	-1.29120700
C	3.76120000	0.42902100	0.36325300
H	3.91323200	-1.59320300	1.09650200
H	3.32685600	2.36892600	-0.47528900
H	4.74395200	0.71658900	0.72280000

COM_{R₃}-Pd(dppp)

P	2.61493600	-0.68567000	-0.17729400
C	2.78077100	-2.53596500	-0.27201800
H	3.02024600	-2.74746500	-1.32071800
H	3.64982800	-2.86193600	0.31113900
C	1.53342300	-3.33410500	0.15287500
H	1.83801000	-4.38442600	0.23329900
H	1.22236600	-3.03951100	1.16103700
C	0.31937200	-3.28122500	-0.79629700
H	-0.30841900	-4.15607600	-0.59738300
H	0.64799700	-3.33863700	-1.84040100
P	-0.72873300	-1.74454000	-0.62390400
Pd	0.61451100	0.12164400	-1.06619800
C	4.29740200	-0.14773500	-0.68821100
C	5.39320700	-0.12314500	0.18553800
C	4.47522300	0.26409600	-2.01675500
C	6.64373500	0.29966100	-0.26482000
H	5.26390400	-0.42186500	1.22127400
C	5.72824900	0.67646000	-2.46967300

H	3.62086300	0.26643700	-2.68808600
C	6.81425100	0.69716000	-1.59259900
H	7.48551600	0.32141500	0.42129400
H	5.85472800	0.99111500	-3.50146300
H	7.78819800	1.02857800	-1.94016500
C	2.57795200	-0.32261900	1.62294400
C	2.90798000	-1.24422200	2.62462600
C	2.07719800	0.93698200	1.99790900
C	2.72835800	-0.92247100	3.97205200
H	3.28964700	-2.22525900	2.36243300
C	1.90877500	1.26090900	3.34197800
H	1.79319600	1.64760600	1.22631600
C	2.22673900	0.32791900	4.33325200
H	2.97506900	-1.65226500	4.73750900
H	1.51357900	2.23453900	3.61574500
H	2.08102500	0.57439700	5.38071900
C	-2.15766500	-2.08142000	-1.73143400
C	-2.46567000	-3.33745600	-2.27311000
C	-2.97845600	-0.98812800	-2.05384300
C	-3.57298600	-3.49706500	-3.10898500
H	-1.84723300	-4.19963600	-2.04848900
C	-4.09282100	-1.15118000	-2.87315900
H	-2.73703400	-0.00812500	-1.65846700
C	-4.39146300	-2.40739900	-3.40613400
H	-3.79630700	-4.47541400	-3.52474900
H	-4.72205500	-0.29578200	-3.09985600
H	-5.25397400	-2.53446300	-4.05348900
C	-1.42643400	-2.03496500	1.05676900
C	-2.54982800	-2.84223600	1.28273600
C	-0.79396900	-1.42775300	2.15080100
C	-3.02784400	-3.03732900	2.57839900
H	-3.06167800	-3.30437800	0.44457400
C	-1.26521700	-1.63351700	3.44734100
H	0.05599700	-0.77867300	1.98458900
C	-2.38617400	-2.43612800	3.66365700
H	-3.90553600	-3.65633300	2.74083600
H	-0.75794200	-1.15613600	4.28025900
H	-2.76330400	-2.58788000	4.67074800
C	-1.00569800	2.76227800	-1.11100100
C	-0.41417300	1.89179900	-2.06624500
C	-0.29499600	3.68802400	-0.38887200
C	0.99799700	2.00443300	-2.25498600
H	-1.05392600	1.41005500	-2.79684400
C	1.10655500	3.78041400	-0.59808400
H	-0.78998000	4.34610200	0.31069800
C	1.73772700	2.96961500	-1.51290900
H	1.45126800	1.55527400	-3.13345200
H	1.67076900	4.51610800	-0.03389900

H	2.80708500	3.05073500	-1.68097700
S	-3.32916500	2.89019900	0.27302800
O	-2.93301000	4.09984800	0.97733200
O	-4.69083300	2.65434800	-0.16353100
C	-2.83195600	1.44993700	1.35652800
F	-3.41820200	1.60324600	2.54210700
F	-1.50880300	1.43093800	1.51210200
F	-3.24677400	0.32006400	0.79486900
O	-2.42105900	2.61658700	-1.04638900

TS5_b

P	-1.66208500	1.20703800	-0.80519200
C	-1.14746800	2.36349200	-2.16802300
H	-1.25470800	1.79280100	-3.09673600
H	-1.87449300	3.18046400	-2.22791900
C	0.28032900	2.93633400	-2.06863100
H	0.32538700	3.80189600	-2.74007200
H	0.46356600	3.33145700	-1.06350900
C	1.43083900	1.99104600	-2.46295100
H	2.31812300	2.59636300	-2.67650200
H	1.17915700	1.43976500	-3.37626200
P	1.85130300	0.73333800	-1.15560200
Pd	-0.10166200	-0.47829200	-0.48039300
C	-3.38330000	0.80764600	-1.27233300
C	-4.48226100	1.08592600	-0.44800900
C	-3.58834600	0.09725400	-2.46633000
C	-5.75939600	0.66310400	-0.81314900
H	-4.33766100	1.62922100	0.47927700
C	-4.86765800	-0.30639900	-2.83746500
H	-2.73981900	-0.16222200	-3.09295200
C	-5.95583500	-0.03382200	-2.00606800
H	-6.60313300	0.88022300	-0.16464600
H	-5.01339000	-0.85356800	-3.76413900
H	-6.95180500	-0.36190400	-2.28800200
C	-1.81834400	2.28435000	0.67002500
C	-1.75251800	3.68327000	0.62963000
C	-1.91489100	1.64768500	1.91939000
C	-1.76211500	4.42771000	1.81056500
H	-1.68396100	4.20325100	-0.31914500
C	-1.94069700	2.39180700	3.09644200
H	-1.96079100	0.56518100	1.95840600
C	-1.85346900	3.78570500	3.04539500
H	-1.69697100	5.51063100	1.76344700
H	-2.01601700	1.88401900	4.05325400
H	-1.85813100	4.36659600	3.96269600
C	3.29419300	-0.16101500	-1.84746500
C	4.12223000	0.34237100	-2.86184200
C	3.55938000	-1.43716800	-1.32345400

C	5.19931100	-0.40948000	-3.33321100
H	3.93263400	1.32083800	-3.29100000
C	4.64166900	-2.18147300	-1.78871200
H	2.91864600	-1.85022600	-0.55216600
C	5.46318300	-1.66978000	-2.79511700
H	5.83148900	-0.00997100	-4.12092200
H	4.83315600	-3.16451600	-1.36990700
H	6.30144900	-2.25337000	-3.16377600
C	2.56171900	1.81839100	0.14686800
C	3.86307500	2.33496300	0.08160300
C	1.73838000	2.17473700	1.22522800
C	4.32441700	3.20373000	1.07008100
H	4.51894100	2.04797800	-0.73454200
C	2.19574000	3.05568900	2.20498900
H	0.74066600	1.75805100	1.29656800
C	3.49010100	3.57131500	2.12889500
H	5.33662900	3.59382300	1.01524100
H	1.53878500	3.33015400	3.02480600
H	3.85251700	4.25077600	2.89470500
C	-1.45324900	-2.14007700	0.06028000
C	-1.94760200	-2.72344900	-1.11720800
C	-2.26314900	-1.99282300	1.19683300
C	-3.31657600	-2.95639100	-1.21588000
H	-1.27121400	-2.94371000	-1.93561400
C	-3.62720200	-2.23203500	1.06225500
H	-1.84475600	-1.66100000	2.13628700
C	-4.16908000	-2.70387000	-0.13804200
H	-3.71634000	-3.34967700	-2.14599900
H	-4.27322000	-2.05513300	1.91766900
H	-5.23395500	-2.88628700	-0.22559900
S	0.78509400	-3.21659700	1.60243400
O	-0.21010400	-3.80300300	2.48830800
O	2.00861900	-3.92322100	1.24424200
C	1.36512300	-1.66594000	2.46765800
F	1.87448800	-2.00604200	3.65059500
F	0.34528800	-0.81298800	2.66717000
F	2.30568000	-1.04891900	1.74660600
O	0.15494000	-2.65825300	0.27061000

6_b

P	-1.61536200	0.96194300	-1.01760400
C	-1.16814200	2.04152300	-2.46047500
H	-1.13876700	1.36343600	-3.32117300
H	-1.99227700	2.73765200	-2.64828100
C	0.15829300	2.81057600	-2.35191300
H	0.21273700	3.49424100	-3.20719100
H	0.16625500	3.44115000	-1.45812200
C	1.43025700	1.95281400	-2.37340300

H	2.30058700	2.58771400	-2.56784100
H	1.37703300	1.22131400	-3.18628400
P	1.78045600	1.00698300	-0.81669900
C	-3.27069300	0.35436700	-1.50753800
C	-4.36571100	1.23244000	-1.54243900
C	-3.44386300	-0.99032700	-1.85991200
C	-5.61785400	0.77094500	-1.93931400
H	-4.24253400	2.26877900	-1.24207700
C	-4.70413800	-1.44642100	-2.25164600
H	-2.61221100	-1.68058300	-1.78817200
C	-5.78775800	-0.57049900	-2.29447600
H	-6.46279000	1.45289000	-1.96201700
H	-4.83400800	-2.49423000	-2.50281300
H	-6.76777800	-0.93127000	-2.59257700
C	-1.98895300	2.15193100	0.33181000
C	-2.01372400	3.54185800	0.15803500
C	-2.25141600	1.62680000	1.60739400
C	-2.26935000	4.38897000	1.23778400
H	-1.83860100	3.98031300	-0.81696100
C	-2.52162700	2.47262500	2.68014800
H	-2.24275200	0.55627100	1.76125300
C	-2.52130100	3.85785300	2.50148200
H	-2.27480300	5.46416400	1.08628700
H	-2.72787500	2.04778700	3.65796600
H	-2.72120400	4.51749900	3.34039700
C	3.51608200	0.49047400	-1.03660000
C	3.99735500	0.11262000	-2.29664000
C	4.34121900	0.34986500	0.08715300
C	5.28828500	-0.39690200	-2.43055200
H	3.36684200	0.19288200	-3.17575400
C	5.62533200	-0.16927900	-0.04983500
H	3.96787200	0.61551300	1.06914400
C	6.10195900	-0.54325000	-1.30749600
H	5.65235600	-0.68854200	-3.41089300
H	6.25012900	-0.29204700	0.82896900
H	7.10181000	-0.95346100	-1.41019000
C	1.82985200	2.27542600	0.49010700
C	2.59689700	3.44155500	0.34223300
C	1.06446900	2.09344600	1.64746400
C	2.57785100	4.41916900	1.33370400
H	3.21368000	3.58082000	-0.54073900
C	1.04865300	3.07342300	2.63993600
H	0.47277000	1.19170700	1.75612600
C	1.79989100	4.23695000	2.48113100
H	3.16948700	5.32167100	1.21443200
H	0.43722300	2.93032300	3.52395500
H	1.78366000	5.00308500	3.25033000
Pd	0.21974000	-0.58688000	-0.46091500

C	2.48525300	-2.53667000	-0.68934900
C	1.76989700	-1.71856000	0.18325100
C	2.09516900	-1.69064300	1.53982400
C	3.13797500	-2.48597000	2.02323000
C	3.86013200	-3.29979200	1.15106800
C	3.52865600	-3.32768000	-0.20478000
H	2.24083600	-2.55716500	-1.74715600
H	3.38150600	-2.46870900	3.08233200
H	4.67459200	-3.91303300	1.52557800
H	4.08312400	-3.96504700	-0.88814300
H	1.53671700	-1.06416800	2.22839700
S	-1.38409700	-3.38131800	0.51305300
O	-2.51764000	-4.19540200	0.06879900
O	-0.23485300	-4.02955000	1.14219700
C	-2.08847500	-2.30185200	1.84833200
F	-2.53377100	-3.02661900	2.87539000
F	-3.10729900	-1.55720100	1.37555300
F	-1.14976500	-1.44162800	2.32020800
O	-1.03473500	-2.33441700	-0.53820600

TS6_b

P	-1.01803400	1.78545500	-0.30159100
C	-1.08821200	1.60244600	-2.13787100
H	-1.73999400	0.73717900	-2.28545700
H	-1.60450800	2.48181500	-2.53842400
C	0.24871300	1.38488800	-2.87290100
H	0.05137800	1.52218900	-3.94226100
H	0.97376400	2.15883200	-2.59785800
C	0.88492300	-0.00404700	-2.69758400
H	1.68142100	-0.14594900	-3.43483000
H	0.13660500	-0.78693700	-2.83269400
P	1.59743200	-0.25345900	-1.01233200
C	-2.75437900	2.10868600	0.15155000
C	-3.33216600	3.37058400	-0.05521400
C	-3.52579500	1.05789200	0.66386000
C	-4.67664500	3.57623500	0.24566800
H	-2.73074900	4.19022300	-0.43731700
C	-4.87437900	1.27081400	0.95252800
H	-3.08230800	0.08116400	0.82790600
C	-5.44910400	2.52496400	0.74745900
H	-5.12110500	4.55505700	0.09173000
H	-5.47062200	0.44965200	1.33738000
H	-6.49745700	2.68742500	0.97990200
C	-0.14659000	3.36138700	0.02664000
C	0.18160000	4.28382000	-0.97404300
C	0.24086600	3.62714800	1.35009900
C	0.90212200	5.43860800	-0.66198500

H	-0.11545100	4.10689400	-2.00136800
C	0.94704700	4.78535900	1.66294300
H	-0.00335700	2.91039100	2.12914800
C	1.28822100	5.69030100	0.65352600
H	1.16085300	6.13970600	-1.44955800
H	1.23779400	4.97936100	2.69097000
H	1.85009700	6.58771600	0.89372000
C	2.35674400	-1.90871600	-1.04298800
C	1.54462800	-3.00363600	-1.37751600
C	3.67350600	-2.12492200	-0.61559900
C	2.05649600	-4.29687900	-1.30270100
H	0.50705600	-2.85971400	-1.65277300
C	4.17850400	-3.42316200	-0.54574200
H	4.29848500	-1.28523600	-0.33228000
C	3.37368900	-4.50950400	-0.89180400
H	1.41117900	-5.13389300	-1.54896300
H	5.20029000	-3.58445700	-0.21488900
H	3.76906200	-5.51924000	-0.83055600
C	2.97322300	0.94847000	-0.96277600
C	3.96687800	0.98046900	-1.95407300
C	2.99087500	1.91214100	0.05282700
C	4.95154900	1.96591100	-1.92910300
H	3.97438900	0.23001500	-2.73893700
C	3.96977500	2.90590400	0.07155000
H	2.22178100	1.88874400	0.81568100
C	4.94986000	2.93376300	-0.92004300
H	5.71788600	1.98339300	-2.69819400
H	3.95391900	3.65959100	0.85218000
H	5.71274500	3.70649800	-0.91025600
Pd	0.05772600	0.02767300	0.78843600
C	0.69444100	-2.71132700	1.97233400
C	0.89374500	-1.35194500	2.24093100
C	2.08206900	-0.90334100	2.83555700
C	3.08692300	-1.81907700	3.13967300
C	2.89877100	-3.17529600	2.85802300
C	1.70627900	-3.61892100	2.28454900
H	-0.22594500	-3.04721200	1.51111300
H	4.01455100	-1.47735900	3.58942400
H	3.68665500	-3.88721100	3.08511900
H	1.56810000	-4.67027800	2.05536700
H	2.21999000	0.15196800	3.05178600
C	-0.60941100	-0.27097600	2.55992400
O	-1.19300400	-0.23876300	3.56518200
S	-2.08502700	-2.40986700	-0.50678000
O	-1.50614400	-3.75907900	-0.63517000
O	-2.23801600	-1.91499300	0.88789700
C	-3.83829900	-2.56951700	-1.09328400
F	-4.51763600	-3.42790000	-0.32383500

F	-3.87116700	-3.00737700	-2.35945100
F	-4.45453300	-1.37427100	-1.04334500
O	-1.51673900	-1.39348500	-1.44069800
7 _b			
P	-2.06316300	-0.46486700	-0.36291600
C	-1.80047100	-0.63850800	-2.17484000
H	-1.21189400	-1.55598000	-2.28531600
H	-2.77469100	-0.82917000	-2.63816300
C	-1.09673600	0.54571900	-2.85913200
H	-1.18470700	0.39189200	-3.94023000
H	-1.61284700	1.48766000	-2.64222400
C	0.39808800	0.69455600	-2.54184100
H	0.85356300	1.39579700	-3.24875400
H	0.92073500	-0.25768500	-2.65018000
P	0.76935100	1.36337400	-0.85816900
C	-2.78170200	-2.05885900	0.15009300
C	-4.16367000	-2.28947500	0.14645400
C	-1.90047600	-3.08162600	0.53198400
C	-4.65927300	-3.53720900	0.52406700
H	-4.84775100	-1.49701600	-0.14067100
C	-2.40298000	-4.32925400	0.89472900
H	-0.83191700	-2.90550200	0.52598700
C	-3.78029400	-4.55712600	0.89509300
H	-5.73083700	-3.71297300	0.52741900
H	-1.71187500	-5.11955600	1.16952500
H	-4.17005800	-5.52856100	1.18419600
C	-3.38965900	0.77505300	-0.14341200
C	-4.06460500	1.37128600	-1.21546800
C	-3.68477100	1.19932100	1.16316200
C	-4.99958000	2.38338000	-0.98866500
H	-3.86134300	1.05863500	-2.23298800
C	-4.62550000	2.19987900	1.38970400
H	-3.16624800	0.74914100	2.00399600
C	-5.27978600	2.80192400	0.31094600
H	-5.50687400	2.84355500	-1.83096500
H	-4.84354800	2.51505500	2.40554000
H	-6.00493500	3.59079700	0.48541700
C	2.57211300	1.59590100	-0.86181600
C	3.40104000	0.58280900	-1.36597300
C	3.13758400	2.72569300	-0.25422300
C	4.78579700	0.71807500	-1.27214000
H	2.98813600	-0.32149400	-1.79899700
C	4.52144300	2.84639200	-0.16045600
H	2.49954800	3.49600600	0.16303000
C	5.34821500	1.84408100	-0.67100700
H	5.42107900	-0.07082400	-1.66267500
H	4.95234300	3.71883100	0.32084700

H	6.42731100	1.93826100	-0.59272600
C	0.03034200	3.03280600	-0.91214600
C	0.45678100	3.98542500	-1.85068200
C	-1.03649900	3.34014400	-0.05895100
C	-0.18261800	5.22020100	-1.93423900
H	1.29533900	3.76449900	-2.50407500
C	-1.68358300	4.57269200	-0.15134800
H	-1.36453700	2.60503700	0.66723600
C	-1.25714500	5.51279100	-1.08891200
H	0.15445100	5.95438000	-2.65965900
H	-2.52115700	4.78806500	0.50433500
H	-1.75734900	6.47378000	-1.16260600
Pd	-0.13864800	0.12930000	0.93670200
C	2.68332900	0.00543100	1.91754000
C	1.52318000	0.78053800	1.97972200
C	1.51517900	1.98348000	2.68657300
C	2.68175600	2.42492700	3.32154000
C	3.84619100	1.66055200	3.25351600
C	3.84382100	0.45174600	2.55354100
H	2.69010200	-0.91608300	1.34364800
H	2.67720900	3.36719400	3.86343500
H	4.75366500	2.00607300	3.74019300
H	4.75111300	-0.14232900	2.49042700
H	0.61646800	2.59278700	2.73024900
C	-0.73121800	-0.59790700	2.64028000
O	-1.06346500	-0.98133600	3.66365300
S	1.32875600	-2.73652100	-1.43199100
O	0.07547400	-3.29460700	-1.98006700
O	2.35394500	-2.34166100	-2.41916900
C	2.07397000	-4.13220400	-0.46627400
F	2.38466200	-5.16502500	-1.25576400
F	1.19998000	-4.55712300	0.46855900
F	3.18589400	-3.71982400	0.16176200
O	1.12179200	-1.72482000	-0.35078700

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P	1.31831100	-2.23604100	-0.54495400
C	1.15376400	-3.28824800	0.98167500
H	0.17038300	-3.07405000	1.41499000
H	1.15187300	-4.33565200	0.66493200
C	2.24606100	-3.09178400	2.03822000
H	2.18982500	-3.93464400	2.73615300
H	3.23777000	-3.15099600	1.57436500
C	2.11012800	-1.79710000	2.85054200
H	2.61491300	-1.88743000	3.81659000
H	1.05732000	-1.58900300	3.06575700
P	2.78028400	-0.30617500	1.99261800

C	-0.20071500	-2.70932000	-1.46690400
C	-0.53566300	-1.99279400	-2.62673300
C	-1.03317300	-3.76306600	-1.05782100
C	-1.67239300	-2.33227100	-3.35845000
H	0.08788300	-1.16267300	-2.94125700
C	-2.18017000	-4.08621000	-1.78453000
H	-0.81145800	-4.33151000	-0.16280800
C	-2.50241200	-3.37182000	-2.93805400
H	-1.92063600	-1.77127100	-4.25323200
H	-2.82640700	-4.88669200	-1.43987100
H	-3.40058300	-3.61644600	-3.49666600
C	2.66000400	-3.10961300	-1.43721700
C	2.51006900	-4.42127000	-1.90957100
C	3.87966300	-2.44748400	-1.61638700
C	3.57535100	-5.06522000	-2.53466200
H	1.55541200	-4.92918000	-1.80387900
C	4.94792300	-3.09706300	-2.23561500
H	3.98078500	-1.42063700	-1.28356800
C	4.79833300	-4.40563300	-2.69291500
H	3.45330800	-6.07951200	-2.90257700
H	5.89085500	-2.57473500	-2.36378000
H	5.62697800	-4.91008200	-3.18075400
C	2.60344900	0.99832800	3.25886700
C	1.32635800	1.28216600	3.76727200
C	3.68982600	1.79516100	3.64198500
C	1.14550700	2.33418700	4.66151600
H	0.46615400	0.70533500	3.44196600
C	3.50186700	2.85178300	4.53420200
H	4.67520300	1.59859700	3.23414200
C	2.23333400	3.12111200	5.04648000
H	0.15178100	2.55311900	5.03777200
H	4.34899700	3.46670900	4.82355500
H	2.08857800	3.94860300	5.73458500
C	4.57999500	-0.62729800	1.86732300
C	5.26844800	-1.39095900	2.82106900
C	5.28552400	-0.09840600	0.77463300
C	6.63343800	-1.63732800	2.67574100
H	4.74487900	-1.79992400	3.67879700
C	6.65227200	-0.34157700	0.63762400
H	4.76988700	0.52492600	0.05345800
C	7.32628700	-1.11610200	1.58142100
H	7.15448700	-2.23686100	3.41579000
H	7.18696500	0.07703000	-0.20940400
H	8.38891400	-1.31085800	1.46930400
Pd	1.94268500	0.11794000	-0.12457100
C	1.57401400	4.09937500	1.43946400
C	1.28856700	2.85909900	0.84993700
C	-0.00522100	2.32952900	0.93772900

C	-0.99319300	3.01952200	1.63432100
C	-0.70203700	4.24547800	2.23438300
C	0.58008900	4.79187700	2.12516800
H	2.58764200	4.47951700	1.37406900
H	-1.98439600	2.59138300	1.70627100
H	-1.47392400	4.77625000	2.78447300
H	0.80655900	5.74548900	2.59265200
I	1.78446300	1.04226600	-2.67845200
H	-0.24012000	1.38136800	0.46140100
Cu	-2.45053400	1.69304100	-1.34856100
B	-4.10056200	-1.80262500	0.66491200
C	-3.31033600	0.54821000	-0.00169800
C	-1.10608700	4.87763300	-1.35536500
O	-3.86474700	-1.73380400	2.02219800
O	-5.13757000	-2.66121100	0.35751500
C	-1.59856600	2.82744100	-2.68315100
N	-1.05671300	4.06972100	-2.56515600
N	-1.33343000	2.47681900	-3.97059800
C	-0.42889500	4.46365000	-3.73644300
C	-0.60186900	3.45272800	-4.62617700
C	-5.00354700	-2.33254800	2.68562000
C	-5.54882400	-3.31329600	1.58539900
C	-1.68905400	1.19186200	-4.55111100
H	0.07384900	5.41273600	-3.83163800
H	-0.27654200	3.34557800	-5.64786800
H	-2.31760100	0.66413900	-3.83337200
H	-0.78714500	0.60430200	-4.73745600
H	-2.24314600	1.33854300	-5.48168400
H	-1.78709500	4.40168700	-0.65530100
H	-1.47250900	5.87932600	-1.59411100
H	-0.11775300	4.94878700	-0.89171800
C	-4.68361000	1.08655200	0.24109600
C	-5.82916000	0.56513700	-0.39168200
C	-7.10606200	1.06686500	-0.12930700
C	-7.29547100	2.10910800	0.77865200
C	-4.90412500	2.14699300	1.15304300
C	-6.17334400	2.64622600	1.41904400
H	-5.72455200	-0.26075300	-1.08645400
H	-6.29332000	3.45239000	2.13927600
H	-2.74504900	0.67637800	0.93143600
H	-7.96174400	0.62734300	-0.63671700
H	-8.28989300	2.49170600	0.98788400
H	-4.05072700	2.57845900	1.67005800
C	-5.97162500	-1.18688700	3.01147200
H	-6.83724900	-1.53754900	3.58236100
H	-5.43929400	-0.44116000	3.60779600
H	-6.32059400	-0.69155500	2.10254400
C	-4.52214100	-3.00482400	3.96551300

H	-4.12618200	-2.24636600	4.64663100
H	-5.34604900	-3.51883000	4.47187500
H	-3.72978400	-3.72924600	3.76550300
C	-7.06628700	-3.47619500	1.56522900
H	-7.35346900	-4.16644800	0.76656700
H	-7.42869100	-3.88488300	2.51472400
H	-7.56047000	-2.52124000	1.38203400
C	-4.86039300	-4.68394600	1.60519100
H	-5.16339900	-5.28210200	2.46985500
H	-5.13464400	-5.22554000	0.69567400
H	-3.77210200	-4.57191600	1.61994200
C	-3.30079800	-0.95101600	-0.37405800
H	-3.70845800	-1.12926300	-1.37573700
H	-2.27634400	-1.32648000	-0.43629500
C	2.42309000	2.06815700	0.27491200
O	3.54372900	2.51869300	0.18238800

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P	1.22174900	-1.13323800	1.74484100
C	1.25758700	-0.05570100	3.27006700
H	0.32633000	0.52015200	3.29011200
H	1.26344600	-0.69065600	4.16088200
C	2.46548800	0.89508600	3.33088900
H	2.51477600	1.29572400	4.35047600
H	3.38641500	0.32507500	3.18371600
C	2.43537600	2.10210800	2.38189200
H	3.24621300	2.79209700	2.63899400
H	1.49737400	2.64835600	2.52657800
P	2.50480900	1.75077600	0.56409600
C	0.25247300	-2.59773700	2.29642200
C	0.46417200	-3.80454500	1.60662200
C	-0.61266400	-2.58641700	3.39701600
C	-0.13475400	-4.98162500	2.04701300
H	1.11567100	-3.81930600	0.73842400
C	-1.21963800	-3.76828900	3.83089400
H	-0.81258200	-1.66291200	3.92911400
C	-0.96810500	-4.96980800	3.16938400
H	0.05164700	-5.90902700	1.51417100
H	-1.87973700	-3.74719600	4.69306300
H	-1.42638200	-5.89036800	3.51851900
C	2.89430000	-1.90299900	1.83719300
C	3.40466500	-2.35753800	3.06551600
C	3.65102000	-2.07811700	0.67786800
C	4.66396100	-2.94632600	3.13067200
H	2.81528100	-2.26319400	3.97249500
C	4.90862400	-2.68231300	0.74287600
H	3.24719100	-1.76183800	-0.27517700
C	5.42116500	-3.10689700	1.96584100

H	5.05193100	-3.28797200	4.08596700
H	5.48346400	-2.80747100	-0.16827700
H	6.40289800	-3.56892000	2.01651700
C	2.65009500	3.44380600	-0.14991000
C	2.24106800	4.58887000	0.54648400
C	3.08753800	3.58094800	-1.47595800
C	2.25937900	5.83937000	-0.07033200
H	1.88084000	4.51852600	1.56499000
C	3.10772000	4.83058100	-2.08858800
H	3.39170700	2.70881200	-2.04091200
C	2.68953200	5.96413100	-1.39003300
H	1.92380700	6.71229900	0.48095100
H	3.44134100	4.91477300	-3.11828300
H	2.69426700	6.93654600	-1.87309300
C	4.17058800	1.07915000	0.22228100
C	5.23256600	1.14660600	1.13204600
C	4.37778500	0.50530000	-1.04113800
C	6.48476100	0.64081200	0.78415100
H	5.09292900	1.58930500	2.11238700
C	5.63714100	0.02520300	-1.39354300
H	3.54342600	0.39173100	-1.72737500
C	6.69103100	0.08710300	-0.48035300
H	7.29977800	0.68266200	1.50050400
H	5.78192600	-0.42161500	-2.37226200
H	7.66840300	-0.30308400	-0.74851000
Pd	0.61780000	0.44102600	-0.06595700
C	-0.60321600	4.19557100	-1.96873800
C	-0.38597200	3.19905100	-1.00731100
C	-0.76053300	3.43609500	0.31907600
C	-1.34537800	4.64613500	0.68425800
C	-1.55972600	5.63358600	-0.27834300
C	-1.18704300	5.40579300	-1.60701200
H	-0.29110500	3.99905400	-2.98852500
H	-1.64039600	4.80958500	1.71562500
H	-2.01613400	6.57848800	0.00324300
H	-1.34780800	6.17605900	-2.35571400
I	1.64009200	-1.79092100	-2.45961000
H	-0.58783600	2.66707000	1.06385300
Cu	-0.61452700	-1.73637300	-1.04197900
B	-3.42511700	0.80857600	1.74673400
C	-1.71837300	0.25394400	-0.03949900
C	-1.62684400	-3.19059600	-3.90855900
O	-3.32723500	2.18165300	1.81330000
O	-4.71674400	0.36518600	1.89609600
C	-1.95607200	-3.20156200	-1.42198500
N	-2.28173000	-3.61976300	-2.67875900
N	-2.86332300	-3.84721900	-0.63280200
C	-3.36786900	-4.47989600	-2.67167100

C	-3.73784100	-4.62508300	-1.37557400
C	-4.66668000	2.70481900	1.60417800
C	-5.56204300	1.52561600	2.13184800
C	-2.98935400	-3.66769200	0.80003700
H	-3.76649800	-4.91053600	-3.57628800
H	-4.52351500	-5.20679100	-0.92039900
H	-2.10440200	-3.15254500	1.15791000
H	-3.05691300	-4.63666700	1.29668300
H	-3.87686200	-3.07348500	1.03533200
H	-0.70641100	-2.66819400	-3.65320500
H	-2.28620200	-2.51902400	-4.46171400
H	-1.38594400	-4.06632300	-4.51701700
C	-2.64495400	-0.13659200	-1.15734600
C	-3.88088200	-0.78088100	-0.93913200
C	-4.74458000	-1.07912200	-1.99230400
C	-4.41471200	-0.73500000	-3.30336000
C	-2.32926200	0.20147300	-2.49236300
C	-3.20060100	-0.08510500	-3.53990600
H	-4.18185100	-1.04529300	0.06469100
H	-2.91830700	0.19228600	-4.55213300
H	-1.68293100	1.33593300	-0.09246500
H	-5.68368400	-1.58414500	-1.78130200
H	-5.08941800	-0.96476700	-4.12285500
H	-1.37491700	0.66035500	-2.71199500
C	-4.80494100	2.94640600	0.09655400
H	-5.77125400	3.39499500	-0.15201100
H	-4.01160800	3.62691800	-0.22195800
H	-4.69393400	2.01514900	-0.46537900
C	-4.81014700	4.01539400	2.36714600
H	-4.14701200	4.76487000	1.92779300
H	-5.83648500	4.39081200	2.30137700
H	-4.54683400	3.89982900	3.41997500
C	-6.86704900	1.32397600	1.37116600
H	-7.41792300	0.48245800	1.80066400
H	-7.49918800	2.21524100	1.43980500
H	-6.67778700	1.10557700	0.31928900
C	-5.81681200	1.58816100	3.63946500
H	-6.50553200	2.39720600	3.89921400
H	-6.25734000	0.64167500	3.96380600
H	-4.88273000	1.73486500	4.18838600
C	-2.18617800	-0.08548000	1.39574100
H	-2.38438400	-1.14791700	1.53202300
H	-1.37432000	0.16619200	2.08361500
C	0.29215300	1.92097800	-1.43732300
O	0.72116500	1.80858600	-2.56642800

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P	0.90183600	-0.80579000	1.89859700
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C	0.58576600	0.43258200	3.27523000
H	-0.43000400	0.81247700	3.12477400
H	0.58780200	-0.10988200	4.22558400
C	1.57443200	1.60169600	3.38041600
H	1.37036100	2.10709900	4.33264000
H	2.58606100	1.19921400	3.46289400
C	1.52110200	2.67925700	2.28643400
H	2.19282700	3.49708000	2.56700600
H	0.51231700	3.09872300	2.22921800
P	1.90782900	2.12742500	0.55908900
C	0.28470100	-2.34175400	2.72450800
C	0.98958000	-3.54545100	2.56381600
C	-0.85116600	-2.33307400	3.54709200
C	0.59088000	-4.69743200	3.23916600
H	1.86648700	-3.57363800	1.92702200
C	-1.25755000	-3.49117400	4.21217300
H	-1.42215100	-1.42141000	3.68122000
C	-0.53096100	-4.67402600	4.07147600
H	1.16024200	-5.61406300	3.11634200
H	-2.13531400	-3.46237300	4.85104400
H	-0.83762000	-5.57021900	4.60238700
C	2.70282600	-1.12523900	2.04422400
C	3.31783300	-1.28221200	3.29782800
C	3.46871200	-1.26390800	0.88391100
C	4.68139900	-1.54603900	3.38370300
H	2.72830600	-1.20993700	4.20696700
C	4.83313300	-1.54823400	0.97204800
H	3.00597100	-1.13901600	-0.08908200
C	5.44214500	-1.67881200	2.21739600
H	5.15136900	-1.65411000	4.35693300
H	5.41467500	-1.63731100	0.06100600
H	6.50672000	-1.88236000	2.28504000
C	1.79837300	3.68961700	-0.40736300
C	1.56510200	4.94005300	0.17781100
C	1.93264900	3.60242200	-1.80181600
C	1.46459700	6.08284900	-0.61544200
H	1.44020300	5.03565800	1.24948000
C	1.84242900	4.74737200	-2.58908500
H	2.05953800	2.63568400	-2.27684300
C	1.60626100	5.99058600	-1.99946000
H	1.26917600	7.04362700	-0.14855400
H	1.93744900	4.66171300	-3.66717200
H	1.52365300	6.88049600	-2.61649200
C	3.73754500	1.88133100	0.56772100
C	4.52993700	2.07143900	1.70771900
C	4.36412100	1.51901400	-0.63394000
C	5.91187400	1.88706800	1.65106400
H	4.08709000	2.36723400	2.65019500

C	5.74502100	1.35155800	-0.69190800
H	3.76963000	1.33057500	-1.51906400
C	6.52504700	1.52903700	0.45161700
H	6.50687200	2.02818100	2.54860800
H	6.20701500	1.06788100	-1.63278900
H	7.60099600	1.38753500	0.40916900
Pd	0.08995900	0.54579400	0.00132500
C	-1.57760600	4.31940800	-1.37990300
C	-1.32918500	3.17756200	-0.60657100
C	-1.69001700	3.17018000	0.74268300
C	-2.28523800	4.28908500	1.32253800
C	-2.51097100	5.43197300	0.55270700
C	-2.15665500	5.44414500	-0.80065700
H	-1.28544800	4.30654300	-2.42359500
H	-2.58607000	4.26222700	2.36538200
H	-2.96564400	6.30993700	1.00312400
H	-2.32845500	6.33464100	-1.39839000
I	2.09446000	-0.66756100	-2.69008400
H	-1.51835400	2.27018200	1.32099900
Cu	0.38756900	-1.97377400	-1.18467600
B	-4.04731400	0.18203800	1.15128200
C	-1.99254200	-0.10255500	-0.22869600
C	1.17858400	-4.32865000	-3.30137300
O	-4.25886600	1.50823700	1.45938700
O	-5.18029300	-0.44031700	0.68744900
C	-0.08754500	-3.90909800	-1.18592000
N	0.31350500	-4.73225400	-2.19945400
N	-0.95016700	-4.68528200	-0.47227700
C	-0.29710700	-5.97241900	-2.12709500
C	-1.09499100	-5.94447500	-1.03012400
C	-5.51438500	1.88852600	0.83562800
C	-6.27536900	0.51482100	0.78127900
C	-1.68622200	-4.26011200	0.70440500
H	-0.10755300	-6.75204400	-2.84746500
H	-1.73669500	-6.69560600	-0.59826700
H	-1.41861100	-3.23103100	0.91566500
H	-1.42494300	-4.88259200	1.55968000
H	-2.75833300	-4.31911300	0.51214700
H	1.86283500	-3.55405000	-2.95873000
H	0.58031600	-3.91720300	-4.11855400
H	1.73872300	-5.19813400	-3.65268300
C	-2.25661500	-1.12669600	-1.30305900
C	-3.16967700	-2.18499900	-1.13925100
C	-3.38478500	-3.12289400	-2.14955100
C	-2.71112200	-3.02565500	-3.36709800
C	-1.62793400	-1.00952600	-2.56414900
C	-1.84656700	-1.94930700	-3.57250500
H	-3.73951800	-2.26777600	-0.22304800

H	-1.32349200	-1.83364000	-4.51752900
H	-2.45546200	0.82385400	-0.57577100
H	-4.09121100	-3.93264300	-1.98312100
H	-2.87573300	-3.76203900	-4.14850400
H	-0.96259700	-0.17689600	-2.75177500
C	-5.16829600	2.43958200	-0.55234200
H	-6.05987000	2.80119500	-1.07261500
H	-4.46603100	3.26868300	-0.44252500
H	-4.69153700	1.67489800	-1.17171000
C	-6.17287600	2.96828600	1.68418400
H	-5.54806100	3.86545900	1.67174800
H	-7.15661800	3.23138100	1.28229600
H	-6.29168400	2.64907600	2.72095700
C	-7.17985400	0.32660000	-0.42990400
H	-7.65054700	-0.65954700	-0.38869100
H	-7.97174700	1.08250400	-0.44260900
H	-6.61500900	0.39294100	-1.36050700
C	-7.03165400	0.19647300	2.07341700
H	-7.91826700	0.82706100	2.18568800
H	-7.35070000	-0.84881300	2.04979000
H	-6.38983800	0.33810300	2.94719800
C	-2.60315600	-0.41792500	1.16559400
H	-2.55171900	-1.48425700	1.39097000
H	-2.03383000	0.09876800	1.94200100
C	-0.65406700	1.99175600	-1.25197600
O	-0.54876100	1.94521300	-2.46072800

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P	0.04428500	-1.59878700	1.49657000
C	1.19952000	-1.91130800	2.93529100
H	1.15416400	-1.02223900	3.57414100
H	0.79250900	-2.74059700	3.52151300
C	2.65679400	-2.22081900	2.55763000
H	3.14998500	-2.63416200	3.44580800
H	2.67581800	-3.01438600	1.80454900
C	3.49367900	-1.02288200	2.08620000
H	4.54741000	-1.30695300	1.99358400
H	3.45526200	-0.22734500	2.83830100
P	2.94501500	-0.22191200	0.50715100
C	-1.56979300	-1.83223800	2.33599300
C	-2.50769300	-2.78030800	1.90732400
C	-1.90312600	-0.97792600	3.39878500
C	-3.75331100	-2.86967200	2.52935300
H	-2.26814300	-3.43675800	1.07897000
C	-3.14403900	-1.07548800	4.02450800
H	-1.19812700	-0.21797700	3.72501100
C	-4.07481700	-2.01998900	3.58752700
H	-4.47513800	-3.60246200	2.18099500

H	-3.38959800	-0.40548000	4.84292200
H	-5.04711800	-2.08766600	4.06574400
C	0.25442500	-3.11740400	0.49664900
C	0.37166500	-4.39144600	1.07592600
C	0.32853900	-2.98880400	-0.89457900
C	0.57786600	-5.51214800	0.27473700
H	0.29595000	-4.50977200	2.15275300
C	0.52830800	-4.11269500	-1.69598700
H	0.22505300	-2.01097000	-1.34742800
C	0.66059300	-5.37192700	-1.11399400
H	0.67233100	-6.49346100	0.73054900
H	0.58368500	-3.99325800	-2.77224700
H	0.82366600	-6.24626300	-1.73745100
C	4.15763800	1.14070600	0.35072400
C	4.16182000	2.13733500	1.33968200
C	4.99258000	1.28088300	-0.76319000
C	4.99652500	3.24455100	1.22442400
H	3.48028600	2.07077800	2.18195700
C	5.82165700	2.39773800	-0.88097900
H	4.98574100	0.52722500	-1.54260300
C	5.82757500	3.37855900	0.11025000
H	4.97300600	4.01671600	1.98641800
H	6.46111500	2.50035900	-1.75271200
H	6.46755800	4.25005400	0.01063400
C	3.35683700	-1.40160500	-0.82733000
C	4.10078000	-2.57032900	-0.62496600
C	2.82809100	-1.13392700	-2.10297000
C	4.30181900	-3.46849300	-1.67400400
H	4.52242400	-2.79365800	0.34885800
C	3.05306900	-2.02271000	-3.15162000
H	2.24032000	-0.23447300	-2.26640100
C	3.78033200	-3.19595200	-2.93838700
H	4.86643800	-4.37980800	-1.50132000
H	2.64228200	-1.80509900	-4.13299700
H	3.93721300	-3.89642900	-3.75332600
Pd	0.67116400	0.39114300	0.24604900
C	1.29457200	1.98763000	-0.86169300
O	1.57157300	1.89242400	-2.05181500
C	1.52018600	3.28911900	-0.14726400
C	1.05591200	3.47283600	1.15921900
C	2.26508100	4.30050000	-0.76650900
C	1.33652900	4.65272900	1.84602600
H	0.48499700	2.67029800	1.61961900
C	2.55744600	5.47404300	-0.07824900
H	2.62255200	4.12902000	-1.77620500
C	2.09420600	5.65159600	1.22926800
H	0.96916900	4.79558800	2.85836500
H	3.15082600	6.25039000	-0.55293200

H	2.32235500	6.56849800	1.76572000
B	-3.67997600	1.64048400	0.12751100
C	-1.26839400	1.06616900	-0.42234700
O	-3.95808000	2.55940300	-0.85702600
O	-4.77118900	0.87159400	0.45984900
C	-5.23776600	2.19892500	-1.43821600
C	-5.91408100	1.37358400	-0.27916300
C	-1.65837500	-0.04366400	-1.33483400
C	-2.57513700	-1.04950900	-0.97152800
C	-2.88634200	-2.09434600	-1.84346100
C	-2.29764600	-2.16808000	-3.10534900
C	-1.08222600	-0.12547900	-2.62299700
C	-1.39350600	-1.16960200	-3.48789300
H	-3.06123000	-1.00897200	-0.00618600
H	-0.93178800	-1.20423600	-4.47158700
H	-1.11541400	1.96267100	-1.02273300
H	-3.59696200	-2.85469700	-1.52891600
H	-2.54093900	-2.98148600	-3.78230500
H	-0.36616100	0.63427100	-2.92002800
C	-4.93198200	1.35967700	-2.68376000
H	-5.84533900	1.10171800	-3.22817000
H	-4.28618300	1.94210300	-3.34576200
H	-4.40047600	0.44100000	-2.42648300
C	-5.97177500	3.47614500	-1.83010200
H	-5.41446200	3.98943800	-2.61835900
H	-6.97124900	3.24682200	-2.21404100
H	-6.06873200	4.15921100	-0.98481300
C	-6.74212600	0.18034900	-0.74369500
H	-7.15177600	-0.34230600	0.12539200
H	-7.57766900	0.50632100	-1.37158500
H	-6.13128900	-0.52553200	-1.30832900
C	-6.71921900	2.24059100	0.69249600
H	-7.63882100	2.61621900	0.23443500
H	-6.98648200	1.63863700	1.56519200
H	-6.12731800	3.09276200	1.03708700
C	-2.24269000	1.41532900	0.71720000
H	-2.28076100	0.64331600	1.48762700
H	-1.88252900	2.32968300	1.20423700

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P	-1.11618200	-1.39477700	1.43472600
C	-0.39868500	-2.53273800	2.72142000
H	-0.14270600	-1.88172900	3.56552600
H	-1.18304400	-3.20608100	3.08490300
C	0.83540700	-3.34550600	2.29405400
H	1.00556100	-4.10867200	3.06286900
H	0.63068000	-3.89185800	1.36744400
C	2.14101400	-2.54731500	2.13891300

H	2.99484100	-3.23214900	2.17593200
H	2.25048900	-1.84703800	2.97426400
P	2.24208200	-1.56651900	0.56271000
C	-2.57785000	-0.77087700	2.35941300
C	-3.64847200	-1.60122500	2.71952100
C	-2.60033500	0.57635200	2.73726100
C	-4.71716600	-1.09391700	3.45685800
H	-3.65432200	-2.64093200	2.40557800
C	-3.66665000	1.08383700	3.48149900
H	-1.78665400	1.22745900	2.43521200
C	-4.72613200	0.24977800	3.84151900
H	-5.54530100	-1.74272000	3.72671800
H	-3.67273600	2.13038700	3.77112700
H	-5.55977400	0.64539100	4.41392500
C	-1.84273200	-2.53965900	0.19382000
C	-1.99423600	-3.91866700	0.38488100
C	-2.19285300	-1.98660600	-1.04951800
C	-2.47467200	-4.73075000	-0.64481000
H	-1.72914200	-4.37501100	1.33230100
C	-2.68105200	-2.79589900	-2.07275900
H	-2.07674100	-0.91943900	-1.20325800
C	-2.81698700	-4.17259100	-1.87544300
H	-2.57538800	-5.80004600	-0.48411800
H	-2.94039900	-2.35515800	-3.03068600
H	-3.18301500	-4.80547200	-2.67826500
C	3.99462100	-1.05896100	0.49011300
C	4.78340600	-0.90763600	1.63803800
C	4.51753800	-0.67085000	-0.75429400
C	6.07364100	-0.38411300	1.54311400
H	4.39734000	-1.18871900	2.61226400
C	5.80345200	-0.14879700	-0.84459600
H	3.90193600	-0.75271300	-1.64434700
C	6.58488000	-0.00161600	0.30391400
H	6.67580900	-0.27171200	2.44009100
H	6.18725600	0.16620900	-1.80938600
H	7.58417600	0.41689200	0.23241600
C	2.12634300	-2.87933200	-0.71221600
C	2.97868900	-3.99379800	-0.70402100
C	1.12563600	-2.78514700	-1.68649900
C	2.81251700	-5.01027500	-1.64179800
H	3.77585900	-4.06081700	0.03099500
C	0.95822700	-3.80590100	-2.62319700
H	0.49435400	-1.90507000	-1.71069400
C	1.79608000	-4.92000100	-2.59808500
H	3.47360600	-5.87197200	-1.62960000
H	0.16984600	-3.72728500	-3.36468700
H	1.66530400	-5.71634700	-3.32508100
Pd	0.51375800	-0.03315600	0.29792400

C	1.41781800	1.10751000	-1.16714900
O	1.24041400	0.63876300	-2.29577700
C	2.65268400	1.89537900	-0.86157200
C	3.08549000	2.12745500	0.44725300
C	3.39708500	2.40783200	-1.93132200
C	4.24235200	2.86091900	0.68639100
H	2.50768900	1.71994000	1.26928000
C	4.55305800	3.14703400	-1.69427700
H	3.04914400	2.20910100	-2.93964300
C	4.97818400	3.37512500	-0.38376600
H	4.57241800	3.03213900	1.70632500
H	5.12437900	3.54500500	-2.52851800
H	5.88017400	3.95070700	-0.19595200
B	-2.61170400	1.91112900	-1.63799700
C	-0.29920100	2.12200500	-0.49240400
O	-3.16440100	1.21615400	-0.58116000
O	-3.55714400	2.31115900	-2.55294700
C	-4.61011700	1.34802700	-0.67956900
C	-4.80548200	1.65536200	-2.20621500
C	0.26190200	3.36859100	0.07583300
C	0.77069600	4.41047500	-0.71769100
C	1.35160700	5.53697500	-0.14048100
C	1.43838300	5.66044100	1.24730200
C	0.35282400	3.51365100	1.47178300
C	0.93042300	4.63856400	2.05238500
H	0.74235400	4.32176000	-1.79864900
H	0.98795400	4.71745900	3.13488200
H	-0.92881500	1.66899500	0.28292100
H	1.75085600	6.31904400	-0.78035300
H	1.89661200	6.53758700	1.69414500
H	-0.00972600	2.70612900	2.10448000
C	-5.00393100	2.51963400	0.22374200
H	-6.08891400	2.65513600	0.25476000
H	-4.65122600	2.31269200	1.23585200
H	-4.54458600	3.45129100	-0.11763700
C	-5.26151900	0.06004000	-0.19279500
H	-5.09129300	-0.05925500	0.87826500
H	-6.34253400	0.09115600	-0.36577900
H	-4.85010500	-0.81449500	-0.69853000
C	-5.95940500	2.59528300	-2.53280800
H	-6.00370400	2.76123200	-3.61267500
H	-6.91316200	2.16153100	-2.21502800
H	-5.83523700	3.56375900	-2.04670200
C	-4.89148300	0.38933100	-3.06426400
H	-5.84109900	-0.13367600	-2.92028100
H	-4.80235100	0.66876200	-4.11710900
H	-4.07878400	-0.29965800	-2.82322600
C	-1.07901600	2.15559600	-1.79946100

H	-0.91560000	3.09228900	-2.34302300
H	-0.68194700	1.37820700	-2.47432600
P₁			
P	-0.73022700	-1.45610000	-1.33741500
C	-1.40033200	-0.96896300	-3.00616000
H	-0.63986800	-0.31203600	-3.44177500
H	-1.43440000	-1.85998500	-3.64294600
C	-2.76563500	-0.25551100	-3.03103800
H	-3.11233900	-0.26579700	-4.07132500
H	-3.50656300	-0.82726600	-2.46330500
C	-2.78520400	1.21114800	-2.55628600
H	-3.68241300	1.70704400	-2.94292700
H	-1.91580200	1.74328300	-2.95811500
P	-2.75029100	1.37887000	-0.69925300
C	0.89999200	-2.15603200	-1.83023700
C	1.28989800	-3.46906900	-1.53257100
C	1.83503600	-1.29719800	-2.43496000
C	2.57572300	-3.91283300	-1.84598700
H	0.59218300	-4.14534900	-1.05315700
C	3.11921900	-1.73974900	-2.74244100
H	1.57765300	-0.26203300	-2.63878300
C	3.49293300	-3.05360000	-2.45236200
H	2.86147600	-4.93273500	-1.60617800
H	3.83001300	-1.04464800	-3.17580000
H	4.49601600	-3.39969900	-2.68299500
C	-1.72766100	-2.90966900	-0.84107900
C	-2.79930900	-3.41231200	-1.59015800
C	-1.46599200	-3.45850400	0.42781700
C	-3.60979100	-4.42598300	-1.07575900
H	-3.01852800	-3.01465700	-2.57408800
C	-2.26618200	-4.48311000	0.92861700
H	-0.63291800	-3.08224300	1.01572800
C	-3.34855800	-4.96159500	0.18490800
H	-4.44546900	-4.79530400	-1.66291000
H	-2.04852300	-4.90223600	1.90678400
H	-3.98051500	-5.74931700	0.58441900
C	-3.20551100	3.13186700	-0.42944600
C	-2.79861900	4.14951500	-1.30483600
C	-3.87216200	3.48843900	0.75616900
C	-3.05961400	5.48806500	-1.00834800
H	-2.27516600	3.90236800	-2.22314200
C	-4.13129200	4.82503200	1.04941100
H	-4.19311200	2.71092800	1.44182200
C	-3.72640500	5.83094600	0.16810000
H	-2.74343800	6.26314500	-1.70060100
H	-4.65420800	5.08293200	1.96595200
H	-3.92982700	6.87259600	0.39703400

C	-4.30198200	0.49337400	-0.25594400
C	-5.56100200	0.94360500	-0.68248600
C	-4.21424000	-0.70653700	0.46225900
C	-6.70651100	0.20107500	-0.40293300
H	-5.64394600	1.88135900	-1.22449200
C	-5.36050100	-1.45533100	0.73294400
H	-3.24363900	-1.04978500	0.80370500
C	-6.60672600	-1.00351300	0.30029900
H	-7.67709900	0.55849500	-0.73486400
H	-5.27014100	-2.39168400	1.27462700
H	-7.50061800	-1.58374400	0.51051900
Pd	-0.97187400	0.24231600	0.27253300
C	1.01949100	-0.89120700	2.03271400
O	1.15100500	-2.11407400	1.97398900
C	-0.28313800	-0.29460500	2.43795300
C	-0.58439800	1.10346400	2.40008000
C	-1.25404100	-1.16017400	3.02978800
C	-1.77590900	1.59029700	2.99937700
H	0.18050000	1.82283500	2.12910500
C	-2.41744900	-0.66620400	3.57595800
H	-1.02012100	-2.21640100	3.07299300
C	-2.68532200	0.72365700	3.56657500
H	-1.96482600	2.65904900	2.98419200
H	-3.12699800	-1.34722500	4.03670500
H	-3.60069900	1.10222400	4.01117000
B	3.42957300	1.39370800	-0.13249600
C	2.22528100	0.03853700	1.75604400
O	4.24827800	2.17135400	0.64504700
O	3.87885300	1.26626000	-1.42697500
C	5.48774000	2.35671600	-0.09436900
C	5.01909700	2.15428300	-1.58117200
C	3.52706100	-0.72851100	1.86868400
C	3.87196200	-1.68586500	0.90499400
C	5.08796500	-2.36169200	0.98113500
C	5.97612000	-2.09896300	2.02715800
C	4.42011000	-0.47402700	2.91229600
C	5.63625800	-1.15448200	2.99607500
H	3.18544200	-1.90834200	0.09947300
H	6.31946000	-0.94110300	3.81330900
H	2.22429000	0.82483100	2.51900300
H	5.33548300	-3.09899400	0.22283000
H	6.92394000	-2.62624700	2.08672300
H	4.16543500	0.27292400	3.65947300
C	6.45160800	1.26830300	0.38488800
H	7.43607300	1.37268200	-0.08073300
H	6.56662700	1.34972300	1.46740300
H	6.06205700	0.26997400	0.17417400
C	6.04180000	3.73937000	0.22516700

H	6.31266600	3.78741400	1.28324400
H	6.94160400	3.94147700	-0.36502400
H	5.30924200	4.52340100	0.02703500
C	6.03628500	1.47412700	-2.48942200
H	5.61695100	1.36461400	-3.49388000
H	6.95015100	2.07170300	-2.56758300
H	6.29639400	0.48199900	-2.11790500
C	4.49280600	3.43722500	-2.22980300
H	5.30080900	4.14155700	-2.44717300
H	3.99540100	3.18090700	-3.16905900
H	3.76353700	3.93190900	-1.58266400
C	2.11149600	0.70594000	0.35953300
H	1.84756700	-0.05755600	-0.37083300
H	1.28482800	1.42961600	0.33745300

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P	-1.90703400	0.46694400	-1.82808800
C	-0.69981700	1.39816500	-2.88210400
H	0.16830200	0.74735700	-2.99718800
H	-1.12343200	1.51918400	-3.88336400
C	-0.23954100	2.74942500	-2.31515500
H	0.27715300	3.28561300	-3.11953300
H	-1.10121500	3.36837000	-2.04281500
C	0.73239500	2.64864600	-1.13092200
H	1.21840100	3.61637100	-0.97051000
H	1.52652700	1.92839100	-1.34221200
P	-0.06440000	2.18422800	0.47722000
C	-2.18897100	-1.03172600	-2.84725000
C	-3.48078400	-1.52514700	-3.07065600
C	-1.09162500	-1.72509200	-3.38054100
C	-3.67200800	-2.67624000	-3.83525800
H	-4.33650100	-1.00923600	-2.65145400
C	-1.28868100	-2.86369200	-4.16110600
H	-0.07959200	-1.39392900	-3.18145800
C	-2.57928400	-3.34275600	-4.39187000
H	-4.67902100	-3.04718800	-4.00096400
H	-0.42998100	-3.38161000	-4.57826500
H	-2.73165400	-4.23127800	-4.99720000
C	-3.45767200	1.44435400	-2.00271600
C	-3.61684500	2.44319900	-2.97365200
C	-4.50237400	1.21754000	-1.09219000
C	-4.78241700	3.20846000	-3.02231500
H	-2.83424400	2.64157900	-3.69604500
C	-5.67274300	1.97254100	-1.15289800
H	-4.38982800	0.45025200	-0.33247400
C	-5.81312900	2.97728300	-2.11160700
H	-4.88268500	3.98553100	-3.77423100

H	-6.47054500	1.77775500	-0.44223500
H	-6.71911400	3.57476700	-2.15040600
C	1.26482600	2.49124200	1.69308400
C	2.61528700	2.31080600	1.36366100
C	0.91669000	2.87570700	2.99742600
C	3.59879400	2.51931300	2.33339000
H	2.91598400	1.98613300	0.37412200
C	1.90251200	3.06951600	3.95919700
H	-0.12508900	2.99842900	3.26535500
C	3.24827800	2.89360300	3.62916000
H	4.64220700	2.37278800	2.07338800
H	1.61694800	3.34804000	4.96871100
H	4.01813900	3.04302800	4.38045200
C	-1.21372100	3.58791600	0.74361900
C	-0.73755000	4.90491500	0.83392700
C	-2.59233500	3.35306200	0.78693700
C	-1.63212000	5.96640100	0.94972300
H	0.33149700	5.09562100	0.82724300
C	-3.48836600	4.41727200	0.89238400
H	-2.95592400	2.33374100	0.73116600
C	-3.00916700	5.72410200	0.97236000
H	-1.25739700	6.98314000	1.02155900
H	-4.55524300	4.21858400	0.90333400
H	-3.70365900	6.55485000	1.05600900
Pd	-1.31190000	0.22938100	0.49430300
C	0.23148800	-0.42640400	2.95934100
C	-0.92751900	0.19879800	2.49539700
C	-1.77311600	0.82594900	3.41619200
C	-1.45218800	0.83737200	4.77803100
C	-0.28364300	0.22327800	5.23328200
C	0.55616900	-0.41413800	4.31809400
H	0.89186200	-0.91592000	2.25375400
H	-2.11877500	1.32841900	5.48288200
H	-0.03149700	0.24093700	6.28983400
H	1.47283800	-0.89302100	4.65434300
I	-3.16758700	-1.71007000	0.95931400
H	-2.68689200	1.30596900	3.07968600
Cu	0.71813300	-2.36168500	0.00731800
B	3.69143600	-0.00661100	-2.20071800
C	2.08866300	-1.02319500	-0.47900500
C	0.75083700	-3.80751600	3.00071600
O	3.90983200	1.16769700	-1.50202000
O	4.74034900	-0.31693000	-3.03032100
C	-0.25508200	-3.89412500	0.72134000
N	-0.15356600	-4.35522100	1.99835300
N	-1.20938800	-4.68412500	0.16260300
C	-1.05665900	-5.37658200	2.24231100
C	-1.72756900	-5.58228300	1.07918900

C	5.31953900	1.49430400	-1.64213900
C	5.67264900	0.79834300	-3.00399900
C	-1.71888100	-4.50433200	-1.18604500
H	-1.13382500	-5.86367900	3.20097800
H	-2.50896600	-6.28042000	0.82582300
H	-0.99423100	-3.92315800	-1.74966400
H	-2.66121800	-3.95260700	-1.16186900
H	-1.85880300	-5.47702100	-1.66431900
H	1.16462700	-4.62241600	3.59975800
H	0.22478600	-3.09991300	3.64459000
H	1.56481100	-3.28858600	2.49329300
C	3.26536400	-1.48669700	0.30965400
C	4.19126100	-2.42379300	-0.20296400
C	5.28870400	-2.85316800	0.54328900
C	5.51020000	-2.36721900	1.83395900
C	3.51597300	-1.00558600	1.61497600
C	4.60863300	-1.43747000	2.36100800
H	4.04857000	-2.81928100	-1.20363000
H	4.76749000	-1.02744000	3.35570700
H	1.77037100	-0.05560800	-0.08105700
H	5.97968000	-3.57136000	0.10832900
H	6.36763900	-2.69899600	2.41167200
H	2.85329400	-0.25864600	2.03404500
C	6.04474500	0.86713700	-0.44767000
H	7.10764700	1.12591200	-0.44771500
H	5.59737800	1.23669500	0.47655800
H	5.94050000	-0.21965300	-0.44183900
C	5.46701600	3.01040900	-1.62433900
H	5.17536800	3.39447000	-0.64250000
H	6.50624500	3.30187200	-1.80694100
H	4.83317200	3.48487400	-2.37556600
C	7.09013900	0.24778000	-3.09540200
H	7.23718700	-0.23059800	-4.06766700
H	7.82563600	1.05299500	-2.99687800
H	7.27641400	-0.49552600	-2.31933000
C	5.35453300	1.66972400	-4.22229500
H	6.05800400	2.50190800	-4.31861000
H	5.41838000	1.05554100	-5.12419400
H	4.34124100	2.07582400	-4.15771400
C	2.39519700	-0.86145300	-1.98951100
H	2.48429500	-1.82197400	-2.50993400
H	1.54740800	-0.35773800	-2.46621800

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P	-1.17469800	-0.76113400	-1.86735200
C	-1.14798800	0.45508300	-3.28129200
H	-0.16058100	0.91800900	-3.33644400
H	-1.30452100	-0.10869400	-4.20576100

C	-2.22646500	1.54337800	-3.15329800
H	-2.29175200	2.05808300	-4.11925700
H	-3.20647900	1.08403100	-2.98729700
C	-1.94797700	2.60337400	-2.08101800
H	-2.58482700	3.47964800	-2.23808700
H	-0.91904300	2.96659700	-2.17036700
P	-2.11689800	2.08513500	-0.29940600
C	-0.14221700	-2.13980000	-2.50063300
C	-0.45761000	-3.44892700	-2.09444400
C	0.90627000	-1.94223000	-3.40895400
C	0.22830800	-4.53412600	-2.63376000
H	-1.25027100	-3.60858300	-1.37048100
C	1.60801000	-3.03336300	-3.92782800
H	1.16826800	-0.94175400	-3.73573300
C	1.25773000	-4.33153700	-3.55722300
H	-0.04154800	-5.54105500	-2.32940300
H	2.41288700	-2.86528000	-4.63720400
H	1.78738800	-5.18026500	-3.97970800
C	-2.86265900	-1.43370500	-2.16732100
C	-3.16857300	-2.07727700	-3.37721600
C	-3.88427500	-1.19792800	-1.24589300
C	-4.47751900	-2.46280100	-3.65717100
H	-2.38265600	-2.28553300	-4.09693100
C	-5.19843600	-1.57055000	-1.53097100
H	-3.64164900	-0.74429700	-0.29886300
C	-5.49740200	-2.20245700	-2.73643800
H	-4.70343100	-2.96486100	-4.59343500
H	-5.97754300	-1.36624800	-0.80346300
H	-6.51817000	-2.49899200	-2.95975500
C	-1.59427500	3.67519100	0.46296200
C	-0.22336100	3.87120900	0.68503800
C	-2.49364200	4.69977100	0.77902800
C	0.24267900	5.08048400	1.19372700
H	0.47811300	3.07176400	0.48361200
C	-2.02549300	5.90449600	1.30724100
H	-3.55808800	4.55467400	0.62579100
C	-0.65875000	6.09912900	1.51073000
H	1.30860600	5.21342000	1.35132900
H	-2.73123900	6.69047700	1.56024300
H	-0.29862100	7.03787500	1.92129400
C	-3.93074200	1.99058200	-0.02171700
C	-4.87621500	2.64846500	-0.82037300
C	-4.38100900	1.16067800	1.01867900
C	-6.24173700	2.48650900	-0.58130000
H	-4.55698600	3.28564500	-1.63818600
C	-5.74437700	1.00896200	1.26336100
H	-3.66072400	0.60234300	1.60926800
C	-6.67827100	1.67021700	0.46255000

H	-6.96311500	2.99634400	-1.21303400
H	-6.07370800	0.35890200	2.06808800
H	-7.74112200	1.54306900	0.64543700
Pd	-0.75924300	0.20125400	0.30793700
C	0.50095700	0.31746500	3.05326300
C	-0.53805600	0.83413300	2.26704900
C	-1.44762700	1.68112000	2.91741700
C	-1.31938800	2.00476800	4.27146300
C	-0.26844000	1.48934400	5.02665300
C	0.64219300	0.63551700	4.40568200
H	1.21659800	-0.36334600	2.61162700
H	-2.04798700	2.66952500	4.72912600
H	-0.16228900	1.74539400	6.07693900
H	1.46842600	0.21292900	4.97367400
I	-1.95919100	-2.39271000	1.55280500
H	-2.28207600	2.12023700	2.38839500
Cu	0.62713100	-1.85282200	0.80866000
B	2.92937500	2.16400300	-1.42124800
C	1.60197200	0.56445800	0.04207800
C	1.38256200	-2.86489000	3.89743400
O	3.30191900	3.04446700	-0.43233600
O	3.82300200	2.11774100	-2.46234000
C	1.90123000	-3.21217100	1.48256600
N	2.10106700	-3.49853400	2.79986400
N	2.77535500	-4.03215100	0.83989600
C	3.08901000	-4.45541700	2.97195200
C	3.51381000	-4.79725700	1.72927600
C	4.68504700	3.40968700	-0.68738300
C	4.81210000	3.15932600	-2.23424100
C	2.84903100	-4.17688700	-0.60247100
H	3.39394300	-4.80176800	3.94649100
H	4.25507700	-5.50900300	1.40314400
H	2.29414000	-3.36211700	-1.05738900
H	2.40765200	-5.12775200	-0.90950000
H	3.88859600	-4.12669800	-0.92995300
H	1.95802600	-2.02792500	4.30009300
H	1.21117300	-3.60075500	4.68627200
H	0.42225600	-2.50368000	3.52957900
C	2.84374400	-0.22722900	0.25780600
C	3.49966500	-0.90074600	-0.79602800
C	4.72649700	-1.53272900	-0.60620200
C	5.34071100	-1.54281800	0.64743800
C	3.51543100	-0.20043000	1.50326100
C	4.71997200	-0.86547600	1.70165200
H	3.04283800	-0.92778700	-1.77842300
H	5.20011900	-0.82157100	2.67580600
H	1.53794800	1.29496400	0.84273300
H	5.20716700	-2.02206800	-1.44988700

H	6.29473000	-2.04010200	0.79341300
H	3.08901400	0.37995300	2.31306400
C	5.55074900	2.46113100	0.14718500
H	6.61175400	2.71725600	0.07142200
H	5.24778800	2.53792800	1.19396700
H	5.41285900	1.42188300	-0.15872400
C	4.89448900	4.85306000	-0.24736300
H	4.76665600	4.92586500	0.83623700
H	5.90620100	5.19180200	-0.49321400
H	4.17567300	5.52443500	-0.71997500
C	6.17031500	2.64090000	-2.69060500
H	6.15989500	2.48306800	-3.77274700
H	6.95958200	3.36364200	-2.45936400
H	6.41056400	1.69142100	-2.21051200
C	4.38420300	4.36397900	-3.07675700
H	5.11397700	5.17667900	-3.01921800
H	4.29421700	4.05221700	-4.12065000
H	3.41283400	4.74460500	-2.74934300
C	1.62835000	1.29120800	-1.31438600
H	1.58389200	0.59488100	-2.15447200
H	0.75264600	1.93818600	-1.40770000

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P	-0.81312600	-0.11754300	-2.12226400
C	-0.58969600	1.45219200	-3.11581100
H	0.44521400	1.79370900	-3.02439500
H	-0.75705500	1.18939400	-4.16553900
C	-1.55981600	2.59255800	-2.75009400
H	-1.46923300	3.34582400	-3.54232500
H	-2.58901200	2.22419400	-2.80684000
C	-1.32472100	3.30972500	-1.40907300
H	-1.84042100	4.27601900	-1.41560500
H	-0.26390700	3.53841400	-1.28736700
P	-1.81498500	2.36910200	0.13175100
C	0.17970500	-1.36127700	-3.04115300
C	0.11271000	-2.68634700	-2.58205200
C	0.97893300	-1.06875100	-4.15232200
C	0.82630700	-3.69275700	-3.22730500
H	-0.51146400	-2.92607400	-1.72444300
C	1.71323400	-2.07592400	-4.78314100
H	1.04620600	-0.05364200	-4.52787500
C	1.63766600	-3.39013600	-4.32380000
H	0.74912400	-4.71600300	-2.87249500
H	2.33733100	-1.83112200	-5.63770800
H	2.20186200	-4.17471900	-4.81904900
C	-2.50357200	-0.53090300	-2.74969800
C	-2.68570500	-1.17860700	-3.98012400
C	-3.63047100	-0.08505100	-2.05080000

C	-3.96871500	-1.37173400	-4.49337800
H	-1.82869300	-1.53828100	-4.53870100
C	-4.91168200	-0.26080600	-2.57072400
H	-3.51394800	0.38365600	-1.08772400
C	-5.08452400	-0.90913100	-3.79331300
H	-4.09442100	-1.88403600	-5.44297000
H	-5.76503000	0.10006000	-2.00537200
H	-6.08158800	-1.05923200	-4.19722300
C	-1.36401200	3.62891000	1.40292400
C	-0.26849300	3.38001000	2.24195500
C	-2.06541400	4.83629000	1.53916900
C	0.13112900	4.32993700	3.18332000
H	0.25525500	2.43439500	2.17402600
C	-1.66818100	5.78188100	2.48287900
H	-2.93248700	5.03015700	0.91488900
C	-0.56558700	5.53196000	3.30396000
H	0.98054300	4.12161500	3.82689000
H	-2.22040900	6.71225700	2.58089000
H	-0.25827200	6.26899500	4.04023400
C	-3.65474600	2.49433000	0.11285800
C	-4.39182400	3.30535700	-0.76197100
C	-4.35425400	1.64131200	0.98421100
C	-5.78729100	3.27270400	-0.76063700
H	-3.88587900	3.96226000	-1.46070400
C	-5.74728000	1.61360500	0.99072400
H	-3.80458100	0.96025900	1.62537700
C	-6.46943700	2.42938700	0.11665000
H	-6.34033000	3.90454300	-1.44973700
H	-6.26658400	0.94032000	1.66582400
H	-7.55497800	2.40047900	0.11297300
Pd	-0.38756800	-0.04188600	0.33845000
C	0.87209400	-0.86786100	3.04401800
C	-0.17427100	-0.21165100	2.37747100
C	-1.19278100	0.33154400	3.18020500
C	-1.16480600	0.23247900	4.57181200
C	-0.11280000	-0.42629900	5.21361400
C	0.90594000	-0.97974400	4.43988600
H	1.67476600	-1.31547900	2.47392000
H	-1.96754600	0.67560000	5.15583100
H	-0.08759000	-0.49966500	6.29725900
H	1.73767400	-1.49551700	4.91556900
I	-2.71812900	-1.98363200	0.68480300
H	-2.02509800	0.84819400	2.71766600
Cu	-0.19026300	-2.54378000	0.89530200
B	3.25314300	2.48595700	-0.47410000
C	1.66265500	0.64486300	0.37036000
C	-0.39521800	-4.19221200	3.68202700
O	4.09358700	2.59104200	0.60630900

O	3.84810600	2.85926600	-1.65593700
C	0.89213800	-4.00945800	1.56129400
N	0.68008800	-4.58719200	2.77665200
N	1.98926300	-4.64817800	1.07696000
C	1.63110500	-5.55763900	3.04774600
C	2.45750700	-5.60121000	1.96911700
C	5.43309600	2.81712600	0.08963200
C	5.14479600	3.42856900	-1.33029100
C	2.54236700	-4.40788500	-0.24682000
H	1.63710900	-6.12169000	3.96677600
H	3.31704200	-6.21767400	1.75973000
H	2.19042400	-3.44151700	-0.60202800
H	2.22272500	-5.18987600	-0.94148300
H	3.63018500	-4.38268800	-0.19565400
H	-0.03891000	-3.45708800	4.40668600
H	-0.77715700	-5.07719200	4.19591800
H	-1.19247000	-3.73767300	3.09183900
C	2.67887300	-0.34850600	-0.09220200
C	2.92355500	-0.56771600	-1.45977000
C	3.95855700	-1.38801900	-1.90127400
C	4.80839600	-2.00751800	-0.98115100
C	3.55491800	-0.97611300	0.81686200
C	4.59714900	-1.79313000	0.38273400
H	2.30531200	-0.06661600	-2.18967900
H	5.26569300	-2.23967300	1.11430900
H	1.83913000	0.84100800	1.42498100
H	4.10240300	-1.53396100	-2.96752000
H	5.62818100	-2.63343500	-1.32183700
H	3.45501200	-0.76355600	1.87462100
C	6.11754000	1.44956000	0.02502400
H	7.16005100	1.53836400	-0.29512100
H	6.09660800	0.99713400	1.01894200
H	5.59366600	0.77450800	-0.65432100
C	6.17498100	3.73898400	1.04981300
H	6.30240000	3.23612600	2.01228000
H	7.16828800	3.98523700	0.66038600
H	5.62642500	4.66613400	1.22270800
C	6.13517100	3.02526900	-2.41609800
H	5.84523600	3.48208600	-3.36653800
H	7.14469600	3.36816500	-2.16720400
H	6.15492200	1.94295900	-2.55092600
C	4.96341200	4.94893100	-1.30822600
H	5.91116300	5.46710700	-1.13617700
H	4.56257800	5.27113100	-2.27287600
H	4.25613500	5.24710100	-0.52970000
C	1.77095600	1.97480600	-0.38926800
H	1.38904800	1.89656600	-1.40623900
H	1.16063400	2.72783800	0.11717900

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P	0.25660800	1.80656500	-1.14282900
C	1.33409700	2.29960700	-2.58481000
H	0.96724400	1.71505900	-3.43617200
H	1.11867400	3.34628800	-2.82202400
C	2.85025400	2.09658600	-2.43146800
H	3.33697200	2.61969800	-3.26333700
H	3.20986200	2.58135700	-1.51793900
C	3.31993300	0.63609200	-2.45456000
H	4.40056400	0.59022800	-2.62335100
H	2.83906800	0.10451500	-3.28259300
P	2.92067900	-0.28334400	-0.88917000
C	-1.34944500	2.44495600	-1.76689900
C	-2.01616800	3.52215500	-1.17099600
C	-1.94926000	1.78853000	-2.85199100
C	-3.26602800	3.92390600	-1.64271300
H	-1.56955000	4.03208500	-0.32554400
C	-3.19745300	2.19127300	-3.32254200
H	-1.45025800	0.94296000	-3.31725200
C	-3.86223800	3.25722000	-2.71337300
H	-3.77751500	4.75482400	-1.16568400
H	-3.65676500	1.66341400	-4.15247200
H	-4.84107600	3.56290800	-3.06995200
C	0.71127300	3.01093500	0.16782800
C	1.47147700	4.16471300	-0.06699500
C	0.28295000	2.73651100	1.47577100
C	1.81928500	5.01013500	0.98731100
H	1.80061200	4.41393300	-1.06926600
C	0.61313100	3.59262200	2.52438700
H	-0.30163800	1.84883600	1.67544200
C	1.39262500	4.72589300	2.28526100
H	2.42142700	5.89259300	0.79237400
H	0.25911000	3.36349400	3.52457300
H	1.66263500	5.38724200	3.10334000
C	3.75519400	-1.88827900	-1.14400800
C	3.62254000	-2.56475800	-2.36442600
C	4.40178100	-2.52696000	-0.07753000
C	4.13975800	-3.84989000	-2.51953000
H	3.09997200	-2.10024400	-3.19475800
C	4.90828900	-3.81506900	-0.23219400
H	4.47934900	-2.02990400	0.88191000
C	4.78257200	-4.47893900	-1.45289600
H	4.03279500	-4.36219600	-3.47117300
H	5.38938000	-4.30480000	0.60859800
H	5.17489600	-5.48461600	-1.57004000
C	3.96740000	0.58664300	0.33422500
C	5.35539300	0.71744800	0.17452900

C	3.34375700	1.19124500	1.43153200
C	6.09988400	1.45443800	1.09286800
H	5.85298500	0.23194800	-0.66000500
C	4.08780000	1.93698300	2.34637600
H	2.27275800	1.08478900	1.55239600
C	5.46537100	2.07025900	2.17641500
H	7.17408200	1.55104800	0.96526400
H	3.58504400	2.41653600	3.17988900
H	6.04816000	2.64991000	2.88628500
Pd	0.62048900	-0.43221700	-0.29476200
C	1.03483500	-3.42379700	-0.03015500
C	1.12088000	-2.18814400	0.62626100
C	1.64334000	-2.17063600	1.92790100
C	2.07609200	-3.34683300	2.55021300
C	1.99553100	-4.56648600	1.87768200
C	1.47092900	-4.59994700	0.58363300
H	0.63487700	-3.47193800	-1.03969300
H	2.47876700	-3.30730000	3.55998700
H	2.33609500	-5.48086000	2.35562800
H	1.40537400	-5.54436400	0.04887600
H	1.72748700	-1.22920300	2.46531900
B	-3.69457100	-1.57025500	-0.58868400
C	-1.37214700	-1.00453400	0.26485400
O	-4.05036600	-2.59701100	0.25378300
O	-4.76307700	-0.77808500	-0.94100200
C	-5.38701300	-2.31297700	0.74161500
C	-5.96283800	-1.37253700	-0.38206900
C	-1.89868400	-0.00988200	1.23358000
C	-2.76942700	1.03677700	0.87479400
C	-3.21200900	1.96567200	1.81838900
C	-2.81305300	1.87253600	3.15177100
C	-1.52131500	-0.09978300	2.59191700
C	-1.96749600	0.82285000	3.53278500
H	-3.11258100	1.12237600	-0.14704100
H	-1.66008800	0.72273300	4.57069700
H	-1.25152900	-1.95100900	0.78694000
H	-3.87458500	2.76653600	1.50108300
H	-3.16037200	2.59462800	3.88462300
H	-0.85983100	-0.90828600	2.89029000
C	-5.21885700	-1.61055000	2.09328600
H	-6.18558700	-1.41512900	2.56702700
H	-4.63397500	-2.25714800	2.75230200
H	-4.67750900	-0.66818600	1.98716700
C	-6.13193000	-3.63082200	0.92111700
H	-5.64323000	-4.22175800	1.70037500
H	-7.16765000	-3.45203200	1.22844000
H	-6.13564700	-4.21988600	0.00267100
C	-6.86128100	-0.24884700	0.12319700

H	-7.19910800	0.35911000	-0.72096700
H	-7.74473600	-0.65324900	0.62796700
H	-6.32549400	0.40061700	0.81681100
C	-6.64621800	-2.13541900	-1.52040600
H	-7.60173200	-2.56457400	-1.20487700
H	-6.83218000	-1.44418300	-2.34679200
H	-6.00623400	-2.94140000	-1.88940900
C	-2.21202400	-1.26053900	-1.00059500
H	-2.19953900	-0.41277000	-1.68770700
H	-1.77012400	-2.11105800	-1.53406900

TS8'

P	0.18080800	1.51212700	-1.47425200
C	1.35347900	1.75654700	-2.90549600
H	1.24642400	0.88853200	-3.56466500
H	1.04511200	2.63805100	-3.47691700
C	2.82318000	1.91580000	-2.47161500
H	3.37177600	2.33755200	-3.32269100
H	2.88547900	2.66459200	-1.67479100
C	3.56160000	0.63343500	-2.04890400
H	4.63917800	0.82728300	-1.99580900
H	3.42989400	-0.14250500	-2.81217900
P	3.00938700	-0.17422600	-0.46249900
C	-1.46891400	1.71936400	-2.24635200
C	-2.44788800	2.56026000	-1.69471500
C	-1.83537500	0.86126300	-3.29727300
C	-3.75716400	2.53576100	-2.17581400
H	-2.18584500	3.22598500	-0.87966000
C	-3.13935900	0.85122800	-3.78703800
H	-1.10134500	0.18013800	-3.71979800
C	-4.10823600	1.68282100	-3.22133700
H	-4.50512200	3.18307200	-1.72701500
H	-3.40372200	0.18160800	-4.60024900
H	-5.12942600	1.65943300	-3.58894300
C	0.43139300	3.07443600	-0.54441700
C	0.37516500	4.33788700	-1.15443100
C	0.74492700	2.98915800	0.81648600
C	0.64089000	5.48962300	-0.41654500
H	0.11518300	4.42159900	-2.20578800
C	1.01401400	4.14149900	1.55542900
H	0.77775200	2.01877100	1.29363700
C	0.96586000	5.39126300	0.94014100
H	0.59615300	6.46292200	-0.89671000
H	1.26629600	4.05274900	2.60676300
H	1.17836400	6.28970600	1.51251900
C	4.24257800	-1.52942900	-0.35218000
C	3.89667000	-2.76290500	-0.92177800
C	5.49445700	-1.38350700	0.26282100

C	4.79731300	-3.82689100	-0.89446300
H	2.91493900	-2.89719200	-1.36275600
C	6.39010900	-2.45195300	0.29422900
H	5.76499500	-0.43741400	0.72102000
C	6.04421400	-3.67427400	-0.28701600
H	4.50831000	-4.77979900	-1.32665800
H	7.35726900	-2.33142400	0.77421900
H	6.74146600	-4.50665500	-0.25658900
C	3.53689400	0.99049100	0.85585100
C	4.40692600	2.07031700	0.65859700
C	2.97257900	0.80225500	2.12836600
C	4.69916200	2.94669000	1.70589500
H	4.85795000	2.23957800	-0.31330200
C	3.27685500	1.66528900	3.17742800
H	2.26126000	-0.00494800	2.27648600
C	4.13766000	2.74585700	2.96651900
H	5.36499300	3.78741900	1.53446600
H	2.82577800	1.50700800	4.15256800
H	4.36387200	3.43055000	3.77856100
Pd	0.69284500	-0.54840100	-0.38161500
C	0.24244900	-3.31905000	-1.27984600
C	0.43099000	-2.64031000	-0.05933000
C	1.12468100	-3.32271200	0.96342500
C	1.62314900	-4.60570700	0.76531400
C	1.44422900	-5.25990300	-0.46059900
C	0.75951800	-4.60341400	-1.48267600
H	-0.30279900	-2.83320600	-2.08337300
H	2.17104700	-5.09568000	1.56607100
H	1.83131900	-6.26321500	-0.61054300
H	0.61296900	-5.09286100	-2.44263700
H	1.29839900	-2.82981100	1.91521800
B	-3.77818600	-1.50050600	0.01195600
C	-1.28056900	-1.67811700	0.52661200
O	-4.28938000	-2.23189500	1.05523100
O	-4.64001200	-0.53047400	-0.43763700
C	-5.49105200	-1.55480800	1.51531700
C	-5.90276300	-0.70260500	0.25507800
C	-1.27414200	-0.49992500	1.45822500
C	-1.98978500	0.68610900	1.19123200
C	-2.00301900	1.73821500	2.10183800
C	-1.29384100	1.65237800	3.30339900
C	-0.58786300	-0.58102800	2.68714600
C	-0.58472200	0.48391500	3.58721600
H	-2.53793200	0.78721400	0.26390700
H	-0.04036500	0.39130000	4.52331100
H	-1.38938800	-2.57122300	1.13604800
H	-2.56136800	2.63915700	1.86339000
H	-1.29842800	2.47982500	4.00602500

H	-0.06277300	-1.49724400	2.93640100
C	-5.07871300	-0.70385400	2.72005700
H	-5.94079500	-0.20463600	3.17219100
H	-4.62444300	-1.35664200	3.46983900
H	-4.33630500	0.04744200	2.44316300
C	-6.50808700	-2.60895100	1.93838900
H	-6.12223900	-3.16288800	2.79829700
H	-7.45300200	-2.14018700	2.23187300
H	-6.70570000	-3.32300500	1.13745700
C	-6.46367600	0.67989600	0.56849400
H	-6.68732900	1.20258900	-0.36571300
H	-7.38862900	0.60438500	1.14906400
H	-5.74503000	1.28015600	1.12809400
C	-6.82922200	-1.44910400	-0.70858100
H	-7.83522300	-1.56699200	-0.29575000
H	-6.89906400	-0.88029900	-1.63948500
H	-6.43097200	-2.43911500	-0.94608300
C	-2.33635500	-1.69588500	-0.57587600
H	-2.15665300	-0.93238500	-1.33521900
H	-2.28117000	-2.66444500	-1.08559100

P₃

C	3.50045800	-1.54304500	0.95706800
C	2.80154400	-0.62856600	0.15986600
C	3.49724800	0.04227700	-0.85250300
C	4.85450500	-0.19964000	-1.06510500
C	5.54029600	-1.11606400	-0.26671800
C	4.85733500	-1.78814300	0.74794200
H	2.97207600	-2.06733100	1.74991600
H	5.37843600	0.33343300	-1.85341500
H	6.59776200	-1.30110800	-0.43030200
H	5.38162100	-2.49906300	1.38020200
H	2.97607500	0.76814300	-1.46859200
B	-1.05587600	-1.16661200	-0.27705700
C	1.30736900	-0.43173700	0.37833400
O	-1.62329300	-1.06823700	0.96957900
O	-1.94629400	-0.94256900	-1.29495000
C	-2.94004100	-0.47482700	0.79748300
C	-3.26980500	-0.82427300	-0.70118600
C	0.86607800	1.01164800	0.18419900
C	0.38019900	1.49032300	-1.03955000
C	-0.03182500	2.81824500	-1.17610200
C	0.03376800	3.68987900	-0.08983900
C	0.93501600	1.90160700	1.26370800
C	0.52223800	3.22573000	1.13377000
H	0.29694900	0.82204200	-1.88917900
H	0.57533200	3.89451900	1.98793700
H	1.09860800	-0.67885000	1.42499900

H	-0.41056400	3.16655000	-2.13268600
H	-0.29359800	4.72003100	-0.19329500
H	1.30947900	1.54264700	2.21873000
C	-2.78199400	1.02788600	1.04934700
H	-3.74797500	1.54032600	1.01806200
H	-2.34327400	1.17452300	2.03923200
H	-2.11464200	1.48997700	0.31948400
C	-3.88590700	-1.08679900	1.82382900
H	-3.56102300	-0.80985700	2.83037000
H	-4.90519200	-0.71356000	1.68160300
H	-3.89965500	-2.17589800	1.75999300
C	-4.03885300	0.25321300	-1.45622200
H	-4.20636400	-0.06867000	-2.48769800
H	-5.01424900	0.43050100	-0.99190700
H	-3.48503100	1.19275300	-1.47880700
C	-3.94914900	-2.18571300	-0.87018900
H	-4.98052100	-2.16880500	-0.50685400
H	-3.95931600	-2.44690000	-1.93147500
H	-3.40282500	-2.96592000	-0.33346700
C	0.47973500	-1.42666800	-0.48048600
H	0.75661300	-1.34704200	-1.53666600
H	0.74806300	-2.44493300	-0.17380800

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P	1.41283900	-0.30623300	2.17231700
C	1.20072200	0.83495600	3.62736900
H	0.13488400	1.07200900	3.72135300
H	1.49510700	0.31257500	4.54275900
C	2.02044400	2.13072300	3.48911700
H	2.04274800	2.61552000	4.47194700
H	3.05830600	1.88325900	3.24728000
C	1.47330000	3.16751600	2.49420400
H	1.95604400	4.13659300	2.65989100
H	0.40440700	3.31118700	2.68517800
P	1.59626800	2.75174900	0.69238200
C	0.84109900	-1.93046800	2.80370600
C	1.46606000	-3.09313800	2.31963200
C	-0.18521000	-2.04662400	3.75104000
C	1.08140700	-4.34265000	2.80151900
H	2.25527600	-3.02619000	1.57856300
C	-0.57261900	-3.30298900	4.22147900
H	-0.68327800	-1.16203800	4.13311100
C	0.06630900	-4.45257000	3.75516100
H	1.58047900	-5.23037200	2.42507900
H	-1.36553200	-3.37867200	4.95974500
H	-0.22697900	-5.42834100	4.13129900
C	3.22794400	-0.54865400	2.16357100

C	3.93217900	-0.81319900	3.35011700
C	3.91963000	-0.49483000	0.95362600
C	5.31138800	-0.99549000	3.31866700
H	3.40352000	-0.89061200	4.29561200
C	5.29964200	-0.69374600	0.92045100
H	3.36897800	-0.33125900	0.04111600
C	5.99736400	-0.93450300	2.10061000
H	5.85133700	-1.19677400	4.23930500
H	5.81314200	-0.67335100	-0.03374200
H	7.07202200	-1.08979500	2.07676200
C	0.97657900	4.27597300	-0.11903100
C	0.08608500	5.15026100	0.51880800
C	1.28867500	4.49368900	-1.46973100
C	-0.48542000	6.21324200	-0.18075100
H	-0.18381300	5.00529800	1.55857400
C	0.71283800	5.55215600	-2.16611700
H	1.96475300	3.82084400	-1.98536100
C	-0.18063800	6.41291200	-1.52615000
H	-1.17627800	6.87937900	0.32743500
H	0.95400100	5.69688500	-3.21452600
H	-0.63704300	7.23144300	-2.07394500
C	3.37239300	2.73016900	0.26533900
C	4.35839900	3.32094400	1.06474300
C	3.74242000	2.07396400	-0.91982200
C	5.69932200	3.25067100	0.68775700
H	4.08995500	3.83136200	1.98391600
C	5.08098500	2.02843700	-1.30366800
H	2.99145300	1.57071000	-1.52140200
C	6.06124900	2.60988100	-0.49820000
H	6.46065000	3.69688600	1.32044600
H	5.35489000	1.50448800	-2.21356300
H	7.10648600	2.55481800	-0.78715400
Pd	0.56706800	0.73789900	0.16063900
C	-1.30712500	2.48062200	-3.42151000
C	-0.99195500	2.26795600	-2.07086600
C	-1.77871300	2.86055100	-1.07921000
C	-2.86926900	3.65390400	-1.42689600
C	-3.18791900	3.84999700	-2.77135900
C	-2.40399500	3.26202800	-3.77002300
H	-0.67886100	2.01553400	-4.17406100
H	-3.46804700	4.11286800	-0.64711600
H	-4.04449400	4.46008800	-3.04326300
H	-2.65125000	3.41763400	-4.81619300
H	-1.52925400	2.70233100	-0.03668300
Cu	-0.37241000	-1.49615200	-0.50491300
B	-3.70123300	0.21380800	1.80205000
C	-1.99086400	-0.34130000	0.07063800
C	-0.73471000	-2.58209900	-3.59818800

O	-3.97095500	1.50943400	1.41521900
O	-4.81011200	-0.44226000	2.27217000
C	-1.08711900	-3.26118000	-1.24803900
N	-1.24419100	-3.48387600	-2.57561200
N	-1.59131300	-4.37536900	-0.66313200
C	-1.82080000	-4.71905300	-2.82059000
C	-2.04954500	-5.28502800	-1.60762600
C	-5.41561800	1.62640700	1.30852900
C	-5.91088400	0.50810600	2.29739900
C	-1.69471900	-4.55177700	0.77271400
H	-1.25938000	-3.67932600	1.25543200
H	-1.14327100	-5.43853400	1.09268500
H	-2.74305800	-4.64610100	1.07225000
H	0.29319500	-2.84819300	-3.84897900
H	-0.75338500	-1.56481700	-3.20710500
H	-1.37698900	-2.63295100	-4.47991000
C	-3.01332400	-0.97159700	-0.81912600
C	-3.84161100	-2.02714400	-0.39426200
C	-4.79335700	-2.58835000	-1.24456300
C	-4.94799600	-2.11355500	-2.54794400
C	-3.19563700	-0.49577200	-2.13181500
C	-4.14190600	-1.05739500	-2.98273100
H	-3.74979500	-2.40570200	0.61650100
H	-4.25857400	-0.66082400	-3.98793800
H	-1.95309000	0.70441000	-0.19421600
H	-5.41811900	-3.40145400	-0.88439300
H	-5.68901400	-2.55148800	-3.20996200
H	-2.58682900	0.32917400	-2.48108400
C	-5.77636700	1.34430200	-0.15417400
H	-6.84429400	1.49711400	-0.33633600
H	-5.21051400	2.02531200	-0.79426700
H	-5.51098400	0.32607300	-0.44487200
C	-5.81853900	3.04620600	1.68753700
H	-5.41883100	3.74771900	0.94973300
H	-6.90818500	3.15127300	1.69590200
H	-5.43144000	3.32718600	2.66835500
C	-7.17601400	-0.21954300	1.85826700
H	-7.43831300	-0.98058900	2.59846600
H	-8.01631200	0.47713100	1.77320300
H	-7.02900800	-0.71554100	0.89790500
C	-6.04058100	0.99208600	3.74378000
H	-6.89456600	1.66365400	3.87108100
H	-6.18211800	0.12568200	4.39508700
H	-5.13498000	1.51402800	4.06479200
C	-2.28713400	-0.43046700	1.58026200
H	-2.23410500	-1.44993000	1.97014800
H	-1.52350800	0.14632500	2.11124600
C	0.17427800	1.38664600	-1.72954500

O	0.96046500	1.04499700	-2.60008200
S	2.49620200	-2.88986800	-1.35502200
O	3.53115300	-3.35903700	-0.42014200
O	1.72963900	-3.91181600	-2.08431100
C	3.41705700	-1.98780900	-2.69478300
F	4.28533800	-2.80534000	-3.30293200
F	4.11102200	-0.94223100	-2.19342500
F	2.56195300	-1.51358200	-3.61238200
O	1.67561500	-1.75840900	-0.78712800
H	-2.49124100	-6.23068200	-1.33740300
H	-2.01362800	-5.08055800	-3.81786000

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P	-0.88520700	-0.73630800	-2.39523600
C	-0.71353300	0.44465500	-3.83744700
H	0.28246900	0.89621200	-3.76742900
H	-0.73419900	-0.13866500	-4.76285200
C	-1.78653300	1.54291600	-3.90674000
H	-1.72330500	1.99962300	-4.90176700
H	-2.77888200	1.08977200	-3.84157800
C	-1.65777800	2.67947400	-2.88467600
H	-2.35247400	3.48851000	-3.13432000
H	-0.64832300	3.09954700	-2.94489600
P	-1.88933400	2.22934900	-1.10312800
C	-0.06899100	-2.23784200	-3.09145400
C	-0.65578000	-3.49850300	-2.89654600
C	1.12236100	-2.15576600	-3.82755700
C	-0.07465500	-4.64279600	-3.44079700
H	-1.57773400	-3.58150100	-2.33208700
C	1.71066900	-3.30436000	-4.35794100
H	1.59710400	-1.19569500	-3.99497500
C	1.11071500	-4.55087100	-4.17231000
H	-0.55092500	-5.60716700	-3.29082900
H	2.63229000	-3.22116000	-4.92626900
H	1.56265100	-5.44239100	-4.59657000
C	-2.63786700	-1.25539200	-2.52645600
C	-3.24862000	-1.48000900	-3.77254800
C	-3.35746900	-1.50162200	-1.35594800
C	-4.56853600	-1.91688000	-3.83472700
H	-2.69318100	-1.32620200	-4.69277700
C	-4.67585400	-1.95825800	-1.41884800
H	-2.89085400	-1.33940900	-0.39529200
C	-5.28404100	-2.15626200	-2.65591900
H	-5.03801400	-2.07977700	-4.80066300
H	-5.20192400	-2.14224300	-0.48904600
H	-6.31262500	-2.50127800	-2.70897400
C	-1.83530400	3.87517900	-0.28101500
C	-1.06031400	4.92648000	-0.78998900

C	-2.48393100	4.05085300	0.95061700
C	-0.92957900	6.12035900	-0.08217100
H	-0.52998300	4.81980800	-1.72870900
C	-2.35111500	5.24412500	1.65570800
H	-3.08317300	3.25144600	1.36821500
C	-1.56984400	6.28146000	1.14530400
H	-0.31322200	6.91723900	-0.48654600
H	-2.85535200	5.35811800	2.61043100
H	-1.45809800	7.20703400	1.70173500
C	-3.63088300	1.74209100	-0.88543000
C	-4.63241400	1.99876800	-1.83000400
C	-3.95918500	1.11068300	0.32285900
C	-5.94898600	1.62412900	-1.56472700
H	-4.39586200	2.48780800	-2.76925500
C	-5.28072600	0.76489600	0.59569400
H	-3.17851700	0.86459500	1.03306900
C	-6.27472200	1.01645100	-0.35023800
H	-6.72071200	1.80985900	-2.30595500
H	-5.50601100	0.25292700	1.52325800
H	-7.30162800	0.72594700	-0.14921000
Pd	-0.23722300	0.62391800	-0.39995800
C	1.03027700	3.81146100	2.32254900
C	0.88955300	3.01957100	1.17501400
C	1.59249300	3.36286300	0.01576600
C	2.43737700	4.46994400	0.00251000
C	2.57738200	5.25103500	1.15096100
C	1.86843300	4.92222000	2.31063100
H	0.46419400	3.53726500	3.20619600
H	2.98591400	4.71649700	-0.90099200
H	3.23599100	6.11500700	1.14416900
H	1.97097400	5.53470100	3.20165600
H	1.47154600	2.75778900	-0.87611500
Cu	0.04436200	-1.74175800	0.86170600
B	3.97529400	0.33986600	-1.39149000
C	1.90559500	0.05448200	-0.01194200
C	0.49570200	-3.23964100	3.83192300
O	4.16758400	1.70232600	-1.29958900
O	5.15013500	-0.36544100	-1.33286200
C	0.98386300	-3.39696600	1.38277200
N	1.10237000	-3.85517000	2.65841600
N	1.72034100	-4.28064200	0.65238700
C	1.89303800	-4.99010600	2.72207000
C	2.28818800	-5.26005600	1.45267800
C	5.50124600	1.89518200	-0.75602300
C	6.24100800	0.59342700	-1.23665700
C	1.99449400	-4.14672500	-0.76556100
H	1.42131900	-3.30595300	-1.14689000
H	1.69734100	-5.04865100	-1.30244300

H	3.05926500	-3.95901000	-0.92962500
H	-0.35979900	-3.82425500	4.16987000
H	0.15008200	-2.24677300	3.56372200
H	1.25059900	-3.15483000	4.61622100
C	2.51795900	-0.65234600	1.16269700
C	3.52228700	-1.63069500	1.02433800
C	4.15152900	-2.19439100	2.13386700
C	3.80728500	-1.79679700	3.42510200
C	2.18415200	-0.26524200	2.47944900
C	2.81939700	-0.82169200	3.58522500
H	3.83457600	-1.94664600	0.03872400
H	2.53216300	-0.49500000	4.58103200
H	2.11964000	1.10144600	0.17696300
H	4.91730400	-2.95034000	1.98222700
H	4.29955700	-2.23362800	4.28894100
H	1.40269500	0.46579700	2.63873800
C	5.34092300	1.97334700	0.76668400
H	6.29415600	2.18294100	1.26040000
H	4.63973200	2.77728200	1.00311100
H	4.93305900	1.04306200	1.17054400
C	6.06966100	3.19997000	-1.29846700
H	5.47715300	4.03779700	-0.92137700
H	7.10330700	3.33947200	-0.96594100
H	6.04589200	3.22711100	-2.38919100
C	7.26873400	0.04456200	-0.25444900
H	7.73089100	-0.85601000	-0.66852500
H	8.05935400	0.77886800	-0.06933200
H	6.80126000	-0.21960100	0.69515200
C	6.84228600	0.72224000	-2.63769200
H	7.72115400	1.37341500	-2.64077900
H	7.14513500	-0.26864000	-2.98610900
H	6.10868000	1.12251700	-3.34268300
C	2.52884400	-0.26843100	-1.38862400
H	2.49810000	-1.33384300	-1.62067800
H	1.94054000	0.24127700	-2.15907900
C	-0.03225700	1.83014400	1.22550000
O	-0.70997000	1.61393700	2.21184200
S	-2.81011000	-1.93888800	2.30185000
O	-4.20765400	-1.89465800	1.84117900
O	-2.29791400	-3.23090800	2.77968100
C	-2.77565600	-0.82301700	3.78508700
F	-3.48341000	-1.35740600	4.78955800
F	-3.30288800	0.37459300	3.48591400
F	-1.51340100	-0.63870500	4.20966800
O	-1.86878800	-1.19419500	1.38191900
H	2.91329800	-6.04276500	1.05366400
H	2.10047400	-5.49515900	3.65176600

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P	1.70050100	-2.80786500	-0.39173900
C	3.05688900	-3.73245300	0.50089000
H	2.59727700	-4.11390300	1.42004400
H	3.30737900	-4.61147900	-0.10110400
C	4.33455500	-2.95750000	0.83782300
H	5.07332200	-3.68125600	1.20204900
H	4.75796700	-2.52296400	-0.07347300
C	4.17060400	-1.87207000	1.91466700
H	5.14476100	-1.59456500	2.32865600
H	3.56906100	-2.25871800	2.74465400
P	3.31031000	-0.35831400	1.29058500
C	0.57813400	-4.23609100	-0.63267600
C	0.32853800	-4.81104500	-1.88166700
C	-0.05852600	-4.75938100	0.50277000
C	-0.54601600	-5.89269700	-1.99324700
H	0.79424800	-4.39779300	-2.76880500
C	-0.93408900	-5.83647700	0.39012100
H	0.11026800	-4.30305100	1.47428900
C	-1.18159200	-6.40454900	-0.86222400
H	-0.74147000	-6.32509000	-2.97006300
H	-1.43308700	-6.22257900	1.27368500
H	-1.86998800	-7.23924900	-0.95401000
C	2.41290700	-2.43832700	-2.02953900
C	3.28414800	-3.30622400	-2.70700500
C	2.08930400	-1.20356100	-2.60782800
C	3.81995500	-2.93755900	-3.93926000
H	3.54230900	-4.26963600	-2.27785200
C	2.62425800	-0.83424100	-3.84176200
H	1.42804900	-0.52639300	-2.08090500
C	3.49089300	-1.70198900	-4.50499100
H	4.49709400	-3.61109200	-4.45657400
H	2.38125800	0.13890000	-4.25492300
H	3.91859300	-1.41486500	-5.46111000
C	3.57840300	0.88162300	2.61390100
C	3.85669700	0.52364400	3.93877300
C	3.39569800	2.23557000	2.29335300
C	3.95599300	1.50332400	4.92664100
H	3.97780900	-0.51775500	4.21438400
C	3.49888800	3.21056500	3.28191400
H	3.15966800	2.52269300	1.27392400
C	3.77958000	2.84749000	4.60101000
H	4.16173600	1.21211600	5.95212500
H	3.35504200	4.25477200	3.02122000
H	3.85350400	3.60879400	5.37182900
C	4.41117900	0.25750700	-0.03577300
C	5.79754700	0.03484900	-0.00476300
C	3.85939600	1.01641600	-1.07384400

C	6.61337700	0.55138200	-1.00784300
H	6.24690500	-0.53497100	0.80195000
C	4.68223300	1.54419800	-2.07149300
H	2.79258400	1.20487600	-1.10987800
C	6.05497400	1.30678100	-2.04256700
H	7.68369000	0.36819700	-0.97983200
H	4.22529400	2.12158200	-2.86625900
H	6.69264300	1.70867100	-2.82466800
Pd	1.00085800	-0.82526700	0.78719900
C	0.43366500	1.58243600	4.35161700
C	0.51369500	0.49800600	3.46783400
C	0.66030700	-0.79717900	3.98168200
C	0.72705200	-1.00829900	5.35689200
C	0.65378600	0.07957700	6.23066200
C	0.50756800	1.37459800	5.72576400
H	0.34897300	2.58004200	3.93524500
H	0.83588600	-2.01519600	5.74968200
H	0.71306300	-0.08110400	7.30341100
H	0.46481200	2.22001300	6.40641000
H	0.72419200	-1.62470800	3.27939600
Cu	-0.81638000	2.32823000	-0.28716000
B	-3.43338200	-1.71772500	1.24384800
C	-1.13824900	-0.94100600	0.45125500
C	-2.85206300	2.37645700	2.41453500
O	-4.20949700	-0.58320800	1.10898100
O	-4.13043100	-2.86850400	0.96935100
C	-2.71085300	2.64086600	-0.05520200
N	-3.41050400	2.70024300	1.10988000
N	-3.64802400	2.87537700	-1.01264700
C	-4.75894600	2.96792400	0.89272000
C	-4.91259200	3.07868700	-0.46008200
C	-5.40335200	-0.97097700	0.37185000
C	-5.50284100	-2.51286900	0.67305400
C	-3.37688400	2.85704600	-2.44336200
H	-2.30429000	2.76934400	-2.60295000
H	-3.73902400	3.77813000	-2.90775800
H	-3.86986800	1.99850900	-2.90907900
H	-3.16981400	3.11519400	3.15457200
H	-1.76719200	2.38272900	2.33645400
H	-3.18964200	1.38167200	2.71851000
C	-1.44278400	-1.36244400	-0.95198500
C	-1.99456800	-2.60913500	-1.29492100
C	-2.33577900	-2.90936800	-2.61677200
C	-2.12733200	-1.98322700	-3.63733100
C	-1.23865500	-0.44607700	-2.00275200
C	-1.56788300	-0.74065900	-3.31953000
H	-2.18189000	-3.35045400	-0.53143900
H	-1.38309400	0.00809800	-4.08326300

H	-1.42371300	0.11131500	0.51859100
H	-2.76029000	-3.88402200	-2.84091500
H	-2.39374400	-2.22278800	-4.66280600
H	-0.80511900	0.52079100	-1.78268300
C	-5.12652500	-0.64407200	-1.09957000
H	-6.00620800	-0.83041400	-1.72321100
H	-4.86441200	0.41368500	-1.16805500
H	-4.28604700	-1.21958800	-1.49043300
C	-6.59150400	-0.15779100	0.86989500
H	-6.45468200	0.88840400	0.59367900
H	-7.51858700	-0.51358800	0.40894400
H	-6.69739300	-0.21922800	1.95451600
C	-5.96944100	-3.35894200	-0.50672300
H	-5.99387100	-4.41277300	-0.21531100
H	-6.97725700	-3.06878000	-0.82130800
H	-5.29053500	-3.25581800	-1.35432500
C	-6.31948200	-2.83853200	1.92665100
H	-7.38871600	-2.66748200	1.77253400
H	-6.17091200	-3.89189000	2.17827700
H	-5.98721700	-2.23774100	2.77759600
C	-1.89571500	-1.69931300	1.56125600
H	-1.53655800	-2.72762100	1.66704800
H	-1.70101400	-1.20118700	2.51704600
C	0.48441500	0.72728900	1.98427600
O	0.20624600	1.86933400	1.59016800
S	0.81728600	2.71291900	-2.87581600
O	2.08801700	2.46945400	-3.57281500
O	-0.41819500	2.36530500	-3.59957900
C	0.72186700	4.55494900	-2.65851700
F	0.73919800	5.16934200	-3.84544600
F	1.74963100	4.99774100	-1.92481100
F	-0.42275800	4.88296000	-2.02590500
O	0.84304700	2.24492800	-1.43625600
C	-6.11947900	3.34802500	-1.29119500
H	-6.01160800	4.26321100	-1.88455600
H	-6.31889400	2.52620500	-1.98856800
H	-6.99913200	3.46516100	-0.65459500
C	-5.73546700	3.10901300	2.00882500
H	-5.77318900	2.20471400	2.62504300
H	-5.48026300	3.94933000	2.66508300
H	-6.73870100	3.28760100	1.61629100

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P	-2.97796700	0.39785700	-1.46787800
C	-3.77165900	1.71591600	-2.51116300
H	-3.19268000	1.78133100	-3.43294200
H	-4.77734700	1.39232200	-2.78627500

C	-3.82966700	3.08515900	-1.80441100
H	-4.54639000	3.70694300	-2.35302100
H	-4.23096300	2.96765600	-0.79582200
C	-2.49385700	3.85315400	-1.76839300
H	-2.68046900	4.90820000	-1.50076900
H	-2.04374100	3.86608600	-2.76178300
P	-1.20716900	3.19330000	-0.61001400
C	-3.10002200	-1.07058000	-2.54617600
C	-3.95628600	-2.15742200	-2.29982000
C	-2.25010600	-1.11564000	-3.66765300
C	-3.98862800	-3.24444600	-3.18181200
H	-4.59098500	-2.15212100	-1.42705000
C	-2.29010600	-2.19707600	-4.54176100
H	-1.53879400	-0.30820000	-3.82241400
C	-3.16248100	-3.25904300	-4.30151100
H	-4.64353200	-4.08178300	-2.97149000
H	-1.62619200	-2.22369100	-5.40395100
H	-3.17929700	-4.11299500	-4.98193400
C	-4.18563200	0.18897700	-0.12170100
C	-5.56417900	0.01672700	-0.35752500
C	-3.71556300	0.24039900	1.19628200
C	-6.44974000	-0.10448200	0.71338400
H	-5.94575000	-0.03145900	-1.37358000
C	-4.60428000	0.13346900	2.26900500
H	-2.66618700	0.36176300	1.38970900
C	-5.96937400	-0.04453400	2.02698000
H	-7.51346600	-0.23843400	0.52552900
H	-4.20151300	0.15698300	3.27494600
H	-6.66401500	-0.13175100	2.85844600
C	0.15425500	4.40526200	-0.76828600
C	0.63278200	4.76722300	-2.03588700
C	0.84498700	4.85081400	0.37236100
C	1.76990800	5.55100100	-2.17156300
H	0.14215800	4.39372100	-2.93251000
C	1.98535800	5.64211300	0.23286000
H	0.49538600	4.57271100	1.35702300
C	2.45698600	5.98641900	-1.03164500
H	2.13812800	5.81008100	-3.15920800
H	2.50943700	5.97517800	1.12342200
H	3.35181600	6.59341100	-1.12930800
C	-1.86616300	3.41536200	1.06990700
C	-2.90357900	4.32164500	1.36403300
C	-1.31200500	2.62907900	2.09288900
C	-3.38155500	4.41929200	2.66598400
H	-3.33709700	4.94107000	0.58595400
C	-1.79369800	2.75496200	3.39646300
H	-0.53133200	1.91972800	1.87029100
C	-2.82716000	3.63626200	3.68067400

H	-4.19456600	5.11463200	2.88664600
H	-1.37650800	2.12278600	4.16931100
H	-3.21345000	3.71919000	4.70291500
Pd	-0.67549700	1.00738500	-0.96038600
C	3.56802100	1.88352600	-1.40387400
C	2.20025800	1.73784800	-1.65393200
C	1.71429700	1.86558400	-2.96286200
C	2.59209300	2.14399500	-4.01472300
C	3.95601800	2.29942700	-3.74953800
C	4.44698100	2.15576600	-2.44558000
H	3.91377000	1.73464400	-0.39000700
H	2.21952600	2.24636800	-5.02994600
H	4.64390600	2.51999400	-4.56081800
H	5.50984400	2.25232700	-2.24551600
H	0.64921100	1.73918900	-3.14308500
Cu	-1.01643300	-1.95087200	0.32384100
C	-3.81126100	-3.45023300	1.63183100
C	-1.96664400	-3.58403700	-0.02638500
N	-3.10756100	-4.09135200	0.51167200
N	-1.64142000	-4.47329200	-1.00708900
C	-3.49883600	-5.24784800	-0.12376800
C	-2.57413100	-5.49370500	-1.08701800
C	-0.52049200	-4.25515100	-1.91631200
H	-4.37607500	-5.81649800	0.17678300
H	-2.49209600	-6.29787200	-1.80086300
H	-0.86210800	-3.45356600	-2.74369900
H	-0.25925700	-5.33200500	-2.40050500
H	0.41076100	-3.82404500	-1.28907800
H	-4.43656200	-4.20152300	2.12511200
H	-4.45372900	-2.63662800	1.27082500
H	-3.07652800	-3.06441900	2.32871500
C	1.26304400	1.48985000	-0.51666000
O	1.61429300	1.51866600	0.64212500
B	3.41972400	-1.56383800	1.09603200
C	2.17882700	-1.80028900	-1.14874700
O	4.06709600	-0.39144500	0.79285300
O	4.00195700	-2.24010300	2.13822600
C	5.01795300	-0.12326000	1.85098700
C	5.23127200	-1.55129400	2.48354700
C	3.43526500	-2.09256600	-1.86884300
C	3.84319500	-1.33520700	-2.98413200
C	5.05132400	-1.58909200	-3.62598300
C	5.90214300	-2.59861700	-3.16850300
C	4.30833000	-3.09130500	-1.41667300
C	5.52211400	-3.35103300	-2.05644200
H	3.22801800	-0.50986900	-3.32115000
H	6.17204300	-4.13762100	-1.67227700
H	5.34232700	-0.98438900	-4.47381800

H	6.85060100	-2.78680800	-3.66304600
H	4.03523600	-3.68646000	-0.54089200
C	4.36143200	0.87926500	2.79884600
H	5.04028400	1.18812900	3.58965700
H	4.06711400	1.76139900	2.21527800
H	3.45470000	0.46606400	3.24136200
C	6.26816700	0.48979400	1.21701300
H	6.04269700	1.48080200	0.81774300
H	7.05932100	0.60898900	1.96442000
H	6.64364200	-0.13518700	0.40775100
C	5.37375300	-1.56238800	4.00106900
H	5.50849900	-2.59020200	4.34928700
H	6.24390800	-0.97765600	4.30709800
H	4.48114400	-1.15845500	4.48046500
C	6.36952700	-2.33878400	1.82697900
H	7.34854100	-1.93250200	2.07202500
H	6.32059300	-3.37235900	2.18162000
H	6.26224400	-2.34907900	0.73936900
C	2.13120100	-2.05438200	0.33928600
H	1.29570000	-1.49988000	0.78475200
H	1.95251600	-3.11562900	0.58102300
C	1.11337400	-1.29300500	-1.81183100
O	-0.08101800	-0.99375900	-1.28564100
H	1.19086000	-1.11771000	-2.88670000
S	-0.93990100	-1.08194300	3.26901200
O	-1.97485400	-0.30020600	3.96636500
O	-1.01605000	-2.54757500	3.39665300
C	0.64485200	-0.58712800	4.09419800
F	0.58732400	-0.85024500	5.40459100
F	0.85347300	0.73443700	3.94439500
F	1.68517900	-1.23782200	3.57406300
O	-0.68038300	-0.60328700	1.85767900

TS10

P	2.62065000	0.97839500	-1.21106700
C	3.06317700	0.37857900	-2.91923800
H	2.12396300	0.20167900	-3.45437900
H	3.59816500	1.16775600	-3.45585200
C	3.91544900	-0.90198900	-2.89885500
H	4.35447600	-1.03004200	-3.89529800
H	4.75765900	-0.76837300	-2.21254600
C	3.16414200	-2.20223800	-2.57196000
H	3.80541600	-3.06644800	-2.77580500
H	2.29827400	-2.29778200	-3.23495100
P	2.48725800	-2.39390300	-0.85473400
C	1.96201600	2.65340500	-1.54171200
C	2.43264700	3.77717200	-0.84813600
C	0.91630200	2.81176800	-2.46390000

C	1.88440900	5.03616900	-1.09491300
H	3.22462400	3.66470700	-0.11656400
C	0.37299800	4.07043800	-2.70765300
H	0.51122900	1.94750000	-2.97721700
C	0.85720200	5.18803200	-2.02524700
H	2.25972400	5.90035500	-0.55478200
H	-0.43534100	4.17548300	-3.42513300
H	0.42626700	6.16804800	-2.20503300
C	4.28730900	1.28108200	-0.51058300
C	5.26416400	1.99763900	-1.22187700
C	4.61368200	0.73274900	0.73441300
C	6.54769900	2.14569000	-0.70140300
H	5.01900000	2.44845700	-2.17904700
C	5.90136900	0.87823900	1.25296800
H	3.85440400	0.20697800	1.29717900
C	6.86935800	1.57910400	0.53581400
H	7.29663700	2.70142200	-1.25812200
H	6.14053200	0.43648500	2.21450900
H	7.87211100	1.69070300	0.93817200
C	1.77196800	-4.07926300	-0.92527600
C	0.84967200	-4.39293900	-1.93557500
C	2.02311200	-5.01839900	0.08257300
C	0.20052900	-5.62414000	-1.94354400
H	0.60203900	-3.66272900	-2.69845400
C	1.36669600	-6.24906100	0.07505000
H	2.71963500	-4.78445900	0.87919400
C	0.45551800	-6.55502500	-0.93539000
H	-0.52526200	-5.84274900	-2.72000300
H	1.56615400	-6.96640800	0.86542600
H	-0.06184000	-7.50957200	-0.93271800
C	3.93548200	-2.55659200	0.24860000
C	5.23205500	-2.80577700	-0.21764000
C	3.71502500	-2.38957000	1.62681000
C	6.29988300	-2.87145300	0.67776100
H	5.42107100	-2.94128500	-1.27699400
C	4.78273700	-2.47916500	2.51798400
H	2.71326100	-2.17910700	1.99064800
C	6.07685700	-2.71053300	2.04549000
H	7.30458700	-3.04812300	0.30574900
H	4.60247000	-2.34949900	3.58067200
H	6.90940400	-2.76293800	2.74089300
Pd	1.15458100	-0.67611200	-0.15120600
C	-1.68788500	-3.87478300	0.68735000
C	-1.08214700	-2.75687700	0.09546600
C	-1.50566300	-2.32718100	-1.16358900
C	-2.54225500	-2.98618200	-1.82025800
C	-3.13338800	-4.10418100	-1.23376000
C	-2.69740500	-4.55472400	0.01663400

H	-1.32953300	-4.20280600	1.65673100
H	-2.89219500	-2.62546200	-2.78184500
H	-3.93542600	-4.62602600	-1.74805800
H	-3.14781300	-5.43639400	0.46403600
I	1.19519600	1.03486900	2.37078700
H	-1.00253400	-1.48564600	-1.61836100
Cu	-0.33509100	2.40957100	0.65342700
C	0.82429000	5.08729400	2.33064900
C	-0.88297100	4.27255700	0.71120900
N	-0.29665700	5.27868000	1.42144200
N	-1.85160900	4.90850100	-0.00840300
C	-0.87018700	6.50783800	1.13851500
C	-1.85697100	6.27315500	0.23483300
C	-2.75856200	4.24546800	-0.93467200
H	-0.53911700	7.42298700	1.60336900
H	-2.55640300	6.94320100	-0.23947000
H	-2.67513300	4.69841600	-1.92631100
H	-3.79122200	4.32928900	-0.58567100
H	-2.48903700	3.19244200	-1.00088000
H	0.58753300	5.51072100	3.31033200
H	1.72128300	5.57049000	1.93259500
H	1.00616000	4.01653500	2.42943400
C	0.07156200	-2.11864600	0.79848500
O	0.42256200	-2.48867100	1.89985500
B	-4.25617600	-0.17369800	1.07981400
C	-2.88950200	0.75061900	-0.91968900
O	-4.31599300	-1.51337100	0.78933800
O	-5.29269700	0.24496100	1.88510400
C	-5.34220700	-2.09671800	1.63237100
C	-6.23699100	-0.85309300	1.98539200
C	-4.03074200	0.74971900	-1.84389400
C	-3.95234900	0.21216300	-3.14745200
C	-5.04295200	0.23516300	-4.01030400
C	-6.26460900	0.77715200	-3.59971100
C	-5.27392700	1.28617000	-1.44799200
C	-6.37031100	1.29711600	-2.30981100
H	-3.02725300	-0.25048800	-3.47521400
H	-7.31287900	1.71622600	-1.96749300
H	-4.94661100	-0.19253000	-5.00501200
H	-7.11890500	0.78206200	-4.26988400
H	-5.38351900	1.69376700	-0.44865000
C	-4.62505200	-2.68918300	2.84882800
H	-5.31943500	-3.21286200	3.51268600
H	-3.87174200	-3.39714800	2.49748300
H	-4.11338400	-1.91027200	3.42028100
C	-6.05849800	-3.19247600	0.85181200
H	-5.36872000	-4.01672900	0.66161100
H	-6.90982700	-3.57815300	1.42237200

H	-6.41669700	-2.82260300	-0.11001200
C	-6.82586700	-0.86100300	3.39134700
H	-7.41287900	0.04834000	3.54803100
H	-7.48856300	-1.72161800	3.52950600
H	-6.04458400	-0.89438700	4.15192600
C	-7.33680100	-0.58859500	0.95154800
H	-8.13197600	-1.33742400	1.01159600
H	-7.77386000	0.39453300	1.14774800
H	-6.93343900	-0.58083200	-0.06330800
C	-3.12873100	0.79025800	0.57507400
H	-2.18886200	0.50910500	1.06702600
H	-3.35235800	1.81017700	0.92328500
C	-1.61051000	0.78347200	-1.38717000
O	-0.52577200	0.85601600	-0.64410100
H	-1.44782800	0.77737500	-2.47457600

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P	-2.76486300	-0.02349700	-1.43865400
C	-3.55631400	1.08921200	-2.70366200
H	-2.85525200	1.15835300	-3.54319500
H	-4.46283300	0.60727000	-3.08288800
C	-3.89656400	2.48592800	-2.16039800
H	-4.59471200	2.96020800	-2.86003200
H	-4.43698000	2.38693700	-1.21343700
C	-2.70688200	3.44416800	-1.99344000
H	-3.06664400	4.45771500	-1.78692900
H	-2.14667400	3.50317600	-2.93274400
P	-1.45265400	3.02452200	-0.69518700
C	-2.68654200	-1.61339700	-2.33709000
C	-3.60877600	-2.65363000	-2.17197900
C	-1.61996100	-1.77664700	-3.23413500
C	-3.48225200	-3.82777600	-2.91377700
H	-4.41583800	-2.55611100	-1.45550000
C	-1.50245600	-2.94629300	-3.98157400
H	-0.87036500	-0.99757200	-3.32034200
C	-2.43523400	-3.97385000	-3.82434400
H	-4.19657100	-4.63207200	-2.77103000
H	-0.67274900	-3.06223800	-4.67241600
H	-2.33986700	-4.88860300	-4.40212300
C	-4.07855900	-0.15243400	-0.17615400
C	-5.42906900	-0.38518200	-0.48885900
C	-3.71225800	0.06465900	1.15711600
C	-6.38719500	-0.41872100	0.52289400
H	-5.73474800	-0.53962900	-1.51931600
C	-4.67321100	0.03816300	2.16805200
H	-2.67394000	0.23176200	1.41469600
C	-6.00906500	-0.20619300	1.85341500
H	-7.42832300	-0.60395100	0.27524100

H	-4.36261600	0.20651400	3.19355600
H	-6.75962300	-0.22789600	2.63816400
C	-0.29669900	4.43849500	-0.81377000
C	0.32918400	4.70922400	-2.03965500
C	0.05217100	5.19176400	0.31369300
C	1.28462100	5.71709300	-2.13740400
H	0.09576300	4.11621900	-2.91716900
C	1.01199700	6.19861200	0.21300200
H	-0.41344100	4.98276700	1.26970700
C	1.63077100	6.46256400	-1.00900700
H	1.76963500	5.90729400	-3.08976400
H	1.28013600	6.77231200	1.09488100
H	2.38360000	7.24149300	-1.08166000
C	-2.28154200	3.20720900	0.91532500
C	-3.52366400	3.83699700	1.07529400
C	-1.63558500	2.64536400	2.02853000
C	-4.12041900	3.89109100	2.33407900
H	-4.03325100	4.28091900	0.22677200
C	-2.23339900	2.71324100	3.28574400
H	-0.68314500	2.13608500	1.91236500
C	-3.47608900	3.32992000	3.43897200
H	-5.08882700	4.36828300	2.45067900
H	-1.73351500	2.25030800	4.12970700
H	-3.94656800	3.36883900	4.41703600
Pd	-0.58717000	0.91454200	-0.83295800
C	3.57693500	1.97226300	-1.20475100
C	2.21445300	1.84193200	-1.49949300
C	1.78562900	1.87327500	-2.83058300
C	2.70186300	2.07956400	-3.85979600
C	4.05875100	2.22909600	-3.56001700
C	4.49475900	2.15866200	-2.23449300
H	3.88925400	1.89072000	-0.17255600
H	2.36383700	2.11810200	-4.89143000
H	4.77743300	2.37937000	-4.36042200
H	5.55327200	2.23807300	-2.00716500
I	-0.50546200	-0.80407100	3.03662700
H	0.72672600	1.74008200	-3.03957000
Cu	-0.69086900	-1.94748100	0.70200600
C	-3.61345300	-3.36488100	1.69807300
C	-1.60379500	-3.63106000	0.26647800
N	-2.77455400	-4.11186600	0.77061600
N	-1.16321200	-4.63248000	-0.54430600
C	-3.06059900	-5.37712500	0.28161600
C	-2.03629900	-5.70835500	-0.54825300
C	0.10365000	-4.59403900	-1.26241100
H	-3.94844200	-5.92088100	0.56292700
H	-1.85427300	-6.60039900	-1.12601900
H	-0.04737000	-4.93120700	-2.28956400

H	0.84234500	-5.23205400	-0.76865900
H	0.46735900	-3.56871000	-1.27340900
H	-4.02015800	-4.04470100	2.45068400
H	-4.43410800	-2.87040000	1.17130900
H	-2.99139800	-2.61339800	2.18574400
C	1.23140500	1.70944200	-0.37830400
O	1.49655900	2.03171100	0.75790800
B	3.45481600	-1.44851600	1.52038800
C	2.55158600	-1.79705100	-0.85484100
O	3.72397500	-0.11250300	1.35256100
O	4.10658200	-1.99569200	2.59938600
C	4.37909200	0.34237400	2.56632200
C	5.02408300	-0.98574800	3.09954200
C	3.84147900	-1.92989300	-1.55982200
C	4.13956200	-1.22734000	-2.74706600
C	5.37780400	-1.33980600	-3.36753400
C	6.37955400	-2.14965500	-2.82426800
C	4.86937500	-2.73266400	-1.02263800
C	6.11446600	-2.83973500	-1.64272100
H	3.41020100	-0.54834600	-3.16979600
H	6.87961300	-3.46782000	-1.19416000
H	5.56969100	-0.76958800	-4.27288100
H	7.34958300	-2.22844200	-3.30621400
H	4.69942400	-3.27823900	-0.10165100
C	3.28166000	0.89667800	3.47709000
H	3.70107800	1.34026300	4.38573400
H	2.72876600	1.65874300	2.92448900
H	2.56765300	0.11717900	3.75379000
C	5.37744500	1.43623600	2.20441600
H	4.83920400	2.32850600	1.87210700
H	5.97972300	1.71384300	3.07584800
H	6.04746300	1.11713300	1.40357700
C	5.09489400	-1.09807600	4.61670800
H	5.53562200	-2.05941600	4.89578500
H	5.72017200	-0.30183300	5.03443800
H	4.10185200	-1.03514500	5.06350200
C	6.38692500	-1.28575400	2.46697300
H	7.16117800	-0.60555000	2.83395800
H	6.67675200	-2.30891900	2.72158300
H	6.33625300	-1.20919800	1.37733900
C	2.48909700	-2.25061000	0.58219100
H	1.48591900	-2.07344600	0.98846900
H	2.66752300	-3.32893000	0.68446200
C	1.48159600	-1.22535300	-1.46281800
O	0.27652500	-1.02062500	-0.93090700
H	1.57003100	-0.90725800	-2.50275500

P	0.35829900	2.42961600	-0.51998500
C	1.71915800	3.67103200	-0.78097300
H	2.07308600	3.51096200	-1.80524400
H	1.29306300	4.67826100	-0.75426800
C	2.88650200	3.55478100	0.21135300
H	3.45634200	4.49077900	0.18058600
H	2.50605000	3.46569700	1.23499700
C	3.86865300	2.41237800	-0.07880600
H	4.75186800	2.50490200	0.56133400
H	4.22098700	2.47340000	-1.11408300
P	3.18741400	0.70046400	0.13660700
C	-0.85661500	2.98602800	-1.76640200
C	-2.06747600	3.59898800	-1.42856800
C	-0.55895700	2.73604400	-3.11523200
C	-2.97136200	3.95823000	-2.42955100
H	-2.31303600	3.77717800	-0.38762100
C	-1.45863700	3.10580500	-4.11101200
H	0.35464600	2.20961800	-3.37790300
C	-2.66938200	3.71467300	-3.76929900
H	-3.91550600	4.42149400	-2.15902300
H	-1.22537700	2.89977200	-5.15113400
H	-3.37745300	3.98933000	-4.54530000
C	-0.35014800	2.91314100	1.09486100
C	-0.25349500	4.20634600	1.63139900
C	-1.02522000	1.92517700	1.82111100
C	-0.81856700	4.49621500	2.87307600
H	0.25633200	4.99350800	1.08621400
C	-1.59973700	2.21774100	3.05629000
H	-1.11016500	0.92752500	1.41404100
C	-1.49260200	3.50299600	3.58764700
H	-0.73502500	5.49911800	3.28135000
H	-2.12118600	1.43304200	3.59495300
H	-1.93113400	3.73345800	4.55407300
C	4.67401300	-0.32780600	-0.13609800
C	5.33263200	-0.23327600	-1.37141400
C	5.08758600	-1.29310300	0.78973600
C	6.39700100	-1.08081500	-1.66710000
H	4.98897500	0.47288300	-2.12067100
C	6.14595100	-2.14801600	0.48479500
H	4.56884000	-1.39261400	1.73614300
C	6.80398800	-2.04255600	-0.74028000
H	6.89595000	-1.00234500	-2.62807400
H	6.44740600	-2.90464100	1.20242400
H	7.62313000	-2.71438300	-0.97773600
C	2.82296300	0.58220100	1.92376700
C	1.61461900	-0.00206500	2.32546700
C	3.71471600	1.05433800	2.89990400
C	1.29711800	-0.11627600	3.67867700

H	0.91681500	-0.36007500	1.57659500
C	3.39406900	0.94610400	4.25159100
H	4.66342900	1.49448400	2.60769000
C	2.18512500	0.36125900	4.64155400
H	0.35563100	-0.57507900	3.96210400
H	4.08694500	1.31557900	5.00165800
H	1.93986500	0.28019100	5.69635300
Pd	1.30264500	0.21437600	-1.06784600
C	2.29554500	-1.27061400	-2.02864800
O	2.58824900	-1.03336200	-3.17980000
C	2.66657200	-2.55392800	-1.35772100
C	2.26266800	-2.82856500	-0.04976900
C	3.50278300	-3.45582400	-2.03021600
C	2.68345200	-3.99378500	0.58645900
H	1.62320600	-2.12046600	0.46044000
C	3.93030700	-4.61638200	-1.39278600
H	3.81424400	-3.21517100	-3.04081300
C	3.52114700	-4.88725000	-0.08337800
H	2.36728600	-4.19810900	1.60506700
H	4.58662700	-5.30970800	-1.91059100
H	3.85824400	-5.79262800	0.41324400
B	-4.93652400	-0.47399200	-0.47692100
C	-2.40155200	-0.23760900	-0.67645500
O	-5.16339800	-1.58377400	-1.25329100
O	-5.83606500	-0.35776100	0.55944800
C	-6.08859600	-2.43459800	-0.52955900
C	-6.82874100	-1.40578700	0.40251300
C	-2.08742800	-1.04953000	0.50009700
C	-2.80250300	-0.88256800	1.71257000
C	-2.51029900	-1.63910500	2.84630000
C	-1.50231300	-2.60531500	2.81612400
C	-1.08135400	-2.04614400	0.48801700
C	-0.80310000	-2.80531100	1.62182400
H	-3.59708000	-0.14917200	1.77119000
H	-0.04121500	-3.57747600	1.56455500
H	-3.08338500	-1.47671600	3.75607200
H	-1.28075800	-3.20393300	3.69489900
H	-0.54737200	-2.21845400	-0.43618600
C	-5.23503900	-3.44679300	0.24237100
H	-5.85462800	-4.18081400	0.76624600
H	-4.59441500	-3.97532500	-0.46788000
H	-4.58595100	-2.94773600	0.96569900
C	-6.98240600	-3.15200700	-1.53444200
H	-6.37433700	-3.81911200	-2.15133200
H	-7.73676200	-3.75665300	-1.02018600
H	-7.48915700	-2.44819400	-2.19658100
C	-7.19055600	-1.93793300	1.78429200
H	-7.67953100	-1.15133500	2.36606800

H	-7.88166800	-2.78353300	1.70538600
H	-6.30157700	-2.26083600	2.32797200
C	-8.04910700	-0.76004400	-0.25921100
H	-8.87777400	-1.46715100	-0.35866400
H	-8.38194000	0.08022700	0.35592500
H	-7.79742700	-0.37610900	-1.25139800
C	-3.72986700	0.50539500	-0.70200800
H	-3.76016300	1.31236200	0.04480100
H	-3.83046200	0.99834900	-1.67627800
C	-1.58610200	-0.12359700	-1.77500700
O	-0.40078400	-0.64275000	-1.98224200
H	-1.98568400	0.48066600	-2.60097400

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P	0.54899800	1.95727600	-1.09927100
C	1.69659200	2.69085900	-2.36906200
H	1.45669600	2.15895600	-3.29683300
H	1.41628400	3.73743800	-2.53411600
C	3.20707700	2.59416000	-2.08753300
H	3.71370400	3.23096100	-2.82275200
H	3.43778200	3.02478000	-1.10806600
C	3.84079100	1.19459000	-2.18431800
H	4.93101500	1.29138700	-2.22117900
H	3.53080100	0.69471500	-3.10827700
P	3.38937600	0.06298100	-0.77596700
C	-1.07354800	2.30528200	-1.87336900
C	-1.80359200	3.47328700	-1.62030400
C	-1.58726700	1.34819200	-2.75986400
C	-3.02743500	3.68568300	-2.25406200
H	-1.42044000	4.20565000	-0.91751600
C	-2.80065900	1.57391200	-3.40923000
H	-1.04853100	0.41822500	-2.91745900
C	-3.52529700	2.73984600	-3.15260000
H	-3.59317300	4.58915200	-2.04603000
H	-3.18932400	0.83164000	-4.09917200
H	-4.47931300	2.90505300	-3.64389200
C	0.62155200	3.09171300	0.33172200
C	1.36561700	4.27706400	0.37207100
C	-0.07763200	2.68292200	1.47876100
C	1.42713900	5.03015500	1.54630400
H	1.90400300	4.61966100	-0.50451900
C	-0.03221700	3.44664100	2.64141800
H	-0.65339000	1.76381300	1.45926000
C	0.73080300	4.61690700	2.68221100
H	2.01798200	5.94103300	1.57071000
H	-0.59165700	3.12065800	3.51261800
H	0.77963100	5.20555000	3.59360500
C	4.54160200	-1.34054600	-0.96832700

C	4.41165300	-2.14251800	-2.11397000
C	5.45431400	-1.71173900	0.02663200
C	5.21022400	-3.27187500	-2.27550300
H	3.66077400	-1.90501700	-2.86138600
C	6.24327200	-2.85068000	-0.13422900
H	5.53671800	-1.12391100	0.93354300
C	6.13115100	-3.62726500	-1.28689600
H	5.10125800	-3.88412800	-3.16559600
H	6.94043400	-3.13406000	0.64853900
H	6.74601000	-4.51386400	-1.40936500
C	3.98910600	1.01086000	0.67204600
C	3.10379900	1.25059500	1.73029300
C	5.27408800	1.57460100	0.71519600
C	3.48459100	2.05316900	2.80543000
H	2.10859900	0.82172800	1.68941000
C	5.65813800	2.36900400	1.79389500
H	5.97600100	1.38830100	-0.09226300
C	4.76069000	2.61418200	2.83714900
H	2.77602100	2.25203600	3.60235000
H	6.65410400	2.80119200	1.81935300
H	5.05805300	3.24388500	3.67044700
Pd	1.14524700	-0.33832100	-0.64505900
C	1.24483500	-2.40772200	-0.60366700
O	1.10843500	-2.92736800	-1.69312600
C	1.94726400	-2.99268100	0.57278500
C	1.88100600	-2.41463400	1.84786000
C	2.79984100	-4.07749700	0.34431300
C	2.66623600	-2.91845100	2.87937900
H	1.21164000	-1.57829400	2.01150900
C	3.59215900	-4.57332500	1.37933500
H	2.85040800	-4.49968000	-0.65228600
C	3.52948800	-3.99512700	2.64644300
H	2.60905500	-2.47202400	3.86789400
H	4.26764500	-5.40205100	1.18960800
H	4.15035500	-4.37728400	3.45161800
B	-5.07002300	-1.51752200	-0.70315000
C	-2.56422900	-1.15271400	-0.55610200
O	-5.26204600	-2.42445900	0.30917600
O	-6.14779300	-0.68455800	-0.88719900
C	-6.43708000	-2.00258000	1.04959800
C	-7.21484800	-1.14512000	-0.01635700
C	-2.74202900	-0.15080900	0.51361500
C	-3.49293100	1.01808000	0.27984100
C	-3.72735600	1.94305400	1.29610400
C	-3.23911800	1.71750300	2.58446600
C	-2.23417900	-0.35032000	1.81414600
C	-2.49121300	0.56356200	2.83497700
H	-3.89284500	1.20805000	-0.70858600

H	-2.10949800	0.36962300	3.83408500
H	-4.29709200	2.84180100	1.07742500
H	-3.43694600	2.42982300	3.38016300
H	-1.66067200	-1.24573000	2.01547400
C	-5.93350500	-1.17880400	2.23919500
H	-6.75627900	-0.88026000	2.89599700
H	-5.23170400	-1.78744100	2.81426500
H	-5.40165900	-0.28462200	1.90920200
C	-7.17419600	-3.24341300	1.54042100
H	-6.54405000	-3.78319700	2.25238700
H	-8.10329900	-2.96661500	2.04949500
H	-7.41316400	-3.92112200	0.71934800
C	-7.93463600	0.07591300	0.54481700
H	-8.42986900	0.61659300	-0.26675500
H	-8.69743300	-0.22187900	1.27158900
H	-7.23394600	0.75710100	1.02957100
C	-8.16491700	-1.97506700	-0.88393000
H	-9.03843400	-2.31126700	-0.31778400
H	-8.50872800	-1.36072700	-1.72029600
H	-7.65600900	-2.85197200	-1.29283500
C	-3.72635400	-1.38227000	-1.50811800
H	-3.82841900	-0.56213300	-2.22964500
H	-3.53537800	-2.29115800	-2.09193500
C	-1.43205600	-1.88431000	-0.67818200
O	-0.37727700	-1.78470700	0.14334500
H	-1.32153500	-2.60872100	-1.49026000

P₂

C	3.36089100	-1.48935900	-0.32272700
O	3.39486400	-2.69502000	-0.45429800
C	4.50873800	-0.63668500	0.07371600
C	4.40679800	0.75870900	0.16757000
C	5.72408500	-1.27224900	0.35986300
C	5.51799900	1.50712200	0.54917900
H	3.46564900	1.24454100	-0.06145600
C	6.83037500	-0.51893400	0.74092400
H	5.77544300	-2.35232100	0.27808600
C	6.72808600	0.87133100	0.83634600
H	5.44120000	2.58767300	0.62093000
H	7.77139100	-1.01227000	0.96359100
H	7.59168800	1.45914000	1.13316500
B	-2.53059100	-1.07747600	-0.61523300
C	-0.06538800	-0.70323800	-1.08183400
O	-2.49444800	-1.17551600	0.75052800
O	-3.70456400	-0.55832500	-1.09397500
C	-3.62740000	-0.42017500	1.26358900
C	-4.61243100	-0.41868500	0.03575700
C	-0.20914100	0.75102700	-0.82488200

C	-1.06967800	1.52490700	-1.62276800
C	-1.26741000	2.88051400	-1.36142200
C	-0.61920100	3.49166500	-0.28810600
C	0.43077700	1.37998300	0.25857700
C	0.22897900	2.73254400	0.52129400
H	-1.59349100	1.06450900	-2.45285800
H	0.72520200	3.19259000	1.37099100
H	-1.93280000	3.45716200	-1.99722200
H	-0.77797800	4.54533800	-0.07944300
H	1.06907700	0.79494700	0.90866700
C	-3.09636900	0.97233600	1.61692200
H	-3.86901500	1.58702500	2.08771800
H	-2.26463700	0.86268400	2.31677400
H	-2.72024800	1.49312600	0.73425700
C	-4.15327800	-1.12055000	2.51027700
H	-3.39182000	-1.09112300	3.29414900
H	-5.04940200	-0.61739700	2.88743000
H	-4.39544400	-2.16567400	2.31229500
C	-5.40732700	0.86874000	-0.14665300
H	-6.04601500	0.78470300	-1.03019200
H	-6.04871400	1.05478700	0.72075400
H	-4.74665200	1.72567200	-0.28509400
C	-5.54316600	-1.63347600	0.00201100
H	-6.30556200	-1.57833200	0.78415900
H	-6.04428100	-1.66869400	-0.96873900
H	-4.98095600	-2.56256200	0.12807600
C	-1.30579700	-1.45145800	-1.53500800
H	-1.55110900	-1.21098700	-2.57711900
H	-1.11463900	-2.53029000	-1.50366800
C	1.07489900	-1.38436100	-0.90454000
O	2.23599400	-0.74171400	-0.51970600
H	1.18106900	-2.45052000	-1.05799000

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O	-4.62007000	-0.71734500	0.86137400
C	-5.68850400	0.05654600	0.30937700
C	-4.93560500	1.07077300	-0.62578000
O	-3.81479200	0.29268200	-1.06944800
B	-3.51740800	-0.66118500	-0.04216600
C	-6.47680000	0.69732500	1.44939700
H	-6.95892500	-0.08337500	2.04546000
H	-5.82078900	1.26625600	2.11049400
H	-7.25830800	1.36340200	1.06692100
C	-6.59780900	-0.89659700	-0.48155200
H	-6.91539300	-1.70594400	0.18172900
H	-7.49011800	-0.39396000	-0.86856400
H	-6.05231100	-1.33829600	-1.31969800

C	-5.72509000	1.52578800	-1.85107700
H	-6.64296600	2.04670800	-1.55752800
H	-5.11884200	2.21695800	-2.44513300
H	-5.98979300	0.67983200	-2.48720800
C	-4.41914700	2.29928800	0.13846200
H	-3.77380100	2.88016300	-0.52751200
H	-5.23742700	2.94868900	0.46522100
H	-3.83574500	1.99543500	1.01005500
C	-1.56728400	-2.18940200	0.46569600
C	-2.76000500	-2.01387500	-0.49453000
H	-3.41772800	-2.88736900	-0.47970500
H	-2.39080500	-1.90321300	-1.52065200
H	-1.89661500	-2.72423000	1.37087100
C	-1.24551800	-0.77917900	0.98953500
O	-2.21837900	0.00568100	0.85894700
I	3.41216600	0.85479400	-2.01962700
C	2.35355600	0.15009900	2.04104700
C	4.61885000	0.07711700	2.07542400
C	4.24154000	1.22915000	2.69026500
H	5.59699600	-0.32988000	1.87563300
H	4.82566200	2.01402300	3.14352500
N	2.85580600	1.25205700	2.66115300
N	3.45414400	-0.56830600	1.69697000
Cu	0.51730200	-0.28017800	1.57721000
C	-0.34283400	-2.88561800	-0.07256400
C	0.32621300	-2.35853300	-1.18822600
C	0.17973000	-4.03913400	0.52506200
C	1.46613700	-2.97176400	-1.70356100
H	-0.06493600	-1.46361000	-1.65807200
C	1.32053800	-4.66187700	0.01153400
H	-0.32174400	-4.45952400	1.39299100
C	1.96634400	-4.13233100	-1.10712500
H	1.96618700	-2.54095000	-2.56596500
H	1.70000200	-5.56416300	0.48288000
H	2.84911900	-4.61932000	-1.51106000
C	0.39190700	1.25552200	-1.74578200
C	1.62205400	1.70142600	-1.25829200
C	1.70054800	2.68229200	-0.27078800
C	0.51302400	3.20510000	0.24808500
C	-0.72280300	2.74226200	-0.20162800
C	-0.78615400	1.77303200	-1.20414000
H	0.35161500	0.51216000	-2.53278100
H	2.66289300	3.02906300	0.08778900
H	0.56075800	3.97643900	1.01142400
H	-1.64009200	3.12238400	0.23170800
H	-1.75121700	1.39306200	-1.52865700
C	2.03607100	2.29880100	3.25349300
H	1.00332500	2.13463300	2.94972700

H	2.10704300	2.26870700	4.34431500
H	2.36305900	3.27800400	2.89563300
C	3.40396300	-1.83184600	0.96872300
H	4.10766300	-2.53893600	1.41322200
H	2.39549100	-2.23491900	1.03742600
H	3.64697900	-1.67182100	-0.08270600

TS12

P	-1.17469800	-0.76113400	-1.86735200
C	-1.14798800	0.45508300	-3.28129200
H	-0.16058100	0.91800900	-3.33644400
H	-1.30452100	-0.10869400	-4.20576100
C	-2.22646500	1.54337800	-3.15329800
H	-2.29175200	2.05808300	-4.11925700
H	-3.20647900	1.08403100	-2.98729700
C	-1.94797700	2.60337400	-2.08101800
H	-2.58482700	3.47964800	-2.23808700
H	-0.91904300	2.96659700	-2.17036700
P	-2.11689800	2.08513500	-0.29940600
C	-0.14221700	-2.13980000	-2.50063300
C	-0.45761000	-3.44892700	-2.09444400
C	0.90627000	-1.94223000	-3.40895400
C	0.22830800	-4.53412600	-2.63376000
H	-1.25027100	-3.60858300	-1.37048100
C	1.60801000	-3.03336300	-3.92782800
H	1.16826800	-0.94175400	-3.73573300
C	1.25773000	-4.33153700	-3.55722300
H	-0.04154800	-5.54105500	-2.32940300
H	2.41288700	-2.86528000	-4.63720400
H	1.78738800	-5.18026500	-3.97970800
C	-2.86265900	-1.43370500	-2.16732100
C	-3.16857300	-2.07727700	-3.37721600
C	-3.88427500	-1.19792800	-1.24589300
C	-4.47751900	-2.46280100	-3.65717100
H	-2.38265600	-2.28553300	-4.09693100
C	-5.19843600	-1.57055000	-1.53097100
H	-3.64164900	-0.74429700	-0.29886300
C	-5.49740200	-2.20245700	-2.73643800
H	-4.70343100	-2.96486100	-4.59343500
H	-5.97754300	-1.36624800	-0.80346300
H	-6.51817000	-2.49899200	-2.95975500
C	-1.59427500	3.67519100	0.46296200
C	-0.22336100	3.87120900	0.68503800
C	-2.49364200	4.69977100	0.77902800
C	0.24267900	5.08048400	1.19372700
H	0.47811300	3.07176400	0.48361200
C	-2.02549300	5.90449600	1.30724100

H	-3.55808800	4.55467400	0.62579100
C	-0.65875000	6.09912900	1.51073000
H	1.30860600	5.21342000	1.35132900
H	-2.73123900	6.69047700	1.56024300
H	-0.29862100	7.03787500	1.92129400
C	-3.93074200	1.99058200	-0.02171700
C	-4.87621500	2.64846500	-0.82037300
C	-4.38100900	1.16067800	1.01867900
C	-6.24173700	2.48650900	-0.58130000
H	-4.55698600	3.28564500	-1.63818600
C	-5.74437700	1.00896200	1.26336100
H	-3.66072400	0.60234300	1.60926800
C	-6.67827100	1.67021700	0.46255000
H	-6.96311500	2.99634400	-1.21303400
H	-6.07370800	0.35890200	2.06808800
H	-7.74112200	1.54306900	0.64543700
Pd	-0.75924300	0.20125400	0.30793700
C	0.50095700	0.31746500	3.05326300
C	-0.53805600	0.83413300	2.26704900
C	-1.44762700	1.68112000	2.91741700
C	-1.31938800	2.00476800	4.27146300
C	-0.26844000	1.48934400	5.02665300
C	0.64219300	0.63551700	4.40568200
H	1.21659800	-0.36334600	2.61162700
H	-2.04798700	2.66952500	4.72912600
H	-0.16228900	1.74539400	6.07693900
H	1.46842600	0.21292900	4.97367400
I	-1.95919100	-2.39271000	1.55280500
H	-2.28207600	2.12023700	2.38839500
Cu	0.62713100	-1.85282200	0.80866000
B	2.92937500	2.16400300	-1.42124800
C	1.60197200	0.56445800	0.04207800
C	1.38256200	-2.86489000	3.89743400
O	3.30191900	3.04446700	-0.43233600
O	3.82300200	2.11774100	-2.46234000
C	1.90123000	-3.21217100	1.48256600
N	2.10106700	-3.49853400	2.79986400
N	2.77535500	-4.03215100	0.83989600
C	3.08901000	-4.45541700	2.97195200
C	3.51381000	-4.79725700	1.72927600
C	4.68504700	3.40968700	-0.68738300
C	4.81210000	3.15932600	-2.23424100
C	2.84903100	-4.17688700	-0.60247100
H	3.39394300	-4.80176800	3.94649100
H	4.25507700	-5.50900300	1.40314400
H	2.29414000	-3.36211700	-1.05738900
H	2.40765200	-5.12775200	-0.90950000
H	3.88859600	-4.12669800	-0.92995300

H	1.95802600	-2.02792500	4.30009300
H	1.21117300	-3.60075500	4.68627200
H	0.42225600	-2.50368000	3.52957900
C	2.84374400	-0.22722900	0.25780600
C	3.49966500	-0.90074600	-0.79602800
C	4.72649700	-1.53272900	-0.60620200
C	5.34071100	-1.54281800	0.64743800
C	3.51543100	-0.20043000	1.50326100
C	4.71997200	-0.86547600	1.70165200
H	3.04283800	-0.92778700	-1.77842300
H	5.20011900	-0.82157100	2.67580600
H	1.53794800	1.29496400	0.84273300
H	5.20716700	-2.02206800	-1.44988700
H	6.29473000	-2.04010200	0.79341300
H	3.08901400	0.37995300	2.31306400
C	5.55074900	2.46113100	0.14718500
H	6.61175400	2.71725600	0.07142200
H	5.24778800	2.53792800	1.19396700
H	5.41285900	1.42188300	-0.15872400
C	4.89448900	4.85306000	-0.24736300
H	4.76665600	4.92586500	0.83623700
H	5.90620100	5.19180200	-0.49321400
H	4.17567300	5.52443500	-0.71997500
C	6.17031500	2.64090000	-2.69060500
H	6.15989500	2.48306800	-3.77274700
H	6.95958200	3.36364200	-2.45936400
H	6.41056400	1.69142100	-2.21051200
C	4.38420300	4.36397900	-3.07675700
H	5.11397700	5.17667900	-3.01921800
H	4.29421700	4.05221700	-4.12065000
H	3.41283400	4.74460500	-2.74934300
C	1.62835000	1.29120800	-1.31438600
H	1.58389200	0.59488100	-2.15447200
H	0.75264600	1.93818600	-1.40770000

TS13

P	0.18080800	1.51212700	-1.47425200
C	1.35347900	1.75654700	-2.90549600
H	1.24642400	0.88853200	-3.56466500
H	1.04511200	2.63805100	-3.47691700
C	2.82318000	1.91580000	-2.47161500
H	3.37177600	2.33755200	-3.32269100
H	2.88547900	2.66459200	-1.67479100
C	3.56160000	0.63343500	-2.04890400
H	4.63917800	0.82728300	-1.99580900
H	3.42989400	-0.14250500	-2.81217900
P	3.00938700	-0.17422600	-0.46249900
C	-1.46891400	1.71936400	-2.24635200

C	-2.44788800	2.56026000	-1.69471500
C	-1.83537500	0.86126300	-3.29727300
C	-3.75716400	2.53576100	-2.17581400
H	-2.18584500	3.22598500	-0.87966000
C	-3.13935900	0.85122800	-3.78703800
H	-1.10134500	0.18013800	-3.71979800
C	-4.10823600	1.68282100	-3.22133700
H	-4.50512200	3.18307200	-1.72701500
H	-3.40372200	0.18160800	-4.60024900
H	-5.12942600	1.65943300	-3.58894300
C	0.43139300	3.07443600	-0.54441700
C	0.37516500	4.33788700	-1.15443100
C	0.74492700	2.98915800	0.81648600
C	0.64089000	5.48962300	-0.41654500
H	0.11518300	4.42159900	-2.20578800
C	1.01401400	4.14149900	1.55542900
H	0.77775200	2.01877100	1.29363700
C	0.96586000	5.39126300	0.94014100
H	0.59615300	6.46292200	-0.89671000
H	1.26629600	4.05274900	2.60676300
H	1.17836400	6.28970600	1.51251900
C	4.24257800	-1.52942900	-0.35218000
C	3.89667000	-2.76290500	-0.92177800
C	5.49445700	-1.38350700	0.26282100
C	4.79731300	-3.82689100	-0.89446300
H	2.91493900	-2.89719200	-1.36275600
C	6.39010900	-2.45195300	0.29422900
H	5.76499500	-0.43741400	0.72102000
C	6.04421400	-3.67427400	-0.28701600
H	4.50831000	-4.77979900	-1.32665800
H	7.35726900	-2.33142400	0.77421900
H	6.74146600	-4.50665500	-0.25658900
C	3.53689400	0.99049100	0.85585100
C	4.40692600	2.07031700	0.65859700
C	2.97257900	0.80225500	2.12836600
C	4.69916200	2.94669000	1.70589500
H	4.85795000	2.23957800	-0.31330200
C	3.27685500	1.66528900	3.17742800
H	2.26126000	-0.00494800	2.27648600
C	4.13766000	2.74585700	2.96651900
H	5.36499300	3.78741900	1.53446600
H	2.82577800	1.50700800	4.15256800
H	4.36387200	3.43055000	3.77856100
Pd	0.69284500	-0.54840100	-0.38161500
C	0.24244900	-3.31905000	-1.27984600
C	0.43099000	-2.64031000	-0.05933000
C	1.12468100	-3.32271200	0.96342500
C	1.62314900	-4.60570700	0.76531400

C	1.44422900	-5.25990300	-0.46059900
C	0.75951800	-4.60341400	-1.48267600
H	-0.30279900	-2.83320600	-2.08337300
H	2.17104700	-5.09568000	1.56607100
H	1.83131900	-6.26321500	-0.61054300
H	0.61296900	-5.09286100	-2.44263700
H	1.29839900	-2.82981100	1.91521800
B	-3.77818600	-1.50050600	0.01195600
C	-1.28056900	-1.67811700	0.52661200
O	-4.28938000	-2.23189500	1.05523100
O	-4.64001200	-0.53047400	-0.43763700
C	-5.49105200	-1.55480800	1.51531700
C	-5.90276300	-0.70260500	0.25507800
C	-1.27414200	-0.49992500	1.45822500
C	-1.98978500	0.68610900	1.19123200
C	-2.00301900	1.73821500	2.10183800
C	-1.29384100	1.65237800	3.30339900
C	-0.58786300	-0.58102800	2.68714600
C	-0.58472200	0.48391500	3.58721600
H	-2.53793200	0.78721400	0.26390700
H	-0.04036500	0.39130000	4.52331100
H	-1.38938800	-2.57122300	1.13604800
H	-2.56136800	2.63915700	1.86339000
H	-1.29842800	2.47982500	4.00602500
H	-0.06277300	-1.49724400	2.93640100
C	-5.07871300	-0.70385400	2.72005700
H	-5.94079500	-0.20463600	3.17219100
H	-4.62444300	-1.35664200	3.46983900
H	-4.33630500	0.04744200	2.44316300
C	-6.50808700	-2.60895100	1.93838900
H	-6.12223900	-3.16288800	2.79829700
H	-7.45300200	-2.14018700	2.23187300
H	-6.70570000	-3.32300500	1.13745700
C	-6.46367600	0.67989600	0.56849400
H	-6.68732900	1.20258900	-0.36571300
H	-7.38862900	0.60438500	1.14906400
H	-5.74503000	1.28015600	1.12809400
C	-6.82922200	-1.44910400	-0.70858100
H	-7.83522300	-1.56699200	-0.29575000
H	-6.89906400	-0.88029900	-1.63948500
H	-6.43097200	-2.43911500	-0.94608300
C	-2.33635500	-1.69588500	-0.57587600
H	-2.15665300	-0.93238500	-1.33521900
H	-2.28117000	-2.66444500	-1.08559100

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Cu	1.61162500	-1.74622700	0.64677500
B	0.13329800	2.74293500	-0.98239800

C	-2.12232800	1.52889400	-0.96072700
C	2.07418500	-2.26241900	-2.73533400
O	1.35425700	2.92936900	-1.57113500
O	0.13559200	2.96874900	0.36879700
C	3.09791200	-1.53708000	-0.58084400
N	3.16532600	-1.73710600	-1.92205000
N	4.31132400	-1.00353000	-0.26229300
C	4.38412300	-1.32395500	-2.43443800
C	5.11249200	-0.86204900	-1.38487300
C	2.25794600	3.43560900	-0.55179500
C	1.52595900	3.04465900	0.78838000
C	4.72173300	-0.65307100	1.09022800
H	3.87830000	-0.82735400	1.75844500
H	5.00608700	0.40113000	1.13476100
H	5.56611800	-1.27293400	1.40361400
H	1.34085200	-2.72281100	-2.07757800
H	2.47054000	-3.00272400	-3.43453400
H	1.58176500	-1.44887400	-3.26911600
C	-3.29740300	2.18657900	-0.34760400
C	-4.53922300	1.53301100	-0.28298200
C	-5.63687300	2.15260900	0.30962000
C	-5.51141700	3.43230000	0.85310300
C	-3.18482600	3.47877100	0.19251800
C	-4.28117700	4.08983600	0.79609200
H	-4.64477000	0.54635500	-0.72322300
H	-4.17359700	5.08058000	1.22755600
H	-6.59250500	1.63795700	0.34206300
H	-6.36691900	3.91432000	1.31660800
H	-2.22267400	3.97859300	0.18197800
C	2.36331300	4.94698400	-0.76921000
H	3.07614800	5.40611900	-0.07833900
H	2.70028100	5.13556300	-1.79187600
H	1.39174100	5.43091800	-0.63828600
C	3.61558200	2.76978500	-0.75268200
H	4.04281700	3.08716900	-1.70793800
H	4.31061500	3.05677200	0.04371000
H	3.51924200	1.68369500	-0.76914000
C	1.63753200	4.06923900	1.91059500
H	1.08051800	3.71449200	2.78153200
H	2.68252400	4.20528600	2.20738500
H	1.22883400	5.03727300	1.61609100
C	1.89664500	1.65264900	1.29857300
H	2.90757900	1.63789600	1.71555500
H	1.19493700	1.35118600	2.07869100
H	1.82914500	0.91243300	0.49849900
C	-1.18127500	2.38069000	-1.77492200
H	-0.86430900	1.85028900	-2.67639600
H	-1.69371500	3.29583300	-2.09080700

C	-1.93974000	0.20174900	-0.75819000
O	-0.89548300	-1.89573600	-1.37434200
H	-2.64439200	-0.35327900	-0.15308900
H	6.11115600	-0.45847400	-1.33765800
H	4.62227400	-1.39465500	-3.48365200
C	-0.78289600	-0.52756700	-1.26523800
O	0.29136500	-0.03818900	-1.57584000
C	-3.09777400	-2.30799900	-2.27124500
C	-4.32332800	-2.96734000	-2.17620300
C	-4.57646000	-3.82861000	-1.10599100
C	-3.60034800	-4.02941500	-0.12789200
C	-2.37208300	-3.37141900	-0.20648300
C	-2.14089400	-2.51550000	-1.27842700
H	-2.87948300	-1.63893300	-3.09687100
H	-5.07716900	-2.81063200	-2.94174600
H	-5.53094200	-4.34085900	-1.03570500
H	-3.79482600	-4.69326800	0.70869100
H	-1.60863900	-3.47928000	0.55573100
I	0.00245600	-1.82687900	2.51994200

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P	-0.88520700	-0.73630800	-2.39523600
C	-0.71353300	0.44465500	-3.83744700
H	0.28246900	0.89621200	-3.76742900
H	-0.73419900	-0.13866500	-4.76285200
C	-1.78653300	1.54291600	-3.90674000
H	-1.72330500	1.99962300	-4.90176700
H	-2.77888200	1.08977200	-3.84157800
C	-1.65777800	2.67947400	-2.88467600
H	-2.35247400	3.48851000	-3.13432000
H	-0.64832300	3.09954700	-2.94489600
P	-1.88933400	2.22934900	-1.10312800
C	-0.06899100	-2.23784200	-3.09145400
C	-0.65578000	-3.49850300	-2.89654600
C	1.12236100	-2.15576600	-3.82755700
C	-0.07465500	-4.64279600	-3.44079700
H	-1.57773400	-3.58150100	-2.33208700
C	1.71066900	-3.30436000	-4.35794100
H	1.59710400	-1.19569500	-3.99497500
C	1.11071500	-4.55087100	-4.17231000
H	-0.55092500	-5.60716700	-3.29082900
H	2.63229000	-3.22116000	-4.92626900
H	1.56265100	-5.44239100	-4.59657000
C	-2.63786700	-1.25539200	-2.52645600
C	-3.24862000	-1.48000900	-3.77254800
C	-3.35746900	-1.50162200	-1.35594800
C	-4.56853600	-1.91688000	-3.83472700
H	-2.69318100	-1.32620200	-4.69277700

C	-4.67585400	-1.95825800	-1.41884800
H	-2.89085400	-1.33940900	-0.39529200
C	-5.28404100	-2.15626200	-2.65591900
H	-5.03801400	-2.07977700	-4.80066300
H	-5.20192400	-2.14224300	-0.48904600
H	-6.31262500	-2.50127800	-2.70897400
C	-1.83530400	3.87517900	-0.28101500
C	-1.06031400	4.92648000	-0.78998900
C	-2.48393100	4.05085300	0.95061700
C	-0.92957900	6.12035900	-0.08217100
H	-0.52998300	4.81980800	-1.72870900
C	-2.35111500	5.24412500	1.65570800
H	-3.08317300	3.25144600	1.36821500
C	-1.56984400	6.28146000	1.14530400
H	-0.31322200	6.91723900	-0.48654600
H	-2.85535200	5.35811800	2.61043100
H	-1.45809800	7.20703400	1.70173500
C	-3.63088300	1.74209100	-0.88543000
C	-4.63241400	1.99876800	-1.83000400
C	-3.95918500	1.11068300	0.32285900
C	-5.94898600	1.62412900	-1.56472700
H	-4.39586200	2.48780800	-2.76925500
C	-5.28072600	0.76489600	0.59569400
H	-3.17851700	0.86459500	1.03306900
C	-6.27472200	1.01645100	-0.35023800
H	-6.72071200	1.80985900	-2.30595500
H	-5.50601100	0.25292700	1.52325800
H	-7.30162800	0.72594700	-0.14921000
Pd	-0.23722300	0.62391800	-0.39995800
C	1.03027700	3.81146100	2.32254900
C	0.88955300	3.01957100	1.17501400
C	1.59249300	3.36286300	0.01576600
C	2.43737700	4.46994400	0.00251000
C	2.57738200	5.25103500	1.15096100
C	1.86843300	4.92222000	2.31063100
H	0.46419400	3.53726500	3.20619600
H	2.98591400	4.71649700	-0.90099200
H	3.23599100	6.11500700	1.14416900
H	1.97097400	5.53470100	3.20165600
H	1.47154600	2.75778900	-0.87611500
Cu	0.04436200	-1.74175800	0.86170600
B	3.97529400	0.33986600	-1.39149000
C	1.90559500	0.05448200	-0.01194200
C	0.49570200	-3.23964100	3.83192300
O	4.16758400	1.70232600	-1.29958900
O	5.15013500	-0.36544100	-1.33286200
C	0.98386300	-3.39696600	1.38277200
N	1.10237000	-3.85517000	2.65841600

N	1.72034100	-4.28064200	0.65238700
C	1.89303800	-4.99010600	2.72207000
C	2.28818800	-5.26005600	1.45267800
C	5.50124600	1.89518200	-0.75602300
C	6.24100800	0.59342700	-1.23665700
C	1.99449400	-4.14672500	-0.76556100
H	1.42131900	-3.30595300	-1.14689000
H	1.69734100	-5.04865100	-1.30244300
H	3.05926500	-3.95901000	-0.92962500
H	-0.35979900	-3.82425500	4.16987000
H	0.15008200	-2.24677300	3.56372200
H	1.25059900	-3.15483000	4.61622100
C	2.51795900	-0.65234600	1.16269700
C	3.52228700	-1.63069500	1.02433800
C	4.15152900	-2.19439100	2.13386700
C	3.80728500	-1.79679700	3.42510200
C	2.18415200	-0.26524200	2.47944900
C	2.81939700	-0.82169200	3.58522500
H	3.83457600	-1.94664600	0.03872400
H	2.53216300	-0.49500000	4.58103200
H	2.11964000	1.10144600	0.17696300
H	4.91730400	-2.95034000	1.98222700
H	4.29955700	-2.23362800	4.28894100
H	1.40269500	0.46579700	2.63873800
C	5.34092300	1.97334700	0.76668400
H	6.29415600	2.18294100	1.26040000
H	4.63973200	2.77728200	1.00311100
H	4.93305900	1.04306200	1.17054400
C	6.06966100	3.19997000	-1.29846700
H	5.47715300	4.03779700	-0.92137700
H	7.10330700	3.33947200	-0.96594100
H	6.04589200	3.22711100	-2.38919100
C	7.26873400	0.04456200	-0.25444900
H	7.73089100	-0.85601000	-0.66852500
H	8.05935400	0.77886800	-0.06933200
H	6.80126000	-0.21960100	0.69515200
C	6.84228600	0.72224000	-2.63769200
H	7.72115400	1.37341500	-2.64077900
H	7.14513500	-0.26864000	-2.98610900
H	6.10868000	1.12251700	-3.34268300
C	2.52884400	-0.26843100	-1.38862400
H	2.49810000	-1.33384300	-1.62067800
H	1.94054000	0.24127700	-2.15907900
C	-0.03225700	1.83014400	1.22550000
O	-0.70997000	1.61393700	2.21184200
S	-2.81011000	-1.93888800	2.30185000
O	-4.20765400	-1.89465800	1.84117900
O	-2.29791400	-3.23090800	2.77968100

C	-2.77565600	-0.82301700	3.78508700
F	-3.48341000	-1.35740600	4.78955800
F	-3.30288800	0.37459300	3.48591400
F	-1.51340100	-0.63870500	4.20966800
O	-1.86878800	-1.19419500	1.38191900
H	2.91329800	-6.04276500	1.05366400
H	2.10047400	-5.49515900	3.65176600

COM_{R3}-Pd(dppp)

O	4.25864600	-1.05614300	-1.29435800
C	5.43255400	-1.00033500	-0.44433500
C	5.80314100	0.52921700	-0.48019600
O	4.52809000	1.15557200	-0.76767600
B	3.69625000	0.20038500	-1.30988700
C	6.49412000	-1.93191200	-1.01931600
H	6.13923400	-2.96490200	-0.96772000
H	6.70984700	-1.70016900	-2.06357000
H	7.42354500	-1.86269800	-0.44445500
C	5.00084500	-1.48390500	0.94376500
H	4.56124700	-2.47955200	0.84694200
H	4.24297100	-0.82955000	1.37705200
C	6.32656600	1.09133800	0.83741700
H	6.54798300	2.15618600	0.72093700
C	6.74549800	0.89762500	-1.63005500
H	6.79297800	1.98673700	-1.71282300
H	7.75763000	0.51770100	-1.46232400
H	6.37658200	0.50117700	-2.57975300
C	1.20181300	-0.30354000	-0.92953600
C	2.23195000	0.50095800	-1.78679000
H	2.05734200	1.58313800	-1.74513900
H	2.09223200	0.21804600	-2.83719700
H	1.16237500	-1.33338600	-1.29685200
I	-3.71706100	-2.27087800	-0.60930300
C	-2.07447200	1.80349600	-0.90479000
C	-3.36944500	3.50616200	-0.14131200
C	-4.05246300	2.89480900	-1.14369200
H	-3.63036900	4.34573500	0.48283700
H	-5.02595200	3.09486800	-1.56213000
N	-3.24306800	1.86401800	-1.59746400
N	-2.16784000	2.82835000	-0.01334600
Cu	-0.55458600	0.59299900	-1.01343200
H	5.58629100	0.98285500	1.63134200
H	7.24784600	0.58288200	1.13989300
H	5.85231700	-1.54470800	1.62857900
C	-3.59037300	0.96540600	-2.68885300
H	-3.73771700	1.53313800	-3.61196000
H	-2.76982700	0.26118400	-2.81846900

H	-4.49802300	0.40757000	-2.44838600
C	-1.10530800	3.20073700	0.91218700
H	-1.53700500	3.44581800	1.88387500
H	-0.42848200	2.35486900	1.03104400
H	-0.54948000	4.06101100	0.52796200
C	1.49482700	-0.32478800	0.52537500
C	1.34138100	-1.50267000	1.29128700
C	1.93294000	0.82506200	1.22549100
C	1.58086400	-1.52863700	2.66225300
H	1.04563700	-2.41608100	0.78009900
C	2.17991600	0.79905200	2.59742000
H	2.10696500	1.74301400	0.67258900
C	2.00044100	-0.37511600	3.33484500
H	1.45532900	-2.45937400	3.20987800
H	2.52432500	1.70320900	3.09397800
H	2.19830000	-0.39653700	4.40202100
C	-1.64570700	0.02997200	2.46852500
C	-1.96093800	-0.88570000	1.46226100
C	-3.23617500	-0.86055400	0.89781400
C	-4.19211900	0.07234700	1.29894900
C	-3.86196900	0.98350800	2.30465700
C	-2.59731200	0.95717200	2.89504600
H	-0.65164700	0.00651800	2.90282300
H	-1.21621600	-1.59924700	1.13641200
H	-5.17573700	0.08834500	0.84381700
H	-4.60263500	1.70999600	2.62577800
H	-2.35290900	1.65960900	3.68642300

TS5_c

P	1.42249900	0.47740600	1.06019200
C	0.70721500	0.98237600	2.70149600
H	0.60123400	0.05049900	3.26796200
H	1.43691400	1.59165500	3.24608900
C	-0.64605700	1.71660400	2.62984500
H	-0.79263500	2.22447800	3.59059800
H	-0.60702900	2.51315600	1.87793600
C	-1.88445000	0.83491800	2.38655400
H	-2.77677200	1.39899400	2.67822000
H	-1.84254200	-0.06195900	3.01535600
P	-2.08962900	0.25150700	0.62532100
Pd	-0.12791700	-0.75472100	-0.20969600
C	3.00905600	-0.28307900	1.58035500
C	4.22338200	0.41224700	1.64012300
C	2.98601900	-1.65023800	1.90004100
C	5.39235500	-0.24615600	2.02485700
H	4.25478900	1.46537700	1.37991600
C	4.15209800	-2.30263400	2.29683400

H	2.05339600	-2.20228300	1.80882000
C	5.35886600	-1.60135500	2.35729200
H	6.33043100	0.30014700	2.06397900
H	4.12247300	-3.36009400	2.54240800
H	6.27041300	-2.11165200	2.65386500
C	1.91966200	2.06691700	0.28736200
C	2.04052800	3.27935000	0.98025400
C	2.11178800	2.06127400	-1.10443700
C	2.33881100	4.46039200	0.29784700
H	1.89612900	3.31338600	2.05477000
C	2.42294600	3.23777600	-1.78251800
H	1.99822200	1.13631800	-1.65798700
C	2.53065800	4.44297900	-1.08405300
H	2.41907000	5.39393400	0.84710500
H	2.56908900	3.21173000	-2.85829600
H	2.75904800	5.36322300	-1.61353600
C	-3.64755700	-0.71706200	0.69675000
C	-4.70536100	-0.45606900	1.58110900
C	-3.75606100	-1.79868400	-0.19003100
C	-5.85415100	-1.24704000	1.56370400
H	-4.63853500	0.36341900	2.28952100
C	-4.90767400	-2.58488600	-0.21163600
H	-2.91870300	-2.02866000	-0.84339100
C	-5.95922600	-2.30916500	0.66356200
H	-6.66605100	-1.03520400	2.25340800
H	-4.97781400	-3.41938300	-0.90289000
H	-6.85360600	-2.92508200	0.65231900
C	-2.54577900	1.83318900	-0.20067300
C	-3.83706400	2.37863300	-0.18058400
C	-1.51830900	2.54359400	-0.84025300
C	-4.08877700	3.61446400	-0.77690800
H	-4.64987800	1.83355100	0.28786900
C	-1.76724300	3.78685400	-1.42069900
H	-0.52355000	2.11636700	-0.88442300
C	-3.05445600	4.32477300	-1.39073500
H	-5.09500300	4.02355700	-0.76294700
H	-0.95340600	4.32475500	-1.89788200
H	-3.25481600	5.28862100	-1.84953000
C	1.10931000	-1.76315000	-1.65303600
C	2.51260500	-1.82677700	-1.54366700
C	0.50137000	-1.20510100	-2.79519300
C	3.28745500	-1.19007400	-2.49990100
H	2.96700100	-2.31110300	-0.68873200
C	1.30915500	-0.55561300	-3.73940000
H	-0.57009800	-1.28511200	-2.93851700
C	2.69379100	-0.53939900	-3.59734500
H	4.36798900	-1.18704900	-2.38744400
H	0.84184200	-0.09156500	-4.60354400

H	3.31539700	-0.05514800	-4.34368100
Br	0.00567800	-3.37870100	-0.78215700

6_c

P	-1.48694900	-0.19921000	-1.13580400
C	-0.82436600	-0.40295900	-2.86898600
H	-0.63952700	-1.47442900	-2.99514900
H	-1.63491900	-0.14458500	-3.55665200
C	0.45498700	0.37983700	-3.20457400
H	0.53266700	0.45400800	-4.29538900
H	0.39159600	1.40925200	-2.83060700
C	1.72836800	-0.29531200	-2.67256300
H	2.60933900	0.09028100	-3.19225200
H	1.68717100	-1.37080000	-2.86965900
P	1.98432300	-0.03222900	-0.84255300
Pd	0.03702100	0.27657100	0.49349500
C	-2.23313800	-1.84310300	-0.84780300
C	-3.46476500	-2.21377000	-1.40258900
C	-1.49358800	-2.78410400	-0.11586100
C	-3.95222300	-3.50816500	-1.22166800
H	-4.04755900	-1.48869200	-1.96131200
C	-1.98030600	-4.07918100	0.05562900
H	-0.54760800	-2.48917300	0.33097000
C	-3.21122800	-4.44165900	-0.49458300
H	-4.91163200	-3.78679200	-1.64707400
H	-1.40453600	-4.79841200	0.63001100
H	-3.59512000	-5.44736100	-0.35246300
C	-2.88379400	0.95841300	-1.33961900
C	-2.82952800	1.97139500	-2.30778500
C	-3.97380700	0.91237000	-0.45693400
C	-3.85499300	2.91171200	-2.40427200
H	-1.98511400	2.04099600	-2.98592300
C	-4.99906100	1.84928200	-0.56276800
H	-4.01289600	0.15978500	0.32167200
C	-4.94423100	2.84947600	-1.53461000
H	-3.80086900	3.69121400	-3.15819100
H	-5.83297100	1.80390400	0.13038700
H	-5.74232700	3.58189200	-1.60914800
C	2.91214000	-1.51563200	-0.32074300
C	2.39982900	-2.78450600	-0.63185300
C	4.03481200	-1.41611900	0.51011100
C	3.01832800	-3.93451500	-0.14625000
H	1.50380700	-2.88021200	-1.23900300
C	4.65116000	-2.56971400	0.99459000
H	4.41483200	-0.44009100	0.78710500
C	4.14940100	-3.82905800	0.66586000
H	2.61481800	-4.91104500	-0.39725100

H	5.52075200	-2.48146600	1.63861700
H	4.63050100	-4.72440100	1.04764800
C	3.18297000	1.34777100	-0.82213300
C	4.41077000	1.24895400	-1.49580000
C	2.85698700	2.53454600	-0.15467900
C	5.29611200	2.32410700	-1.50517400
H	4.68235900	0.32464400	-1.99794100
C	3.74301300	3.61307800	-0.17322000
H	1.92993500	2.59254700	0.40374900
C	4.95994900	3.50992600	-0.84626700
H	6.24731000	2.23744200	-2.02183800
H	3.48425300	4.52856100	0.34970000
H	5.65048700	4.34807200	-0.85374900
C	-1.58454500	0.58078600	1.69897100
C	-2.26828800	-0.46201300	2.33123900
C	-2.03458200	1.89290200	1.88419300
C	-3.39670200	-0.20004700	3.11619900
H	-1.93751300	-1.48768600	2.20735300
C	-3.15570000	2.15768000	2.67350500
H	-1.51774700	2.71760200	1.40156100
C	-3.84719100	1.11015800	3.28526600
H	-3.92161400	-1.02289900	3.59530000
H	-3.49329800	3.18279300	2.80354300
H	-4.72432600	1.31373400	3.89315500
Br	1.52815500	0.57101200	2.49395400

TS6_c

P	-2.02702300	-0.03441400	-0.44878000
C	-1.89677300	0.14820600	-2.28481700
H	-1.68422200	-0.87093600	-2.62440200
H	-2.88396400	0.42896400	-2.66783200
C	-0.82062400	1.11023100	-2.82460000
H	-1.00914800	1.22485800	-3.89836100
H	-0.93747200	2.10844800	-2.38914400
C	0.63609800	0.64293200	-2.66182200
H	1.29752500	1.24598700	-3.29148400
H	0.73245400	-0.40669900	-2.95475900
P	1.21983000	0.71857600	-0.91072500
C	-3.44608600	-1.16535200	-0.23062400
C	-4.74475800	-0.68496200	-0.01177400
C	-3.21241800	-2.54795200	-0.29004100
C	-5.80195400	-1.58058500	0.14734400
H	-4.92896500	0.38284100	0.04440300
C	-4.27694800	-3.43488100	-0.13686800
H	-2.20589200	-2.91669800	-0.47130000
C	-5.56937100	-2.95536600	0.08564500
H	-6.80520600	-1.20366400	0.32313900
H	-4.09192700	-4.50360500	-0.18518700

H	-6.39337700	-3.65119200	0.21364500
C	-2.62075900	1.56823300	0.20255500
C	-3.04517600	2.62507300	-0.61090200
C	-2.61066400	1.74304500	1.59600600
C	-3.42816400	3.84277600	-0.04424700
H	-3.07716600	2.50861900	-1.68810000
C	-3.01295500	2.94941400	2.16122600
H	-2.26950300	0.92875800	2.22946900
C	-3.41216500	4.00785700	1.33965000
H	-3.74046900	4.66001200	-0.68720000
H	-3.00509300	3.06956000	3.24043400
H	-3.71003500	4.95532300	1.77834800
C	3.00199100	0.33341200	-0.96715900
C	3.41677900	-0.86988400	-1.56094900
C	3.94535100	1.15534500	-0.33660800
C	4.76513000	-1.22085500	-1.54766900
H	2.67944200	-1.54636700	-1.98297800
C	5.29138500	0.78982200	-0.31789300
H	3.62938100	2.07623200	0.14118700
C	5.70497500	-0.39381500	-0.92928000
H	5.07847500	-2.15159000	-2.01123500
H	6.01562500	1.43215900	0.17441400
H	6.75400300	-0.67500500	-0.91676300
C	1.11049100	2.49678200	-0.49546700
C	1.60324100	3.49590400	-1.34924900
C	0.46058900	2.86799200	0.68728500
C	1.43426000	4.84093400	-1.02698700
H	2.12273200	3.22241100	-2.26264000
C	0.28797500	4.21443100	1.00857000
H	0.07264900	2.09092000	1.33623500
C	0.77159400	5.20114300	0.15007800
H	1.81580900	5.60869700	-1.69349100
H	-0.23785500	4.48681200	1.91766100
H	0.63358000	6.25033600	0.39398500
Pd	-0.01893200	-0.74535400	0.49833500
C	2.42365900	-2.28636000	1.41861200
C	1.52872000	-1.33636600	1.92063000
C	1.96154000	-0.34084200	2.80539400
C	3.30710300	-0.27918900	3.16592100
C	4.20818100	-1.21543300	2.65232500
C	3.76623300	-2.22045300	1.78964200
H	2.07308600	-3.02417400	0.70357100
H	3.65349900	0.50067200	3.83797400
H	5.25850200	-1.15810200	2.92188300
H	4.47240700	-2.93654000	1.38137600
H	1.25436000	0.38317800	3.19840800
C	-0.30790800	-1.79996300	2.05237500
O	-0.74835500	-2.46517000	2.90254000

Br	0.28259800	-2.77093300	-1.52000600
7c			
P	-2.02699700	-0.03439500	-0.44867600
C	-1.89669800	0.14811200	-2.28471200
H	-1.68401800	-0.87103300	-2.62420100
H	-2.88389400	0.42875000	-2.66780300
C	-0.82061300	1.11021900	-2.82448400
H	-1.00913700	1.22482900	-3.89824600
H	-0.93756400	2.10843000	-2.38903500
C	0.63617300	0.64311100	-2.66169000
H	1.29750300	1.24636600	-3.29126400
H	0.73279400	-0.40647400	-2.95469500
P	1.21987800	0.71870800	-0.91057800
C	-3.44595100	-1.16544900	-0.23043600
C	-4.74480000	-0.68516500	-0.01241200
C	-3.21200300	-2.54804200	-0.28893000
C	-5.80190600	-1.58088900	0.14673400
H	-4.92921500	0.38263900	0.04308300
C	-4.27644200	-3.43507700	-0.13574200
H	-2.20530500	-2.91669000	-0.46941300
C	-5.56905200	-2.95566400	0.08589600
H	-6.80530300	-1.20405100	0.32187600
H	-4.09120700	-4.50379600	-0.18334800
H	-6.39299300	-3.65156200	0.21390600
C	-2.62087600	1.56823000	0.20257200
C	-3.04535700	2.62500000	-0.61094300
C	-2.61086700	1.74308600	1.59601800
C	-3.42849700	3.84268200	-0.04434500
H	-3.07727000	2.50850900	-1.68814000
C	-3.01330400	2.94943400	2.16117800
H	-2.26966400	0.92884900	2.22952500
C	-3.41258400	4.00780900	1.33954800
H	-3.74085200	4.65986700	-0.68734000
H	-3.00550700	3.06961700	3.24038200
H	-3.71057300	4.95525800	1.77820000
C	3.00206200	0.33360700	-0.96701300
C	3.41683900	-0.86987000	-1.56044000
C	3.94547300	1.15581400	-0.33689100
C	4.76521800	-1.22073100	-1.54729100
H	2.67946100	-1.54657500	-1.98204100
C	5.29154200	0.79040100	-0.31829700
H	3.62953000	2.07684300	0.14064500
C	5.70511600	-0.39340600	-0.92936800
H	5.07854500	-2.15160800	-2.01058300
H	6.01582100	1.43295800	0.17366800
H	6.75416900	-0.67451000	-0.91694900
C	1.11046600	2.49690300	-0.49530900

C	1.60342500	3.49603400	-1.34896100
C	0.46030300	2.86809900	0.68730200
C	1.43438100	4.84106000	-1.02671600
H	2.12313600	3.22254600	-2.26222800
C	0.28761600	4.21453300	1.00856400
H	0.07225400	2.09101500	1.33617200
C	0.77143900	5.20125500	0.15019800
H	1.81609600	5.60883200	-1.69311600
H	-0.23841700	4.48690300	1.91754200
H	0.63337700	6.25044500	0.39409100
Pd	-0.01889700	-0.74534800	0.49835000
C	2.42343600	-2.28675500	1.41845000
C	1.52869900	-1.33657800	1.92047300
C	1.96174200	-0.34110800	2.80518500
C	3.30733700	-0.27967600	3.16562600
C	4.20821700	-1.21611200	2.65202900
C	3.76603700	-2.22109800	1.78942600
H	2.07267900	-3.02455800	0.70348700
H	3.65391200	0.50015100	3.83762400
H	5.25856200	-1.15896500	2.92153400
H	4.47205600	-2.93734200	1.38116700
H	1.25471100	0.38304000	3.19823200
C	-0.30782500	-1.80027300	2.05220300
O	-0.74818600	-2.46577600	2.90218200
Br	0.28244000	-2.77051900	-1.52028600

R₄

C	-1.57298700	-1.20726500	0.00000200
C	-0.17771500	-1.21605700	0.00000400
C	0.50374600	-0.00001500	-0.00001200
C	-0.17771000	1.21605100	-0.00000500
C	-1.57296100	1.20728300	0.00001000
C	-2.27304700	0.00000300	-0.00000500
H	-2.11087200	-2.15037800	0.00000500
H	0.37624500	-2.14787300	0.00000200
H	0.37629600	2.14784100	-0.00000800
H	-2.11086600	2.15038300	0.00001400
H	-3.35833000	0.00002700	-0.00001000
Cl	2.26185700	0.00000000	0.00000200

COM_{R₄-Pd(dppp)}

P	1.60529900	0.14145100	-1.04486000
C	1.07827400	0.05727500	-2.83262700
H	1.38279800	0.96037000	-3.37249300
H	1.66375100	-0.76291200	-3.26102400
C	-0.41952600	-0.23406300	-3.04809500
H	-0.61868500	-0.17441100	-4.12447500

H	-0.61816400	-1.27315100	-2.75997500
C	-1.40092900	0.69653000	-2.30419300
H	-2.32580500	0.81714000	-2.87586200
H	-0.97159000	1.69329700	-2.17669800
P	-1.82846200	0.01501200	-0.61188500
C	1.49882700	1.92948400	-0.59689800
C	1.38203700	2.98495200	-1.51085800
C	1.47152500	2.22509300	0.77744900
C	1.22972700	4.30132200	-1.06584700
H	1.39444700	2.79291800	-2.57819400
C	1.33239000	3.53790300	1.22083400
H	1.53121000	1.41495300	1.49754500
C	1.20419700	4.58107500	0.30030400
H	1.12808900	5.10516100	-1.78914100
H	1.30309600	3.74312500	2.28663400
H	1.08057300	5.60327500	0.64540400
C	3.41905200	-0.13575000	-1.16787200
C	3.90213900	-1.39456700	-0.78221200
C	4.32311700	0.83895700	-1.61286100
C	5.26588100	-1.68016400	-0.85939200
H	3.20511400	-2.14045200	-0.41088400
C	5.68615400	0.55371700	-1.68309900
H	3.96248200	1.82482100	-1.89013200
C	6.15904200	-0.70677400	-1.30955000
H	5.63023100	-2.65799300	-0.55827000
H	6.38087300	1.31522800	-2.02590100
H	7.22161400	-0.92529700	-1.36180700
C	-2.71561300	1.42005900	0.16511000
C	-3.93595300	1.25179800	0.83630900
C	-2.08241000	2.67341900	0.21906900
C	-4.51883200	2.31654200	1.52438800
H	-4.43439800	0.28833000	0.81692900
C	-2.66820400	3.73431200	0.90533200
H	-1.12130200	2.82298200	-0.25852100
C	-3.89042300	3.56201700	1.55872400
H	-5.46715600	2.17093600	2.03385900
H	-2.16122000	4.69439500	0.93276300
H	-4.34583000	4.38925100	2.09495100
C	-3.15110100	-1.18097900	-1.05576500
C	-4.32879000	-0.80308200	-1.71954400
C	-2.94551400	-2.53231300	-0.75058100
C	-5.28205600	-1.75859800	-2.06477900
H	-4.50580400	0.24325500	-1.95135000
C	-3.89646100	-3.49189600	-1.10427900
H	-2.03074900	-2.81845800	-0.23779900
C	-5.06540300	-3.10558700	-1.75945800
H	-6.19312500	-1.45576800	-2.57273600
H	-3.72406400	-4.53731800	-0.86629300

H	-5.80824900	-3.84950200	-2.03194600
Pd	0.07925400	-0.85261600	0.43292600
C	2.15368200	-1.26154700	2.68009100
C	1.08700800	-2.00985600	2.10893100
C	-0.26395700	-1.76946900	2.50527600
C	-0.50301400	-0.71161600	3.42941200
C	0.53365500	0.04515400	3.93296500
C	1.87210800	-0.23807800	3.55924900
H	3.17206700	-1.49796500	2.39295700
H	-1.52451800	-0.52582400	3.74724400
H	0.32921700	0.84428500	4.63852200
H	2.68585500	0.35126000	3.97099100
H	-1.03039700	-2.51277500	2.31988100
Cl	1.48985900	-3.60243500	1.39348200

COM_{R₄}-Pd(dppp)

P	1.25647800	0.31857400	-1.09289600
C	0.61641200	0.21298300	-2.84404000
H	0.78584600	1.19203000	-3.30361900
H	1.24737300	-0.50070100	-3.37836400
C	-0.85541700	-0.19647500	-2.99674600
H	-1.11856100	-0.10161200	-4.05599300
H	-0.96613100	-1.25873100	-2.74819500
C	-1.83073100	0.64030200	-2.14788600
H	-2.81269900	0.69653200	-2.62547800
H	-1.45653400	1.66207900	-2.03090000
P	-2.00573200	-0.12249400	-0.46242900
C	1.11743800	2.10157800	-0.69090500
C	1.67156300	3.08684500	-1.52340700
C	0.40797100	2.49036900	0.45222700
C	1.49506100	4.43602900	-1.22576500
H	2.25160700	2.79893300	-2.39553900
C	0.22023100	3.84239300	0.74247200
H	-0.00583400	1.72931400	1.10374800
C	0.76085300	4.81502500	-0.09733700
H	1.92761900	5.19303000	-1.87298500
H	-0.35487400	4.12549600	1.61814400
H	0.61646100	5.86798000	0.12530700
C	3.04869200	0.02090700	-1.27524700
C	3.51926700	-1.03148800	-2.07163600
C	3.95557200	0.73702900	-0.48284600
C	4.87628700	-1.34668600	-2.09418400
H	2.82990900	-1.63155200	-2.65710400
C	5.30961800	0.41132900	-0.49812900
H	3.59925000	1.53194700	0.16160700
C	5.77425800	-0.62676600	-1.30617900
H	5.22858400	-2.16371200	-2.71640000

H	6.00018900	0.96377200	0.13108700
H	6.82974300	-0.88077100	-1.31340700
C	-2.75819800	1.20131500	0.55262200
C	-2.68435900	1.07560700	1.94992000
C	-3.33040800	2.35293200	-0.00509500
C	-3.17217300	2.09363300	2.76774600
H	-2.23267900	0.18597200	2.38168600
C	-3.81478900	3.36949900	0.81898900
H	-3.39306800	2.47119200	-1.08144100
C	-3.73296100	3.24341900	2.20606300
H	-3.10795300	1.98948600	3.84666700
H	-4.25120700	4.25999700	0.37629400
H	-4.10542200	4.03725000	2.84684600
C	-3.32174500	-1.36153000	-0.73318400
C	-4.61531600	-0.97640700	-1.11511500
C	-3.01652500	-2.71952500	-0.58323500
C	-5.58821600	-1.94168600	-1.36159200
H	-4.86491900	0.07744700	-1.20303300
C	-3.99426200	-3.68399600	-0.83520400
H	-2.03119200	-3.00718200	-0.23387900
C	-5.27579400	-3.29766400	-1.22604700
H	-6.58989800	-1.63948800	-1.65262800
H	-3.75478400	-4.73572600	-0.71218300
H	-6.03618900	-4.04954000	-1.41567000
Pd	0.09316100	-0.87285400	0.46299900
C	2.69937300	-2.31886300	0.94902600
C	1.88376100	-1.25596000	1.34383900
C	2.33113100	-0.39455400	2.35069100
C	3.58248800	-0.58607600	2.94434000
C	4.39730600	-1.64329700	2.53844200
C	3.94894800	-2.51291600	1.54287500
H	2.37390700	-2.99388100	0.16246500
H	3.91802600	0.09234600	3.72506600
H	5.37255000	-1.78961000	2.99420400
H	4.57560500	-3.34064900	1.22069000
H	1.70736500	0.43139300	2.68145500
Cl	-0.99886600	-2.08392900	2.22239000

TS5_d

P	1.35155800	-0.00818400	-1.19616700
C	0.64207300	-0.26416300	-2.90228300
H	0.90637300	0.58017000	-3.54733200
H	1.17924900	-1.12854300	-3.30407400
C	-0.87048200	-0.54549500	-2.95879700
H	-1.16013700	-0.58012200	-4.01538500
H	-1.05908000	-1.54895100	-2.55942100
C	-1.76651600	0.47192600	-2.22335400
H	-2.73150300	0.57494100	-2.72728200

H	-1.30977500	1.46527000	-2.21062900
P	-2.05225200	-0.03221700	-0.44759800
C	1.45526300	1.80828700	-0.94975000
C	1.10241900	2.76884000	-1.90613400
C	1.81808800	2.24009600	0.33944600
C	1.09008100	4.12732600	-1.57919500
H	0.82046600	2.47112500	-2.90967900
C	1.82368100	3.59544300	0.65753300
H	2.07713800	1.51054900	1.09854300
C	1.44822400	4.54442500	-0.29765900
H	0.79862200	4.85705800	-2.32872300
H	2.10437700	3.90735300	1.65894600
H	1.43452200	5.60012800	-0.04403000
C	3.09593900	-0.52040600	-1.42778700
C	3.34084000	-1.88768300	-1.63863300
C	4.18463400	0.34978600	-1.29633100
C	4.64359400	-2.36872500	-1.74157500
H	2.50439800	-2.58016700	-1.69967300
C	5.49024300	-0.13582500	-1.38677500
H	4.01433300	1.40567600	-1.11771200
C	5.72440200	-1.49242400	-1.61207900
H	4.81653300	-3.42803100	-1.90668200
H	6.32579300	0.55037500	-1.28332200
H	6.74107700	-1.86737100	-1.68024600
C	-2.77689700	1.49432100	0.26920000
C	-4.06390600	1.55465200	0.81901400
C	-1.95409400	2.63239100	0.33520400
C	-4.52460100	2.73530900	1.40585000
H	-4.70681100	0.68178200	0.79094700
C	-2.42098300	3.81002800	0.91179400
H	-0.94202000	2.59564200	-0.05102000
C	-3.70953300	3.86617900	1.44957400
H	-5.52448700	2.76827500	1.82889400
H	-1.77088600	4.67922400	0.94757900
H	-4.07188800	4.78266000	1.90565500
C	-3.44531200	-1.21590900	-0.58236800
C	-4.60560100	-0.95568000	-1.32837100
C	-3.32640200	-2.43752100	0.09476200
C	-5.62853700	-1.89940400	-1.39353800
H	-4.71787600	-0.00776400	-1.84652200
C	-4.35189300	-3.38282200	0.02700400
H	-2.42757500	-2.64156000	0.67075300
C	-5.50136000	-3.11548400	-0.71606500
H	-6.52423300	-1.68846100	-1.97043600
H	-4.24918700	-4.32644500	0.55415200
H	-6.29863300	-3.85103600	-0.76910100
Pd	-0.03205100	-0.83284300	0.52886900
C	2.76087600	-1.57989300	1.71836900

C	1.42749100	-1.27524000	2.03594400
C	1.12127700	-0.31038800	3.01294800
C	2.15877600	0.46673300	3.54072200
C	3.48027100	0.24240700	3.15643000
C	3.77193800	-0.79284900	2.25322600
H	2.98567300	-2.36608500	1.00919600
H	1.92391600	1.23616400	4.27133900
H	4.28232600	0.84067500	3.57678400
H	4.79802000	-0.97791800	1.94851300
H	0.09559000	-0.17119700	3.33713800
Cl	0.10979400	-2.91741600	2.12843500

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P	1.25647800	0.31857400	-1.09289600
C	0.61641200	0.21298300	-2.84404000
H	0.78584600	1.19203000	-3.30361900
H	1.24737300	-0.50070100	-3.37836400
C	-0.85541700	-0.19647500	-2.99674600
H	-1.11856100	-0.10161200	-4.05599300
H	-0.96613100	-1.25873100	-2.74819500
C	-1.83073100	0.64030200	-2.14788600
H	-2.81269900	0.69653200	-2.62547800
H	-1.45653400	1.66207900	-2.03090000
P	-2.00573200	-0.12249400	-0.46242900
C	1.11743800	2.10157800	-0.69090500
C	1.67156300	3.08684500	-1.52340700
C	0.40797100	2.49036900	0.45222700
C	1.49506100	4.43602900	-1.22576500
H	2.25160700	2.79893300	-2.39553900
C	0.22023100	3.84239300	0.74247200
H	-0.00583400	1.72931400	1.10374800
C	0.76085300	4.81502500	-0.09733700
H	1.92761900	5.19303000	-1.87298500
H	-0.35487400	4.12549600	1.61814400
H	0.61646100	5.86798000	0.12530700
C	3.04869200	0.02090700	-1.27524700
C	3.51926700	-1.03148800	-2.07163600
C	3.95557200	0.73702900	-0.48284600
C	4.87628700	-1.34668600	-2.09418400
H	2.82990900	-1.63155200	-2.65710400
C	5.30961800	0.41132900	-0.49812900
H	3.59925000	1.53194700	0.16160700
C	5.77425800	-0.62676600	-1.30617900
H	5.22858400	-2.16371200	-2.71640000
H	6.00018900	0.96377200	0.13108700
H	6.82974300	-0.88077100	-1.31340700
C	-2.75819800	1.20131500	0.55262200
C	-2.68435900	1.07560700	1.94992000

C	-3.33040800	2.35293200	-0.00509500
C	-3.17217300	2.09363300	2.76774600
H	-2.23267900	0.18597200	2.38168600
C	-3.81478900	3.36949900	0.81898900
H	-3.39306800	2.47119200	-1.08144100
C	-3.73296100	3.24341900	2.20606300
H	-3.10795300	1.98948600	3.84666700
H	-4.25120700	4.25999700	0.37629400
H	-4.10542200	4.03725000	2.84684600
C	-3.32174500	-1.36153000	-0.73318400
C	-4.61531600	-0.97640700	-1.11511500
C	-3.01652500	-2.71952500	-0.58323500
C	-5.58821600	-1.94168600	-1.36159200
H	-4.86491900	0.07744700	-1.20303300
C	-3.99426200	-3.68399600	-0.83520400
H	-2.03119200	-3.00718200	-0.23387900
C	-5.27579400	-3.29766400	-1.22604700
H	-6.58989800	-1.63948800	-1.65262800
H	-3.75478400	-4.73572600	-0.71218300
H	-6.03618900	-4.04954000	-1.41567000
Pd	0.09316100	-0.87285400	0.46299900
C	2.69937300	-2.31886300	0.94902600
C	1.88376100	-1.25596000	1.34383900
C	2.33113100	-0.39455400	2.35069100
C	3.58248800	-0.58607600	2.94434000
C	4.39730600	-1.64329700	2.53844200
C	3.94894800	-2.51291600	1.54287500
H	2.37390700	-2.99388100	0.16246500
H	3.91802600	0.09234600	3.72506600
H	5.37255000	-1.78961000	2.99420400
H	4.57560500	-3.34064900	1.22069000
H	1.70736500	0.43139300	2.68145500
Cl	-0.99886600	-2.08392900	2.22239000

TS6_d

P	-2.04331600	-0.11548800	-0.58072500
C	-1.87599900	0.17576500	-2.39179200
H	-1.66980600	-0.81932400	-2.79814500
H	-2.84426500	0.50599300	-2.78253100
C	-0.75801200	1.15202200	-2.79874700
H	-0.90229100	1.38826100	-3.85924500
H	-0.85292900	2.10183400	-2.26106300
C	0.66546800	0.60048100	-2.64014400
H	1.37353800	1.22379900	-3.19543500
H	0.71896900	-0.42141900	-3.02324000
P	1.27772600	0.51228300	-0.89711400
C	-3.45271300	-1.27019100	-0.43995100
C	-4.75799900	-0.81800300	-0.20165100

C	-3.20024500	-2.64496900	-0.57399900
C	-5.80442800	-1.73414200	-0.09700500
H	-4.95529900	0.24296600	-0.08889000
C	-4.25489900	-3.55158800	-0.47401800
H	-2.18647300	-2.98738100	-0.77172200
C	-5.55427500	-3.10062300	-0.23266200
H	-6.81326400	-1.37991300	0.09323400
H	-4.05702600	-4.61375800	-0.58126400
H	-6.37028700	-3.81228500	-0.14803300
C	-2.66136500	1.45326300	0.13461400
C	-3.08939700	2.53927800	-0.63850800
C	-2.65772000	1.57816300	1.53352900
C	-3.48488800	3.73130800	-0.02795100
H	-3.11288500	2.46665100	-1.71974900
C	-3.06766000	2.76051800	2.14322500
H	-2.31373500	0.74677600	2.14142100
C	-3.47337900	3.84568100	1.36131300
H	-3.80221800	4.56922100	-0.64114800
H	-3.06157900	2.83956500	3.22614100
H	-3.77972300	4.77371600	1.83420900
C	3.02001000	0.01892900	-1.08788700
C	3.33393500	-1.08146900	-1.90002000
C	4.03050800	0.65122600	-0.35233600
C	4.65336100	-1.52064200	-1.99024300
H	2.54364400	-1.62577300	-2.40568300
C	5.34533200	0.19857400	-0.44141300
H	3.78965400	1.48075300	0.30223800
C	5.66044200	-0.88305500	-1.26439600
H	4.88955100	-2.37512500	-2.61713000
H	6.12116500	0.68704100	0.14015100
H	6.68560700	-1.23544900	-1.32994300
C	1.29955400	2.26287500	-0.37256500
C	2.00532800	3.23848400	-1.09401400
C	0.52535300	2.64975100	0.72661600
C	1.92455200	4.57864000	-0.72220500
H	2.62484000	2.94752900	-1.93696300
C	0.43553800	3.99304200	1.09198000
H	-0.01507900	1.88960100	1.27836200
C	1.13422800	4.95794400	0.36716800
H	2.47435400	5.32871500	-1.28275600
H	-0.18662000	4.27949300	1.93371500
H	1.06693900	6.00472800	0.64822900
Pd	-0.03451200	-0.85419400	0.50503800
C	2.52429200	-2.30279200	1.09148300
C	1.75055900	-1.21090300	1.48784000
C	2.21191100	-0.34720700	2.48285800
C	3.46555100	-0.56190500	3.06660900
C	4.24885200	-1.64272200	2.66260100

C	3.77434300	-2.51279300	1.67839200
H	2.16388200	-2.95633500	0.30266800
H	3.82707900	0.11920300	3.83291400
H	5.22521600	-1.80584000	3.10999200
H	4.38291200	-3.35324800	1.35598300
H	1.61564100	0.50572800	2.79447900
C	-0.86536100	-1.77384600	1.99375400
O	-1.32890000	-2.32631600	2.88229800
Cl	0.16579000	-2.66698400	-1.65624600

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P	-1.85926500	0.11868300	-0.60153400
C	-1.62961900	0.43063200	-2.41632100
H	-1.55051800	-0.57987300	-2.83161600
H	-2.56077200	0.86715700	-2.79458800
C	-0.42853900	1.27653700	-2.88178500
H	-0.58962700	1.48744800	-3.94553000
H	-0.42453900	2.24921200	-2.37918200
C	0.96003900	0.62350400	-2.75069100
H	1.69722800	1.19353800	-3.32529400
H	0.93853700	-0.40159900	-3.13405900
P	1.49488900	0.47026100	-0.98877100
C	-3.41422400	-0.82977600	-0.57116800
C	-4.64658700	-0.24793500	-0.24644200
C	-3.34566700	-2.19249200	-0.90109500
C	-5.80601300	-1.02293700	-0.26054500
H	-4.70022300	0.80273800	0.01923200
C	-4.51113600	-2.95552500	-0.92312300
H	-2.38430700	-2.64475400	-1.13265400
C	-5.73953700	-2.37506200	-0.60081000
H	-6.75984900	-0.57044300	-0.00561400
H	-4.45518400	-4.00907100	-1.17886800
H	-6.64368400	-2.97676700	-0.60908500
C	-2.25184100	1.71889300	0.18262700
C	-2.46955100	2.90120400	-0.53412300
C	-2.29172600	1.75346700	1.58599100
C	-2.70165600	4.10141400	0.14051800
H	-2.45712000	2.89480500	-1.61808400
C	-2.54773800	2.94540100	2.25662700
H	-2.10873500	0.83857100	2.14294200
C	-2.74179000	4.12631400	1.53366500
H	-2.85357600	5.01550100	-0.42530100
H	-2.58387600	2.95829000	3.34187600
H	-2.92331500	5.06065700	2.05608500
C	3.23282200	-0.09041300	-1.02121200
C	3.49778100	-1.38288100	-1.50656600
C	4.27330800	0.66825300	-0.46896500
C	4.79421000	-1.89113000	-1.45423600

H	2.68167000	-1.99483200	-1.88353800
C	5.56682500	0.14644500	-0.41118300
H	4.07413800	1.66023100	-0.07810500
C	5.83117700	-1.13077900	-0.90579100
H	4.99179300	-2.88934100	-1.83380000
H	6.36678200	0.74052000	0.02115100
H	6.83839400	-1.53456300	-0.86056800
C	1.53351000	2.19515500	-0.38345000
C	2.05071900	3.25547100	-1.14348400
C	0.96500900	2.46571900	0.86800100
C	1.99126100	4.56183400	-0.66091800
H	2.50025900	3.06034400	-2.11255500
C	0.90617600	3.77262600	1.35118200
H	0.54881900	1.64480600	1.44322500
C	1.41527500	4.82148700	0.58561900
H	2.39000700	5.37741800	-1.25687600
H	0.44464700	3.97032300	2.31290800
H	1.36158200	5.84107200	0.95561400
Pd	-0.01102800	-1.01300200	0.14744800
C	1.65987900	-2.54099100	1.50211300
C	0.49870200	-2.13575900	2.20211100
C	0.62141700	-1.40323300	3.40371900
C	1.87964700	-1.10310900	3.90209100
C	3.03160300	-1.48174500	3.19194900
C	2.92327900	-2.19488500	2.00491200
H	1.56304700	-3.13280700	0.59680100
H	1.97505500	-0.56155900	4.83851800
H	4.01148500	-1.21447300	3.57563800
H	3.81021700	-2.47594300	1.44701600
H	-0.27765800	-1.08760700	3.92417200
C	-0.83944300	-2.19141600	1.51909200
O	-1.89225200	-2.66089800	1.83224800
Cl	0.26969600	-2.82962700	-1.76386500

TS1'

O	-2.44971200	1.97799900	-0.57866500
C	-3.05763000	2.98818300	0.26982900
C	-2.34796800	2.72630900	1.64102600
O	-1.04918600	2.22661900	1.21871400
B	-1.21630700	1.65178700	-0.03624300
C	-4.56688600	2.77870100	0.26942700
H	-4.96329000	2.99023900	-0.72801100
H	-4.82078900	1.74866700	0.52037800
H	-5.05600100	3.45388300	0.97971900
C	-2.70403300	4.35067000	-0.33429400
H	-3.04683600	4.37619700	-1.37210500
H	-3.18157600	5.17209300	0.20839800
H	-1.62255300	4.51128200	-0.32876300

C	-2.13997800	3.95836400	2.51142700
H	-3.10063800	4.41247400	2.77693900
H	-1.63117700	3.67429900	3.43694300
H	-1.52767100	4.70581700	2.00474900
C	-3.01698600	1.60341100	2.43936700
H	-2.35799600	1.30768200	3.26022000
H	-3.97603700	1.91908300	2.86131600
H	-3.18147600	0.73504400	1.79951300
C	6.73785600	2.12577800	0.12266300
C	5.44680600	2.29979100	-0.37767600
C	4.95901500	1.50087700	-1.42000800
C	5.79979300	0.50156900	-1.93261800
C	7.08967800	0.31925700	-1.43451000
C	7.56742800	1.13632600	-0.40654400
H	7.09737400	2.76550400	0.92392000
H	4.80669100	3.07499700	0.03607700
H	5.43863100	-0.12977600	-2.74075100
H	7.72698900	-0.45409800	-1.85469400
H	8.57422900	1.00129500	-0.02245800
C	3.55831800	1.67382600	-1.94934200
H	3.17473800	2.66218100	-1.67060100
H	3.56568600	1.63611400	-3.04607100
C	2.57655200	0.58759100	-1.43079000
H	2.61305400	0.59761300	-0.33343000
H	2.97422700	-0.39135500	-1.72334800
C	1.15402600	0.74655200	-1.91487300
C	0.31766500	1.80209800	-1.28657300
H	-0.31054800	2.36661500	-1.97583700
H	0.83785200	2.45872900	-0.58412300
H	1.01919700	0.64040200	-2.99094600
C	-0.72846200	-1.71296100	0.07072000
C	-1.74894700	-3.66071500	0.67308900
C	-0.48395500	-3.69912600	1.16126900
H	-2.55169600	-4.37756400	0.72101000
H	0.04047500	-4.45228800	1.72634400
N	0.12165900	-2.50224800	0.78729800
N	-1.88954300	-2.43590300	0.01795700
C	-3.11511400	-1.88206200	-0.47595100
C	-4.13464000	-1.58455400	0.44389200
C	-3.23214800	-1.57570300	-1.83893100
C	-5.29138900	-0.96879400	-0.03708600
C	-4.40577400	-0.94783500	-2.26742500
C	-5.43971100	-0.63017000	-1.38593900
H	-6.08706600	-0.72949600	0.66430500
H	-4.50743100	-0.69750900	-3.32008700
C	1.45834500	-2.08480700	1.10242500
C	1.65307900	-1.19651600	2.16846400
C	2.50986100	-2.51383700	0.28115500

C	2.95987700	-0.77014800	2.42495900
C	3.79629500	-2.06453600	0.58016000
C	4.04139600	-1.19629700	1.64923600
H	3.13301900	-0.07856400	3.24546200
H	4.62221600	-2.36707900	-0.05770400
Cu	-0.23763600	-0.06052700	-0.68491600
C	2.23528500	-3.35318300	-0.93872100
H	3.16747400	-3.63822700	-1.43167600
H	1.68010100	-4.26569800	-0.69871300
H	1.62775400	-2.77868400	-1.64807900
C	0.49404900	-0.67128300	2.97915600
H	-0.02997100	0.12415200	2.43682700
H	-0.23773100	-1.45534200	3.19675200
H	0.84661300	-0.25726000	3.92730700
C	5.44306400	-0.73421800	1.95153500
H	5.96540200	-1.45882300	2.58911200
H	6.02542100	-0.61319300	1.03601600
H	5.44136100	0.22590900	2.47353600
C	-2.13401100	-1.89605400	-2.81959100
H	-1.29872900	-1.18977500	-2.73125600
H	-1.71614900	-2.89146400	-2.64180000
H	-2.51157200	-1.85299600	-3.84414200
C	-3.99025800	-1.88901100	1.91528400
H	-4.72967600	-1.32986300	2.49325300
H	-4.13831100	-2.95280500	2.13201700
H	-2.99547200	-1.62149500	2.28205200
C	-6.67314600	0.09465300	-1.86249400
H	-6.60034500	1.16641400	-1.64202100
H	-6.80771800	-0.01118900	-2.94228700
H	-7.57479000	-0.27854300	-1.36693500

3'

O	-1.88911700	3.21821200	-0.47876600
C	-3.21245500	3.30488900	0.09705500
C	-3.04881500	2.51292000	1.44628100
O	-1.64049400	2.67742400	1.73313800
B	-0.99537000	2.95003700	0.54088200
C	-4.21536200	2.69977100	-0.88059300
H	-4.25272400	3.30590600	-1.79032600
H	-3.93805800	1.68260700	-1.15939100
H	-5.21914000	2.68231900	-0.44167900
C	-3.50772500	4.79385800	0.30614400
H	-3.40310400	5.31133900	-0.65108800
H	-4.52174300	4.95970400	0.68225900
H	-2.79740500	5.23659400	1.00947900
C	-3.85634800	3.06073100	2.61798000
H	-4.92963800	3.01697000	2.40470300
H	-3.66216200	2.45784900	3.50968700

H	-3.58626200	4.09346900	2.84361000
C	-3.29759900	1.01222800	1.28893800
H	-2.96949500	0.50240900	2.19922700
H	-4.35340700	0.78612100	1.12402600
H	-2.72186300	0.60559400	0.45418100
C	6.99028900	2.08071500	-0.04872100
C	5.66209800	2.51079300	-0.10119000
C	4.76499900	1.98445600	-1.03984800
C	5.24029300	1.00106300	-1.92145100
C	6.56248900	0.56235400	-1.87036700
C	7.44630300	1.10247000	-0.93266800
H	7.66799300	2.51083000	0.68362600
H	5.31352600	3.27294900	0.59118400
H	4.56057000	0.58134800	-2.65898900
H	6.90800500	-0.19515700	-2.56896400
H	8.47836400	0.76660100	-0.89470000
C	3.32015600	2.41437500	-1.07721000
H	3.19383400	3.33478700	-0.49808600
H	3.02571600	2.64614300	-2.10948800
C	2.37056200	1.31805700	-0.53409400
H	2.68923400	1.06587800	0.48700000
H	2.55144700	0.41036300	-1.12368600
C	0.87383800	1.66911800	-0.54533200
C	0.54984300	2.88857500	0.36035900
H	0.95127800	3.83110600	-0.04791900
H	1.01263600	2.74643700	1.34643800
H	0.59495400	1.94288200	-1.57545700
C	-0.59283800	-1.86208600	0.08807700
C	-1.42008100	-3.98228900	-0.05228100
C	-0.11988900	-4.08048100	0.32641900
H	-2.16733700	-4.73523900	-0.24205000
H	0.49938200	-4.93615300	0.54146200
N	0.36298400	-2.77944800	0.40642000
N	-1.68999400	-2.62161400	-0.19050800
C	-2.95604200	-2.07744300	-0.59078500
C	-4.03120700	-2.14690800	0.30546800
C	-3.07216200	-1.47591200	-1.85327400
C	-5.25485400	-1.60539400	-0.09625700
C	-4.31242900	-0.93454300	-2.20114300
C	-5.41177200	-0.98629300	-1.33882000
H	-6.09634400	-1.64622000	0.59043600
H	-4.41963900	-0.45903800	-3.17252200
C	1.71482100	-2.39580500	0.71835100
C	2.02437900	-2.01974600	2.03051400
C	2.65442100	-2.34235000	-0.32047600
C	3.32990800	-1.59672600	2.29296300
C	3.94550200	-1.91494500	-0.00946700
C	4.29938100	-1.53116600	1.28796100

H	3.58958300	-1.29455100	3.30418000
H	4.68193700	-1.83549000	-0.80357200
Cu	-0.08601900	0.00957000	-0.12586100
C	2.25578900	-2.65580900	-1.73917300
H	3.12286400	-2.61816800	-2.40205600
H	1.79443900	-3.64443300	-1.83151900
H	1.52151700	-1.92305800	-2.09434400
C	0.96803500	-2.01629100	3.10490900
H	0.23742300	-1.22102000	2.91703400
H	0.41483500	-2.96052400	3.13755500
H	1.41355500	-1.84354000	4.08711300
C	5.67808400	-0.99744700	1.57523500
H	6.43766200	-1.50368100	0.97342800
H	5.73227800	0.06655300	1.32242700
H	5.93939000	-1.10929800	2.63142700
C	-1.90452700	-1.38531000	-2.80102600
H	-1.22022500	-0.58477300	-2.49481000
H	-1.32416800	-2.31246200	-2.81827900
H	-2.24907400	-1.17056800	-3.81533500
C	-3.86248400	-2.73701400	1.68280600
H	-4.73485700	-2.51888800	2.30257900
H	-3.73500400	-3.82462800	1.65597200
H	-2.97752700	-2.32296000	2.17613100
C	-6.72059800	-0.34516500	-1.72572200
H	-6.69081500	0.73451100	-1.53606700
H	-6.93412600	-0.48139900	-2.79004000
H	-7.55496600	-0.75887300	-1.15295100

2''

Cu	0.91944700	-0.95325800	-0.21060100
B	-1.03161200	-0.38985300	0.00338700
C	4.13819000	-1.08703300	1.15483200
O	-1.58551200	0.61430300	-0.80305000
O	-1.96749600	-0.80504400	0.94042200
C	2.47026500	0.31900500	-0.03313100
N	3.68629500	0.16223200	0.56253600
N	2.45553100	1.63089100	-0.39796200
C	4.40931900	1.34556200	0.57343400
C	3.63073500	2.27333400	-0.04214600
C	-3.25530000	-0.22048100	0.61560900
C	1.35040200	2.27023700	-1.10629100
H	5.39141000	1.42400200	1.01193900
H	3.80921500	3.31509700	-0.25627300
H	1.18857300	3.26921900	-0.69346100
H	1.57997200	2.35520700	-2.17251100
H	0.44724300	1.67193000	-0.97458500
H	4.03341500	-1.06255300	2.24356800
H	3.52379900	-1.89295400	0.75198600

H	5.18545500	-1.26327000	0.89693500
C	-2.84814100	1.03491900	-0.22186900
C	-2.54954400	2.26461900	0.64436900
H	-2.07546200	3.02885000	0.02170000
H	-3.45979800	2.69060000	1.07755700
H	-1.86099600	2.00946200	1.45394700
C	-3.80896500	1.40718800	-1.34579000
H	-4.79674300	1.66306900	-0.94685100
H	-3.42541900	2.27848100	-1.88482300
H	-3.92158400	0.59109600	-2.06092600
C	-3.99869000	0.08143500	1.91255400
H	-4.94701800	0.59138100	1.71003000
H	-4.22095600	-0.85372900	2.43417100
H	-3.40127000	0.70492700	2.57974100
C	-4.02404800	-1.26469100	-0.20211400
H	-3.50488300	-1.48193800	-1.13905200
H	-4.08029200	-2.19104300	0.37544100
H	-5.04265800	-0.93558300	-0.43100500
C	0.97550900	-2.82779800	-0.68208600
O	0.57062600	-3.86527500	-0.97028100

TS1''

Cu	1.16393100	-1.17168500	-0.40129300
B	-1.09487300	-0.60303200	-0.05283200
C	4.10394900	-1.34308000	1.29160200
O	-1.56946400	0.37203200	-0.91239300
O	-1.84555300	-0.70029000	1.09302300
C	2.56130000	0.06841600	-0.04981600
N	3.71979100	-0.09595000	0.64723200
N	2.59250300	1.37199400	-0.44702000
C	4.45840700	1.07721400	0.68279600
C	3.74923400	2.00182500	-0.01579300
C	-3.09124300	0.02388700	0.85341300
C	1.55800200	1.99435400	-1.26494200
H	5.40375900	1.15084000	1.19590000
H	3.96422300	3.03392100	-0.24178200
H	1.41191900	3.02690700	-0.93969400
H	1.84454500	1.98436100	-2.32058000
H	0.62476400	1.44236300	-1.13937800
H	3.89057400	-1.30964600	2.36385200
H	3.52833400	-2.14956700	0.83376300
H	5.17055600	-1.52415600	1.13887700
C	-2.66099600	1.06687200	-0.23547300
C	-2.06726800	2.34853600	0.35643900
H	-1.61261300	2.93335100	-0.44831700
H	-2.83275800	2.96551700	0.83600800
H	-1.29328200	2.11453800	1.09219400
C	-3.73107800	1.40091800	-1.26684700

H	-4.60400800	1.85761400	-0.78829000
H	-3.33238800	2.11237700	-1.99581100
H	-4.05315500	0.50878500	-1.80521500
C	-3.56672400	0.62456500	2.16950200
H	-4.46521000	1.23215700	2.01665400
H	-3.81518000	-0.17797700	2.86912900
H	-2.79717400	1.24716700	2.62876800
C	-4.09509500	-1.00799300	0.33320100
H	-3.72541500	-1.48357800	-0.57894900
H	-4.21807900	-1.78949400	1.08740700
H	-5.07285200	-0.55884100	0.13586300
C	-0.32831700	-2.18049200	-0.82984900
O	-1.31289200	-2.79737300	-1.12883400

3"

Cu	1.11774900	-1.12004700	-0.27060000
B	-1.72750300	-1.00992400	-0.41422400
C	4.16321400	-1.29843400	1.41449100
O	-1.74580700	0.25914000	-0.97740000
O	-2.61452900	-1.13062700	0.62934500
C	2.66057300	0.07466200	-0.00737700
N	3.81727100	-0.08342500	0.68884600
N	2.74861200	1.33542600	-0.51219000
C	4.61237700	1.05109300	0.62100800
C	3.93515700	1.94931500	-0.14171600
C	-3.42663400	0.07211500	0.66087800
C	1.72952500	1.94056100	-1.36382700
H	5.56873600	1.12151800	1.11442000
H	4.18948400	2.95268300	-0.44440800
H	1.49007800	2.94230300	-0.99814200
H	2.08545400	2.00724000	-2.39562300
H	0.83270300	1.31995000	-1.33066800
H	4.31160400	-1.07812700	2.47500400
H	3.33846000	-2.00237900	1.30370700
H	5.07498500	-1.74043500	1.00393500
C	-2.51477200	1.10971000	-0.08602700
C	-1.50960600	1.79641600	0.84519500
H	-0.80970700	2.38243100	0.24360600
H	-2.00294400	2.47198300	1.54941000
H	-0.93504700	1.05655700	1.40982100
C	-3.26090900	2.14520000	-0.91798900
H	-3.90111100	2.76671500	-0.28331900
H	-2.54303100	2.80009500	-1.42045300
H	-3.87844800	1.67207300	-1.68239600
C	-3.73488400	0.41166500	2.11469100
H	-4.28254500	1.35739400	2.18680500
H	-4.35657200	-0.37539800	2.54983700
H	-2.82277500	0.48725800	2.70880100

C	-4.71850200	-0.24581000	-0.09786700
H	-4.50906700	-0.48090400	-1.14459100
H	-5.18688800	-1.12193100	0.35745500
H	-5.42680800	0.58719000	-0.05908100
C	-0.55630500	-2.02868400	-0.71619200
O	-0.67095700	-3.15677700	-1.20366900

1A

Cu	-0.03819600	0.97927000	-0.18992200
C	0.46107700	-0.82382200	0.07143900
N	1.67107600	-1.43094100	0.21738900
N	-0.43613800	-1.83733000	0.23014100
C	1.53149700	-2.79430800	0.46503300
C	0.19782000	-3.05111300	0.47295300
C	-2.50149300	2.82160500	1.07770700
H	-1.88140300	3.29915900	1.84338500
H	-3.52901000	3.19449300	1.17709800
H	-2.51087000	1.74211300	1.26625700
C	-1.90545700	3.10106300	-0.31846500
C	-2.75229200	2.36784600	-1.38078300
H	-2.31465100	2.52829600	-2.37166800
H	-2.75522200	1.29088100	-1.17851900
H	-3.79339700	2.71501700	-1.39823700
C	-1.93694400	4.61594500	-0.59461400
H	-1.33355100	5.13899400	0.15395200
H	-1.50303600	4.81836300	-1.57883800
H	-2.95559300	5.02172800	-0.57023600
O	-0.56903200	2.69085600	-0.37485300
H	-0.35417100	-3.96380400	0.62788400
H	2.38425300	-3.43641900	0.61366200
C	2.92259700	-0.73208600	0.13020500
C	3.65823700	-0.81840400	-1.05874300
C	3.34585400	0.03609600	1.22301900
C	4.86899600	-0.12554800	-1.12681300
C	4.56147200	0.71400400	1.10565200
C	5.33753100	0.64113000	-0.05530700
H	5.45173600	-0.17553100	-2.04279000
H	4.90552800	1.31934700	1.94014200
C	-1.85555500	-1.61974000	0.16872900
C	-2.49957800	-1.72082600	-1.07020200
C	-2.52627200	-1.23730300	1.33760400
C	-3.86968100	-1.45304000	-1.11326300
C	-3.89481300	-0.97656100	1.24451000
C	-4.58194200	-1.08130500	0.03101800
H	-4.38646000	-1.51294800	-2.06727700
H	-4.43119300	-0.66431100	2.13642100
C	-1.77617100	-1.05038100	2.63052900
H	-1.18602800	-1.93483300	2.89155300

H	-1.07788800	-0.21015000	2.54397600
H	-2.46381000	-0.83909700	3.45207500
C	-1.71973700	-2.03420400	-2.32015600
H	-1.01910200	-1.22037600	-2.53940100
H	-1.12809800	-2.94937100	-2.21563600
H	-2.38706700	-2.15113300	-3.17665300
C	-6.06262000	-0.80364300	-0.03967500
H	-6.35451000	-0.45747500	-1.03485300
H	-6.64432100	-1.70774500	0.17863900
H	-6.35800000	-0.04113700	0.68641900
C	2.50066000	0.15803800	2.46457000
H	1.61455800	0.77147900	2.26529700
H	2.14424400	-0.81777200	2.80928900
H	3.06565300	0.62612300	3.27369300
C	3.13561900	-1.60139700	-2.23636300
H	3.04330100	-2.66927800	-2.01055300
H	2.13933900	-1.24947700	-2.52448500
H	3.79913600	-1.49459800	-3.09713200
C	6.66115000	1.35961400	-0.14146700
H	7.46756000	0.74967000	0.28400900
H	6.92872000	1.57949400	-1.17856800
H	6.63900500	2.30255100	0.41226600

2A

O	-3.46787000	1.12143100	-0.68943700
C	-4.21138700	2.35865800	-0.80157400
C	-3.22670300	3.39685300	-0.16921800
O	-1.93598400	2.78740200	-0.42210400
B	-2.10397100	1.40813700	-0.59364400
C	-5.54038700	2.19554800	-0.07059400
H	-6.13661400	1.42286500	-0.56502600
H	-5.39010600	1.89328800	0.96709000
H	-6.11526400	3.12810200	-0.08272400
C	-4.46021700	2.59649400	-2.29550500
H	-4.97821100	1.72617700	-2.70767700
H	-5.07606400	3.48375300	-2.47391400
H	-3.51377800	2.71106200	-2.82993500
C	-3.24896700	4.78265600	-0.80536900
H	-4.23419800	5.24966200	-0.69666700
H	-2.51294700	5.42493100	-0.31303700
H	-2.99916700	4.73709200	-1.86643400
C	-3.37154600	3.51868100	1.35288800
H	-2.52443600	4.09039800	1.74172500
H	-4.29552100	4.03200800	1.63764500
H	-3.35856500	2.53379900	1.82652800
C	6.52562600	1.04749400	-1.43221700
C	5.28320500	0.86493200	-2.03932000
C	4.69734800	-0.40459200	-2.11414700

C	5.38894400	-1.48871300	-1.55790600
C	6.62857600	-1.31177300	-0.94273000
C	7.20218400	-0.04010100	-0.87722300
H	6.96635200	2.03916600	-1.39261200
H	4.75882100	1.71642200	-2.46553700
H	4.94944100	-2.48164800	-1.61271200
H	7.15110900	-2.16684400	-0.52314300
H	8.17091600	0.09979600	-0.40692200
C	3.32622700	-0.59152400	-2.71537900
H	3.14945300	0.14907100	-3.50299500
H	3.25443100	-1.57973900	-3.18545100
C	2.21845100	-0.46166500	-1.64179700
H	2.27917200	0.53742300	-1.19508500
H	2.44200800	-1.16643900	-0.83849000
C	0.83385800	-0.72011800	-2.17395600
C	0.00394100	0.26205100	-2.66598600
H	-0.88253900	0.01820000	-3.24183600
H	0.31963100	1.30136600	-2.69606300
H	0.56227400	-1.76186900	-2.33838200
C	-0.18330600	-1.02341100	0.99265400
C	-0.62021400	-2.39487600	2.76766100
C	0.49878500	-1.68930000	3.06881300
H	-1.16626800	-3.14081400	3.32203100
H	1.13060200	-1.69009600	3.94181300
N	0.75141500	-0.86055100	1.97577500
N	-1.01721100	-1.97556300	1.50086300
C	-2.19155500	-2.39945100	0.79281200
C	-3.39981600	-1.73686600	1.04423300
C	-2.07132800	-3.40739000	-0.17121400
C	-4.51357900	-2.11245200	0.29254300
C	-3.21399300	-3.75141600	-0.89760800
C	-4.43814900	-3.10915500	-0.68475300
H	-5.45514900	-1.59692700	0.46007500
H	-3.14396800	-4.53192500	-1.65104700
C	1.85620000	0.04883600	1.86826300
C	1.61131800	1.42853000	1.94906800
C	3.13990200	-0.47044300	1.64685600
C	2.69766300	2.28796700	1.76209400
C	4.19305400	0.42942500	1.46666700
C	3.98743300	1.81069600	1.51053100
H	2.52736500	3.36029400	1.81944800
H	5.18579600	0.04253800	1.25916800
Cu	-0.61747800	0.02560500	-0.63739200
C	3.38827900	-1.95706300	1.58191600
H	4.33526600	-2.15965900	1.07783200
H	3.43692000	-2.40336600	2.58238400
H	2.59002600	-2.47451700	1.04166000
C	0.23741100	1.98067600	2.22728300

H	-0.35776500	2.05640000	1.31121300
H	-0.31870600	1.34153500	2.91899200
H	0.31271300	2.98025500	2.66391100
C	5.12583500	2.77294200	1.27965000
H	5.08774200	3.60997600	1.98416500
H	6.09370800	2.27687500	1.38172800
H	5.08075100	3.19348300	0.26861500
C	-0.74516400	-4.07993400	-0.42010200
H	0.00365000	-3.35132000	-0.74659600
H	-0.35546200	-4.54930300	0.48992000
H	-0.83754400	-4.85064700	-1.18890400
C	-3.47198000	-0.63731500	2.06880900
H	-4.47901900	-0.21869000	2.11511800
H	-3.19829800	-0.99512100	3.06750300
H	-2.78045400	0.16525700	1.79865100
C	-5.64718400	-3.45764900	-1.51736800
H	-5.75790800	-2.75688800	-2.35360000
H	-5.56742100	-4.46348200	-1.93934400
H	-6.56723900	-3.40637300	-0.92727100

TS1A

O	-2.44971200	1.97799900	-0.57866500
C	-3.05763000	2.98818300	0.26982900
C	-2.34796800	2.72630900	1.64102600
O	-1.04918600	2.22661900	1.21871400
B	-1.21630700	1.65178700	-0.03624300
C	-4.56688600	2.77870100	0.26942700
H	-4.96329000	2.99023900	-0.72801100
H	-4.82078900	1.74866700	0.52037800
H	-5.05600100	3.45388300	0.97971900
C	-2.70403300	4.35067000	-0.33429400
H	-3.04683600	4.37619700	-1.37210500
H	-3.18157600	5.17209300	0.20839800
H	-1.62255300	4.51128200	-0.32876300
C	-2.13997800	3.95836400	2.51142700
H	-3.10063800	4.41247400	2.77693900
H	-1.63117700	3.67429900	3.43694300
H	-1.52767100	4.70581700	2.00474900
C	-3.01698600	1.60341100	2.43936700
H	-2.35799600	1.30768200	3.26022000
H	-3.97603700	1.91908300	2.86131600
H	-3.18147600	0.73504400	1.79951300
C	6.73785600	2.12577800	0.12266300
C	5.44680600	2.29979100	-0.37767600
C	4.95901500	1.50087700	-1.42000800
C	5.79979300	0.50156900	-1.93261800
C	7.08967800	0.31925700	-1.43451000
C	7.56742800	1.13632600	-0.40654400

H	7.09737400	2.76550400	0.92392000
H	4.80669100	3.07499700	0.03607700
H	5.43863100	-0.12977600	-2.74075100
H	7.72698900	-0.45409800	-1.85469400
H	8.57422900	1.00129500	-0.02245800
C	3.55831800	1.67382600	-1.94934200
H	3.17473800	2.66218100	-1.67060100
H	3.56568600	1.63611400	-3.04607100
C	2.57655200	0.58759100	-1.43079000
H	2.61305400	0.59761300	-0.33343000
H	2.97422700	-0.39135500	-1.72334800
C	1.15402600	0.74655200	-1.91487300
C	0.31766500	1.80209800	-1.28657300
H	-0.31054800	2.36661500	-1.97583700
H	0.83785200	2.45872900	-0.58412300
H	1.01919700	0.64040200	-2.99094600
C	-0.72846200	-1.71296100	0.07072000
C	-1.74894700	-3.66071500	0.67308900
C	-0.48395500	-3.69912600	1.16126900
H	-2.55169600	-4.37756400	0.72101000
H	0.04047500	-4.45228800	1.72634400
N	0.12165900	-2.50224800	0.78729800
N	-1.88954300	-2.43590300	0.01795700
C	-3.11511400	-1.88206200	-0.47595100
C	-4.13464000	-1.58455400	0.44389200
C	-3.23214800	-1.57570300	-1.83893100
C	-5.29138900	-0.96879400	-0.03708600
C	-4.40577400	-0.94783500	-2.26742500
C	-5.43971100	-0.63017000	-1.38593900
H	-6.08706600	-0.72949600	0.66430500
H	-4.50743100	-0.69750900	-3.32008700
C	1.45834500	-2.08480700	1.10242500
C	1.65307900	-1.19651600	2.16846400
C	2.50986100	-2.51383700	0.28115500
C	2.95987700	-0.77014800	2.42495900
C	3.79629500	-2.06453600	0.58016000
C	4.04139600	-1.19629700	1.64923600
H	3.13301900	-0.07856400	3.24546200
H	4.62221600	-2.36707900	-0.05770400
Cu	-0.23763600	-0.06052700	-0.68491600
C	2.23528500	-3.35318300	-0.93872100
H	3.16747400	-3.63822700	-1.43167600
H	1.68010100	-4.26569800	-0.69871300
H	1.62775400	-2.77868400	-1.64807900
C	0.49404900	-0.67128300	2.97915600
H	-0.02997100	0.12415200	2.43682700
H	-0.23773100	-1.45534200	3.19675200
H	0.84661300	-0.25726000	3.92730700

C	5.44306400	-0.73421800	1.95153500
H	5.96540200	-1.45882300	2.58911200
H	6.02542100	-0.61319300	1.03601600
H	5.44136100	0.22590900	2.47353600
C	-2.13401100	-1.89605400	-2.81959100
H	-1.29872900	-1.18977500	-2.73125600
H	-1.71614900	-2.89146400	-2.64180000
H	-2.51157200	-1.85299600	-3.84414200
C	-3.99025800	-1.88901100	1.91528400
H	-4.72967600	-1.32986300	2.49325300
H	-4.13831100	-2.95280500	2.13201700
H	-2.99547200	-1.62149500	2.28205200
C	-6.67314600	0.09465300	-1.86249400
H	-6.60034500	1.16641400	-1.64202100
H	-6.80771800	-0.01118900	-2.94228700
H	-7.57479000	-0.27854300	-1.36693500

3A

O	-1.88911700	3.21821200	-0.47876600
C	-3.21245500	3.30488900	0.09705500
C	-3.04881500	2.51292000	1.44628100
O	-1.64049400	2.67742400	1.73313800
B	-0.99537000	2.95003700	0.54088200
C	-4.21536200	2.69977100	-0.88059300
H	-4.25272400	3.30590600	-1.79032600
H	-3.93805800	1.68260700	-1.15939100
H	-5.21914000	2.68231900	-0.44167900
C	-3.50772500	4.79385800	0.30614400
H	-3.40310400	5.31133900	-0.65108800
H	-4.52174300	4.95970400	0.68225900
H	-2.79740500	5.23659400	1.00947900
C	-3.85634800	3.06073100	2.61798000
H	-4.92963800	3.01697000	2.40470300
H	-3.66216200	2.45784900	3.50968700
H	-3.58626200	4.09346900	2.84361000
C	-3.29759900	1.01222800	1.28893800
H	-2.96949500	0.50240900	2.19922700
H	-4.35340700	0.78612100	1.12402600
H	-2.72186300	0.60559400	0.45418100
C	6.99028900	2.08071500	-0.04872100
C	5.66209800	2.51079300	-0.10119000
C	4.76499900	1.98445600	-1.03984800
C	5.24029300	1.00106300	-1.92145100
C	6.56248900	0.56235400	-1.87036700
C	7.44630300	1.10247000	-0.93266800
H	7.66799300	2.51083000	0.68362600
H	5.31352600	3.27294900	0.59118400
H	4.56057000	0.58134800	-2.65898900

H	6.90800500	-0.19515700	-2.56896400
H	8.47836400	0.76660100	-0.89470000
C	3.32015600	2.41437500	-1.07721000
H	3.19383400	3.33478700	-0.49808600
H	3.02571600	2.64614300	-2.10948800
C	2.37056200	1.31805700	-0.53409400
H	2.68923400	1.06587800	0.48700000
H	2.55144700	0.41036300	-1.12368600
C	0.87383800	1.66911800	-0.54533200
C	0.54984300	2.88857500	0.36035900
H	0.95127800	3.83110600	-0.04791900
H	1.01263600	2.74643700	1.34643800
H	0.59495400	1.94288200	-1.57545700
C	-0.59283800	-1.86208600	0.08807700
C	-1.42008100	-3.98228900	-0.05228100
C	-0.11988900	-4.08048100	0.32641900
H	-2.16733700	-4.73523900	-0.24205000
H	0.49938200	-4.93615300	0.54146200
N	0.36298400	-2.77944800	0.40642000
N	-1.68999400	-2.62161400	-0.19050800
C	-2.95604200	-2.07744300	-0.59078500
C	-4.03120700	-2.14690800	0.30546800
C	-3.07216200	-1.47591200	-1.85327400
C	-5.25485400	-1.60539400	-0.09625700
C	-4.31242900	-0.93454300	-2.20114300
C	-5.41177200	-0.98629300	-1.33882000
H	-6.09634400	-1.64622000	0.59043600
H	-4.41963900	-0.45903800	-3.17252200
C	1.71482100	-2.39580500	0.71835100
C	2.02437900	-2.01974600	2.03051400
C	2.65442100	-2.34235000	-0.32047600
C	3.32990800	-1.59672600	2.29296300
C	3.94550200	-1.91494500	-0.00946700
C	4.29938100	-1.53116600	1.28796100
H	3.58958300	-1.29455100	3.30418000
H	4.68193700	-1.83549000	-0.80357200
Cu	-0.08601900	0.00957000	-0.12586100
C	2.25578900	-2.65580900	-1.73917300
H	3.12286400	-2.61816800	-2.40205600
H	1.79443900	-3.64443300	-1.83151900
H	1.52151700	-1.92305800	-2.09434400
C	0.96803500	-2.01629100	3.10490900
H	0.23742300	-1.22102000	2.91703400
H	0.41483500	-2.96052400	3.13755500
H	1.41355500	-1.84354000	4.08711300
C	5.67808400	-0.99744700	1.57523500
H	6.43766200	-1.50368100	0.97342800
H	5.73227800	0.06655300	1.32242700

H	5.93939000	-1.10929800	2.63142700
C	-1.90452700	-1.38531000	-2.80102600
H	-1.22022500	-0.58477300	-2.49481000
H	-1.32416800	-2.31246200	-2.81827900
H	-2.24907400	-1.17056800	-3.81533500
C	-3.86248400	-2.73701400	1.68280600
H	-4.73485700	-2.51888800	2.30257900
H	-3.73500400	-3.82462800	1.65597200
H	-2.97752700	-2.32296000	2.17613100
C	-6.72059800	-0.34516500	-1.72572200
H	-6.69081500	0.73451100	-1.53606700
H	-6.93412600	-0.48139900	-2.79004000
H	-7.55496600	-0.75887300	-1.15295100

TS2A

Cu	0.75897100	-0.61833900	-0.28272200
B	-3.45583300	-0.86241100	0.90191900
C	-1.05315500	-1.41075900	1.47359100
O	-4.23791600	0.02541400	0.19063800
O	-3.88891700	-2.15835300	0.76769500
C	1.69313000	1.03559400	-0.64301800
N	1.13977000	2.26916100	-0.79642200
N	3.00128100	1.21843400	-0.97893200
C	2.07779400	3.20299000	-1.22647800
C	3.25522900	2.53830900	-1.34247800
C	-5.11248000	-0.74768300	-0.67272100
C	-5.14388300	-2.14762000	0.04586400
H	1.81615500	4.23247800	-1.40862800
H	4.23427400	2.86786500	-1.64883100
C	0.25662600	-1.19808700	2.02348200
C	0.60857600	-0.05537000	2.80821700
C	1.90868600	0.15593900	3.23768000
C	2.94603700	-0.72914600	2.89501400
C	1.32999200	-2.10123300	1.70841800
C	2.63992100	-1.85129600	2.12755500
H	-0.17188000	0.64566300	3.08488800
H	3.42505600	-2.55185900	1.85541300
H	-1.33274600	-2.45551300	1.36077900
H	2.12650200	1.02075500	3.86129700
H	3.96067200	-0.55211900	3.23451000
H	1.09994000	-3.02631900	1.18641100
C	-4.44531000	-0.79226200	-2.05135600
H	-5.06722000	-1.31946900	-2.78058800
H	-4.29565500	0.23116300	-2.40523200
H	-3.47111700	-1.28179900	-2.00139400
C	-6.45827600	-0.03658300	-0.76331700
H	-6.32867300	0.93279300	-1.25309000
H	-7.16777800	-0.62312700	-1.35584500

H	-6.88930800	0.13860000	0.22384300
C	-5.16870800	-3.34880800	-0.89286500
H	-5.18740200	-4.27088000	-0.30552100
H	-6.06093700	-3.33079000	-1.52761900
H	-4.28051000	-3.37004500	-1.52518200
C	-6.25502800	-2.26204900	1.09362200
H	-7.24424700	-2.32471900	0.63080000
H	-6.08966400	-3.16692500	1.68376600
H	-6.24112000	-1.40685300	1.77483100
C	-2.20497300	-0.46804000	1.75675400
H	-2.49460900	-0.48466300	2.82731100
H	-1.93237400	0.57130000	1.54219500
C	-0.59782700	-1.83443800	-0.82930400
O	-1.42791000	-2.49362800	-1.31289800
C	3.99278300	0.18592400	-0.86206100
C	4.90381600	0.25715800	0.20223500
C	3.99708400	-0.86870700	-1.78435900
C	5.82649900	-0.78117100	0.33858300
C	4.93699900	-1.88688000	-1.60046800
C	5.84991600	-1.86660500	-0.54280400
H	6.53521400	-0.74674300	1.16187200
H	4.95441400	-2.71445100	-2.30492800
C	-0.22748200	2.56251800	-0.46473200
C	-1.23894700	2.23665600	-1.37935600
C	-0.49835500	3.14143500	0.78128100
C	-2.55573000	2.51206900	-1.01233800
C	-1.83472700	3.39944000	1.10086300
C	-2.87465500	3.08604800	0.22253400
H	-3.35579400	2.25700100	-1.69965500
H	-2.06672100	3.83909400	2.06723400
C	0.61104400	3.44149100	1.75622100
H	1.16823600	2.53024900	1.99397100
H	1.32613500	4.16727800	1.35427500
H	0.20599400	3.84644000	2.68643000
C	-0.91702300	1.58551000	-2.69968600
H	-0.11795000	2.11568800	-3.22802200
H	-0.57409100	0.55611800	-2.54995400
H	-1.79953300	1.55992100	-3.34286800
C	-4.31402900	3.30558200	0.60747100
H	-4.40151700	3.92834100	1.50181600
H	-4.87441800	3.78746400	-0.20084300
H	-4.78593300	2.33791400	0.80496000
C	3.02163800	-0.91877500	-2.93214300
H	2.02617800	-1.21965800	-2.58463600
H	2.91025400	0.06000900	-3.40844400
H	3.35261700	-1.63678600	-3.68621500
C	6.82309500	-3.00147400	-0.33998400
H	7.76070200	-2.65047900	0.10080500

H	6.40626700	-3.75594200	0.33813500
H	7.05508300	-3.50339700	-1.28354200
C	4.88163000	1.40865800	1.17460900
H	5.20517400	2.34451600	0.70579600
H	3.87438900	1.56435400	1.56897300
H	5.54807600	1.21076000	2.01692000

4A

Cu	0.81149000	-0.52720900	0.14002400
B	-3.63060300	-0.65103800	0.91265100
C	-1.44537300	-0.15129400	2.12078100
O	-4.37909700	-0.15775100	-0.17518900
O	-4.18042300	-1.85765700	1.37312900
C	2.09260500	0.31941500	-1.04468700
N	1.62702400	1.29151000	-1.87797100
N	3.39396300	0.17255800	-1.39741300
C	2.61982700	1.74241700	-2.73740200
C	3.74114700	1.03472100	-2.43524900
C	-5.18214700	-1.24466300	-0.67394100
C	-5.36723100	-2.13609600	0.61136900
H	2.43654200	2.50804300	-3.47351500
H	4.73598900	1.05827900	-2.84939200
C	-0.37893100	0.80780600	2.59645600
C	-0.50831500	2.19840200	2.51332000
C	0.55136700	3.04034100	2.85728300
C	1.77029400	2.50922400	3.28092600
C	0.85235800	0.28600700	3.03245800
C	1.91585300	1.12295700	3.37117000
H	-1.44329900	2.62824000	2.17487800
H	2.85325800	0.69246300	3.71229100
H	-1.48680100	-0.99222200	2.83168900
H	0.42325200	4.11709600	2.79011200
H	2.59263300	3.16638000	3.54856100
H	0.96712400	-0.79135800	3.11776000
C	-4.39533000	-1.95258100	-1.78596700
H	-4.97439100	-2.76707300	-2.23191400
H	-4.16870100	-1.22755500	-2.57384700
H	-3.45069600	-2.34520800	-1.40796800
C	-6.47373200	-0.66618600	-1.24578500
H	-6.24313900	-0.04589000	-2.11744500
H	-7.15247200	-1.46314100	-1.56787100
H	-6.98917100	-0.04158800	-0.51446200
C	-5.43955500	-3.63690300	0.34223800
H	-5.54873800	-4.17331000	1.28933800
H	-6.29929400	-3.88405800	-0.29025100
H	-4.53026900	-3.99354300	-0.14402700

C	-6.56282600	-1.69865500	1.46779200
H	-7.52024800	-1.94144700	0.99609800
H	-6.50986500	-2.21391100	2.43071400
H	-6.52811400	-0.62258700	1.65796100
C	-2.86572300	0.36747100	1.87276300
H	-3.40677400	0.51671700	2.81312800
H	-2.82123600	1.33445600	1.36107300
C	-0.98485300	-0.82474200	0.79693000
O	-1.93468600	-1.23232200	0.10204200
C	4.28462900	-0.73190200	-0.72632300
C	4.98883100	-0.26807100	0.39227100
C	4.38530000	-2.04953200	-1.18916300
C	5.83600400	-1.16869300	1.04278800
C	5.24456400	-2.91312000	-0.50562900
C	5.97533100	-2.49146700	0.61017500
H	6.39573800	-0.82914100	1.91040200
H	5.34041600	-3.93950100	-0.84999700
C	0.28178600	1.79872200	-1.75514900
C	-0.79216700	1.02628400	-2.22058200
C	0.09356800	2.99099200	-1.03914600
C	-2.08425800	1.47769300	-1.94092100
C	-1.21743000	3.40620800	-0.79996400
C	-2.31785800	2.65647500	-1.23016400
H	-2.92886300	0.86197600	-2.22918900
H	-1.38186200	4.32001200	-0.23491200
C	1.26543200	3.75436700	-0.47735700
H	1.79723500	3.15074300	0.26584500
H	1.98743100	4.03698700	-1.25029200
H	0.92592900	4.66616200	0.01831300
C	-0.60471100	-0.29791400	-2.91554800
H	0.39562200	-0.41185700	-3.33816700
H	-0.77634400	-1.10872300	-2.19849900
H	-1.33709000	-0.41277400	-3.71966200
C	-3.73170000	3.08177200	-0.92491700
H	-3.75939700	3.84063500	-0.13764100
H	-4.21378600	3.50844500	-1.81316100
H	-4.32051700	2.21606300	-0.60791100
C	3.56707900	-2.51833000	-2.36497700
H	2.49679000	-2.46904800	-2.13594000
H	3.73222600	-1.89319400	-3.24866300
H	3.81446400	-3.54990700	-2.62439100
C	6.87082600	-3.45326100	1.35129100
H	7.69786200	-2.93215800	1.84162300
H	6.31207700	-3.98632200	2.12994500
H	7.29151800	-4.20639600	0.67896900
C	4.80793700	1.14293000	0.89084700
H	4.96104400	1.87793500	0.09415600
H	3.79304900	1.29274600	1.27502900

H	5.51182200	1.36140200	1.69718400
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TS3A

Cu	1.10282400	-0.26563800	-0.78624600
B	-2.86964400	-0.25095900	-0.41337400
C	-1.03474500	1.57491000	-0.18469400
O	-2.86973900	-0.33954500	-1.78992000
O	-4.06589800	-0.73038800	0.12089200
C	2.26964700	-1.55938200	0.08913600
N	3.62743500	-1.54005000	0.19892000
N	1.88772400	-2.51628600	0.98205900
C	4.08423900	-2.45914600	1.13960300
C	2.98070100	-3.07778600	1.63471500
C	-4.03043700	-1.08104900	-2.19841500
C	-4.99533600	-0.89347400	-0.97496800
C	-1.94374600	2.72880100	-0.31312600
C	-3.23044200	2.74216200	0.28300800
C	-4.07739500	3.84902000	0.20081400
C	-3.68111200	5.00068700	-0.47844000
C	-1.56261500	3.91695500	-0.99186900
C	-2.41268800	5.01491300	-1.07123400
H	-3.57530600	1.87305000	0.83238600
H	-2.07985400	5.90182700	-1.60845500
H	-5.05472200	3.80596600	0.67933900
H	-4.33755700	5.86539200	-0.54202700
H	-0.59893600	3.92263000	-1.48240500
C	-3.58197900	-2.53568600	-2.39058300
H	-4.39048900	-3.17036200	-2.76858300
H	-2.75810200	-2.55156800	-3.10903100
H	-3.21269100	-2.95068100	-1.44928300
C	-4.54106700	-0.50392300	-3.51464600
H	-3.79456500	-0.66665000	-4.29709400
H	-5.47426300	-0.99053700	-3.82069200
H	-4.70998400	0.57056200	-3.43213600
C	-5.90469300	-2.08359800	-0.68681300
H	-6.51275300	-1.87666200	0.19913300
H	-6.58197500	-2.26536900	-1.52864900
H	-5.33013500	-2.99186400	-0.49894500
C	-5.81973100	0.39693300	-1.05428500
H	-6.58651900	0.34144000	-1.83378200
H	-6.31492800	0.55507800	-0.09173600
H	-5.17772100	1.26096600	-1.24176300
C	-1.67418500	0.30686700	0.41023400
H	-0.89827900	-0.47328900	0.40280300
H	-1.94148100	0.43693600	1.46604400
C	0.00835800	1.28742500	-1.22888800
O	0.32637000	2.10627100	-2.11068200
C	0.81153500	4.15099200	1.95168900

H	0.09411300	4.27805800	1.13619500
H	0.71551800	5.00743800	2.63326700
H	1.81851300	4.16045200	1.51994100
C	0.56978600	2.80472800	2.66777200
C	1.58979800	2.64749700	3.81364700
H	1.43776400	1.69069900	4.32539800
H	2.60970300	2.65936600	3.41588500
H	1.50171100	3.45193400	4.55647600
C	-0.85664700	2.78812600	3.26221300
H	-1.59971300	2.91383600	2.47027300
H	-1.03907900	1.82459500	3.75194300
H	-1.00593400	3.58593700	4.00243000
O	0.73950800	1.74281200	1.77244200
H	-0.11272500	1.79702900	0.80917200
H	2.86585000	-3.84483600	2.38338200
H	5.13166000	-2.57306400	1.36768400
C	0.50909500	-2.77481200	1.29923100
C	-0.06172600	-2.10660800	2.39395200
C	-0.22872600	-3.62523600	0.46734100
C	-1.41183700	-2.35199000	2.65956200
C	-1.57704400	-3.82980700	0.77146900
C	-2.18515100	-3.19663900	1.86026000
H	-1.88025900	-1.82831100	3.48865700
H	-2.16730400	-4.48423400	0.13483700
C	4.43744400	-0.58085000	-0.49710600
C	4.55356300	0.71131500	0.03760800
C	5.03847100	-0.95778800	-1.70368200
C	5.31999600	1.63213800	-0.68473100
C	5.79584400	-0.00293800	-2.38458900
C	5.93855100	1.29821300	-1.89189200
H	5.41992200	2.64195300	-0.29497100
H	6.26726600	-0.27561000	-3.32585700
C	0.70207700	-1.07893600	3.17920500
H	1.74077700	-1.37458700	3.35349600
H	0.71304900	-0.11215800	2.63627500
H	0.22519100	-0.90792000	4.14881900
C	0.39778100	-4.24043800	-0.75676700
H	1.35849700	-4.71444500	-0.53002500
H	-0.26474600	-4.98933800	-1.19856700
H	0.59127800	-3.46561800	-1.50791100
C	-3.65835800	-3.35930300	2.13375600
H	-4.06963600	-4.23040400	1.61390900
H	-3.85762300	-3.47404300	3.20463800
H	-4.19012800	-2.47009300	1.77995400
C	3.86558700	1.10327600	1.31513900
H	2.79134100	1.31678500	1.17807300
H	3.92868700	0.30966800	2.06626400
H	4.32590500	2.00399700	1.73086200

C	4.82918500	-2.34134600	-2.26465500
H	5.15129700	-3.12038900	-1.56488900
H	3.76638300	-2.51560200	-2.46541300
H	5.38203000	-2.46970000	-3.19870000
C	6.71307700	2.33529700	-2.66817100
H	6.03933000	2.93946000	-3.28754700
H	7.24205800	3.02223400	-1.99992200
H	7.44739100	1.87238100	-3.33466700

4A'

Cu	-0.17494400	-0.55521900	-0.23031400
B	2.16446000	2.05706300	-0.58324800
C	-0.14491800	2.39946800	-0.76201400
O	2.68177700	3.17750500	0.05769000
O	2.61313000	0.88612000	0.02494200
C	0.05758100	-2.46679100	0.06911000
N	1.12634300	-3.30295800	-0.09873600
N	-0.89875000	-3.27340700	0.61582000
C	0.83627500	-4.59935800	0.32618400
C	-0.44061900	-4.57590500	0.78270200
C	3.00574000	2.75412600	1.39741400
C	3.40568700	1.25229000	1.17100200
C	-0.48081300	3.79766200	-0.51524200
C	0.28045500	4.86981600	-1.05511900
C	-0.05515300	6.20331900	-0.83694800
C	-1.16579500	6.54914100	-0.06408100
C	-1.59908000	4.17890300	0.28115800
C	-1.92594200	5.51344700	0.49126600
H	1.16991400	4.65511100	-1.63407100
H	-2.79635800	5.75014100	1.10207600
H	0.56718400	6.98326900	-1.27431800
H	-1.42835000	7.59128400	0.10403700
H	-2.18726100	3.38489800	0.72022400
C	1.73500500	2.91502400	2.24337600
H	1.91748600	2.66912400	3.29521200
H	1.40026300	3.95257800	2.17251100
H	0.92261500	2.29292000	1.85955500
C	4.11838900	3.64677100	1.93736300
H	3.74423700	4.67003800	2.03239800
H	4.44534400	3.30890500	2.92735700
H	4.98177900	3.66264700	1.26877800
C	3.04470100	0.31526600	2.31969400
H	3.38128500	-0.69678000	2.08249500
H	3.52619000	0.62901700	3.25294000
H	1.96391000	0.28887100	2.46549000
C	4.87801900	1.07947700	0.78105000
H	5.54976000	1.27471900	1.62392900
H	5.02944600	0.05237300	0.44283700

H	5.13730100	1.75590800	-0.03819500
C	1.05885500	2.08724800	-1.67398200
H	0.92243400	1.09868800	-2.12323800
H	1.18179600	2.81760700	-2.47930700
C	-0.73288700	1.29598700	-0.11250300
O	-1.69491900	1.39326700	0.76892200
C	-3.67667400	2.33911900	-1.98630100
H	-2.61128700	2.41233300	-1.75528600
H	-3.79885200	2.40318400	-3.07533600
H	-4.18252800	3.19377900	-1.52684400
C	-4.25838400	1.02551600	-1.43935200
C	-5.74316400	0.90993400	-1.80507100
H	-6.15709200	-0.03110000	-1.42643400
H	-6.30356700	1.73650700	-1.35530600
H	-5.88786800	0.93922100	-2.89102200
C	-3.47898200	-0.17174200	-2.01381200
H	-2.42360700	-0.09936500	-1.73096300
H	-3.87924100	-1.10626400	-1.61060200
H	-3.54343200	-0.20170400	-3.10961400
O	-4.20866900	1.01308700	-0.02073400
H	-3.25654300	1.11978200	0.26712100
H	-1.05884600	-5.35037300	1.20571000
H	1.55300700	-5.40088000	0.25757100
C	-2.23217200	-2.81884500	0.90874800
C	-3.28712700	-3.32902000	0.13505700
C	-2.43650700	-1.83677900	1.89085500
C	-4.57372700	-2.84202800	0.37280500
C	-3.73901400	-1.36800800	2.06800000
C	-4.81333800	-1.84217000	1.31776900
H	-5.39479300	-3.20683200	-0.23971800
H	-3.90291000	-0.56200700	2.77708700
C	2.39711000	-2.86918300	-0.60033600
C	3.51495300	-2.94106200	0.24544200
C	2.48763300	-2.36618200	-1.90694500
C	4.74564300	-2.50983600	-0.25264500
C	3.73843600	-1.92750800	-2.34971200
C	4.87439300	-1.98678900	-1.54225100
H	5.61739300	-2.55452100	0.39590400
H	3.81887900	-1.51846800	-3.35351500
C	-1.32966200	-1.19265800	2.68261200
H	-0.40756800	-1.77672800	2.68275600
H	-1.14173900	-0.20456300	2.23536800
H	-1.64893300	-1.04116500	3.71937100
C	-3.04023100	-4.30847400	-0.98643300
H	-2.21150800	-3.97390100	-1.61937200
H	-2.78555500	-5.31340000	-0.62903000
H	-3.93112000	-4.39579200	-1.61322300
C	-6.16233300	-1.19074400	1.45454400

H	-6.93537400	-1.73151900	0.89991200
H	-6.47546400	-1.11825700	2.50226700
H	-6.07738500	-0.17609700	1.05031000
C	3.40028200	-3.42949700	1.66887000
H	3.30506000	-4.51951700	1.73165000
H	4.28666100	-3.14247800	2.24004200
H	2.52262600	-3.00090400	2.16104900
C	1.28647600	-2.26155500	-2.80699600
H	0.64545900	-3.14540500	-2.73464500
H	0.67099800	-1.39841700	-2.51857600
H	1.59645600	-2.13457200	-3.84754300
C	6.19647600	-1.44383200	-2.02304700
H	7.03812900	-2.01506600	-1.61820900
H	6.26361800	-1.46046600	-3.11476700
H	6.32178600	-0.40286700	-1.70100000

TS4A

H	0.83217000	-2.36893500	-1.59195200
C	2.09739500	1.29725600	-0.13209300
C	3.68442000	2.83916100	0.42127900
C	2.50465600	3.49906900	0.28628700
H	4.67473500	3.18542500	0.66915900
H	2.25414500	4.54241700	0.38815900
N	1.54996000	2.54211300	-0.04586300
N	3.41204300	1.49873700	0.16251400
C	4.34226600	0.41100000	0.26571200
C	4.45799000	-0.24991900	1.49476900
C	5.02400000	-0.00888800	-0.88231700
C	5.32626600	-1.34204800	1.56300100
C	5.87971600	-1.10527600	-0.76586100
C	6.03546200	-1.78665300	0.44431400
H	5.42182300	-1.87823900	2.50394400
H	6.40164600	-1.46030600	-1.65066500
C	0.14017800	2.79519400	-0.16760000
C	-0.57954600	3.04524200	1.01206900
C	-0.47531500	2.74330000	-1.42576900
C	-1.94727800	3.30591400	0.90154200
C	-1.84798900	3.01399300	-1.47876500
C	-2.59907500	3.28914400	-0.33299800
H	-2.52159900	3.48455900	1.80732000
H	-2.34547200	2.97465800	-2.44422700
Cu	1.23901200	-0.30378700	-0.74612200
C	2.83512200	-2.81673400	-1.17995600
H	2.75732700	-1.67658500	-1.13908800
H	3.59135200	-2.99455300	-1.98047600
H	3.32949300	-3.07747800	-0.21647000
O	1.62939400	-3.40033300	-1.38059900
O	-4.03675200	-2.13149600	-0.51382500

C	-5.39249800	-2.12242900	-0.03265900
C	-5.57934100	-0.63519600	0.44141200
O	-4.64075600	0.07119800	-0.39842000
B	-3.66548500	-0.83661800	-0.81494900
C	-5.52280400	-3.16928100	1.06956000
H	-5.35356500	-4.16421300	0.64819400
H	-4.78206700	-3.00757500	1.85371100
H	-6.52425800	-3.14945600	1.51425300
C	-6.28900300	-2.48985600	-1.22137100
H	-5.95512700	-3.44886800	-1.62586000
H	-7.34105600	-2.57838900	-0.93100400
H	-6.20433400	-1.74231700	-2.01467600
C	-6.97177700	-0.05338700	0.21273200
H	-7.72636900	-0.61160600	0.77778500
H	-6.99357800	0.98635400	0.55311000
H	-7.24357200	-0.06849300	-0.84428900
C	-5.14583600	-0.40856000	1.89457200
H	-5.11189700	0.66824800	2.08592300
H	-5.84767700	-0.86392100	2.60082900
H	-4.14540500	-0.80887200	2.07282200
C	-1.08867600	-1.05130200	-0.96666600
C	-2.34938600	-0.41311100	-1.52133100
H	-2.35176200	-0.70772700	-2.58267400
H	-2.30015400	0.68484100	-1.52266000
C	-0.07620500	-1.42885900	-1.91440100
O	-0.21215900	-1.20796300	-3.16122200
C	-0.85044200	-1.11144400	0.45983400
C	-1.55925400	-0.26892300	1.36873500
C	0.14347700	-1.96804700	1.04766800
C	-1.27183800	-0.24424400	2.73014900
H	-2.30511800	0.41361200	0.97843700
C	0.43187500	-1.90587300	2.40643600
H	0.65132700	-2.69594800	0.41594500
C	-0.25652800	-1.04035000	3.27302500
H	-1.83770400	0.42738900	3.37494100
H	1.19413500	-2.57356900	2.80541100
H	-0.03219000	-1.01556500	4.33613800
C	0.07860200	2.94930900	2.36493900
H	0.38553900	1.91493400	2.55706200
H	0.96650400	3.58340200	2.45230900
H	-0.62460100	3.23643100	3.15101400
C	0.25044700	2.33457400	-2.68110300
H	1.32627000	2.51156500	-2.61573600
H	0.09866400	1.26133600	-2.87379600
H	-0.14168300	2.88477000	-3.54274100
C	-4.09476200	3.45179500	-0.42284300
H	-4.49459800	3.97986700	0.44893500
H	-4.38694200	4.00388800	-1.32253500

H	-4.56313200	2.46122700	-0.46863800
C	6.89148100	-3.02613900	0.51770400
H	7.75560300	-2.95914600	-0.15090300
H	7.25570900	-3.20513600	1.53393900
H	6.30892300	-3.90442900	0.21468700
C	3.60873400	0.14952000	2.67349500
H	3.59391000	1.23374100	2.82198600
H	2.57152600	-0.17221300	2.51897300
H	3.97360400	-0.32115400	3.59033100
C	4.75305500	0.63624700	-2.21507600
H	3.74670700	0.35948500	-2.55241100
H	4.79042100	1.72880400	-2.16054600
H	5.47104600	0.29826100	-2.96627800

5A'

Cu	1.60518800	-0.03995700	1.04431700
B	-2.63710300	1.72942000	0.64576800
C	-1.79559000	-0.22610800	-0.46668100
O	-4.01911600	1.85510200	0.65809700
O	-2.03180300	2.88609600	0.17024100
C	2.13368500	-1.59567300	0.09593100
N	1.65735100	-2.87185100	0.07779700
N	3.25149800	-1.64862700	-0.68129000
C	2.47069100	-3.70320300	-0.68676200
C	3.47689400	-2.93107500	-1.17088500
C	-4.34204300	2.95694700	-0.21770700
C	-3.06149800	3.85744600	-0.09326900
H	2.25285300	-4.75038700	-0.81365200
H	4.31474900	-3.16300700	-1.80767000
C	-2.94318000	-0.97473500	-0.93732000
C	-4.06690500	-1.23117500	-0.10404300
C	-5.15110000	-1.98980200	-0.53764800
C	-5.18556400	-2.53030100	-1.82602800
C	-3.02284500	-1.49919100	-2.25933600
C	-4.10802300	-2.25843400	-2.67979600
H	-4.09588600	-0.81028600	0.89236400
H	-4.11788200	-2.64295500	-3.69894300
H	-5.98553700	-2.15479700	0.14267500
H	-6.03135400	-3.12510000	-2.16165400
H	-2.19423700	-1.29242200	-2.92444700
C	-5.63723100	3.60360300	0.25989600
H	-5.87621100	4.48907000	-0.33985300
H	-6.46008200	2.89003800	0.15762000
H	-5.57241500	3.89852300	1.30905300
C	-4.52192700	2.36038500	-1.61938800
H	-5.28310200	1.57797500	-1.57019400
H	-4.83160300	3.11568300	-2.34933900
H	-3.59648300	1.88880400	-1.95964900

C	-3.10712000	4.80391800	1.11194300
H	-2.10884800	5.22163800	1.26742200
H	-3.81334200	5.62707700	0.95992400
H	-3.38958600	4.25967300	2.01703400
C	-2.69089200	4.62581800	-1.35768300
H	-3.48720000	5.32414300	-1.63954100
H	-1.77622200	5.19973400	-1.18183800
H	-2.50633700	3.94442700	-2.18917700
C	-1.83863300	0.42815400	0.92437900
H	-2.27800700	-0.23566000	1.67648900
H	-0.83160400	0.68605800	1.26392300
C	-0.64290600	0.00198300	-1.23032400
O	-0.32044100	-0.43011400	-2.38498600
C	3.14348600	2.87400700	2.33761200
H	3.80135300	2.18944700	1.79108100
H	3.52075400	3.89701900	2.20156500
H	3.19416700	2.62119500	3.40258900
C	1.69385500	2.70389800	1.83252000
C	0.76112800	3.67772900	2.58191800
H	-0.25858000	3.54976700	2.20852700
H	0.76959700	3.44639000	3.65268900
H	1.05831700	4.72675200	2.44793500
C	1.64227500	3.03127500	0.32361100
H	2.28554300	2.33923800	-0.23318600
H	0.61729600	2.92266100	-0.04101000
H	1.98184700	4.05537600	0.11312100
O	1.24855300	1.40861600	2.09944900
H	0.09659600	0.65270100	-0.71755200
C	4.00563700	-0.46594900	-0.98638800
C	4.91467200	0.01691700	-0.03569000
C	3.73325500	0.20979000	-2.18575100
C	5.56761500	1.22074600	-0.30827300
C	4.41400600	1.41158900	-2.40988700
C	5.31700000	1.93665600	-1.48237000
H	6.26525500	1.61807300	0.42463800
H	4.21048100	1.96025100	-3.32607000
C	0.39470100	-3.24543000	0.65770600
C	0.24790700	-3.22047000	2.04890600
C	-0.67010200	-3.54738300	-0.20938200
C	-1.02117700	-3.49326100	2.57186900
C	-1.91364500	-3.81694400	0.36289800
C	-2.10985900	-3.77862100	1.74693800
H	-1.15935000	-3.46340900	3.65018600
H	-2.75890300	-4.00238700	-0.29263000
C	-0.50322000	-3.53092400	-1.70532300
H	-1.45254500	-3.77066400	-2.18560600
H	-0.21173300	-2.52955600	-2.05051900
H	0.24910100	-4.25131200	-2.04564700

C	1.39566500	-2.88497200	2.96845900
H	2.33684200	-3.32001900	2.61793400
H	1.54914400	-1.80094900	3.02640800
H	1.19629300	-3.25366900	3.97879500
C	-3.48426200	-4.02047300	2.31757600
H	-4.20380400	-3.33926700	1.85271800
H	-3.82876800	-5.04238800	2.11658500
H	-3.50274100	-3.86419700	3.40022500
C	5.12877900	-0.70456900	1.26946400
H	4.26191900	-0.55489800	1.92410300
H	5.24066000	-1.78353200	1.12406300
H	6.01636400	-0.32465100	1.78204200
C	2.71889100	-0.30941500	-3.16670800
H	2.90750900	-1.35792200	-3.42206900
H	1.68591400	-0.26482500	-2.77395700
H	2.75313300	0.27489500	-4.09045400
C	5.97244800	3.27517400	-1.71766100
H	6.97436900	3.31501400	-1.27846000
H	6.05654700	3.49873700	-2.78549500
H	5.38212700	4.07770900	-1.25901400

5A

Cu	0.48894300	0.17453100	-0.22141800
B	-2.13908500	0.21047300	1.32761300
C	-2.98989600	0.72555100	-0.84885500
O	-0.90637200	-0.43525100	1.20467100
O	-2.96186000	-0.47309100	2.18686500
C	2.37317800	0.41774500	-0.32974400
N	3.04002300	1.60473500	-0.35135300
N	3.31699500	-0.49597200	-0.69299800
C	4.37161800	1.43840200	-0.72330200
C	4.54762000	0.10906100	-0.94007100
C	-0.88815200	-1.59265600	2.09433800
C	-2.42385000	-1.81765300	2.32408500
C	-4.42916300	0.49656400	-1.05051300
C	-4.99314800	0.42576400	-2.34387700
C	-6.34932600	0.18053600	-2.53576900
C	-7.20627900	0.02427900	-1.44339400
C	-5.31482300	0.34952900	0.03899600
C	-6.67557700	0.11902300	-0.15657300
H	-4.35747000	0.59515300	-3.20678900
H	-7.32492000	0.00504500	0.70809000
H	-6.74495300	0.13494600	-3.54739100
H	-8.26692700	-0.15444300	-1.59378400
H	-4.92757900	0.38097000	1.05053600
C	-0.13263900	-1.16204400	3.35130700
H	-0.01609700	-1.99414100	4.05113100
H	0.86128200	-0.81078900	3.05939600

H	-0.64989000	-0.34463900	3.86025400
C	-0.16168800	-2.72919900	1.38916900
H	0.88792400	-2.46599700	1.24244000
H	-0.20228200	-3.64311500	1.99050300
H	-0.59385000	-2.93409100	0.40920100
C	-2.79052000	-2.35267800	3.70105500
H	-3.87610600	-2.45727700	3.77450600
H	-2.34153400	-3.33777200	3.86483000
H	-2.45959000	-1.67976300	4.49383500
C	-3.07416400	-2.65531700	1.21853500
H	-2.76497400	-3.70306300	1.26989600
H	-4.15947600	-2.60235500	1.33072100
H	-2.82531300	-2.25666600	0.23105600
C	-2.50902800	1.42132900	0.42780100
H	-1.63957600	2.04879000	0.19881700
H	-3.29719000	2.05228500	0.84566300
C	-2.07403700	0.26302600	-1.76054500
O	-0.77379800	0.38072100	-1.72401800
H	-2.46931800	-0.26902000	-2.63726000
H	5.41216700	-0.45533200	-1.24943900
H	5.05147300	2.27084600	-0.80471800
C	2.38316600	2.84836100	-0.05921900
C	2.52282200	3.38988300	1.22585000
C	1.57625800	3.43765100	-1.04352900
C	1.83998700	4.57274900	1.51434700
C	0.90911700	4.61885000	-0.70314700
C	1.02458500	5.19680000	0.56412200
H	1.93640700	5.00871300	2.50532200
H	0.27823500	5.09351100	-1.45014800
C	3.01182400	-1.89265300	-0.81317300
C	2.26134900	-2.33332100	-1.91281700
C	3.41282300	-2.75426000	0.21927200
C	1.92141900	-3.69060200	-1.95481400
C	3.05620000	-4.09998100	0.12522000
C	2.30833600	-4.58477600	-0.95412600
H	1.33529300	-4.05334200	-2.79515000
H	3.35119300	-4.78017300	0.92018400
C	3.35272000	2.68856100	2.27115400
H	2.97523200	1.67511300	2.44765100
H	4.39947900	2.58795100	1.96517700
H	3.32685400	3.23393200	3.21717400
C	1.38916000	2.81016300	-2.40033300
H	1.07336200	3.56321600	-3.12709000
H	2.31069800	2.34564700	-2.76268700
H	0.61718500	2.03017400	-2.35753600
C	0.25837200	6.45003500	0.90875500
H	-0.76632700	6.20799500	1.21507300
H	0.72858200	6.99298200	1.73339800

H	0.18916300	7.12404600	0.04988100
C	1.80115400	-1.39300200	-2.99795800
H	0.86972700	-0.88263000	-2.71663700
H	2.54519700	-0.61733100	-3.19925400
H	1.62038400	-1.94539600	-3.92394100
C	4.15280600	-2.22481500	1.42154000
H	4.31772600	-3.01739900	2.15480800
H	5.12752500	-1.80413100	1.15320200
H	3.58478000	-1.42147900	1.90399400
C	1.94774700	-6.04700000	-1.04314700
H	1.05257500	-6.20006900	-1.65191200
H	2.75960200	-6.62513800	-1.50113700
H	1.76468800	-6.47333200	-0.05233100

COM4-6a

P	0.05871400	-1.40518200	-1.48015300
C	-0.07579800	-3.22456700	-1.09681500
H	-0.78383600	-3.35310400	-0.27151800
H	-0.50959600	-3.71643800	-1.97283500
C	1.26119600	-3.90019000	-0.77138900
H	1.09691500	-4.98430400	-0.79063000
H	1.97924400	-3.68748700	-1.56950200
C	1.85569700	-3.55101500	0.59898400
H	2.63358200	-4.26959400	0.87841300
H	1.07922500	-3.62730000	1.36730500
P	2.56265000	-1.84563300	0.79094600
C	-1.55947000	-1.10289100	-2.31154900
C	-1.72156600	0.07974900	-3.05085300
C	-2.62855700	-2.00816900	-2.23222000
C	-2.92380900	0.34386300	-3.70214600
H	-0.90737400	0.79568100	-3.10736100
C	-3.83179200	-1.73719100	-2.88968200
H	-2.55307400	-2.91004900	-1.63944900
C	-3.98279400	-0.56451700	-3.62884500
H	-3.03056100	1.26277700	-4.27087700
H	-4.64850200	-2.45061500	-2.82521000
H	-4.91736300	-0.35915300	-4.14278400
C	1.21848200	-1.46626600	-2.90165700
C	0.91254300	-2.21116000	-4.05063100
C	2.45989400	-0.82903600	-2.80796100
C	1.84700200	-2.33484800	-5.07605000
H	-0.06014000	-2.68559600	-4.14482300
C	3.39933000	-0.96056000	-3.83122100
H	2.68092300	-0.22228800	-1.93968000
C	3.09594800	-1.71560200	-4.96268000
H	1.60321300	-2.91124600	-5.96377300
H	4.36269800	-0.47087700	-3.73545600
H	3.82488700	-1.81738600	-5.76151600

C	3.04084100	-1.90612000	2.55661100
C	2.01113300	-2.01790200	3.50398400
C	4.36242800	-1.78454600	2.99543300
C	2.30058900	-2.02181400	4.86549200
H	0.97634900	-2.06009400	3.17353500
C	4.64914700	-1.77443500	4.36124200
H	5.16547600	-1.68718900	2.27380600
C	3.62292800	-1.89475500	5.29754000
H	1.49448600	-2.10145400	5.58861700
H	5.67813200	-1.67006700	4.69207200
H	3.84958400	-1.88310700	6.35935600
C	4.14361100	-1.88178100	-0.12985800
C	4.62185000	-3.02287500	-0.78740200
C	4.86585200	-0.68142000	-0.23750000
C	5.78760600	-2.96218200	-1.55154600
H	4.08851100	-3.96350600	-0.72070400
C	6.03689000	-0.62822400	-0.98985900
H	4.50330700	0.21059500	0.26139300
C	6.49680000	-1.76621800	-1.65681200
H	6.13884500	-3.85171800	-2.06576400
H	6.58303200	0.30739900	-1.06294400
H	7.40198800	-1.72017900	-2.25479800
Pd	1.06746900	-0.09902900	0.30360600
C	2.18587200	1.17217400	2.87785800
C	2.18852800	1.17571900	1.47815600
C	3.07662800	2.05061400	0.82942000
C	3.91362700	2.90485800	1.55665400
C	3.89417500	2.89070900	2.95205700
C	3.02662300	2.01587000	3.60846900
H	1.51708900	0.51817900	3.41769800
H	4.57594400	3.58292300	1.02355900
H	4.54723600	3.54856000	3.51924300
H	3.00103900	1.98372900	4.69480800
I	1.01815000	2.55186900	-2.18459200
H	3.09968000	2.09542700	-0.25308600
Cu	-0.20920300	2.01998900	0.14381200
B	-3.30329900	-2.04502600	1.33095500
C	-2.28173700	0.34104700	1.76808600
C	0.54415900	4.48324200	2.27906500
O	-4.48966300	-1.78745200	1.96240500
O	-3.28736400	-3.27378600	0.70221900
C	-0.96619800	3.85855100	0.41029200
N	-0.51715800	4.76668200	1.31356000
N	-1.84097300	4.55001200	-0.36028500
C	-1.09161600	6.01153900	1.10199500
C	-1.93229300	5.87308700	0.04180100
C	-5.44437800	-2.78747200	1.51215200
C	-4.50463900	-3.97265900	1.08720700

C	-2.47830000	3.98820100	-1.54208900
H	-0.86637000	6.86490200	1.72145900
H	-2.58527600	6.58110000	-0.44293800
H	-1.83071400	4.12473700	-2.41175300
H	-3.44551700	4.46862400	-1.69633400
H	-2.63379800	2.92373200	-1.38062100
H	0.43509500	5.15307000	3.13463700
H	1.52456700	4.62837900	1.81932200
H	0.45938700	3.44940700	2.61116000
C	-3.33144600	1.14285900	1.02479400
C	-3.90033600	0.72887100	-0.18311300
C	-4.91997100	1.47072900	-0.78481300
C	-5.36934300	2.65283000	-0.19996600
C	-3.77538200	2.34748200	1.59136100
C	-4.78107000	3.09705300	0.98834200
H	-3.56566800	-0.18071900	-0.66222100
H	-5.11164900	4.02388100	1.44832500
H	-2.58809200	0.31175900	2.82012800
H	-5.35145300	1.11795800	-1.71598800
H	-6.16482500	3.22778900	-0.66550600
H	-3.32329600	2.68875000	2.51821500
C	-6.20247000	-2.16474200	0.33592200
H	-7.00566600	-2.81877400	-0.01611500
H	-6.63773900	-1.21687900	0.66056900
H	-5.53021700	-1.95074700	-0.49797600
C	-6.40000700	-3.10074200	2.65620600
H	-6.99169900	-2.21223200	2.89154700
H	-7.08834700	-3.90442200	2.37539300
H	-5.86269200	-3.39810900	3.55788700
C	-4.99262700	-4.78792400	-0.10383700
H	-4.26175500	-5.56552200	-0.34256900
H	-5.94536300	-5.27583200	0.12501100
H	-5.12615400	-4.16305300	-0.98813700
C	-4.13463300	-4.89449200	2.25177100
H	-4.98403600	-5.50728400	2.56603100
H	-3.32628000	-5.55911100	1.93566200
H	-3.78483100	-4.31796100	3.11226800
C	-2.06972300	-1.08785700	1.28185700
H	-1.70460700	-1.06568700	0.25524400
H	-1.24524700	-1.53614200	1.85362300
C	-0.92313300	1.11363400	1.80656100
O	-0.57324100	1.52522800	2.89550400

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P	0.30553000	-0.20288100	1.80925500
C	0.25795500	1.36516100	2.83723200
H	-0.46903100	2.04429300	2.38169200
H	-0.13873200	1.09612200	3.82052300

C	1.61294600	2.05907200	3.02250700
H	1.48128400	2.83970900	3.78214900
H	2.33216500	1.34771000	3.43689500
C	2.18598600	2.73634100	1.77389400
H	3.03232800	3.37854500	2.03939300
H	1.42487300	3.39537300	1.34482900
P	2.71901500	1.64881200	0.36203300
C	-1.12809400	-1.08649900	2.56108600
C	-1.02779900	-2.45016600	2.87466800
C	-2.30072800	-0.39170800	2.89623000
C	-2.07058300	-3.09645100	3.53768200
H	-0.13665400	-3.00309900	2.59947100
C	-3.35038100	-1.04986900	3.53955700
H	-2.40145600	0.66123700	2.65673100
C	-3.23433700	-2.40093600	3.87232200
H	-1.97351700	-4.14935600	3.78513600
H	-4.25105500	-0.49822300	3.79360500
H	-4.04468000	-2.90798300	4.38778200
C	1.69817100	-1.09111600	2.61661700
C	1.75531900	-1.19548500	4.01753300
C	2.71927600	-1.65702100	1.85091700
C	2.82505900	-1.83650300	4.63447100
H	0.95578300	-0.78458000	4.62641500
C	3.78520200	-2.31322500	2.46951500
H	2.66801900	-1.60538700	0.77251000
C	3.84469800	-2.39652700	3.85721400
H	2.86135300	-1.90745900	5.71762600
H	4.56641000	-2.75002900	1.85833800
H	4.67768900	-2.90151900	4.33751700
C	3.24015200	2.96149000	-0.81459900
C	2.31001600	3.95033100	-1.17119600
C	4.50188900	2.97437300	-1.41854800
C	2.63462000	4.92898900	-2.10718000
H	1.31418700	3.94191700	-0.74162600
C	4.82225900	3.94904900	-2.36366200
H	5.23476200	2.21902300	-1.16283500
C	3.89292600	4.92811400	-2.71193000
H	1.90027500	5.68358200	-2.37330900
H	5.80289900	3.93822400	-2.82970700
H	4.14481100	5.68370700	-3.44977700
C	4.29867200	0.88920000	0.87756300
C	4.91238500	1.14705200	2.10890900
C	4.88979300	-0.03293300	-0.00352600
C	6.09218800	0.49004500	2.45893700
H	4.47385100	1.85033800	2.80734200
C	6.07980400	-0.66896000	0.34060000
H	4.41053500	-0.25575100	-0.95196000
C	6.68060100	-0.41458400	1.57582500

H	6.55082000	0.68761400	3.42311000
H	6.52858600	-1.37564800	-0.35087300
H	7.59969700	-0.92349800	1.85019000
Pd	0.91632900	0.27339800	-0.54860700
C	1.98878300	1.40487800	-3.21563300
C	1.92414200	0.33189800	-2.32521700
C	2.62970500	-0.84129700	-2.61910800
C	3.42597300	-0.91436800	-3.76770300
C	3.51210400	0.17280800	-4.63894200
C	2.78198000	1.32980400	-4.36308300
H	1.42662800	2.31168700	-3.02447500
H	3.96981600	-1.83140400	-3.98068800
H	4.13122100	0.11387200	-5.52977800
H	2.82689600	2.17946200	-5.03956000
I	0.99054100	-3.77654600	-0.41503900
H	2.54771300	-1.70973500	-1.97138500
Cu	-0.72753600	-1.97241700	-1.15033800
B	-2.47281800	3.11361100	0.20995000
C	-1.73055100	1.50011700	-1.70664000
C	-2.67194400	-2.06419700	-4.12302600
O	-3.39029200	4.02505800	-0.23663200
O	-2.69097200	2.73325600	1.51756900
C	-2.52935500	-2.68299800	-1.70516700
N	-3.17008600	-2.69710700	-2.90791200
N	-3.33767100	-3.43264500	-0.90662900
C	-4.35374700	-3.41687600	-2.84984300
C	-4.46154200	-3.88183200	-1.57910100
C	-4.46992000	4.08560100	0.73657100
C	-3.78542300	3.53188000	2.04569600
C	-3.04253700	-3.70196400	0.48980000
H	-4.99460600	-3.54161600	-3.70774000
H	-5.21513800	-4.49130400	-1.10690900
H	-1.96518100	-3.82772900	0.59958000
H	-3.54871000	-4.61979500	0.79661600
H	-3.37586200	-2.87736700	1.12042500
H	-2.88495700	-0.99518200	-4.11087600
H	-3.15214800	-2.53693600	-4.98215700
H	-1.59354700	-2.19389600	-4.18140700
C	-3.06397500	0.84170600	-1.43821200
C	-3.29113400	0.15617900	-0.23947000
C	-4.51112300	-0.47009600	0.00835600
C	-5.51701600	-0.45087900	-0.95843900
C	-4.07946100	0.85388900	-2.40198800
C	-5.29473100	0.21009700	-2.16817000
H	-2.50531400	0.10785900	0.49836700
H	-6.07141600	0.23189300	-2.92715500
H	-1.80271200	2.00238300	-2.67549900
H	-4.66438200	-0.98110400	0.95365900

H	-6.46410500	-0.94842200	-0.77364800
H	-3.91457700	1.37979000	-3.33801800
C	-5.58934700	3.18725400	0.20460400
H	-6.47406200	3.22993400	0.84663100
H	-5.86985200	3.53266100	-0.79327000
H	-5.26582100	2.14967100	0.11771300
C	-4.95279300	5.52851400	0.83088900
H	-5.38586000	5.82983300	-0.12645000
H	-5.72580600	5.62801400	1.59961800
H	-4.13668000	6.21424000	1.06342400
C	-4.67013700	2.62363700	2.89326500
H	-4.11255100	2.27997300	3.76951900
H	-5.55610800	3.16085500	3.24537900
H	-4.99126300	1.74893500	2.32582800
C	-3.14646800	4.61932500	2.91216900
H	-3.90053400	5.24111700	3.40249000
H	-2.53697000	4.14264400	3.68470900
H	-2.49602800	5.26547600	2.31680800
C	-1.29120300	2.53023900	-0.63517100
H	-0.57567200	2.05106300	0.04143800
H	-0.74745300	3.33664500	-1.13903100
C	-0.69159300	0.33520900	-1.96498300
O	-0.76889500	-0.20218900	-3.05397600

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P	0.53246600	-0.30785700	2.18337500
C	0.53032600	0.67059200	3.76365900
H	-0.43454700	1.18491800	3.83270800
H	0.58629500	-0.03018300	4.60292900
C	1.67372200	1.69567400	3.86578900
H	1.74973500	1.99953700	4.91603600
H	2.62634000	1.21482900	3.61950800
C	1.48385600	2.97174500	3.02667300
H	2.14709500	3.76656300	3.38209200
H	0.46050600	3.33761500	3.15998500
P	1.72236900	2.73362200	1.20440800
C	-0.67381800	-1.64501100	2.52744600
C	-0.54440700	-2.84877500	1.81897600
C	-1.74060200	-1.49512600	3.42398800
C	-1.44632900	-3.89031400	2.02129400
H	0.25961700	-2.96556400	1.10256800
C	-2.64807500	-2.53863900	3.62158900
H	-1.87424200	-0.56897900	3.97243700
C	-2.49747500	-3.74042500	2.92908000
H	-1.32560200	-4.81385800	1.46499700
H	-3.47088300	-2.40869300	4.31786000
H	-3.20160300	-4.55156300	3.08850300
C	2.13704800	-1.18350400	2.27502800

C	2.49609200	-1.96493800	3.38597200
C	3.04516700	-1.02393000	1.22455200
C	3.75989700	-2.54685200	3.44988400
H	1.78735500	-2.12110700	4.19441400
C	4.31219300	-1.60722600	1.28816800
H	2.76464600	-0.45243600	0.34914500
C	4.67311400	-2.35926100	2.40391900
H	4.03685300	-3.14456000	4.31356100
H	4.99021100	-1.47306800	0.45242700
H	5.65946300	-2.81050400	2.46095000
C	1.46805100	4.40364400	0.50041400
C	0.52687600	5.28785300	1.04392100
C	2.09795700	4.73776400	-0.70687400
C	0.22875700	6.48753400	0.39707300
H	0.01076200	5.04661100	1.96732300
C	1.79186900	5.93120700	-1.35382600
H	2.80728600	4.05340800	-1.15639100
C	0.85773000	6.81065100	-0.80444000
H	-0.50057900	7.16503600	0.83150700
H	2.27338300	6.16525500	-2.29779000
H	0.61582100	7.73831000	-1.31417600
C	3.51054200	2.41497800	0.99753400
C	4.46595000	2.70612000	1.98119800
C	3.92560700	1.82198600	-0.20445800
C	5.80987100	2.40155700	1.76754900
H	4.17139200	3.16733000	2.91774500
C	5.27165400	1.53338600	-0.42249800
H	3.19757100	1.55693000	-0.96430900
C	6.21491500	1.81764400	0.56551000
H	6.54049300	2.62186500	2.54040500
H	5.56264300	1.05663900	-1.35243700
H	7.26196100	1.57927000	0.40359300
Pd	0.31450400	1.04847600	0.25554100
C	-0.83864200	3.25143100	-1.50360800
C	0.04649100	2.16475200	-1.46512200
C	0.82846400	1.90517200	-2.59850700
C	0.75934800	2.73627900	-3.72148600
C	-0.11388700	3.82496500	-3.74080700
C	-0.92119300	4.07440100	-2.62953000
H	-1.46056000	3.48421200	-0.64349300
H	1.38433700	2.52043200	-4.58463600
H	-0.17026600	4.46862200	-4.61464100
H	-1.60723000	4.91773200	-2.63097300
I	3.47108700	-1.20802200	-2.59863300
H	1.49232700	1.04566300	-2.62038600
Cu	1.38605300	-2.25479400	-1.56900600
B	-4.38305600	1.15843000	0.50228600
C	-2.42846300	0.10802600	-0.70821700

C	-1.41111700	-4.19936400	-2.06677600
O	-4.93061500	1.88055000	-0.52932900
O	-5.32268700	0.68016400	1.38238100
C	0.84425200	-4.06991600	-1.01686800
N	-0.30279300	-4.74922400	-1.29102100
N	1.59488500	-4.96433700	-0.31365700
C	-0.26735800	-6.03633400	-0.77643300
C	0.93257300	-6.17022300	-0.14962400
C	-6.34597800	2.04247700	-0.24880400
C	-6.62339200	0.86539600	0.75543100
C	2.90243700	-4.64056500	0.24262500
H	-1.07929500	-6.73385500	-0.90788600
H	1.36298300	-7.00140000	0.38594600
H	3.55081400	-5.51798800	0.18730700
H	2.81245700	-4.31606000	1.28260100
H	3.33097800	-3.83016300	-0.34774200
H	-1.34077100	-3.11317300	-2.04962000
H	-2.35792400	-4.49543100	-1.61415400
H	-1.36743900	-4.56104900	-3.09824800
C	-3.28583500	-1.10410800	-0.99771000
C	-3.61022200	-2.01239400	0.01788000
C	-4.41221100	-3.12161800	-0.24482300
C	-4.90529600	-3.34467300	-1.53225200
C	-3.77213100	-1.34456400	-2.28853500
C	-4.57670900	-2.45350900	-2.55659400
H	-3.24699800	-1.84780800	1.02372500
H	-4.95260400	-2.61677700	-3.56254300
H	-2.54109700	0.82068600	-1.53599600
H	-4.65603200	-3.80646900	0.56240500
H	-5.54062500	-4.20182700	-1.73617800
H	-3.52424000	-0.64829100	-3.08450200
C	-7.11111900	1.95803700	-1.56418100
H	-8.19119900	1.98814400	-1.38771700
H	-6.84544600	2.80798700	-2.19863800
H	-6.86864200	1.04288200	-2.10616000
C	-6.51486400	3.42774100	0.38117100
H	-6.10353600	4.17713900	-0.29982900
H	-7.56745000	3.66346300	0.56286200
H	-5.97336400	3.49569200	1.32870100
C	-6.96280000	-0.45336200	0.05434700
H	-6.91556900	-1.26356800	0.78576100
H	-7.96861700	-0.42945700	-0.37516500
H	-6.24610900	-0.68063600	-0.73724400
C	-7.64804200	1.17017800	1.84097300
H	-8.62648400	1.38633400	1.39985200
H	-7.75609700	0.30147900	2.49627300
H	-7.34508000	2.02103200	2.45332700
C	-2.85077000	0.84567500	0.58240400

H	-2.62618800	0.23805600	1.46280300
H	-2.25234300	1.76028700	0.66127900
C	-0.91742500	-0.20373200	-0.75000900
O	-0.52750200	-1.16069900	-1.41514000

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P	0.69232700	-2.15168700	0.66726600
C	1.42159200	-2.54156600	2.32857100
H	0.77147100	-2.04673800	3.05865300
H	1.32512100	-3.61636100	2.51448100
C	2.88009600	-2.09294200	2.53453300
H	3.24999700	-2.58933800	3.43913100
H	3.50745600	-2.45623400	1.71327200
C	3.09386200	-0.57928600	2.71383400
H	4.08167400	-0.40217500	3.15210800
H	2.34912700	-0.17663700	3.40981200
P	2.96288800	0.38100100	1.12685500
C	-1.00106800	-2.83255400	0.83596900
C	-1.45612100	-3.92350800	0.08540900
C	-1.89014000	-2.17972900	1.70365900
C	-2.77801100	-4.35542200	0.20697000
H	-0.78225600	-4.42675400	-0.59899500
C	-3.20649700	-2.61629100	1.82889200
H	-1.55999700	-1.30867300	2.26303300
C	-3.65295100	-3.70678900	1.07902700
H	-3.12368800	-5.19819300	-0.38406600
H	-3.88730800	-2.08273000	2.48198800
H	-4.68127700	-4.04390600	1.16794300
C	1.54194400	-3.27409200	-0.50369800
C	2.34700100	-4.34556100	-0.09662900
C	1.41851000	-2.98885700	-1.87549200
C	3.03325200	-5.11196500	-1.03957300
H	2.45351900	-4.58616700	0.95531000
C	2.09338200	-3.76889700	-2.81345800
H	0.80807400	-2.15086600	-2.20374900
C	2.90841600	-4.82493600	-2.39879800
H	3.66469800	-5.93179500	-0.71048100
H	1.98901700	-3.54198100	-3.87022000
H	3.44353200	-5.42155900	-3.13164900
C	3.54046900	2.05568200	1.57265600
C	3.65782200	2.49921700	2.89677400
C	3.81574300	2.94963800	0.52432500
C	4.05324500	3.81036700	3.16897800
H	3.44444000	1.83062000	3.72399000
C	4.21278600	4.25445600	0.80076500
H	3.69710200	2.63114500	-0.50538700
C	4.33266600	4.68896300	2.12258300
H	4.14290400	4.14191600	4.19936700

H	4.40780200	4.93607900	-0.02091000
H	4.63636300	5.70960400	2.33568700
C	4.37516500	-0.30280000	0.17780700
C	5.69524100	-0.19846200	0.64080900
C	4.11686300	-0.99351800	-1.01138400
C	6.73490100	-0.79650700	-0.06762300
H	5.90724900	0.36087800	1.54776800
C	5.15734200	-1.59965700	-1.71670600
H	3.09821500	-1.05488800	-1.37441800
C	6.46561800	-1.50383800	-1.24383600
H	7.75550500	-0.71140000	0.29396000
H	4.93816300	-2.14768800	-2.62753200
H	7.27811500	-1.97307900	-1.79091300
Pd	0.90269400	0.07530100	-0.07872200
C	-0.73544400	-0.09993000	-1.27260700
O	-0.68320800	-0.56431500	-2.39892200
C	1.03743900	1.93310600	-0.97443300
C	1.53653500	2.03178000	-2.28064500
C	0.74204100	3.12147100	-0.29282000
C	1.76098200	3.27639700	-2.87785300
H	1.73655000	1.12689100	-2.84968800
C	0.94134700	4.36663500	-0.89121000
H	0.34241000	3.08420600	0.71601600
C	1.46245500	4.45052600	-2.18357800
H	2.15736800	3.32826600	-3.88957600
H	0.68982600	5.27259200	-0.34565000
H	1.62376400	5.41929500	-2.64897600
B	-4.59771000	-0.23518800	-0.46502600
C	-2.08142700	0.32973100	-0.66417700
O	-4.67525700	0.09584900	0.87252800
O	-5.83493800	-0.32361800	-1.05611700
C	-6.04844600	0.47976800	1.14620300
C	-6.83044600	-0.25213400	-0.00308000
C	-2.29019100	1.81676600	-0.88512000
C	-2.11615900	2.38819900	-2.15144100
C	-2.30099700	3.75525400	-2.34220200
C	-2.67437600	4.57116400	-1.27226800
C	-2.66437100	2.64074100	0.18117200
C	-2.86058600	4.00881700	-0.00950600
H	-1.79929300	1.76016200	-2.97727700
H	-3.15016900	4.63543800	0.82976600
H	-2.00256900	0.16973100	0.41386400
H	-2.13642500	4.18761700	-3.32448100
H	-2.81203000	5.63818900	-1.42143300
H	-2.80984900	2.19785100	1.16145400
C	-6.11551200	2.00611400	1.04128100
H	-7.11717400	2.37983800	1.27265600
H	-5.40972400	2.44321100	1.75154400

H	-5.83110400	2.34579200	0.04270200
C	-6.40721000	0.03058200	2.55786200
H	-5.78573400	0.56543000	3.28150400
H	-7.45559700	0.25285000	2.78145800
H	-6.24353500	-1.03986000	2.69394400
C	-8.04771600	0.49572900	-0.53320700
H	-8.51126200	-0.08091500	-1.33823600
H	-8.79186700	0.63684200	0.25750900
H	-7.77091300	1.47221900	-0.93291200
C	-7.20162200	-1.69687200	0.34702500
H	-7.99785300	-1.74157500	1.09553000
H	-7.54699000	-2.20144000	-0.55881100
H	-6.33166600	-2.24011100	0.72525200
C	-3.25185200	-0.51210900	-1.21028800
H	-3.36377200	-0.34675100	-2.28546700
H	-3.00722000	-1.57708600	-1.09506600

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P	-1.11618200	-1.39477700	1.43472600
C	-0.39868500	-2.53273800	2.72142000
H	-0.14270600	-1.88172900	3.56552600
H	-1.18304400	-3.20608100	3.08490300
C	0.83540700	-3.34550600	2.29405400
H	1.00556100	-4.10867200	3.06286900
H	0.63068000	-3.89185800	1.36744400
C	2.14101400	-2.54731500	2.13891300
H	2.99484100	-3.23214900	2.17593200
H	2.25048900	-1.84703800	2.97426400
P	2.24208200	-1.56651900	0.56271000
C	-2.57785000	-0.77087700	2.35941300
C	-3.64847200	-1.60122500	2.71952100
C	-2.60033500	0.57635200	2.73726100
C	-4.71716600	-1.09391700	3.45685800
H	-3.65432200	-2.64093200	2.40557800
C	-3.66665000	1.08383700	3.48149900
H	-1.78665400	1.22745900	2.43521200
C	-4.72613200	0.24977800	3.84151900
H	-5.54530100	-1.74272000	3.72671800
H	-3.67273600	2.13038700	3.77112700
H	-5.55977400	0.64539100	4.41392500
C	-1.84273200	-2.53965900	0.19382000
C	-1.99423600	-3.91866700	0.38488100
C	-2.19285300	-1.98660600	-1.04951800
C	-2.47467200	-4.73075000	-0.64481000
H	-1.72914200	-4.37501100	1.33230100
C	-2.68105200	-2.79589900	-2.07275900
H	-2.07674100	-0.91943900	-1.20325800
C	-2.81698700	-4.17259100	-1.87544300

H	-2.57538800	-5.80004600	-0.48411800
H	-2.94039900	-2.35515800	-3.03068600
H	-3.18301500	-4.80547200	-2.67826500
C	3.99462100	-1.05896100	0.49011300
C	4.78340600	-0.90763600	1.63803800
C	4.51753800	-0.67085000	-0.75429400
C	6.07364100	-0.38411300	1.54311400
H	4.39734000	-1.18871900	2.61226400
C	5.80345200	-0.14879700	-0.84459600
H	3.90193600	-0.75271300	-1.64434700
C	6.58488000	-0.00161600	0.30391400
H	6.67580900	-0.27171200	2.44009100
H	6.18725600	0.16620900	-1.80938600
H	7.58417600	0.41689200	0.23241600
C	2.12634300	-2.87933200	-0.71221600
C	2.97868900	-3.99379800	-0.70402100
C	1.12563600	-2.78514700	-1.68649900
C	2.81251700	-5.01027500	-1.64179800
H	3.77585900	-4.06081700	0.03099500
C	0.95822700	-3.80590100	-2.62319700
H	0.49435400	-1.90507000	-1.71069400
C	1.79608000	-4.92000100	-2.59808500
H	3.47360600	-5.87197200	-1.62960000
H	0.16984600	-3.72728500	-3.36468700
H	1.66530400	-5.71634700	-3.32508100
Pd	0.51375800	-0.03315600	0.29792400
C	1.41781800	1.10751000	-1.16714900
O	1.24041400	0.63876300	-2.29577700
C	2.65268400	1.89537900	-0.86157200
C	3.08549000	2.12745500	0.44725300
C	3.39708500	2.40783200	-1.93132200
C	4.24235200	2.86091900	0.68639100
H	2.50768900	1.71994000	1.26928000
C	4.55305800	3.14703400	-1.69427700
H	3.04914400	2.20910100	-2.93964300
C	4.97818400	3.37512500	-0.38376600
H	4.57241800	3.03213900	1.70632500
H	5.12437900	3.54500500	-2.52851800
H	5.88017400	3.95070700	-0.19595200
B	-2.61170400	1.91112900	-1.63799700
C	-0.29920100	2.12200500	-0.49240400
O	-3.16440100	1.21615400	-0.58116000
O	-3.55714400	2.31115900	-2.55294700
C	-4.61011700	1.34802700	-0.67956900
C	-4.80548200	1.65536200	-2.20621500
C	0.26190200	3.36859100	0.07583300
C	0.77069600	4.41047500	-0.71769100
C	1.35160700	5.53697500	-0.14048100

C	1.43838300	5.66044100	1.24730200
C	0.35282400	3.51365100	1.47178300
C	0.93042300	4.63856400	2.05238500
H	0.74235400	4.32176000	-1.79864900
H	0.98795400	4.71745900	3.13488200
H	-0.92881500	1.66899500	0.28292100
H	1.75085600	6.31904400	-0.78035300
H	1.89661200	6.53758700	1.69414500
H	-0.00972600	2.70612900	2.10448000
C	-5.00393100	2.51963400	0.22374200
H	-6.08891400	2.65513600	0.25476000
H	-4.65122600	2.31269200	1.23585200
H	-4.54458600	3.45129100	-0.11763700
C	-5.26151900	0.06004000	-0.19279500
H	-5.09129300	-0.05925500	0.87826500
H	-6.34253400	0.09115600	-0.36577900
H	-4.85010500	-0.81449500	-0.69853000
C	-5.95940500	2.59528300	-2.53280800
H	-6.00370400	2.76123200	-3.61267500
H	-6.91316200	2.16153100	-2.21502800
H	-5.83523700	3.56375900	-2.04670200
C	-4.89148300	0.38933100	-3.06426400
H	-5.84109900	-0.13367600	-2.92028100
H	-4.80235100	0.66876200	-4.11710900
H	-4.07878400	-0.29965800	-2.82322600
C	-1.07901600	2.15559600	-1.79946100
H	-0.91560000	3.09228900	-2.34302300
H	-0.68194700	1.37820700	-2.47432600

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Cu	1.97842400	-0.89773900	-1.52727200
B	-0.61403000	2.59955900	-0.18282200
C	-2.28532900	1.23072800	-1.52938700
C	3.29041300	1.97025700	-2.27405100
O	0.70916400	2.22354600	-0.11483300
O	-1.10163300	3.00966500	1.04012100
C	3.65840000	-0.16548700	-1.03177700
N	4.05655100	1.08378800	-1.39600200
N	4.63584000	-0.59966400	-0.18997100
C	5.25418400	1.42392800	-0.78874700
C	5.62208400	0.36112300	-0.02456600
C	1.19322600	2.55528300	1.21601500
C	-0.13445900	2.61249300	2.04695300
C	4.61092800	-1.88740100	0.48694900
H	3.73877300	-2.43729500	0.13401100
H	4.53276500	-1.74643400	1.56887600
H	5.51720300	-2.45504600	0.25988800

H	2.37069700	1.46724700	-2.58165400
H	3.89339500	2.22875000	-3.14842300
H	3.01566000	2.87562200	-1.72981300
C	-3.68092300	1.20896900	-1.02179300
C	-4.66603300	0.45991800	-1.68629700
C	-5.96244300	0.37261000	-1.18466500
C	-6.30380500	1.03353900	-0.00255000
C	-4.04342200	1.89516800	0.14945600
C	-5.33895300	1.79712000	0.65735800
H	-4.40348100	-0.05076500	-2.60688700
H	-5.59560600	2.32085200	1.57415000
H	-6.70944400	-0.20710000	-1.71990400
H	-7.31359600	0.96557200	0.39151000
H	-3.29956600	2.47924700	0.67958500
C	1.88844800	3.91553900	1.10867900
H	2.33613800	4.21460700	2.06079800
H	2.68490400	3.85012200	0.36285900
H	1.18715100	4.69236500	0.79292500
C	2.18146400	1.48784600	1.67169300
H	3.10799100	1.56755100	1.09936600
H	2.42634400	1.62359600	2.73050800
H	1.77612600	0.48589900	1.52701300
C	-0.15422800	3.63280900	3.17706000
H	-1.12657300	3.60708900	3.67643600
H	0.61511200	3.40133100	3.92078600
H	0.00886900	4.64610000	2.80664700
C	-0.57269600	1.23519900	2.54847800
H	0.06755000	0.87110400	3.35626000
H	-1.59866500	1.30412300	2.92011000
H	-0.55121100	0.50642200	1.73597400
C	-1.51369000	2.54301200	-1.47080000
H	-0.87851700	2.60264300	-2.35516300
H	-2.22027300	3.37889700	-1.46123700
C	-1.73777000	0.07307300	-1.95505700
O	0.18366100	-1.24422800	-1.96350600
H	-2.30681900	-0.84541900	-1.87474100
H	6.48390300	0.20547900	0.60455100
H	5.73504600	2.37479500	-0.95427900
C	-0.31136000	-0.10050500	-2.34303700
O	0.33797800	0.79519800	-2.91523800
C	-1.57238900	-3.32475500	-0.41776200
C	-2.86273100	-3.34508800	-0.95005700
C	-3.87662500	-2.57127800	-0.38365800
C	-3.60507500	-1.77074900	0.72534000
C	-2.32623500	-1.75742900	1.28521700
C	-1.32620700	-2.53589700	0.70318200
H	-0.77693700	-3.89595700	-0.87814800
H	-3.06462200	-3.95713700	-1.82394000

H	-4.87112800	-2.57060400	-0.81631300
H	-4.38028000	-1.13771700	1.14433000
H	-2.11744800	-1.14514400	2.15327900
I	0.62233300	-2.52729500	1.54928400

TS23

Cu	2.07887900	-0.63324300	-0.65353100
B	-1.40592700	2.60184200	-0.34057400
C	-2.81771100	0.73045900	-1.27324600
C	2.51959200	2.20129700	-2.42990000
O	-0.08966900	2.98761500	-0.42744400
O	-1.87746900	2.61253900	0.95091300
C	3.53138600	0.63537300	-0.76536100
N	3.58229700	1.76274200	-1.52662200
N	4.68794500	0.66952300	-0.04331900
C	4.73592000	2.48631800	-1.27907000
C	5.43739500	1.79533300	-0.34192300
C	0.31610300	3.45042200	0.89289100
C	-0.72153600	2.73346600	1.82418700
C	5.08331500	-0.34281700	0.92704000
H	4.31972700	-1.12034100	0.94150000
H	5.16651500	0.10124400	1.92286100
H	6.04383000	-0.78131300	0.64378700
H	1.81115300	1.38545000	-2.56709600
H	2.95834600	2.49321300	-3.38711500
H	1.97556000	3.04005600	-1.99061900
C	-4.22882500	0.58219200	-0.84135000
C	-4.96855100	-0.56174300	-1.18810600
C	-6.28370700	-0.71925200	-0.76030000
C	-6.88903400	0.26236400	0.02733200
C	-4.85101800	1.56539800	-0.05423300
C	-6.16556400	1.40206100	0.38001100
H	-4.50883800	-1.32113900	-1.81158800
H	-6.62424100	2.16719400	0.99972800
H	-6.84015800	-1.60628100	-1.04891700
H	-7.91565700	0.14073700	0.35987400
H	-4.28808400	2.43812700	0.25623400
C	0.17113700	4.97409800	0.88806700
H	0.52582900	5.41529000	1.82382600
H	0.76397200	5.38394600	0.06607000
H	-0.87054100	5.26944800	0.73654700
C	1.76523400	3.04913900	1.13636200
H	2.42808900	3.60302300	0.46600100
H	2.05800100	3.28194100	2.16537700
H	1.91786100	1.98486100	0.95664100
C	-1.12373400	3.51371700	3.06810600
H	-1.86068700	2.94131900	3.63778900
H	-0.25583000	3.68708900	3.71232800

H	-1.56764400	4.47683300	2.81123000
C	-0.30603000	1.30501400	2.18896100
H	0.51870700	1.29275300	2.90684500
H	-1.16462700	0.79827600	2.63628100
H	-0.00641500	0.74129400	1.30173000
C	-2.29054700	2.12690700	-1.55359000
H	-1.67939700	2.11145300	-2.45579500
H	-3.12793900	2.81411900	-1.70990100
C	-2.03225700	-0.36936300	-1.29788600
O	0.18509500	-1.13600700	-0.84317800
H	-2.44089500	-1.31419000	-0.97208800
H	6.38997400	1.99674700	0.12165000
H	4.95747100	3.41040800	-1.78878700
C	-0.58453900	-0.33424100	-1.58496400
O	-0.06894500	0.41822300	-2.41090500
C	-1.04209800	-3.53985500	-0.77147200
C	-2.33694700	-4.03166200	-0.58100600
C	-3.11787500	-3.60400000	0.49588400
C	-2.58719800	-2.68503700	1.40449300
C	-1.29541400	-2.17887300	1.24249600
C	-0.55712600	-2.62938100	0.15695800
H	-0.43524300	-3.85113500	-1.61221700
H	-2.73281600	-4.74935100	-1.29421100
H	-4.12701800	-3.98000600	0.62509400
H	-3.18131800	-2.34170200	2.24641800
H	-0.87938900	-1.46302800	1.93719800
I	1.88995900	-3.02038300	0.78095900

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Cu	1.61162500	-1.74622700	0.64677500
B	0.13329800	2.74293500	-0.98239800
C	-2.12232800	1.52889400	-0.96072700
C	2.07418500	-2.26241900	-2.73533400
O	1.35425700	2.92936900	-1.57113500
O	0.13559200	2.96874900	0.36879700
C	3.09791200	-1.53708000	-0.58084400
N	3.16532600	-1.73710600	-1.92205000
N	4.31132400	-1.00353000	-0.26229300
C	4.38412300	-1.32395500	-2.43443800
C	5.11249200	-0.86204900	-1.38487300
C	2.25794600	3.43560900	-0.55179500
C	1.52595900	3.04465900	0.78838000
C	4.72173300	-0.65307100	1.09022800
H	3.87830000	-0.82735400	1.75844500
H	5.00608700	0.40113000	1.13476100
H	5.56611800	-1.27293400	1.40361400
H	1.34085200	-2.72281100	-2.07757800
H	2.47054000	-3.00272400	-3.43453400

H	1.58176500	-1.44887400	-3.26911600
C	-3.29740300	2.18657900	-0.34760400
C	-4.53922300	1.53301100	-0.28298200
C	-5.63687300	2.15260900	0.30962000
C	-5.51141700	3.43230000	0.85310300
C	-3.18482600	3.47877100	0.19251800
C	-4.28117700	4.08983600	0.79609200
H	-4.64477000	0.54635500	-0.72322300
H	-4.17359700	5.08058000	1.22755600
H	-6.59250500	1.63795700	0.34206300
H	-6.36691900	3.91432000	1.31660800
H	-2.22267400	3.97859300	0.18197800
C	2.36331300	4.94698400	-0.76921000
H	3.07614800	5.40611900	-0.07833900
H	2.70028100	5.13556300	-1.79187600
H	1.39174100	5.43091800	-0.63828600
C	3.61558200	2.76978500	-0.75268200
H	4.04281700	3.08716900	-1.70793800
H	4.31061500	3.05677200	0.04371000
H	3.51924200	1.68369500	-0.76914000
C	1.63753200	4.06923900	1.91059500
H	1.08051800	3.71449200	2.78153200
H	2.68252400	4.20528600	2.20738500
H	1.22883400	5.03727300	1.61609100
C	1.89664500	1.65264900	1.29857300
H	2.90757900	1.63789600	1.71555500
H	1.19493700	1.35118600	2.07869100
H	1.82914500	0.91243300	0.49849900
C	-1.18127500	2.38069000	-1.77492200
H	-0.86430900	1.85028900	-2.67639600
H	-1.69371500	3.29583300	-2.09080700
C	-1.93974000	0.20174900	-0.75819000
O	-0.89548300	-1.89573600	-1.37434200
H	-2.64439200	-0.35327900	-0.15308900
H	6.11115600	-0.45847400	-1.33765800
H	4.62227400	-1.39465500	-3.48365200
C	-0.78289600	-0.52756700	-1.26523800
O	0.29136500	-0.03818900	-1.57584000
C	-3.09777400	-2.30799900	-2.27124500
C	-4.32332800	-2.96734000	-2.17620300
C	-4.57646000	-3.82861000	-1.10599100
C	-3.60034800	-4.02941500	-0.12789200
C	-2.37208300	-3.37141900	-0.20648300
C	-2.14089400	-2.51550000	-1.27842700
H	-2.87948300	-1.63893300	-3.09687100
H	-5.07716900	-2.81063200	-2.94174600
H	-5.53094200	-4.34085900	-1.03570500
H	-3.79482600	-4.69326800	0.70869100

H	-1.60863900	-3.47928000	0.55573100
I	0.00245600	-1.82687900	2.51994200

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P	-0.00862500	-1.07819800	1.73812000
C	0.23340600	-2.86619300	2.18391000
H	0.98039300	-3.27793300	1.49665000
H	0.66229000	-2.92396800	3.18912300
C	-1.05703600	-3.69663100	2.14661400
H	-0.82762900	-4.68311800	2.56725600
H	-1.79170000	-3.24227200	2.81663100
C	-1.67113700	-3.93026400	0.75910800
H	-2.44016100	-4.70855600	0.81395200
H	-0.90220400	-4.30663200	0.07535800
P	-2.41108400	-2.47491700	-0.13073800
C	1.47001900	-0.27709500	2.48152400
C	1.41779900	1.11102800	2.68379700
C	2.63561200	-0.97651500	2.82163900
C	2.50710400	1.78601600	3.22618100
H	0.52758000	1.65557500	2.40312200
C	3.72762600	-0.29247800	3.36392900
H	2.72498300	-2.03993500	2.63854900
C	3.66656400	1.08557700	3.57110700
H	2.44115100	2.85858000	3.37764500
H	4.62488000	-0.84406400	3.62886800
H	4.51622500	1.61060400	3.99781100
C	-1.33085200	-0.54915300	2.89370800
C	-1.32516400	-0.93447800	4.24368300
C	-2.36115100	0.26839800	2.41952800
C	-2.35212700	-0.52786500	5.09180500
H	-0.51572700	-1.54433900	4.63463400
C	-3.37719700	0.69431200	3.27431400
H	-2.35290400	0.59966800	1.39055600
C	-3.38105700	0.28585500	4.60595600
H	-2.34600400	-0.83525600	6.13358900
H	-4.14701500	1.35118600	2.88682100
H	-4.17505700	0.60936700	5.27267300
C	-2.90270200	-3.28985400	-1.69254100
C	-1.87786800	-3.70716300	-2.55603500
C	-4.23588800	-3.47454400	-2.07079300
C	-2.18337000	-4.31434000	-3.77097500
H	-0.84011800	-3.52037000	-2.29138500
C	-4.53929800	-4.07036200	-3.29620100
H	-5.03498200	-3.14490200	-1.41627000
C	-3.51736000	-4.49308500	-4.14564400
H	-1.38264200	-4.62736900	-4.43415400
H	-5.57749500	-4.20212100	-3.58583300

H	-3.75708900	-4.95374900	-5.09917000
C	-3.96735600	-2.08534700	0.73679300
C	-4.40775400	-2.78379800	1.86832400
C	-4.70875900	-0.98224700	0.28158600
C	-5.55594300	-2.37360800	2.54610800
H	-3.86106800	-3.64395200	2.23556400
C	-5.86358000	-0.58740500	0.95110200
H	-4.36876800	-0.42539100	-0.58382400
C	-6.28453500	-1.27518700	2.09135000
H	-5.87820500	-2.91386700	3.43106400
H	-6.42209400	0.27093700	0.59093000
H	-7.17463900	-0.95437300	2.62398400
Pd	-0.90096200	-0.70470200	-0.48939400
C	-2.19451500	-0.49753700	-3.29153000
C	-2.08521300	0.03054100	-2.00111600
C	-2.88115300	1.13751300	-1.66530300
C	-3.74577400	1.71472100	-2.60389300
C	-3.85009900	1.17394400	-3.88566200
C	-3.07278300	0.06260100	-4.22280200
H	-1.58803100	-1.34220900	-3.58665400
H	-4.33307600	2.58275800	-2.31680000
H	-4.52929200	1.60999300	-4.61315800
H	-3.14674600	-0.37296700	-5.21623200
H	-2.84528300	1.57122000	-0.67359300
Cu	0.15288700	1.46346600	-1.11940800
B	3.76393700	-2.30241500	-0.36898300
C	2.39014300	-0.58191200	-1.79050900
C	-0.45649400	2.61484300	-4.23967600
O	4.92320000	-2.11674900	-1.07156500
O	3.93553300	-3.08081200	0.75621700
C	0.73087500	3.09478900	-2.10911300
N	0.42998900	3.41107400	-3.39490800
N	1.45344600	4.15013100	-1.66143200
C	0.94681900	4.64969800	-3.74134300
C	1.59723100	5.11587000	-2.64238700
C	6.01460900	-2.56917200	-0.22397100
C	5.29529800	-3.60092200	0.71696800
C	1.89245400	4.31501900	-0.28363300
H	0.80925400	5.07976400	-4.72050600
H	2.13998700	6.03234300	-2.47523800
H	1.77362500	3.36393100	0.22958300
H	1.26867300	5.06076100	0.20944100
H	2.94383800	4.60437400	-0.26390600
H	-0.35833000	1.56351800	-3.97613700
H	-0.17508300	2.75472900	-5.28593500
H	-1.49469500	2.92051500	-4.09246400
C	3.25565700	0.61279300	-1.44933800
C	3.64892000	0.92543000	-0.14512100

C	4.49304100	2.01033900	0.10326300
C	4.93627500	2.81241600	-0.94658500
C	3.68931500	1.44041100	-2.49538400
C	4.51817500	2.53096200	-2.25079500
H	3.31773800	0.31796800	0.68560400
H	4.84632900	3.15573900	-3.07636300
H	2.76907800	-0.99246100	-2.73256700
H	4.79468600	2.22238300	1.12390700
H	5.59830900	3.65189100	-0.75350300
H	3.37215300	1.21619300	-3.50998600
C	6.52807600	-1.33121200	0.51846000
H	7.41175100	-1.56215400	1.12050900
H	6.79208400	-0.56592100	-0.21499800
H	5.75713000	-0.91044400	1.16842200
C	7.10925600	-3.15461200	-1.10646600
H	7.53238400	-2.36630400	-1.73448100
H	7.91538300	-3.57285800	-0.49504400
H	6.72278100	-3.93771200	-1.76054000
C	5.83631500	-3.65865100	2.13972000
H	5.25861400	-4.37842600	2.72632400
H	6.88252500	-3.98024700	2.14162400
H	5.77113400	-2.68749800	2.63182500
C	5.21107200	-5.00739600	0.11882400
H	6.18605600	-5.50249400	0.11431700
H	4.52155600	-5.60717400	0.71876700
H	4.83211700	-4.97462600	-0.90605000
C	2.37144000	-1.70015500	-0.75112700
H	1.90651900	-1.33767900	0.16467700
H	1.70906400	-2.50350200	-1.10269400
C	0.93820900	-0.12746600	-2.15865400
O	0.60372300	-0.30334000	-3.31431500
S	-1.55317200	3.49316100	0.83574200
O	-1.22226700	4.61583000	-0.05408500
O	-2.97772100	3.16162700	1.01011700
C	-0.99926200	4.05780900	2.51946000
F	-1.62113200	5.18694600	2.87027200
F	0.33366600	4.29121700	2.52253300
F	-1.24933300	3.12130200	3.44643300
O	-0.67686800	2.27442100	0.66403700

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P	0.11103200	-0.59432100	1.95869500
C	0.52883700	-2.24496300	2.71447000
H	1.28398500	-2.71830400	2.07716300
H	0.99912200	-2.06609300	3.68537200
C	-0.67491600	-3.18073800	2.90290900
H	-0.36841300	-3.97808900	3.59007200
H	-1.48826300	-2.64419300	3.40058800

C	-1.18664400	-3.85301900	1.62436000
H	-1.88281100	-4.66151900	1.86947400
H	-0.34266800	-4.31401200	1.10063800
P	-1.99071700	-2.72951000	0.38962400
C	1.53611700	0.43461500	2.51473600
C	1.36079000	1.82589900	2.56875000
C	2.76217100	-0.11309700	2.91304600
C	2.38705000	2.64734300	3.02789200
H	0.41382300	2.26300000	2.26894900
C	3.79253700	0.71571200	3.36381200
H	2.94858700	-1.17722600	2.84502600
C	3.60646800	2.09542400	3.42940600
H	2.23334500	3.72119600	3.07613100
H	4.74005900	0.27413500	3.65722600
H	4.40391600	2.73873900	3.78914900
C	-1.17542000	0.03967700	3.10153200
C	-1.06321300	-0.12541600	4.49276500
C	-2.25359800	0.75436100	2.57940900
C	-2.03537300	0.40178300	5.33742800
H	-0.21422600	-0.65191700	4.91819500
C	-3.22081400	1.29712700	3.42858100
H	-2.33112500	0.89873500	1.51185200
C	-3.11648100	1.11420900	4.80495200
H	-1.94788300	0.26601400	6.41154900
H	-4.04207600	1.85390000	2.99086400
H	-3.86975200	1.52846400	5.46883600
C	-2.61094100	-3.91410900	-0.86247200
C	-1.87853400	-5.05831100	-1.20578200
C	-3.77904700	-3.61294300	-1.57603700
C	-2.30781800	-5.88682000	-2.24201200
H	-0.96150800	-5.30662500	-0.68210800
C	-4.19832500	-4.43598600	-2.61713000
H	-4.34671200	-2.72298500	-1.33254000
C	-3.46546000	-5.57509200	-2.95372000
H	-1.73135500	-6.77137100	-2.49647400
H	-5.09519500	-4.18014000	-3.17225900
H	-3.79267400	-6.21334400	-3.76883200
C	-3.51202800	-2.10420100	1.17835100
C	-4.13610000	-2.76163400	2.24734100
C	-4.07738600	-0.92730000	0.66770600
C	-5.30459500	-2.24069900	2.80072800
H	-3.71738100	-3.67711800	2.65209800
C	-5.25637500	-0.41855500	1.21028100
H	-3.57811200	-0.38601300	-0.12685800
C	-5.86651900	-1.07268000	2.28048600
H	-5.77553200	-2.74719000	3.63806300
H	-5.65091200	0.51451800	0.82435900
H	-6.77347600	-0.66693100	2.71875200

Pd	-0.57607600	-0.97413900	-0.38726300
C	-0.96682200	-2.41035900	-3.01525700
C	-1.39755400	-1.34394500	-2.22061700
C	-2.42580600	-0.52011800	-2.68650100
C	-3.01947700	-0.77003300	-3.92942900
C	-2.58929500	-1.83692200	-4.71726300
C	-1.55579300	-2.65551000	-4.25612500
H	-0.17326000	-3.06697200	-2.66975400
H	-3.82054300	-0.12156600	-4.27606100
H	-3.05318300	-2.03089000	-5.68029400
H	-1.21221700	-3.49237900	-4.85844900
H	-2.75944600	0.32815500	-2.09984800
Cu	-0.18158900	1.50432100	-0.88079000
B	4.09010200	-1.89155400	-0.15490600
C	2.47245800	-0.41699100	-1.55642000
C	-0.98983300	2.82740800	-3.72992100
O	5.03144500	-2.12898400	-1.12030900
O	4.57471900	-2.06435100	1.12264900
C	0.36314600	3.22931400	-1.67880400
N	-0.05184200	3.60486500	-2.91632800
N	1.13637700	4.26040600	-1.25790100
C	0.44480000	4.85149200	-3.25628000
C	1.19883700	5.26934300	-2.20433200
C	6.32316100	-2.22215100	-0.45740300
C	5.91867800	-2.60890000	1.01453300
C	1.71096900	4.32655600	0.07334400
H	0.22786100	5.31957800	-4.20288000
H	1.77046000	6.17059000	-2.05279600
H	2.00498400	3.32463100	0.37510800
H	0.97613400	4.72400500	0.77901700
H	2.59806600	4.96063300	0.05834500
H	-0.72981900	1.77147100	-3.65692100
H	-0.89981400	3.15030200	-4.76898000
H	-2.00625100	2.99391900	-3.36732800
C	3.26249500	0.86901600	-1.36223600
C	3.87606100	1.20504300	-0.15136300
C	4.62829900	2.37710600	-0.02953100
C	4.75747700	3.24532300	-1.11114300
C	3.38676500	1.75959500	-2.44070900
C	4.12179000	2.93451200	-2.31749000
H	3.78578900	0.55451000	0.70685500
H	4.19979500	3.60959900	-3.16464600
H	2.82767700	-0.86825400	-2.48974500
H	5.09737200	2.60792700	0.92203100
H	5.34286100	4.15578900	-1.01835700
H	2.88395900	1.52385600	-3.37248300
C	6.96927200	-0.83810600	-0.56644200
H	7.97720400	-0.83217500	-0.14183800

H	7.03468400	-0.56414300	-1.62223800
H	6.36714500	-0.07639800	-0.06660000
C	7.16878600	-3.25987900	-1.18527200
H	7.37395100	-2.91417900	-2.20171900
H	8.12668600	-3.40497800	-0.67542300
H	6.65765000	-4.22139100	-1.25191200
C	6.77762100	-1.97774300	2.10384000
H	6.40565600	-2.28074800	3.08685000
H	7.81802300	-2.30681300	2.01913000
H	6.75010500	-0.88838000	2.04897600
C	5.79811300	-4.11881300	1.23454400
H	6.77652000	-4.60709900	1.22961200
H	5.32670000	-4.29951300	2.20431400
H	5.17624600	-4.57968800	0.46240200
C	2.61512200	-1.44871900	-0.43839300
H	2.18854600	-1.06001100	0.48437600
H	2.00753400	-2.32564100	-0.70270100
C	0.99401800	-0.03443100	-1.88365400
O	0.76066800	0.22881000	-3.05021200
S	-3.22570500	2.87199300	-0.33422900
O	-3.47628900	3.48211000	-1.64736100
O	-4.38599000	2.59541800	0.52951300
C	-2.28251200	4.18354800	0.61674600
F	-3.13112000	4.99551800	1.25191200
F	-1.52012400	4.92841600	-0.19963500
F	-1.46864100	3.62411500	1.54083200
O	-2.25979700	1.71604000	-0.37134800

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P	-0.10973500	0.42978100	1.95467400
C	-0.47798700	2.02630900	2.85238100
H	-1.22663200	2.57128500	2.26721300
H	-0.94563000	1.76518600	3.80558300
C	0.74105300	2.92017600	3.11627900
H	0.45397800	3.64983000	3.88265700
H	1.55219200	2.32692000	3.54826100
C	1.23881500	3.70526100	1.90007500
H	1.95140300	4.47853300	2.20332900
H	0.39055300	4.22424600	1.44185300
P	1.99751300	2.68842800	0.54993500
C	-1.53624900	-0.59448200	2.51843300
C	-1.36636300	-1.98363400	2.61171000
C	-2.76518400	-0.03379800	2.89184900
C	-2.40170900	-2.79127100	3.07636000
H	-0.41654200	-2.42963700	2.33534400
C	-3.80366100	-0.84759400	3.34974300
H	-2.94721000	1.02978800	2.80272100
C	-3.62428200	-2.22658700	3.44822300

H	-2.25175800	-3.86419000	3.15185600
H	-4.75226400	-0.39510400	3.62160300
H	-4.42860000	-2.85854800	3.81272700
C	1.21586900	-0.28638400	2.99597000
C	1.10770600	-0.29438100	4.39789500
C	2.33295100	-0.86146800	2.39004600
C	2.11966600	-0.85369300	5.17142000
H	0.23046300	0.12337200	4.88285600
C	3.34224900	-1.43678800	3.16638400
H	2.41156500	-0.87495500	1.31290700
C	3.23907200	-1.42576100	4.55464200
H	2.03452400	-0.85280400	6.25423600
H	4.19045600	-1.88752600	2.66373900
H	4.02364300	-1.86720600	5.16230700
C	2.57721200	3.98436200	-0.61174800
C	1.86938900	5.18210000	-0.77982000
C	3.69310500	3.73527600	-1.42241900
C	2.27137400	6.11327800	-1.73715800
H	0.99417600	5.39701300	-0.17687500
C	4.08389600	4.66097200	-2.38535100
H	4.24521000	2.80964900	-1.31560600
C	3.37653900	5.85323200	-2.54581400
H	1.71438400	7.03838700	-1.85317500
H	4.93939200	4.44450400	-3.01718800
H	3.68256100	6.57246700	-3.29940600
C	3.55280200	2.02224900	1.23517100
C	4.17043500	2.55885400	2.37294900
C	4.15048300	0.94044800	0.57224600
C	5.36544800	2.01533200	2.84162100
H	3.72758600	3.39742600	2.89958600
C	5.35669200	0.41290100	1.03063400
H	3.65525300	0.47988900	-0.27501200
C	5.96142900	0.94717900	2.16852100
H	5.83065600	2.42752300	3.73222600
H	5.77816400	-0.44891400	0.52666400
H	6.88975700	0.52306000	2.53941800
Pd	0.48778800	1.02485700	-0.37514300
C	0.75050200	2.78291400	-2.83089700
C	1.21629800	1.63445000	-2.18763200
C	2.23055600	0.87788500	-2.78230500
C	2.78751400	1.28745900	-3.99810900
C	2.32562000	2.43951500	-4.63614800
C	1.30018500	3.18394000	-4.05101900
H	-0.03599800	3.38283100	-2.38107800
H	3.58305000	0.69711300	-4.44646200
H	2.75981200	2.75479800	-5.58075900
H	0.93276800	4.08384900	-4.53713100
H	2.58072600	-0.03485800	-2.31159100

Cu	0.31153100	-1.56779100	-0.80859900
B	-4.17423300	1.87967500	-0.09602500
C	-2.46027400	0.53483100	-1.52164400
C	0.92773200	-2.77796400	-3.76214600
O	-5.11690000	2.12752100	-1.05724700
O	-4.67995100	1.94579300	1.18344200
C	-0.35581600	-3.20993300	-1.66569200
N	-0.00917800	-3.54446900	-2.93708000
N	-1.14060200	-4.23776300	-1.25477400
C	-0.56163200	-4.75871200	-3.30688400
C	-1.27989100	-5.20027300	-2.24051800
C	-6.41862900	2.10947000	-0.40653600
C	-6.04977900	2.42531000	1.09135400
C	-1.66391000	-4.34733200	0.09376900
H	-0.40395900	-5.18943300	-4.28251300
H	-1.87708500	-6.08702200	-2.10307000
H	-1.93479300	-3.35499100	0.44289500
H	-0.90937300	-4.77978300	0.75745400
H	-2.55848600	-4.97126700	0.08907100
H	0.74678600	-1.71587500	-3.60484200
H	0.74629400	-3.02202000	-4.81088800
H	1.95256600	-3.03249500	-3.48353600
C	-3.22030900	-0.77731800	-1.38858400
C	-3.81078000	-1.18562400	-0.18868300
C	-4.52353400	-2.38558000	-0.10947200
C	-4.63846400	-3.20927900	-1.22668100
C	-3.33429700	-1.62136900	-2.50548200
C	-4.03066600	-2.82328600	-2.42537300
H	-3.73325800	-0.57058700	0.69551600
H	-4.09954000	-3.46194600	-3.30101100
H	-2.78920200	1.00027200	-2.45777800
H	-4.97321600	-2.67153500	0.83649300
H	-5.19303900	-4.14168100	-1.16832900
H	-2.85106800	-1.33181600	-3.43131200
C	-6.98671700	0.70217500	-0.60968200
H	-8.00093800	0.61720700	-0.20891400
H	-7.01754100	0.48875600	-1.68087600
H	-6.35420000	-0.05545700	-0.14251000
C	-7.31224200	3.14391900	-1.07953400
H	-7.49197100	2.85053200	-2.11705400
H	-8.27996400	3.20774400	-0.57158600
H	-6.85177000	4.13292700	-1.08278600
C	-6.88512500	1.68382100	2.12812500
H	-6.54444200	1.94947600	3.13311000
H	-7.94169100	1.95716600	2.04558100
H	-6.79329600	0.60306000	2.00993900
C	-6.01057400	3.92294700	1.40424200
H	-7.01321700	4.35909300	1.42004700

H	-5.55518700	4.06782300	2.38758100
H	-5.40869100	4.46151500	0.66742100
C	-2.67386200	1.53557400	-0.38453600
H	-2.22537300	1.15748100	0.53351300
H	-2.12179300	2.45351900	-0.62986300
C	-0.95802000	0.19645200	-1.79901700
O	-0.70996000	-0.23898000	-2.90901800
S	3.38432100	-2.79062000	-0.61893900
O	3.63058500	-3.41530900	-1.92572400
O	4.54442500	-2.53414300	0.25035900
C	2.41638800	-4.09611300	0.33034900
F	3.25157600	-4.85926200	1.03948600
F	1.72314800	-4.88933800	-0.49948500
F	1.53559100	-3.53488900	1.19333000
O	2.44330400	-1.61193700	-0.67438700

COM_{3-R₂}

Cu	0.10418000	0.55419800	0.03431200
B	1.98942700	-1.03708000	-1.75525200
C	0.62391700	1.11734000	-1.81319400
C	-1.46768300	-1.55257000	2.37723900
O	3.32294900	-1.07646700	-1.40774700
O	1.26587800	-2.02752500	-1.11048200
C	0.04232100	0.38279500	1.96880800
N	-0.55435400	-0.50392600	2.81166600
N	0.74704300	1.20298000	2.79892600
C	-0.23273400	-0.24420400	4.13508000
C	0.59591700	0.83341000	4.12475700
C	3.45636200	-1.93229100	-0.24622400
C	2.18959400	-2.85881300	-0.36725200
C	1.60811200	2.28822400	2.32813200
H	-0.62034100	-0.83249000	4.95132100
H	1.08179600	1.35914700	4.93106300
H	1.77285700	2.98894700	3.14810000
H	1.13008800	2.80559500	1.49704300
H	2.56650700	1.89843700	1.97983200
H	-1.30962700	-1.73367400	1.31693100
H	-2.50503400	-1.24882000	2.53355700
H	-1.26635500	-2.46883400	2.93680000
C	1.45144500	2.26721300	-1.37491100
C	2.84646600	2.19049800	-1.15263300
C	3.55920300	3.26949000	-0.62888200
C	2.92353500	4.47252900	-0.31499800
C	0.83339900	3.50865600	-1.07799300
C	1.54863600	4.58212500	-0.55816500
H	3.37137200	1.26847200	-1.37287500
H	1.03266800	5.51597200	-0.34690100

H	-0.27143800	1.49015900	-2.32075700
H	4.63066000	3.16777900	-0.46983800
H	3.48459800	5.31060500	0.08728800
H	-0.23552400	3.60816800	-1.25399800
C	3.41555500	-1.01361500	0.97984900
H	3.56541200	-1.57097600	1.90920900
H	4.20925100	-0.26801200	0.88671100
H	2.46039700	-0.48502700	1.03627400
C	4.79574100	-2.65505000	-0.32215000
H	5.60772600	-1.92551200	-0.26012600
H	4.90554700	-3.35860400	0.50960600
H	4.90399500	-3.20125000	-1.26038700
C	1.53906600	-3.23229500	0.96050600
H	0.64180200	-3.82890000	0.77245900
H	2.22257400	-3.82599800	1.57620600
H	1.24477900	-2.34304400	1.51794700
C	2.43642300	-4.11140000	-1.21238100
H	3.09014300	-4.82398200	-0.70125900
H	1.47923300	-4.60272200	-1.40824800
H	2.88666900	-3.85076600	-2.17364800
C	1.32240300	0.02976300	-2.67777600
H	0.55238000	-0.46853500	-3.28008300
H	2.04185700	0.47147700	-3.38375900
C	-2.05468400	-1.36408500	-1.22392400
C	-3.18182200	-0.81713400	-0.60916600
C	-4.11148000	-1.62420300	0.04990900
C	-3.89588300	-3.00324800	0.10137400
C	-2.76654700	-3.56546700	-0.49979000
C	-1.85192000	-2.74615500	-1.16167700
H	-1.32629900	-0.72957300	-1.71378200
H	-4.98517200	-1.18615700	0.51960400
H	-4.61481300	-3.63552000	0.61428700
H	-2.60368600	-4.63801900	-0.45270300
H	-0.95489200	-3.15438400	-1.61261400
I	-3.45224500	1.28338100	-0.61825700

TS24_a

Cu	-0.83332600	0.34363200	-0.01043800
B	1.84549100	-1.03252600	-1.27446100
C	-0.09319200	0.65124000	-1.89692600
C	-0.27656500	-1.48507600	2.76203900
O	3.19405500	-0.80986600	-1.46815100
O	1.61126600	-1.73576500	-0.10158500
C	0.08618300	0.74644600	1.74254400
N	0.25938000	-0.13112400	2.76998100
N	0.70203600	1.87816100	2.17862900
C	0.97030900	0.43467900	3.81663400
C	1.25359100	1.70867800	3.43963300

C	3.88174600	-1.16351300	-0.24409300
C	2.90250000	-2.21241300	0.37541300
C	0.78613400	3.12269600	1.42193400
H	1.19929800	-0.10531400	4.72138000
H	1.78583400	2.49663500	3.94779200
H	0.59011400	3.96409800	2.09040300
H	0.04292500	3.10560500	0.62918300
H	1.76911600	3.23328300	0.96199500
H	0.06689100	-1.99333900	1.86151800
H	-1.36831900	-1.45196600	2.77848700
H	0.08729700	-2.01690900	3.64238900
C	0.52887700	1.98066500	-1.86976200
C	1.92099900	2.20718600	-1.77695800
C	2.44149500	3.49922400	-1.69925800
C	1.60399100	4.61619200	-1.71665000
C	-0.29906900	3.13122100	-1.91471000
C	0.22251700	4.41632800	-1.83731300
H	2.60193800	1.36605300	-1.78542300
H	-0.44847400	5.27084100	-1.87591200
H	-1.01885000	0.68323600	-2.47447000
H	3.51899400	3.63327300	-1.63382300
H	2.01485900	5.61960500	-1.65985600
H	-1.37429100	2.99034200	-2.00367700
C	3.99085200	0.11483400	0.59688200
H	4.56556000	-0.05360300	1.51200500
H	4.49773200	0.88323000	0.00777600
H	3.00175700	0.49425500	0.86635400
C	5.26552900	-1.69604300	-0.59260000
H	5.86645800	-0.89613000	-1.03348800
H	5.78132300	-2.05392100	0.30440800
H	5.20862200	-2.51218100	-1.31435100
C	2.91716100	-2.26001500	1.89745100
H	2.22985000	-3.03032100	2.25728200
H	3.91981000	-2.51709500	2.25414400
H	2.62878400	-1.30375800	2.33347400
C	3.08842100	-3.62054300	-0.19827800
H	4.00539500	-4.08863000	0.17087000
H	2.23835600	-4.23886100	0.10222700
H	3.12268500	-3.59720400	-1.29046700
C	0.75415700	-0.56683700	-2.29888800
H	0.06399700	-1.40393200	-2.44911100
H	1.25275400	-0.39034700	-3.26679700
C	-1.88396800	-2.31597500	-0.44071200
C	-2.36511300	-1.05127800	-0.80962400
C	-2.89210400	-0.84713000	-2.09604900
C	-2.81763700	-1.86982100	-3.03447200
C	-2.26631400	-3.11311700	-2.69850000
C	-1.80664300	-3.32823800	-1.39993300

H	-1.55943600	-2.50832300	0.57226100
H	-3.32468600	0.11078700	-2.36100400
H	-3.19566000	-1.69504800	-4.03789500
H	-2.21679300	-3.90665300	-3.43695800
H	-1.39247400	-4.29209000	-1.11753600
I	-3.46939600	0.13096500	0.90854000

16_a

Cu	-1.03570000	-0.14874700	-0.09364100
B	2.24672900	-1.02178100	-1.12136900
C	-0.18931100	-0.24368300	-2.00596400
C	0.35486500	-1.42229300	2.47643500
O	3.36872900	-0.28959700	-1.43330900
O	2.38739600	-1.71354000	0.05875900
C	0.24963100	0.70928500	1.21156200
N	0.66365100	-0.00812400	2.29274600
N	0.57300000	1.99122200	1.52186500
C	1.21150600	0.81176400	3.26584000
C	1.16005300	2.07717900	2.77561300
C	4.24773900	-0.30575000	-0.27601100
C	3.78474000	-1.61053100	0.46334300
C	0.21483800	3.15638200	0.72446500
H	1.57734200	0.42907300	4.20493100
H	1.48339600	3.01536200	3.19644800
H	-0.21384200	3.91722600	1.37996200
H	-0.53194100	2.86244100	-0.00780000
H	1.08734400	3.55855800	0.20783700
H	0.74233800	-1.98589400	1.62897400
H	-0.72804500	-1.54592200	2.56202600
H	0.83827700	-1.77156700	3.39011900
C	-0.07128000	1.21729900	-2.20711000
C	1.15860200	1.89783000	-2.28180800
C	1.19485000	3.26638800	-2.54602900
C	0.01476100	3.99446600	-2.70957400
C	-1.25625100	1.96417300	-2.38954500
C	-1.21504700	3.33435300	-2.62571600
H	2.08706700	1.35515100	-2.16129800
H	-2.14149800	3.88595100	-2.75326100
H	-0.98214400	-0.62621500	-2.63837700
H	2.15564200	3.76813300	-2.62384800
H	0.05077800	5.06126600	-2.90808400
H	-2.21291500	1.45336600	-2.33287200
C	3.95887500	0.97210500	0.51602300
H	4.62462900	1.06926200	1.37779000
H	4.11358300	1.83469800	-0.13757700
H	2.92621200	0.99285900	0.86620000
C	5.69163700	-0.31843500	-0.76137900
H	5.91252400	0.61826500	-1.28007500

H	6.38109000	-0.40935300	0.08398300
H	5.87612000	-1.14047200	-1.45427400
C	3.87025800	-1.54691700	1.98219500
H	3.48831900	-2.47635800	2.41334600
H	4.91248200	-1.43290500	2.29676200
H	3.29298100	-0.71505000	2.38399000
C	4.47478100	-2.87570800	-0.05411600
H	5.52241000	-2.91865700	0.25595900
H	3.95815900	-3.75017100	0.34963400
H	4.43164600	-2.92921900	-1.14513500
C	1.01937600	-1.16262200	-2.09303600
H	0.64263700	-2.18694800	-2.00346300
H	1.41688900	-1.07231100	-3.11774200
C	-1.57685200	-2.86178200	-0.64697700
C	-2.06865700	-1.57807700	-0.88696000
C	-3.29573700	-1.41200400	-1.53153100
C	-4.03726000	-2.53062500	-1.91366800
C	-3.55799500	-3.81872700	-1.65723600
C	-2.33007100	-3.98259200	-1.01963200
H	-0.61203800	-3.00739500	-0.16772100
H	-3.69604300	-0.41775800	-1.70286100
H	-4.99885000	-2.39569400	-2.40181000
H	-4.13913900	-4.68648600	-1.95501300
H	-1.94702000	-4.97944900	-0.81685000
I	-3.00510500	0.60006300	1.56172700

COM_{4-R₂}

Cu	-0.07037900	-0.66886900	0.49139600
B	-3.36050200	0.53930700	0.47430000
C	-2.72818300	-1.78790400	-0.34421200
C	0.49306100	1.99483600	2.53756300
O	-4.22001200	1.03641400	-0.46897000
O	-2.51353300	1.50691400	0.98157100
C	1.30311800	-0.23460800	1.80299500
N	1.44524000	0.89215300	2.54982500
N	2.42217000	-0.95690100	2.07438100
C	2.63856500	0.88560500	3.25398000
C	3.25670200	-0.28770400	2.95547100
C	-4.05196900	2.47769500	-0.51686500
C	-2.62538600	2.67311000	0.11336400
C	2.70329900	-2.26215300	1.48987400
H	2.93644100	1.69764500	3.89770800
H	4.19434700	-0.69927100	3.29325100
H	2.83377700	-3.00776300	2.27880600
H	3.59902900	-2.21107400	0.86891900
H	1.85723700	-2.54086400	0.86215500
H	0.88124400	2.81662500	1.92827200
H	0.32145200	2.34520400	3.55832900

H	-0.44674600	1.64542700	2.10903100
C	-2.33429400	-3.21282900	-0.05239100
C	-1.67173600	-3.57773400	1.13048000
C	-1.19210800	-4.87655700	1.31368300
C	-1.35918600	-5.83671000	0.31618300
C	-2.48462800	-4.18784100	-1.05018000
C	-2.00992300	-5.48513600	-0.86953100
H	-1.53824700	-2.84686300	1.92085600
H	-2.14814700	-6.22396300	-1.65409300
H	-3.45422500	-1.76900500	-1.16488300
H	-0.69148200	-5.13825400	2.24229500
H	-0.99158800	-6.84846700	0.46081400
H	-2.97671700	-3.91445400	-1.97943700
C	-5.17588100	3.07827100	0.33252900
H	-5.16836000	4.17156100	0.29932200
H	-6.13574500	2.72657000	-0.05404100
H	-5.09290600	2.75966400	1.37524300
C	-4.17699600	2.92988200	-1.96653100
H	-5.19308200	2.73989600	-2.32264000
H	-3.97883600	4.00293700	-2.05693900
H	-3.48435600	2.38705100	-2.61055800
C	-2.46831400	3.93096500	0.95970200
H	-1.44855300	3.99020100	1.35035200
H	-2.64511900	4.82516700	0.35352600
H	-3.15896600	3.93914500	1.80444600
C	-1.49078800	2.57447800	-0.91080000
H	-1.47064600	3.45012700	-1.56606300
H	-0.53548600	2.52251300	-0.38300300
H	-1.57726000	1.67370300	-1.52098100
C	-3.28649800	-0.98115400	0.85749700
H	-4.27020200	-1.37964900	1.13183600
H	-2.63158100	-1.09560200	1.72718500
C	-1.42393700	-1.08117100	-0.84914700
O	-1.35718700	-0.80591900	-2.04888200
C	1.70995000	-0.38987000	-1.87272500
C	2.86722700	0.23733000	-1.41286800
C	4.09256100	-0.43093500	-1.36190900
C	4.15286800	-1.76086600	-1.78475400
C	3.00131600	-2.41202900	-2.23628500
C	1.78818100	-1.72690300	-2.27793200
H	0.75150400	0.11163700	-1.94465200
H	4.98327500	0.07621400	-1.00841200
H	5.10431900	-2.28456600	-1.75893700
H	3.05353800	-3.44773600	-2.55773000
H	0.87658500	-2.20767300	-2.61515200
I	2.77322400	2.25449300	-0.76055000

TS25_a

Cu	-0.48643200	-0.52785300	0.14494900
B	1.84981800	2.17823000	-0.24053500
C	-0.47802000	2.15042500	-1.31797400
C	0.57027100	0.71324400	3.24076500
O	2.84099500	2.77496500	-0.97112700
O	2.26583900	1.02394700	0.38475000
C	-1.38474600	0.21072200	1.78677800
N	-0.85542800	0.71533900	2.93334200
N	-2.72486300	0.38225900	1.93846200
C	-1.84394300	1.19137900	3.78263600
C	-3.02874000	0.98049700	3.15088400
C	4.08142500	2.06330100	-0.69073100
C	3.56414300	0.66997600	-0.17995400
C	-3.70807500	-0.03553000	0.94814100
H	-1.62090700	1.63582200	4.73949900
H	-4.04010000	1.20753700	3.44774600
H	-4.48261400	0.72568700	0.85694500
H	-4.15297400	-0.99416100	1.23061300
H	-3.20565900	-0.13595900	-0.01285800
H	0.80630300	-0.09221000	3.94123900
H	0.84822200	1.67340900	3.68328700
H	1.13059900	0.56507300	2.31848000
C	-1.97128600	2.38842200	-1.18819300
C	-2.54479700	3.09143000	-0.12238900
C	-3.92469000	3.29870800	-0.05850600
C	-4.76058200	2.79012900	-1.05300600
C	-2.82502500	1.87369500	-2.17848300
C	-4.20273300	2.07061000	-2.11313700
H	-1.91291600	3.49219700	0.66176200
H	-4.84156500	1.66638600	-2.89311700
H	-0.13590200	2.61872000	-2.25017700
H	-4.34419800	3.86120600	0.77127700
H	-5.83324700	2.95393800	-1.00557000
H	-2.39501200	1.31766600	-3.00602900
C	4.81207300	2.86817300	0.38706000
H	5.79206700	2.43878000	0.61348400
H	4.95527000	3.89134500	0.03041300
H	4.22808700	2.90824000	1.31078700
C	4.90700200	2.01112000	-1.96973400
H	5.20413000	3.02333700	-2.25719900
H	5.81495900	1.41859300	-1.81879600
H	4.33762200	1.57696800	-2.79235000
C	4.39940000	0.02115000	0.91573900
H	3.92528100	-0.91615300	1.21779300
H	5.40652200	-0.20512700	0.55136400
H	4.48221300	0.66378200	1.79414200

C	3.30247900	-0.32763900	-1.31020400
H	4.24045300	-0.67494100	-1.75267900
H	2.77411600	-1.18882300	-0.89682500
H	2.67714800	0.10731200	-2.09231100
C	0.37095300	2.69110900	-0.14683000
H	0.33309500	3.78620400	-0.15174300
H	-0.05999900	2.34654100	0.79806500
C	-0.23895200	0.61012100	-1.51024400
O	0.10010600	0.23758200	-2.61839600
C	0.04654800	-2.48426000	-2.11388100
C	-0.51426800	-2.35296900	-0.84038500
C	-1.79849300	-2.84578200	-0.55596800
C	-2.57509700	-3.34775900	-1.60070400
C	-2.04676900	-3.43607600	-2.89114500
C	-0.73616300	-3.01781600	-3.13589200
H	1.05025100	-2.13666800	-2.31606000
H	-2.18312500	-2.82263900	0.45787000
H	-3.58487900	-3.69334500	-1.39606600
H	-2.64419300	-3.85276400	-3.69616800
H	-0.31873900	-3.09236200	-4.13597000
I	0.96570100	-2.69264900	1.07879300

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Cu	1.79592900	-1.41764500	0.98915600
B	-2.97250700	-0.01613600	-0.58157800
C	-0.75116500	0.71047000	-1.67460300
C	-1.18451300	-2.04545700	2.28782600
O	-3.57715100	1.20903800	-0.72990400
O	-3.59463500	-0.81188600	0.35393400
C	0.36282000	-2.58396700	0.42769900
N	-0.82917700	-2.74892700	1.05884700
N	0.25029400	-3.33401500	-0.70128200
C	-1.67781800	-3.56427600	0.33378400
C	-0.99407900	-3.93982500	-0.78064300
C	-4.80614200	1.19198500	0.04113200
C	-4.54143900	0.03388200	1.07116100
C	1.26577800	-3.39796600	-1.74479200
H	-2.68389200	-3.77651800	0.65492900
H	-1.27836300	-4.56950900	-1.60799400
H	0.96388500	-2.79683100	-2.60558700
H	1.41971700	-4.43631900	-2.04806600
H	2.19327800	-2.99220700	-1.34499200
H	-0.37778500	-2.16003000	3.01336000
H	-2.10163600	-2.47841300	2.68759600
H	-1.33806300	-0.99111300	2.06433200
C	0.47811700	0.24809900	-2.45193900
C	1.74429700	0.14193900	-1.86491200
C	2.83385900	-0.34567000	-2.58824300

C	2.67690600	-0.73396400	-3.91798800
C	0.33344300	-0.13926500	-3.79189200
C	1.41956000	-0.62646000	-4.51936500
H	1.91173400	0.45190700	-0.84034700
H	1.28516000	-0.91552400	-5.55786600
H	-1.25045900	1.49873500	-2.25436600
H	3.79865300	-0.41569700	-2.09494100
H	3.52341300	-1.11015400	-4.48461800
H	-0.63935100	-0.05740600	-4.27018900
C	-5.93730200	0.87821300	-0.94321100
H	-6.91660300	0.91052700	-0.45731500
H	-5.92376300	1.62136300	-1.74449500
H	-5.80424500	-0.10916100	-1.39393500
C	-5.00815400	2.57039900	0.65927700
H	-5.17102300	3.30626000	-0.13283600
H	-5.88389500	2.57842300	1.31612000
H	-4.13404200	2.87958900	1.23378500
C	-5.76281500	-0.80532400	1.42609800
H	-5.47472400	-1.59314400	2.12792800
H	-6.52912000	-0.18922600	1.90720100
H	-6.19722000	-1.27881500	0.54436200
C	-3.84199000	0.51936900	2.34414100
H	-4.50293500	1.15176700	2.94316400
H	-3.56266300	-0.34528500	2.95095200
H	-2.93250500	1.07594000	2.10704200
C	-1.75749900	-0.44316200	-1.47586100
H	-2.11514900	-0.76316000	-2.46210900
H	-1.24533800	-1.29580200	-1.03661000
C	-0.40018700	1.33493200	-0.32060800
O	-0.82274200	0.82290700	0.71437000
C	1.00129800	2.91805500	0.96823600
C	0.44484900	2.55381500	-0.26728400
C	0.71977100	3.32957200	-1.40474000
C	1.52470900	4.45978800	-1.30128200
C	2.07657400	4.81385400	-0.06721600
C	1.81793400	4.03940200	1.06558400
H	0.80530400	2.29158400	1.82945500
H	0.31386800	3.04948600	-2.36999200
H	1.73022200	5.05966700	-2.18235800
H	2.71603100	5.68841700	0.00806600
H	2.26457700	4.30002600	2.01950500
I	3.61707700	0.07004700	1.72511100

COM_{5-R₂}

Cu	1.52708100	-0.10747800	0.08152200
B	0.41730900	2.32662100	0.73132400
C	-1.94273700	1.67075600	0.95257200

C	3.50299500	-2.48241400	-1.39229700
O	1.23468200	1.76157700	-0.43265800
O	1.28377100	3.31150200	1.31814400
C	2.14380200	-1.84528800	0.59145500
N	2.90014800	-2.74730200	-0.09524100
N	1.84922400	-2.48055500	1.75712700
C	3.05979900	-3.92461300	0.62062700
C	2.39154400	-3.75465200	1.79109800
C	2.33462600	2.66548800	-0.66400300
C	2.59582500	3.21778500	0.78147900
C	1.03088400	-1.90189500	2.81844300
H	0.03492800	-2.35304000	2.81126100
H	0.94110700	-0.82934400	2.64162000
H	1.50890800	-2.08032100	3.78444600
H	4.59295700	-2.53590600	-1.32286500
H	3.20986300	-1.47849300	-1.69787800
H	3.15367600	-3.20709600	-2.13329900
C	-3.38795700	1.54357300	0.78250300
C	-4.09762100	0.37745300	1.14640500
C	-5.46817200	0.27174900	0.93678100
C	-6.18090800	1.32179500	0.34935900
C	-4.12200800	2.58613600	0.18473100
C	-5.49599800	2.47761400	-0.02541700
H	-3.56325400	-0.46099200	1.58219300
H	-6.03345400	3.30215600	-0.48624900
H	-5.98412400	-0.64021200	1.22512800
H	-7.25021100	1.23494800	0.18202900
H	-3.60034700	3.49051800	-0.10961500
C	1.83130800	3.74763500	-1.62595600
H	2.63125200	4.43293400	-1.92106900
H	1.43771200	3.26217200	-2.52322100
H	1.02635000	4.32377500	-1.16545200
C	3.49806800	1.90784700	-1.29414200
H	3.20895200	1.53758900	-2.28306700
H	4.36553800	2.56459800	-1.41651400
H	3.79724600	1.05300800	-0.68125600
C	3.23758800	4.60474700	0.80637300
H	3.39442900	4.91780600	1.84254400
H	4.20937100	4.60235000	0.30000600
H	2.59119100	5.34247800	0.32845500
C	3.43169900	2.25383700	1.64180600
H	4.48025800	2.21964500	1.32702300
H	3.39078700	2.59787000	2.67845400
H	3.02479700	1.23813500	1.61465800
C	-1.09795300	2.79084400	0.38746600
H	-1.26004400	2.92204000	-0.68992300
H	-1.33486200	3.75297900	0.86253200
C	-1.14461300	0.80228000	1.60977100

O	0.18900400	1.05808100	1.60597400
H	-1.44283100	-0.09371400	2.14608400
H	2.25955400	-4.41638700	2.63208200
H	3.63055800	-4.75902800	0.24567900
C	-1.78762500	-0.18718900	-1.67543700
C	-0.96952000	-1.30699600	-1.53793800
C	0.20726400	-1.44787300	-2.27724500
C	0.57506500	-0.43251200	-3.16344400
C	-0.22295700	0.70345100	-3.30035900
C	-1.40158000	0.81762800	-2.56472100
H	-2.70322600	-0.09059700	-1.10794500
H	0.81144600	-2.33973300	-2.17320800
H	1.48858700	-0.53448900	-3.74225100
H	0.07235900	1.49605100	-3.98019800
H	-2.03058200	1.69580100	-2.66432000
I	-1.51813100	-2.83021000	-0.16926300

TS26_a

Cu	-0.88364200	-0.68705000	-0.22292700
B	0.84233800	2.19909300	0.49079100
C	2.64121100	0.72961600	-0.66548000
C	-4.11884400	-0.61815800	0.97642800
O	-0.20622700	1.87564600	1.35010300
O	0.62426700	3.40480600	-0.14722200
C	-2.67449100	-0.15353900	-0.99770100
N	-3.89879600	-0.22586100	-0.40780300
N	-2.94644300	0.21415000	-2.27666100
C	-4.91334000	0.08888600	-1.29930500
C	-4.30849000	0.36700000	-2.48324300
C	-1.07235100	3.03158100	1.42870200
C	-0.74176900	3.80023300	0.09782600
C	-1.93082800	0.40122100	-3.31060400
H	-1.93593300	-0.44904600	-3.99862100
H	-0.96081100	0.48741400	-2.81657000
H	-2.14428500	1.31820000	-3.86463000
H	-4.78353100	0.09844700	1.46483400
H	-3.15751800	-0.62251300	1.48631700
H	-4.54975800	-1.62114900	1.02692100
C	4.03422600	0.36639600	-0.93145800
C	4.47477200	-0.07057200	-2.19996200
C	5.79265200	-0.45840100	-2.41375000
C	6.72552400	-0.41048300	-1.37350200
C	4.99582500	0.42840700	0.09809300
C	6.31684500	0.04152800	-0.11844200
H	3.77790900	-0.08078200	-3.03155800
H	7.03088600	0.09463700	0.69905600
H	6.09959300	-0.78695700	-3.40300600
H	7.75581000	-0.70761700	-1.54423800

H	4.69358400	0.76660300	1.08267100
C	-0.65788900	3.80453000	2.68609500
H	-1.30252900	4.67028800	2.86397100
H	-0.72676300	3.13646300	3.54893400
H	0.37638700	4.14929300	2.60664500
C	-2.51683900	2.56358600	1.55539200
H	-2.63800700	1.99695500	2.48384100
H	-3.20106200	3.41797500	1.58832200
H	-2.79551300	1.92272700	0.72033000
C	-0.79504700	5.32083900	0.20560700
H	-0.52943900	5.76393600	-0.75818000
H	-1.80300900	5.65870800	0.46907600
H	-0.09307500	5.69477000	0.95242800
C	-1.57712500	3.32510400	-1.09459900
H	-2.62334600	3.63536700	-1.00783300
H	-1.15961800	3.75975600	-2.00691400
H	-1.52656700	2.24150600	-1.18244800
C	2.28045700	1.55264200	0.54477300
H	2.36672600	0.93681400	1.45091500
H	3.00434200	2.37050800	0.66204900
C	1.60829600	0.26951000	-1.43343300
O	0.35736000	0.57522600	-1.18536100
H	1.79842900	-0.40935300	-2.27293700
H	-4.71853400	0.66243600	-3.43574300
H	-5.95350500	0.09589300	-1.01521700
C	1.70347100	-1.92002400	0.64456200
C	0.40281900	-1.58340400	1.03719700
C	0.12417400	-1.17463800	2.34892200
C	1.18158000	-0.98155800	3.23369900
C	2.49098900	-1.28050400	2.84148200
C	2.74687600	-1.76416900	1.55714200
H	1.90076300	-2.30248500	-0.34898400
H	-0.89409800	-0.97950300	2.66503300
H	0.98147000	-0.60295700	4.23149500
H	3.30824300	-1.15698300	3.54550500
H	3.76050900	-1.99878200	1.25168000
I	-1.31144500	-3.26507200	0.24419300

18_a

Cu	-0.88588800	-0.78084800	-0.20276400
B	1.04212600	2.15173500	0.66974200
C	2.66702800	0.56213500	-0.55872300
C	-4.03509400	-0.18525500	1.00269300
O	-0.04988000	1.98254800	1.50455000
O	0.97905600	3.33002800	-0.04206700
C	-2.56893500	0.02429600	-1.00014900
N	-3.77037000	0.17911900	-0.38333100
N	-2.79711200	0.41731200	-2.27844300

C	-4.73274900	0.65230500	-1.26173900
C	-4.11593800	0.80262900	-2.46269000
C	-0.80731800	3.21885800	1.47760200
C	-0.34964200	3.87447000	0.12355100
C	-1.78551300	0.40508400	-3.33111000
H	-1.89349300	-0.49092100	-3.94877300
H	-0.80835800	0.42279700	-2.84860600
H	-1.90361000	1.29408800	-3.95438000
H	-4.76036900	0.51203800	1.42697500
H	-3.10551000	-0.12242000	1.56546300
H	-4.40928500	-1.20946400	1.05934800
C	4.03748800	0.16630900	-0.88604400
C	4.45226000	-0.08155600	-2.21140100
C	5.74518900	-0.51035200	-2.49147200
C	6.66831600	-0.69632800	-1.45863800
C	4.98789300	-0.00732700	0.14009700
C	6.28136300	-0.43880500	-0.14247100
H	3.75884400	0.09297300	-3.02751300
H	6.99034700	-0.57570100	0.66921100
H	6.04011300	-0.68785200	-3.52181500
H	7.67866400	-1.02701900	-1.67943700
H	4.69367700	0.17029900	1.16805900
C	-0.37781300	4.02109600	2.71032800
H	-0.94822400	4.94903700	2.81040700
H	-0.54457600	3.41257100	3.60313600
H	0.68588500	4.26861700	2.66272200
C	-2.29248700	2.89032500	1.55391000
H	-2.51437100	2.40480500	2.50900800
H	-2.89460200	3.80259900	1.48909400
H	-2.58561500	2.22041800	0.74704500
C	-0.25231700	5.39609800	0.14958900
H	0.09405000	5.75611200	-0.82305800
H	-1.23091900	5.84495200	0.34980900
H	0.45325600	5.74062800	0.90706100
C	-1.17945600	3.41574500	-1.07943100
H	-2.19457700	3.82366500	-1.05190700
H	-0.68988400	3.76455800	-1.99286800
H	-1.22365000	2.32831000	-1.11593800
C	2.36811700	1.30173100	0.72089300
H	2.32908900	0.59504500	1.55838800
H	3.19387400	1.99199600	0.93708600
C	1.61131700	0.18752900	-1.34733800
O	0.37221300	0.50896000	-1.06674500
H	1.77932900	-0.44112100	-2.22857200
H	-4.48735200	1.15502500	-3.41152000
H	-5.74815600	0.84756300	-0.95644700
C	1.64199700	-2.12642700	0.51218100
C	0.47205000	-1.53482400	0.97659200

C	0.30467000	-1.22534900	2.32529300
C	1.37884600	-1.40782900	3.20038900
C	2.57805800	-1.95726700	2.73706500
C	2.70529000	-2.32983600	1.39877000
H	1.74302900	-2.42686400	-0.52482500
H	-0.62172500	-0.79771000	2.69293500
H	1.27834900	-1.11037000	4.24033800
H	3.40404000	-2.11323800	3.42483600
H	3.62713500	-2.77467900	1.03811900
I	-1.91622100	-3.15069500	0.17807700

COM_{3-R₃}

Cu	0.47256500	0.09882700	-0.18069100
B	3.26458500	0.64196400	-1.22060200
C	1.04991200	1.85572500	-0.90937800
C	-0.14794800	-3.37147300	-0.35590700
O	4.32174200	0.78186500	-0.34471300
O	3.03477700	-0.69087200	-1.53199400
C	0.05970000	-1.34118300	1.05097900
N	-0.09664100	-2.68708100	0.92522300
N	-0.07446200	-1.11789900	2.38670200
C	-0.34418800	-3.28850600	2.14846400
C	-0.32478900	-2.29264800	3.07372500
C	4.61139900	-0.52454900	0.20842800
C	4.08475800	-1.48092800	-0.92104400
C	0.00614400	0.21289600	2.99202700
H	-0.51227800	-4.34834300	2.25075800
H	-0.46113900	-2.31947500	4.14278000
H	-0.04769600	0.10683700	4.07636200
H	-0.81645900	0.83341800	2.63738000
H	0.94305700	0.69950500	2.71757100
H	0.43482200	-2.79700700	-1.07556000
H	-1.18430000	-3.45261800	-0.69692300
H	0.28435500	-4.36976700	-0.26015300
C	1.05414700	2.59935800	0.37128900
C	2.20461600	2.79177200	1.17169500
C	2.12281000	3.39592100	2.42783000
C	0.90295500	3.84742000	2.93496000
C	-0.16737600	3.09495800	0.89395700
C	-0.24294900	3.69897300	2.14298000
H	3.16725300	2.44670500	0.81382200
H	-1.20339900	4.05974400	2.50467700
H	0.22802200	2.21621600	-1.53285500
H	3.03054400	3.52021800	3.01476800
H	0.84632200	4.31944300	3.91135400
H	-1.07109600	2.96205300	0.30431000
C	3.81014600	-0.63652000	1.51054900

H	4.01592200	-1.57463600	2.03476400
H	4.08007300	0.19662600	2.16387900
H	2.73719400	-0.57165400	1.31078500
C	6.10529400	-0.61826300	0.49299000
H	6.37443700	0.10172800	1.27060500
H	6.37122200	-1.61907700	0.84901200
H	6.69749000	-0.39283200	-0.39524400
C	3.48613600	-2.78942900	-0.41672500
H	3.12238300	-3.37810700	-1.26436900
H	4.24154600	-3.38404800	0.10727100
H	2.65112800	-2.60790000	0.26046500
C	5.12612300	-1.75568100	-2.00977600
H	5.93109000	-2.40108600	-1.64636300
H	4.63643200	-2.25262500	-2.85163200
H	5.56420800	-0.82278100	-2.37411600
C	2.36714800	1.81250400	-1.72981700
H	2.09870100	1.61721000	-2.77525800
H	2.89964700	2.77641000	-1.70632900
C	-1.19503500	-0.52159200	-2.70328800
C	-2.34149600	-0.00115100	-2.11662900
C	-2.78968900	1.28839800	-2.37301300
C	-2.05682200	2.07712200	-3.25966900
C	-0.91116900	1.57050700	-3.87818900
C	-0.48277800	0.27311800	-3.60222300
H	-0.88382300	-1.53055000	-2.46809500
H	-3.68477800	1.66208400	-1.89321200
H	-2.38487700	3.09056400	-3.46595500
H	-0.34430600	2.19423000	-4.56116100
H	0.42115000	-0.11661700	-4.05687800
S	-3.25428100	-0.60984300	0.31024600
O	-3.06184500	-1.88192000	0.98515400
O	-2.60044600	0.62065100	0.72273200
C	-5.09227100	-0.29251800	0.31515500
F	-5.47553600	-0.12372200	1.57911400
F	-5.73220700	-1.32789300	-0.21790700
F	-5.36617900	0.81192500	-0.38310700
O	-3.08764100	-0.88166200	-1.29492400

TS24_b

Cu	-0.01780600	0.08569500	-0.22612000
B	2.72216000	-1.04755400	-0.97172900
C	0.62822400	0.00371700	-2.12760800
C	-0.17851400	-1.03930700	3.06281200
O	3.99335900	-0.51796600	-0.98042900
O	2.39121600	-1.57393300	0.26450900
C	0.04500100	0.94210600	1.58530900
N	-0.02919400	0.38911600	2.82466800
N	0.02414400	2.27953900	1.81921000

C	-0.12220400	1.35818400	3.80850400
C	-0.08539400	2.55750600	3.16959800
C	4.44783900	-0.44531500	0.39681900
C	3.60242400	-1.57617200	1.07315300
C	0.01566200	3.27897200	0.75336100
H	-0.20725600	1.11448000	4.85507300
H	-0.12335900	3.56464100	3.55187600
H	0.02670500	4.27236600	1.20361200
H	-0.88300400	3.15730200	0.14813400
H	0.89245100	3.15816400	0.11738500
H	0.38738800	-1.57427200	2.30319300
H	-1.23088600	-1.31902900	2.99593400
H	0.22040600	-1.28421400	4.04920000
C	0.91793300	1.43578400	-2.27523100
C	2.19534500	2.00989900	-2.07514600
C	2.38833200	3.38751300	-2.17540600
C	1.32551500	4.23933900	-2.48378100
C	-0.14409800	2.31893100	-2.59848000
C	0.05578300	3.68854500	-2.70137700
H	3.04133300	1.37062600	-1.85757400
H	-0.78124600	4.33481500	-2.95135400
H	-0.24201100	-0.28764900	-2.71172600
H	3.38324200	3.79736600	-2.02054200
H	1.48265600	5.31053000	-2.56565200
H	-1.13729700	1.90401600	-2.74054500
C	4.08923800	0.95299500	0.91288400
H	4.46068900	1.11080100	1.92933500
H	4.54554300	1.70088800	0.25961200
H	3.00767200	1.11205600	0.90510200
C	5.95550900	-0.65824500	0.42786000
H	6.45346800	0.17017900	-0.08300600
H	6.32038900	-0.69028700	1.45949200
H	6.23944600	-1.58455600	-0.07368700
C	3.24396100	-1.31047500	2.52902800
H	2.68191100	-2.15534900	2.93601000
H	4.15279100	-1.19439000	3.12813700
H	2.63880200	-0.40969900	2.63282900
C	4.22472100	-2.96670100	0.92162700
H	5.10661600	-3.08476000	1.55750900
H	3.48516100	-3.71763000	1.21170500
H	4.51343600	-3.15652900	-0.11542400
C	1.75861400	-1.03025700	-2.21119200
H	1.28767500	-2.01608500	-2.28573100
H	2.35066700	-0.88356100	-3.12834400
C	-0.66093800	-2.84947300	-0.23730700
C	-1.31202800	-1.71696300	-0.72079400
C	-2.03865500	-1.72283800	-1.91181000
C	-1.95019300	-2.85219500	-2.72227100

C	-1.21656300	-3.97386600	-2.31756100
C	-0.58141500	-3.96525900	-1.07379900
H	-0.17184900	-2.84730300	0.72645800
H	-2.59974600	-0.84983500	-2.21850300
H	-2.46732800	-2.85332200	-3.67778500
H	-1.16239000	-4.85049000	-2.95433000
H	-0.01922600	-4.83240200	-0.73869500
S	-3.00701000	0.35621500	0.61701100
O	-3.07243500	0.98626600	1.93529900
O	-2.61263500	1.15915000	-0.55054200
C	-4.73961200	-0.22212500	0.26007700
F	-5.55175500	0.83772700	0.21789600
F	-5.14917500	-1.05432000	1.21956300
F	-4.78982100	-0.85503500	-0.91698200
O	-2.24574500	-0.99544400	0.69231300

16_b

Cu	-0.63949800	0.28617800	0.29058600
B	3.15719300	-1.53901400	0.21277600
C	0.78933400	-2.71969400	0.85284900
C	1.41035200	2.46730200	1.89139700
O	3.70896800	-1.49360800	-1.04346400
O	3.51279800	-0.44927900	0.98105000
C	0.28446200	1.91572700	-0.24346600
N	1.04590700	2.75455200	0.50951200
N	0.11570500	2.58490000	-1.41617700
C	1.34002200	3.92498500	-0.17235300
C	0.75159000	3.81495700	-1.39343100
C	4.34466900	-0.19601200	-1.20638700
C	4.60356200	0.22321900	0.28082000
C	-0.71709700	2.10920100	-2.51924900
H	1.93106100	4.71560100	0.26120900
H	0.72960800	4.49255200	-2.23179000
H	-1.66649100	2.64857200	-2.53784900
H	-0.93963900	1.05720400	-2.35589800
H	-0.18317900	2.24421200	-3.46322000
H	1.81181100	1.45646000	1.95530400
H	0.53142900	2.54435100	2.53422200
H	2.16732500	3.18324700	2.21553400
C	0.07683900	-2.63796900	-0.48958300
C	0.44807200	-1.70528400	-1.46777100
C	-0.24614900	-1.62334100	-2.67511100
C	-1.33962400	-2.45233300	-2.91662200
C	-1.01207700	-3.47631800	-0.75228700
C	-1.72162100	-3.38080100	-1.94942900
H	1.30366800	-1.06410800	-1.31180500
H	-2.57261100	-4.03166500	-2.12487000
H	0.48673400	-3.68043000	1.29227200

H	0.06942500	-0.90487800	-3.42574400
H	-1.89092700	-2.37423000	-3.84810500
H	-1.31264500	-4.20628700	-0.00487100
C	3.33774900	0.71259800	-1.91854100
H	3.77443600	1.68617000	-2.15765700
H	3.03104200	0.23385600	-2.85232900
H	2.44690700	0.87485300	-1.30759000
C	5.59755700	-0.37329900	-2.05433600
H	5.31573700	-0.68133200	-3.06462700
H	6.15119200	0.56830500	-2.12784400
H	6.25765800	-1.13665600	-1.64000500
C	4.53375300	1.72047700	0.54371100
H	4.65992000	1.91479000	1.61237300
H	5.33951400	2.23347600	0.00895600
H	3.58344400	2.14395900	0.22295200
C	5.90204800	-0.35351800	0.85286800
H	6.78185900	0.13821300	0.42895100
H	5.90943900	-0.20335500	1.93550300
H	5.97564900	-1.42664300	0.65727100
C	2.33456700	-2.78781400	0.71562400
H	2.74976600	-3.08554500	1.68651500
H	2.55297500	-3.61092100	0.02702500
C	1.08990100	-1.12709000	2.84638900
C	0.27815100	-1.65642200	1.83054100
C	-1.08450100	-1.27304900	1.80108400
C	-1.59147000	-0.34869900	2.73306500
C	-0.76291300	0.16469800	3.72990300
C	0.57050700	-0.24404300	3.79250600
H	2.13809700	-1.39149800	2.89599900
H	-1.77052700	-1.73563900	1.09985400
H	-2.62798400	-0.04501000	2.65953200
H	-1.15716300	0.87117000	4.45368500
H	1.22164000	0.14493500	4.57047500
S	-3.46271100	0.94287400	-0.44001900
O	-3.97288900	1.68828500	-1.59885900
O	-2.43552000	-0.10675900	-0.78735400
C	-4.86419700	-0.12681200	0.13382000
F	-5.28647800	-0.93359100	-0.84645500
F	-5.89321000	0.61524000	0.55698700
F	-4.45020600	-0.89958500	1.16323500
O	-3.09078700	1.72354400	0.76021000

COM_{4-R₃}

Cu	0.34818300	0.41478900	0.86941800
B	4.00163500	0.84893800	-0.08883900
C	1.96174800	2.18920900	-0.85803400
C	-0.13598900	-2.19679200	3.03496600

O	4.71017800	0.57196600	-1.22679700
O	4.03576900	-0.17569800	0.82992600
C	-0.82085000	0.10086900	2.39218900
N	-1.00497700	-1.03119500	3.12189000
N	-1.84748000	0.90967700	2.76278800
C	-2.13521900	-0.94021200	3.91997100
C	-2.66910200	0.28942700	3.68896000
C	5.37429200	-0.70491300	-1.04849200
C	4.59194800	-1.34123200	0.16645200
C	-2.09646900	2.21989400	2.16410700
H	-2.44541100	-1.73389000	4.58073400
H	-3.54024100	0.77055300	4.10426900
H	-2.43704100	2.91362600	2.93580800
H	-2.84206000	2.14094900	1.37084200
H	-1.16764100	2.58936200	1.73193200
H	-0.69027900	-3.05398100	2.64673400
H	0.27876800	-2.43433300	4.01828900
H	0.67435400	-1.95819600	2.34682600
C	0.90417000	3.22976500	-0.54185300
C	1.03764800	4.18867000	0.46986200
C	-0.00108300	5.07791600	0.75896900
C	-1.20099800	5.01436600	0.04990800
C	-0.31218100	3.17682200	-1.24562400
C	-1.35285800	4.05637300	-0.95557600
H	1.96035200	4.24889200	1.03658200
H	-2.28749000	3.97698600	-1.50090700
H	2.33056300	2.32882200	-1.88245000
H	0.13043400	5.82070900	1.54129300
H	-2.00978100	5.70262400	0.27836100
H	-0.44367600	2.42413600	-2.01727900
C	6.84039300	-0.39368700	-0.73365300
H	7.43714000	-1.30534500	-0.63705800
H	7.25492000	0.20673700	-1.54751200
H	6.93106500	0.18275000	0.19095800
C	5.26302200	-1.48289100	-2.35531100
H	5.81874300	-0.96103000	-3.13910400
H	5.68474500	-2.48801800	-2.24971000
H	4.22354800	-1.56354600	-2.67545900
C	5.46454300	-2.09669800	1.16311800
H	4.84194600	-2.48153500	1.97587200
H	5.95723400	-2.94703700	0.68058200
H	6.22879700	-1.45160300	1.59888600
C	3.40492900	-2.21254500	-0.26040600
H	3.74379000	-3.14136100	-0.72990900
H	2.82414200	-2.46973700	0.63038200
H	2.74555800	-1.67847000	-0.94655400
C	3.16261200	2.16022700	0.12100200
H	3.77551200	3.05814000	-0.02273000

H	2.79244600	2.17347100	1.15254100
C	1.27616200	0.79577200	-0.78882200
O	1.35441600	0.07210200	-1.78769100
C	-2.59329600	-2.93273000	0.43503100
C	-1.86843200	-1.91164500	-0.17038600
C	-0.61150800	-2.10377200	-0.73416900
C	-0.07555300	-3.39426800	-0.67821600
C	-0.77389900	-4.44027300	-0.07276100
C	-2.03565200	-4.21073000	0.48323200
H	-3.56842100	-2.71536300	0.85628500
H	-0.05581200	-1.29939200	-1.21568400
H	0.90321200	-3.56905300	-1.11215800
H	-0.33959800	-5.43463900	-0.03744400
H	-2.58774200	-5.02162600	0.94805400
S	-2.93092400	0.18241700	-1.41578100
O	-3.38070900	1.47280500	-0.92438200
O	-2.00667100	0.02729700	-2.52192100
C	-4.46341800	-0.80658600	-1.82762700
F	-5.15800600	-0.14344200	-2.74867900
F	-5.20538700	-0.95781700	-0.72806900
F	-4.11799900	-2.00380200	-2.29690000
O	-2.44333300	-0.61943500	-0.08396700

TS25_b

Cu	0.01401500	0.27821300	0.36488000
B	3.29854100	1.04827000	-0.67371400
C	1.09905100	1.82087000	-1.78901000
C	1.73495700	0.26000900	3.36608700
O	4.10171700	0.58174100	-1.67390400
O	3.43442100	0.34218900	0.50164300
C	-0.21235400	1.18259400	2.13306900
N	0.52779400	1.07336400	3.26895100
N	-1.25286100	1.97995800	2.48638300
C	-0.04585900	1.77777100	4.31529300
C	-1.17382400	2.35277600	3.81689100
C	4.96383200	-0.44927000	-1.11616300
C	4.20370400	-0.86177700	0.20047400
C	-2.33810100	2.35376100	1.57993500
H	0.39654600	1.82093000	5.29763500
H	-1.90566600	2.99356500	4.28208700
H	-2.65230400	3.37500300	1.80032900
H	-3.17901900	1.66630200	1.67695300
H	-1.97477300	2.30940900	0.55701300
H	1.47815100	-0.77600000	3.60820600
H	2.37805400	0.66440100	4.15031200
H	2.26350500	0.28865700	2.41265500
C	-0.13341900	2.70135200	-1.67026800
C	-0.10149500	3.97105500	-1.07957500

C	-1.25985400	4.74531300	-0.98962900
C	-2.47496300	4.25436800	-1.46983100
C	-1.36055800	2.22164300	-2.15587300
C	-2.52260100	2.98547700	-2.04918400
H	0.83132700	4.36474200	-0.69109600
H	-3.46303200	2.57283900	-2.39771500
H	1.46419900	1.82719600	-2.82395800
H	-1.21116000	5.73234100	-0.53803600
H	-3.37789900	4.85193700	-1.38664300
H	-1.41949000	1.23415300	-2.60032200
C	6.31906100	0.21305000	-0.85562000
H	7.05694000	-0.50779400	-0.49230700
H	6.68705000	0.64279600	-1.79063700
H	6.22998100	1.02087800	-0.12402900
C	5.10127000	-1.56409100	-2.14598300
H	5.62439400	-1.18474300	-3.02773600
H	5.68032400	-2.39885500	-1.73811200
H	4.12432200	-1.93125300	-2.46226400
C	5.10335300	-1.16791500	1.39213900
H	4.48823900	-1.42973200	2.25810000
H	5.75322300	-2.02100400	1.17385100
H	5.72643800	-0.31358700	1.66097300
C	3.19113200	-1.98910800	-0.00506400
H	3.69197900	-2.94606200	-0.17597200
H	2.57373200	-2.08662900	0.89074400
H	2.52454600	-1.78706300	-0.84381700
C	2.26309200	2.21688500	-0.84108800
H	2.75035600	3.11398800	-1.23992000
H	1.85716400	2.47076200	0.14396800
C	0.70255700	0.34024900	-1.48192200
O	0.91695800	-0.51872900	-2.30756600
C	-0.42506000	-2.22360200	1.57350500
C	-0.60215700	-1.75182700	0.27284100
C	-0.40707400	-2.52267100	-0.86167300
C	0.17242300	-3.78157400	-0.67484100
C	0.47216000	-4.25571000	0.60453500
C	0.17123400	-3.47663500	1.72699800
H	-0.72668400	-1.62510400	2.42470900
H	-0.63912200	-2.14076700	-1.84514600
H	0.38177600	-4.39350800	-1.54739000
H	0.90925200	-5.24110600	0.72991100
H	0.37051800	-3.85114000	2.72717700
S	-3.23614900	-0.62198600	-0.72312000
O	-4.17167700	0.47492600	-0.46476400
O	-2.64828700	-0.76967000	-2.05597700
C	-4.19659800	-2.18581300	-0.42668600
F	-5.16862200	-2.29190200	-1.33706100
F	-4.74148200	-2.16379100	0.79415000

F	-3.39091800	-3.24922500	-0.52246800
O	-2.19468300	-0.69862900	0.42211700
17_b			
Cu	-1.83795600	0.43075900	0.85347400
B	4.35788500	0.50497400	-0.63004000
C	1.93362500	0.42258000	-1.47088400
C	-0.06359400	3.40241000	1.47068700
O	5.06218500	-0.25009700	-1.52194800
O	4.79560200	0.37654000	0.66432700
C	-2.20252100	2.33234200	0.79538800
N	-1.44078800	3.43718900	1.00779900
N	-3.39746900	2.82776900	0.37099100
C	-2.13346500	4.59723400	0.69994600
C	-3.37162800	4.20929600	0.29460500
C	6.17705300	-0.85695500	-0.80634700
C	5.71750000	-0.75590200	0.69778000
C	-4.52366200	1.99468300	-0.04524300
H	-1.69779100	5.57767300	0.80693400
H	-4.22348200	4.78688400	-0.02713200
H	-4.50167300	1.83036900	-1.12419100
H	-5.45692400	2.48466200	0.23954800
H	-4.44844700	1.02443500	0.44245100
H	0.03630900	3.96364300	2.40402200
H	0.59808700	3.82671700	0.71224800
H	0.21216500	2.36420200	1.64067700
C	0.61481500	1.13186900	-1.75975100
C	0.51441000	2.52450100	-1.83971700
C	-0.69139500	3.13520800	-2.19364300
C	-1.81703600	2.36064700	-2.46373800
C	-0.53003300	0.36184200	-2.02377000
C	-1.73732000	0.96916200	-2.37149800
H	1.38473000	3.14280900	-1.64909800
H	-2.60837800	0.35057400	-2.55868900
H	2.25876800	-0.07339600	-2.39226200
H	-0.74686300	4.21805700	-2.25735300
H	-2.75283800	2.83703700	-2.74044000
H	-0.49188000	-0.72220300	-1.97706300
C	7.40995500	-0.00782000	-1.12452600
H	8.31472500	-0.42835500	-0.67689700
H	7.54415200	0.02582600	-2.20859300
H	7.28774300	1.01775300	-0.76555200
C	6.35638800	-2.27867600	-1.32374400
H	6.66312500	-2.25080300	-2.37260900
H	7.13135400	-2.80286100	-0.75551100
H	5.42533200	-2.84243400	-1.25720600
C	6.82972000	-0.44255300	1.69081200
H	6.41059300	-0.36828500	2.69791000

H	7.57769200	-1.24144000	1.69342000
H	7.32626200	0.50076400	1.45877600
C	4.90492100	-1.96363800	1.17308300
H	5.54008600	-2.84554400	1.29351200
H	4.45784800	-1.72761200	2.14242200
H	4.09629400	-2.20647900	0.48080900
C	3.09111000	1.34968300	-1.02050200
H	3.32757600	2.01577400	-1.85792600
H	2.77385000	1.98215500	-0.18598800
C	1.71936700	-0.75626200	-0.50986500
O	1.97531800	-1.89378600	-0.86776800
C	1.75086900	0.24447000	1.84226600
C	1.13207800	-0.53839300	0.85945600
C	-0.04232000	-1.25037300	1.17282900
C	-0.61955400	-1.12227800	2.44487800
C	-0.00386000	-0.32259100	3.41759600
C	1.18785000	0.33651800	3.11913300
H	2.69603800	0.73094900	1.63841900
H	-0.48902800	-1.90656000	0.43138300
H	-1.53061200	-1.66778100	2.66662200
H	-0.44574100	-0.23647700	4.40536800
H	1.68648900	0.92901500	3.88057500
S	-3.39854700	-1.77294600	-0.61993000
O	-4.29016600	-0.99699600	-1.49837000
O	-2.16039700	-2.30576100	-1.21696300
C	-4.37589700	-3.26376300	-0.11106000
F	-4.67800600	-4.00208100	-1.18383100
F	-5.51255700	-2.89147300	0.49195500
F	-3.66287200	-4.01216200	0.74179700
O	-3.16792000	-1.12009100	0.72870900

COM_{5-R₃}

Cu	-1.32528500	-0.04918400	1.32261500
B	-2.67798100	1.22796200	-0.96555300
C	-0.62768100	2.55038700	-0.83426100
C	1.32370100	1.81213900	2.29261100
O	-2.80323300	0.22918300	0.20591100
O	-3.97189400	1.15652600	-1.57579200
C	0.22774300	-0.42845800	2.34810000
N	1.28003700	0.38646100	2.60852800
N	0.62825000	-1.65403500	2.78568100
C	2.33198100	-0.31745400	3.16704400
C	1.91970000	-1.60837700	3.28483300
C	-4.16120400	-0.24426000	0.28879200
C	-4.62698400	-0.04644100	-1.19697700
C	-0.21649800	-2.84067500	2.77266600
H	-0.96843300	-2.72378000	1.99268800

H	-0.71014800	-2.97207000	3.73979700
H	0.38883500	-3.71747100	2.54301000
H	0.36470500	2.10317100	1.87112500
H	2.10118400	2.00883700	1.55543400
H	1.51234600	2.38541800	3.20325000
C	0.41499600	3.49959200	-0.45745600
C	1.77136100	3.32555200	-0.81410800
C	2.75236400	4.20775700	-0.37815400
C	2.42041400	5.30343800	0.42692100
C	0.09877900	4.61624100	0.34128800
C	1.08515200	5.50123800	0.77730300
H	2.06482600	2.47702800	-1.42066800
H	0.80519200	6.35078200	1.39475700
H	3.78697000	4.03593500	-0.66271500
H	3.18941800	5.98972300	0.76842500
H	-0.93563600	4.78257400	0.62272000
C	-4.91198200	0.66166100	1.26893500
H	-5.93756400	0.31935300	1.43592800
H	-4.38689400	0.65773500	2.22985300
H	-4.93684500	1.68673500	0.89358000
C	-4.15878700	-1.68622300	0.78606700
H	-3.81613600	-1.72082900	1.82682000
H	-5.16638000	-2.11303200	0.75246800
H	-3.49445800	-2.30990900	0.18533500
C	-6.13403700	0.14872300	-1.35037900
H	-6.37751900	0.27174600	-2.40934300
H	-6.68893600	-0.71660500	-0.97139100
H	-6.46975000	1.04356800	-0.82388000
C	-4.15565000	-1.19114300	-2.10994600
H	-4.68764200	-2.12752200	-1.90972800
H	-4.34124800	-0.90185300	-3.14729600
H	-3.08188900	-1.35038300	-1.99950500
C	-2.09988900	2.66933800	-0.48787000
H	-2.27449200	2.85204400	0.58184100
H	-2.56649100	3.50643600	-1.02609000
C	-0.45327600	1.43010000	-1.58003200
O	-1.53249400	0.65924600	-1.80787200
H	0.47133400	1.07682100	-2.02494500
H	2.42272900	-2.48003900	3.67107100
H	3.27164400	0.15107900	3.40970700
C	-0.18258400	-2.16338100	-0.98464000
C	1.07668200	-2.27297200	-0.40344400
C	1.61221800	-3.49107200	0.00455400
C	0.85383800	-4.64576200	-0.20167400
C	-0.41570700	-4.57043200	-0.77596800
C	-0.92853500	-3.33078100	-1.16207100
H	-0.58166200	-1.19799500	-1.28628400
H	2.58927400	-3.53868200	0.46408200

H	1.26192700	-5.60588800	0.09870600
H	-0.99995400	-5.47268200	-0.92567600
H	-1.91206600	-3.25942500	-1.61413000
S	3.31604600	-0.76952700	-0.33941500
O	3.53933700	0.56086700	0.19257500
O	4.11674600	-1.91284900	0.07020300
C	3.42904500	-0.67268400	-2.20214400
F	4.70584500	-0.50313900	-2.53121500
F	2.70948400	0.35393100	-2.65144500
F	2.96869300	-1.80605100	-2.72800700
O	1.72466300	-1.03269800	-0.15999900

TS26_b

Cu	-0.13634700	-0.14986800	0.14788700
B	-3.10088800	-0.14501700	-0.27845400
C	-1.82320100	2.06130000	-0.93057300
C	1.20860100	2.74001000	1.32401300
O	-2.59790200	-1.07135700	0.63193900
O	-3.98769200	-0.71118600	-1.15579500
C	0.24387500	0.52790100	1.95469800
N	0.81497000	1.71281600	2.28323500
N	0.04530700	-0.09599500	3.14522100
C	0.99382600	1.82131700	3.65013100
C	0.50582000	0.67690700	4.19848700
C	-3.28589000	-2.33647100	0.40500100
C	-3.88351900	-2.15226200	-1.04091100
C	-0.58920900	-1.40179900	3.27846300
H	-1.39628600	-1.46458700	2.55001800
H	-0.99264800	-1.49886600	4.28779600
H	0.13126100	-2.20254300	3.09440200
H	0.84786200	2.44604100	0.34219200
H	2.29460000	2.82803400	1.28979700
H	0.75024100	3.69333400	1.59443400
C	-1.66186700	3.51971800	-0.90901900
C	-0.50615600	4.15898300	-1.41849200
C	-0.36043600	5.53969300	-1.36828500
C	-1.35375300	6.34009400	-0.79571600
C	-2.64411000	4.34673700	-0.32571200
C	-2.49384300	5.73102100	-0.27306700
H	0.30084800	3.56940700	-1.83924200
H	-3.27474100	6.33534200	0.17997600
H	0.54186000	5.99378400	-1.76761600
H	-1.23445100	7.41825900	-0.75190500
H	-3.54101500	3.90108300	0.08759500
C	-4.35638400	-2.43739500	1.49532300
H	-4.90172700	-3.38362600	1.43945100
H	-3.87463100	-2.37754000	2.47542200
H	-5.07339300	-1.61584200	1.42010600

C	-2.28355000	-3.47660800	0.53498000
H	-1.93180400	-3.55497400	1.56747100
H	-2.75291900	-4.42986000	0.27176300
H	-1.41883400	-3.32372400	-0.10861700
C	-5.27390200	-2.74953800	-1.23351000
H	-5.61805900	-2.54223900	-2.25006000
H	-5.25229300	-3.83574000	-1.09751300
H	-5.99862300	-2.32287300	-0.53835700
C	-2.94691700	-2.62926400	-2.15424300
H	-2.83798100	-3.71780400	-2.14688100
H	-3.37177800	-2.33116900	-3.11641600
H	-1.96755400	-2.16209700	-2.06341100
C	-2.93804900	1.41838000	-0.12610000
H	-2.82484100	1.67037400	0.93795800
H	-3.89413600	1.86063900	-0.43856900
C	-0.99177700	1.25426700	-1.67548100
O	-1.00098000	-0.06091300	-1.59173400
H	-0.25498600	1.68784600	-2.35666700
H	0.43729600	0.35474800	5.22497700
H	1.43741200	2.69191200	4.10536400
C	0.77969200	-2.38285500	-1.50611500
C	1.11402200	-1.72239600	-0.33193600
C	1.69225300	-2.33036400	0.77276700
C	1.76974700	-3.72786600	0.75397400
C	1.36261800	-4.44881400	-0.37045300
C	0.87903900	-3.77598600	-1.49781100
H	0.40951000	-1.82875700	-2.35855100
H	2.07538200	-1.74357200	1.59706000
H	2.17827100	-4.24324700	1.61862600
H	1.44857300	-5.53058400	-0.38041900
H	0.58055300	-4.33084200	-2.38252000
S	3.30658900	0.47194100	-0.27555600
O	3.63434800	1.83148500	-0.71239100
O	3.36997700	0.16514000	1.16022200
C	4.56856200	-0.63493900	-1.07160900
F	5.78200900	-0.34687300	-0.59073800
F	4.56813300	-0.45858000	-2.39510700
F	4.29190300	-1.91855500	-0.80562700
O	2.00460000	-0.01196900	-0.94273700

18_b

Cu	0.07804900	-0.24213600	0.03467800
B	-2.88427200	1.21192400	-0.30371800
C	-0.45702700	2.16330100	-0.69399400
C	2.28999400	1.62256500	1.91579700
O	-3.30843400	0.14216200	0.45619800
O	-3.71872300	1.48308900	-1.35511000
C	0.30819200	0.08074400	1.95361500

N	1.26112100	0.81936300	2.57301700
N	-0.42887800	-0.45895800	2.96074800
C	1.13782400	0.73110400	3.94663000
C	0.07154600	-0.07460200	4.19213800
C	-4.64822400	-0.20612400	-0.00537900
C	-4.66843500	0.38783100	-1.46128800
C	-1.58475600	-1.34288000	2.80551000
H	-2.17017800	-1.02325600	1.94552400
H	-2.19400400	-1.26079400	3.70764600
H	-1.25543900	-2.37408000	2.67027400
H	2.11475100	1.60410800	0.84784600
H	3.27207000	1.19600600	2.11554800
H	2.22592900	2.65356100	2.27006400
C	0.53745600	3.23362400	-0.56988500
C	1.83245600	3.09248100	-1.12299600
C	2.79668300	4.07649300	-0.94283900
C	2.50363900	5.22877000	-0.20882500
C	0.26546400	4.39705300	0.17900300
C	1.23365800	5.38204000	0.35172100
H	2.11598700	2.17061700	-1.61406300
H	0.99683600	6.27093100	0.92896400
H	3.79016200	3.92046300	-1.35033300
H	3.26123100	5.99270600	-0.06289800
H	-0.70987700	4.53367800	0.63076900
C	-5.61931900	0.49793200	0.94758400
H	-6.65945800	0.24776400	0.72201600
H	-5.40235700	0.18070000	1.97111500
H	-5.50333600	1.58379000	0.89626400
C	-4.83491700	-1.71483300	0.08027900
H	-4.77119100	-2.03777400	1.12339700
H	-5.82136000	-1.99692500	-0.30076200
H	-4.07670600	-2.25271100	-0.48612700
C	-6.01423300	0.95838100	-1.89517800
H	-5.92505000	1.37492300	-2.90173600
H	-6.77666300	0.17315800	-1.91927500
H	-6.35114500	1.75387100	-1.22895100
C	-4.13352900	-0.57228000	-2.52633300
H	-4.80724700	-1.42085000	-2.67488400
H	-4.04775000	-0.03182100	-3.47248100
H	-3.13807100	-0.93504100	-2.26819000
C	-1.74067900	2.21809500	0.11299700
H	-1.53239800	2.15482000	1.18627800
H	-2.17314400	3.21550600	-0.05061600
C	-0.30011400	1.17120700	-1.67602300
O	-0.94637100	0.04682300	-1.61724800
H	0.45773100	1.27857900	-2.45292900
H	-0.37566900	-0.39810000	5.11793400
H	1.80525800	1.25155500	4.61414900

C	-1.28619800	-2.72874700	-0.41846000
C	-0.16501300	-2.17068700	0.17460600
C	0.79671400	-2.92712000	0.82862700
C	0.60263900	-4.31290000	0.90336200
C	-0.52819500	-4.90271600	0.33567100
C	-1.46742200	-4.11413200	-0.33049200
H	-2.00164500	-2.10957800	-0.94119600
H	1.68671200	-2.46694200	1.24407900
H	1.34705400	-4.92565600	1.40447200
H	-0.67146000	-5.97720900	0.40257400
H	-2.33946300	-4.57043500	-0.79212100
S	3.42040300	-0.46890100	-0.42280700
O	4.44009900	0.56528500	-0.64768300
O	3.37266500	-1.07160200	0.92776300
C	3.86328400	-1.87840200	-1.54314100
F	5.05677300	-2.38309100	-1.20517300
F	3.91544000	-1.46507000	-2.81611500
F	2.94541400	-2.85167800	-1.44745600
O	2.06427700	-0.07979200	-0.95371800

IMes'CuCl_{sol}

C	2.92797600	0.67944500	0.00020100
C	2.92803100	-0.67929900	0.00024300
N	1.59968800	-1.07375100	0.00008000
N	1.59960100	1.07378900	0.00006700
C	0.76355100	-0.00001600	0.00009700
C	1.14837700	2.46003700	-0.00019300
H	1.51074700	2.97561800	-0.89322100
H	0.05850700	2.46206500	0.00025700
H	1.51149500	2.97614900	0.89222100
C	1.14856800	-2.46003300	0.00013400
H	0.05869900	-2.46214000	-0.00063900
H	1.51199200	-2.97608400	-0.89219100
H	1.51071100	-2.97562100	0.89325000
Cu	-1.15603400	-0.00003700	-0.00004200
Cl	-3.29502600	-0.00001100	-0.00017200
H	3.74206200	1.38667400	0.00022200
H	3.74217400	-1.38646300	0.00032600

NaO'Bu_{sol}

Na	-2.73314100	-0.00006600	-0.00228700
O	-0.75125900	-0.00403000	-0.00970500
C	0.62156200	-0.00009400	-0.00032300
C	1.16920000	0.26532900	-1.42418500
H	0.79691300	1.23071500	-1.78595000
H	2.26597200	0.28001700	-1.46763600
H	0.80797400	-0.51243700	-2.10692100
C	1.15762200	-1.36777700	0.48885300

H	2.25393000	-1.41667200	0.51650700
H	0.77791300	-1.57074400	1.49696500
H	0.79392200	-2.16151100	-0.17403000
C	1.14897700	1.10600400	0.94611800
H	0.77619500	2.08144000	0.61270100
H	0.77257400	0.93057600	1.96059800
H	2.24507100	1.15081600	0.98777800

NaCl_{sol}

Na	0.00000000	0.00000000	-1.50216700
Cl	0.00000000	0.00000000	0.97199000

B₂pin_{2sol}

B	-0.84986300	0.00000100	0.00000100
C	-2.99632000	-0.76816300	0.09531000
O	-1.60474100	-1.13827900	0.13359600
C	-2.99632100	0.76816200	-0.09531000
O	-1.60474200	1.13827900	-0.13359600
H	-3.48105300	-1.29613000	-0.73135500
H	-3.47125600	-1.07707300	1.03143400
H	-3.48105400	1.29612800	0.73135500
H	-3.47125700	1.07707300	-1.03143400
B	0.84986300	-0.00000100	-0.00000100
O	1.60474100	1.13828500	0.13354400
O	1.60474100	-1.13828600	-0.13354400
C	2.99632000	0.76815500	0.09536700
C	2.99632100	-0.76815500	-0.09536700
H	3.48114700	1.29618000	-0.73120500
H	3.47116200	1.07698700	1.03156600
H	3.47116100	-1.07698600	-1.03156700
H	3.48114700	-1.29618000	0.73120400

BpinO'Bu_{sol}

C	1.58979400	0.80747700	0.07189900
C	1.97795100	-0.70993800	-0.06004800
O	0.16312600	0.73202200	0.34371300
B	-0.27633700	-0.46940400	-0.18252300
O	0.75389900	-1.29782300	-0.57320500
C	2.26019400	-1.37043900	1.29275300
H	1.46274000	-1.15357800	2.00886200
H	2.30908000	-2.45339500	1.15384800
H	3.20983100	-1.03154000	1.71592100
C	3.10888200	-0.99906000	-1.03906000
H	4.02912800	-0.49726200	-0.72380500
H	3.30214700	-2.07480300	-1.07064300
H	2.85771200	-0.66951900	-2.04821000
C	2.26593500	1.54974900	1.21735800
H	1.92161600	2.58747900	1.23803700

H	2.03354200	1.09495000	2.18142900
H	3.35227100	1.55493700	1.08412900
C	1.75354000	1.58184800	-1.23896300
H	1.28009600	1.05201300	-2.07003900
H	1.27257100	2.55824900	-1.13728300
H	2.80758900	1.73970500	-1.48312800
O	-1.56399100	-0.85796700	-0.32533800
C	-2.71362800	-0.03662800	0.00460700
C	-3.92233800	-0.90363000	-0.34972500
H	-3.90617700	-1.83193000	0.22846500
H	-4.85348900	-0.37264900	-0.13129700
H	-3.90761800	-1.15997000	-1.41289100
C	-2.69806100	0.28298000	1.50304400
H	-3.60074500	0.83513100	1.78218200
H	-2.66945200	-0.64383000	2.08419600
H	-1.82624700	0.88739800	1.76174000
C	-2.69464700	1.23953100	-0.84268300
H	-2.66302300	0.98447100	-1.90640500
H	-3.59738400	1.82966500	-0.65761500
H	-1.82251300	1.85029600	-0.60132500

R_{1(sol)}

C	-0.40725500	-1.28305600	0.00000200
C	0.51473200	-0.22305200	-0.00012300
C	0.01295000	1.09130800	-0.00017400
C	-1.35745800	1.33095900	-0.00005600
C	-2.26240000	0.26454400	0.00010000
C	-1.78102800	-1.04469900	0.00012400
H	-0.03653200	-2.30482100	0.00002300
H	0.69999500	1.93143700	-0.00034600
H	-1.72399000	2.35331300	-0.00010400
H	-3.33125300	0.45520700	0.00018200
H	-2.47387000	-1.88094100	0.00023000
C	1.95266100	-0.53264200	-0.00020200
H	2.18533700	-1.59699000	-0.00067500
C	2.97062200	0.33664700	0.00028000
H	2.82476100	1.41278400	0.00082900
H	3.99860400	-0.01004900	0.00015300

I_{1(sol)}

Cu	0.24266100	-0.02581400	-0.51797800
B	-1.70817300	-0.33969100	-0.04916300
C	1.70914100	-1.09427700	-1.80267900
C	-0.35203300	3.08666200	-1.31540500
O	-2.29992000	-1.37327300	0.66937800
O	-2.69095000	0.55076700	-0.49284900
C	1.12310500	1.65708300	0.07886700

N	0.70865000	2.88764500	-0.33409300
N	2.09091500	1.92798400	0.99540400
C	1.40871100	3.90224200	0.30165000
C	2.28201200	3.29524900	1.14636700
C	-3.69457400	-1.03877100	0.91064900
C	-3.99924900	-0.03561400	-0.24866000
C	2.81898800	0.91453700	1.74760600
H	1.22083000	4.94588400	0.10631300
H	3.00203300	3.70547700	1.83628900
H	2.81135600	1.16994400	2.81008100
H	3.84879200	0.83317100	1.39516100
H	2.32857900	-0.04512600	1.60135300
H	-1.12169600	2.32688100	-1.16302000
H	0.04224700	3.01139900	-2.33295500
H	-0.78757000	4.07755600	-1.17401500
C	2.77815400	-1.46234900	-0.87336200
C	2.57678000	-2.34346400	0.21041600
C	3.61240600	-2.63726600	1.09511700
C	4.87826900	-2.07112000	0.92408500
C	4.06298400	-0.90533800	-1.03397800
C	5.09740600	-1.20695400	-0.15379800
H	1.60089900	-2.79121800	0.36721700
H	6.07830400	-0.76489000	-0.30564800
H	1.98661600	-0.39282600	-2.58552500
H	3.42865000	-3.31384800	1.92506100
H	5.68287600	-2.30487700	1.61433900
H	4.23858000	-0.22387900	-1.86245700
C	-3.76374600	-0.39167200	2.29856800
H	-4.79381500	-0.16772100	2.59288500
H	-3.33730600	-1.08213200	3.03116400
H	-3.18156900	0.53320800	2.32478400
C	-4.51934900	-2.32081100	0.88759700
H	-4.22692200	-2.96231000	1.72392600
H	-5.58705400	-2.09814000	0.98834100
H	-4.36541400	-2.87964900	-0.03684600
C	-4.98072800	1.07830400	0.09876700
H	-5.11460200	1.73434700	-0.76643700
H	-5.96011600	0.66623100	0.36497400
H	-4.62015500	1.68493700	0.93116700
C	-4.42610800	-0.72795500	-1.54778400
H	-5.43602600	-1.14292200	-1.47581700
H	-4.41181500	0.00424700	-2.35992300
H	-3.73308400	-1.53346700	-1.80388500
C	0.43570700	-1.64953600	-1.82672700
H	-0.22354500	-1.44150700	-2.66287800
H	0.17737100	-2.52476900	-1.24167200

Cu	0.47936400	0.27894000	-0.84569100
B	-1.36623600	-0.52967000	-0.40205900
C	1.38814000	-1.37705000	-1.77546800
C	-1.03325200	3.28498700	-0.91084400
O	-1.64251800	-1.13455900	0.81276800
O	-2.52096800	-0.08652200	-1.02627100
C	0.95797300	1.99510000	-0.16620000
N	0.23454700	3.14833800	-0.20586200
N	2.06172700	2.31321700	0.56306900
C	0.87629200	4.16736600	0.48169900
C	2.02593600	3.63578800	0.97565400
C	-3.02952900	-0.84180400	1.14391500
C	-3.66014600	-0.60473600	-0.27004100
C	3.10778200	1.35292400	0.90484500
H	0.46908000	5.16307900	0.55220300
H	2.80872000	4.07542300	1.57260500
H	2.79726400	0.72373400	1.74155900
H	4.01534500	1.89682500	1.16965500
H	3.30157300	0.70853500	0.04815700
H	-1.49899000	2.30054200	-0.98159600
H	-0.87669300	3.68429500	-1.91700000
H	-1.68674100	3.95993900	-0.35411100
C	2.34638200	-1.74254300	-0.75986800
C	1.95677500	-2.06108800	0.57166900
C	2.90539000	-2.32810200	1.55826400
C	4.27211900	-2.30192300	1.27437400
C	3.74198200	-1.74529600	-1.02932000
C	4.67562600	-2.01251300	-0.03842500
H	0.90336700	-2.08446300	0.83390400
H	5.73425200	-2.00050100	-0.28779400
H	1.74646500	-1.20742300	-2.78485800
H	2.56648300	-2.56161200	2.56515200
H	5.00566300	-2.51208500	2.04649000
H	4.07622700	-1.51649900	-2.03886300
C	-3.02066700	0.41739600	2.01688600
H	-4.02399200	0.67266400	2.36971700
H	-2.38306500	0.23800500	2.88634400
H	-2.61235400	1.27021600	1.46799400
C	-3.60540800	-2.02137700	1.91707800
H	-3.09390800	-2.11590600	2.87887800
H	-4.67226700	-1.87160700	2.11250800
H	-3.47753700	-2.95754200	1.37147700
C	-4.78219700	0.42378400	-0.31253400
H	-5.14586500	0.53199200	-1.33817700
H	-5.62207400	0.10456700	0.31313900
H	-4.44219700	1.40141200	0.03313000
C	-4.09046400	-1.90101700	-0.96015000
H	-4.97938600	-2.33241100	-0.49099500

H	-4.32197700	-1.68667000	-2.00671000
H	-3.28841700	-2.64355800	-0.93310900
C	-0.05630900	-1.54801900	-1.56471000
H	-0.64414400	-1.49383100	-2.47942700
H	-0.34980400	-2.40152400	-0.94829600

3_(sol)

Cu	0.60516800	0.65781800	-1.20743800
B	-1.02054900	-1.86631400	-0.92711600
C	1.24729800	-1.10657200	-1.86035900
C	-1.62214000	3.28867800	-1.46596800
O	-1.20196400	-2.51524400	0.27684200
O	-1.92856100	-0.83455800	-1.09369900
C	0.21112000	2.23796200	-0.15738300
N	-0.73596500	3.20194300	-0.31226000
N	0.80992400	2.54754400	1.02630800
C	-0.73235900	4.09330400	0.74990700
C	0.24412600	3.67583400	1.59880500
C	-2.06987200	-1.68572300	1.09387000
C	-2.87247000	-0.88579600	0.00892700
C	1.85990900	1.74235800	1.64693300
H	-1.40621300	4.93326600	0.80438500
H	0.58025400	4.07789500	2.54119300
H	1.44033000	1.11132500	2.43449600
H	2.61860400	2.40087900	2.07414000
H	2.31665500	1.10514500	0.88998100
H	-1.53999800	2.35694800	-2.02476300
H	-1.33660500	4.12714400	-2.10667600
H	-2.65361900	3.42078700	-1.13216900
C	2.27420400	-1.29175000	-0.80373700
C	2.05274200	-2.02098100	0.38791600
C	3.00956900	-2.06671900	1.40349400
C	4.23204300	-1.40577500	1.27518000
C	3.53606100	-0.65407000	-0.92279000
C	4.48787400	-0.70484100	0.08910900
H	1.11187300	-2.53850000	0.52954100
H	5.43997600	-0.19697500	-0.04697500
H	1.74055300	-0.98615700	-2.83052800
H	2.79359800	-2.63289500	2.30710400
H	4.97314200	-1.44470100	2.06792500
H	3.74785600	-0.09288400	-1.83088500
C	-1.15300200	-0.79327900	1.93889100
H	-1.72455200	-0.17279600	2.63512100
H	-0.47309600	-1.42733000	2.51302500
H	-0.54828000	-0.14226200	1.30196700
C	-2.91072600	-2.58537700	1.98996200
H	-2.26146100	-3.10931800	2.69674800
H	-3.63138600	-1.99429300	2.56416000

H	-3.45395300	-3.33297200	1.41001500
C	-3.23940200	0.53865100	0.40813600
H	-3.78655600	1.01928800	-0.40791400
H	-3.88379200	0.53769300	1.29300200
H	-2.35007400	1.13229200	0.62026100
C	-4.10802200	-1.63440800	-0.49901100
H	-4.90054100	-1.66225200	0.25417700
H	-4.49170900	-1.12354700	-1.38608200
H	-3.85609600	-2.66058500	-0.77935700
C	0.12083100	-2.17257900	-1.95196800
H	-0.30476700	-2.11733400	-2.96143600
H	0.51250500	-3.19451000	-1.82211800

6_{a(sol)}

P	-2.03782400	0.08687000	-0.41027700
C	-1.95465100	0.11220900	-2.25135600
H	-1.77443600	-0.93498800	-2.51583300
H	-2.93868600	0.38589300	-2.64805000
C	-0.86736100	1.00127300	-2.87847300
H	-1.04956500	1.00748900	-3.96184600
H	-0.97046600	2.03785100	-2.55054200
C	0.58594800	0.53967900	-2.66344700
H	1.25656700	1.09339100	-3.32725900
H	0.68087900	-0.52709000	-2.88964200
P	1.19042000	0.76951400	-0.93211200
C	-3.47852800	-0.98564400	-0.05493300
C	-4.78306500	-0.48676500	-0.18325600
C	-3.28632800	-2.31892400	0.32678300
C	-5.87646100	-1.31683500	0.05762600
H	-4.94369400	0.55048500	-0.46048100
C	-4.38510000	-3.14573100	0.56943000
H	-2.27762100	-2.72630200	0.39312400
C	-5.68157100	-2.64725500	0.43386800
H	-6.88396600	-0.91812000	-0.04300200
H	-4.22421200	-4.17871800	0.85525300
H	-6.53461200	-3.28528700	0.62413600
C	-2.59220300	1.74135200	0.13055300
C	-2.99991600	2.74106900	-0.75688200
C	-2.59995400	2.01025900	1.50777400
C	-3.37254400	4.00146900	-0.28370700
H	-3.02366000	2.54946800	-1.82340300
C	-2.98848900	3.26067700	1.98557700
H	-2.28114100	1.24661800	2.21142900
C	-3.36608500	4.26747600	1.08454900
H	-3.66862900	4.77286800	-0.98782400
H	-2.98818500	3.45947800	3.05294300
H	-3.65460100	5.24177600	1.44995200
C	2.97740600	0.41395400	-0.97659300

C	3.42856400	-0.78623000	-1.54005900
C	3.89136200	1.27486900	-0.34549600
C	4.78130100	-1.11660400	-1.48385000
H	2.72001700	-1.48593900	-1.97428700
C	5.24240500	0.93360000	-0.29223300
H	3.54236800	2.19534500	0.10740000
C	5.69081600	-0.25878800	-0.86144600
H	5.12173300	-2.05128200	-1.91898700
H	5.94330600	1.60069700	0.20054700
H	6.74337400	-0.52193300	-0.81524200
C	1.06047500	2.57849800	-0.67275000
C	1.52998500	3.49841500	-1.62663900
C	0.45356900	3.04940000	0.49379100
C	1.37211700	4.87163700	-1.41204300
H	2.01738600	3.15321200	-2.53319600
C	0.30038000	4.41758800	0.70755700
H	0.09637200	2.33641400	1.22464900
C	0.75302100	5.33196600	-0.24342000
H	1.72936400	5.57671300	-2.15028100
H	-0.19031600	4.76947300	1.61125000
H	0.63119600	6.39738700	-0.08419100
Pd	-0.01895100	-0.55088800	0.62755400
C	2.61958300	-1.77036500	1.63172000
C	1.72459600	-0.73082400	1.85914800
C	1.95879600	0.25521900	2.81962300
C	3.25598400	0.37945400	3.33507600
C	4.23792400	-0.54084700	2.95045200
C	3.91320600	-1.64790000	2.16214400
H	2.35559300	-2.57021700	0.94460900
H	3.50757400	1.19917400	4.00358100
H	5.25647300	-0.41349200	3.29842000
H	4.68089500	-2.37979600	1.91216500
I	0.26575800	-3.07865400	-1.18714700
H	1.18991300	0.99015200	3.05450000
C	-0.60254600	-1.52607000	2.21497200
O	-0.71602800	-2.14273500	3.19246500

TS6_{a(sol)}

P	-2.03782400	0.08047000	-0.38467700
C	-1.94185100	0.10580900	-2.23215600
H	-1.76163600	-0.94138800	-2.49663300
H	-2.93228600	0.37309300	-2.61605000
C	-0.86736100	1.00127300	-2.87847300
H	-1.06876500	1.00748900	-3.95544600
H	-0.97686600	2.03785100	-2.54414200
C	0.59234800	0.55247900	-2.68904700
H	1.24376700	1.10619100	-3.37205900
H	0.69367900	-0.51429000	-2.90884200

P	1.19042000	0.78231400	-0.95771200
C	-3.48492800	-0.98564400	-0.04853300
C	-4.78946500	-0.48676500	-0.18325600
C	-3.28632800	-2.31892400	0.33318300
C	-5.88286100	-1.31683500	0.05762600
H	-4.95009400	0.55048500	-0.46048100
C	-4.38510000	-3.14573100	0.56943000
H	-2.27762100	-2.70710200	0.42512400
C	-5.68157100	-2.64725500	0.43386800
H	-6.89036600	-0.92452000	-0.04300200
H	-4.22421200	-4.17871800	0.86165300
H	-6.53461200	-3.29168700	0.62413600
C	-2.59860300	1.74135200	0.13695300
C	-2.99991600	2.74106900	-0.75688200
C	-2.59995400	2.01665900	1.51417400
C	-3.37254400	4.00146900	-0.28370700
H	-3.02366000	2.54946800	-1.82340300
C	-2.98848900	3.26707700	1.98557700
H	-2.28114100	1.24661800	2.21142900
C	-3.36608500	4.26747600	1.08454900
H	-3.66862900	4.77286800	-0.98782400
H	-2.98818500	3.46587800	3.05294300
H	-3.65460100	5.24817600	1.44995200
C	2.97740600	0.42035400	-0.98299300
C	3.42856400	-0.78623000	-1.54005900
C	3.89136200	1.27486900	-0.35189600
C	4.78130100	-1.11660400	-1.48385000
H	2.72001700	-1.47953900	-1.98068700
C	5.24240500	0.93360000	-0.29223300
H	3.54876800	2.20174500	0.09460000
C	5.69081600	-0.25878800	-0.86144600
H	5.12173300	-2.05128200	-1.91898700
H	5.94330600	1.60069700	0.20054700
H	6.74337400	-0.52193300	-0.81524200
C	1.06687500	2.58489800	-0.68555000
C	1.52998500	3.51121500	-1.63303900
C	0.45996900	3.04940000	0.48739100
C	1.37211700	4.87803700	-1.41204300
H	2.01738600	3.16601200	-2.53959600
C	0.30038000	4.41758800	0.70755700
H	0.09637200	2.33001400	1.21184900
C	0.75302100	5.33196600	-0.24342000
H	1.72936400	5.58951300	-2.15028100
H	-0.19031600	4.76307300	1.61125000
H	0.62479600	6.39738700	-0.07779100
Pd	-0.01255100	-0.54448800	0.60195400
C	2.52998300	-1.82796500	1.70852000
C	1.55179600	-0.90362400	2.08954800

C	1.88199600	0.19761900	2.89002300
C	3.20478400	0.38585400	3.29027600
C	4.18672400	-0.52804700	2.89925200
C	3.84920600	-1.63510000	2.11734400
H	2.25959300	-2.65981700	1.06620900
H	3.46917400	1.24397400	3.90118100
H	5.21807300	-0.37509200	3.20242000
H	4.61689500	-2.33499600	1.80336500
I	0.26575800	-3.07865400	-1.18714700
H	1.11311300	0.90055200	3.19530000
C	-0.25694600	-1.47487000	2.24697200
O	-0.65842800	-2.09793500	3.14766500

$7_{a(sol)}$

P	1.24398500	0.84131900	1.17131500
C	0.57833600	1.60839600	2.72440000
H	0.61122200	0.80560300	3.46911300
H	1.29999300	2.36413200	3.05183700
C	-0.83138300	2.21892000	2.67696900
H	-0.99506900	2.71326200	3.64141300
H	-0.87773000	3.00734700	1.92075000
C	-1.98924700	1.23788600	2.45143900
H	-2.93990500	1.73272200	2.67290100
H	-1.91110600	0.38428000	3.13394600
P	-2.07031900	0.51412200	0.74061600
C	2.95033700	0.42157300	1.68442300
C	4.07577500	1.03490500	1.12107700
C	3.12225600	-0.58299000	2.64954100
C	5.35645900	0.64898200	1.51863800
H	3.95428400	1.80237000	0.36558500
C	4.40231300	-0.96005800	3.04879700
H	2.25926700	-1.09539100	3.06143300
C	5.52264600	-0.34667500	2.48147000
H	6.22328600	1.12518200	1.07077400
H	4.52512100	-1.74217000	3.79138000
H	6.51993900	-0.64869300	2.78630600
C	1.44592600	2.20550100	-0.02849200
C	1.29877100	3.55637400	0.31066300
C	1.76599600	1.86359800	-1.35185500
C	1.44272600	4.54539700	-0.66360600
H	1.07427600	3.84971300	1.32916300
C	1.93761300	2.85405900	-2.31478800
H	1.88212100	0.82114700	-1.62379000
C	1.76312100	4.19768700	-1.97575000
H	1.30897100	5.58809700	-0.39297200
H	2.19399100	2.57394100	-3.33193500
H	1.87746200	4.96990400	-2.73020600
C	-3.70782400	-0.29536600	0.77545600

C	-3.81859500	-1.50166700	1.48351500
C	-4.83446200	0.23348100	0.13526400
C	-5.04710600	-2.15124000	1.57567500
H	-2.93804100	-1.94328700	1.94016800
C	-6.06110700	-0.42812400	0.21829500
H	-4.75587700	1.15513300	-0.43086100
C	-6.17114900	-1.61555500	0.94210700
H	-5.12267800	-3.08480700	2.12457300
H	-6.92939200	-0.01466000	-0.28608700
H	-7.12601800	-2.12877100	1.00373100
C	-2.23977100	1.97336400	-0.34392800
C	-2.94393600	3.12924500	0.02746400
C	-1.58493400	1.93914300	-1.58254500
C	-2.98303800	4.23281000	-0.82390100
H	-3.46247800	3.17136300	0.98019900
C	-1.62850400	3.04169500	-2.43462000
H	-1.03076700	1.04897000	-1.86109800
C	-2.32316900	4.19029900	-2.05450800
H	-3.52647900	5.12482000	-0.52728200
H	-1.10660700	3.00817400	-3.38507100
H	-2.34915900	5.05287400	-2.71350800
Pd	-0.09880000	-0.84173900	0.28293600
C	2.10975300	-1.51752200	-2.22580000
C	2.50251300	-1.88697500	-0.93331300
C	3.86470600	-2.00653900	-0.62398400
C	4.82546200	-1.73362500	-1.59525000
C	4.43212800	-1.37289800	-2.88629600
C	3.07387300	-1.27822700	-3.20364000
H	1.05110900	-1.43811900	-2.45018700
H	5.88007900	-1.80016200	-1.34518400
H	5.18190400	-1.16649100	-3.64443100
H	2.76731100	-1.01270500	-4.21096100
I	-1.41897800	-2.69921600	-1.20491200
H	4.15202000	-2.28160400	0.38451800
C	1.51082500	-2.07124400	0.16947400
O	1.69384000	-2.85037800	1.08221800

COM_{R3-Pd(dppp)(sol)}

P	-2.56929400	0.75001300	-0.11527000
C	-2.71283800	2.60324900	-0.07573600
H	-2.95757700	2.89408000	-1.10395800
H	-3.57254300	2.89564400	0.53793600
C	-1.45260000	3.35225300	0.39593900
H	-1.74184100	4.39827800	0.55051800
H	-1.14202300	2.98423400	1.37972000
C	-0.24600000	3.34981100	-0.56376500
H	0.39525300	4.20008800	-0.31015300
H	-0.58216300	3.48474900	-1.59816300

P	0.78526400	1.79325400	-0.51358800
Pd	-0.58302000	-0.02808400	-1.07014700
C	-4.26147600	0.26785300	-0.65000400
C	-5.35130200	0.20256300	0.22941300
C	-4.45480800	-0.05312900	-2.00130900
C	-6.61148700	-0.17213000	-0.23714600
H	-5.21034100	0.43404800	1.28068500
C	-5.71730500	-0.41755300	-2.47003900
H	-3.60596200	-0.02367100	-2.67875600
C	-6.79728900	-0.48005000	-1.58698600
H	-7.44866000	-0.22574500	0.45274400
H	-5.85589700	-0.66234000	-3.51899600
H	-7.77843400	-0.77413000	-1.94748000
C	-2.52237400	0.25766600	1.65390000
C	-2.82187500	1.11478300	2.72081500
C	-2.04782600	-1.03625000	1.93486700
C	-2.63475400	0.69640700	4.04061400
H	-3.18529600	2.11923500	2.53224100
C	-1.87230700	-1.45637000	3.25131600
H	-1.79331800	-1.70005200	1.11297700
C	-2.15705300	-0.58670600	4.30845000
H	-2.85719100	1.37641800	4.85749100
H	-1.49810200	-2.45557400	3.45280300
H	-2.00492300	-0.90799200	5.33439900
C	2.19753800	2.18902000	-1.62455400
C	2.52967200	3.48092000	-2.05771000
C	2.97641300	1.10773900	-2.06868100
C	3.61972000	3.68606800	-2.90659600
H	1.94418400	4.33571800	-1.73749500
C	4.07353000	1.31422300	-2.90216800
H	2.71480700	0.10343900	-1.75429700
C	4.39658300	2.60571800	-3.32604200
H	3.86212600	4.69193900	-3.23692100
H	4.67023300	0.46709100	-3.22689800
H	5.24523400	2.76770400	-3.98374000
C	1.51810600	1.95401200	1.17017400
C	2.68496200	2.68776200	1.42527100
C	0.87064900	1.31448400	2.23757200
C	3.19083100	2.78001300	2.72231600
H	3.20771800	3.17524300	0.60870800
C	1.37030000	1.41716700	3.53585100
H	-0.01411500	0.71998700	2.04894400
C	2.53459100	2.14740800	3.78085100
H	4.10097200	3.34370000	2.90585900
H	0.85163800	0.91602700	4.34757600
H	2.93298600	2.21842200	4.78859700
C	0.89977700	-2.76008500	-1.28981700
C	0.38519800	-1.77877400	-2.17990200

C	0.12074300	-3.70038500	-0.66302600
C	-1.02796800	-1.79049300	-2.39934300
H	1.06660900	-1.28367200	-2.86188100
C	-1.27915300	-3.69063300	-0.90122100
H	0.56191700	-4.44416500	-0.01508600
C	-1.83935200	-2.76800900	-1.75460700
H	-1.43505200	-1.24601500	-3.24628200
H	-1.89836800	-4.43416100	-0.40999300
H	-2.90760500	-2.76813000	-1.94638100
S	3.15599000	-3.04994500	0.16683400
O	2.65149600	-4.22296400	0.86580200
O	4.54899500	-2.92444900	-0.21960000
C	2.72604600	-1.57087300	1.22495700
F	3.29729800	-1.73144400	2.41609300
F	1.40508300	-1.49149600	1.36860200
F	3.19845800	-0.47373900	0.64456400
O	2.32330700	-2.72688500	-1.18741600

TS6_{b(sol)}

P	-1.65239900	1.23309000	-0.77212400
C	-1.13605100	2.42401200	-2.10363500
H	-1.23774200	1.87719600	-3.04704200
H	-1.86577500	3.23945500	-2.14350200
C	0.28826100	3.00107700	-1.98765800
H	0.32893300	3.88217400	-2.63831300
H	0.46891800	3.37357400	-0.97357500
C	1.44362000	2.07308100	-2.40629600
H	2.33133100	2.68823000	-2.58719700
H	1.20155500	1.55846200	-3.34316600
P	1.85719400	0.76922400	-1.14535700
Pd	-0.09312700	-0.47685500	-0.52016200
C	-3.38175900	0.86777400	-1.24115800
C	-4.46933000	1.11522600	-0.39183900
C	-3.60731000	0.21977700	-2.46679800
C	-5.75490800	0.72252700	-0.76236500
H	-4.30988800	1.61163200	0.55902400
C	-4.89444000	-0.15549700	-2.84163300
H	-2.77017400	-0.01216100	-3.11893000
C	-5.97129700	0.08592500	-1.98554100
H	-6.58932200	0.91624400	-0.09464900
H	-5.05546100	-0.65434300	-3.79271100
H	-6.97341100	-0.21882300	-2.27181600
C	-1.79103300	2.26705000	0.73528400
C	-1.72915000	3.66691700	0.73272500
C	-1.87544400	1.59604100	1.96721700
C	-1.73000900	4.37804600	1.93430700
H	-1.67121300	4.21377700	-0.20148400
C	-1.89306300	2.30655800	3.16534400

H	-1.91825200	0.51282700	1.97619100
C	-1.80915500	3.70171400	3.15187700
H	-1.66787200	5.46192700	1.91678300
H	-1.95997600	1.77247500	4.10832000
H	-1.80690600	4.25694800	4.08482800
C	3.32832500	-0.07292000	-1.84768900
C	4.13277700	0.46008100	-2.86581500
C	3.64098500	-1.34078800	-1.32904300
C	5.23227600	-0.25416300	-3.34554900
H	3.90833500	1.43166600	-3.29276800
C	4.74535400	-2.04718200	-1.80158500
H	3.01733500	-1.77438600	-0.55450900
C	5.54318600	-1.50571000	-2.81228400
H	5.84515500	0.16878200	-4.13614100
H	4.97470500	-3.02404700	-1.38715200
H	6.39855300	-2.05958300	-3.18713500
C	2.53835600	1.80879600	0.20993900
C	3.79989300	2.41632600	0.13700600
C	1.73211200	2.04057800	1.33343100
C	4.23772900	3.25189600	1.16412000
H	4.44333300	2.22807100	-0.71715400
C	2.16436900	2.88834400	2.35365500
H	0.76650800	1.55454200	1.40488800
C	3.41834100	3.49511600	2.27021100
H	5.21859400	3.71418100	1.10250300
H	1.51953700	3.06854600	3.20842700
H	3.76116500	4.15031500	3.06552400
C	-1.44745000	-2.15772000	-0.01977900
C	-1.93481800	-2.69758300	-1.22193600
C	-2.27285800	-2.02741400	1.10911400
C	-3.30717400	-2.89439200	-1.34981300
H	-1.25048600	-2.90722300	-2.03672000
C	-3.63904900	-2.23226100	0.94547800
H	-1.86477100	-1.72318300	2.06238500
C	-4.17097300	-2.65786200	-0.27698600
H	-3.70046100	-3.24821900	-2.29827600
H	-4.29568900	-2.06289700	1.79424800
H	-5.23816100	-2.81195300	-0.38706500
S	0.73874700	-3.30847900	1.51472800
O	-0.27213700	-3.91224100	2.37369300
O	1.95008800	-4.03348100	1.14626700
C	1.34240100	-1.80059100	2.43709300
F	1.83379400	-2.19575700	3.61071500
F	0.33835900	-0.93767900	2.65619000
F	2.30199000	-1.18289100	1.74404100
O	0.13204800	-2.69898700	0.19820200

P	-1.81372300	1.00920000	-0.84996900
C	-1.39219300	2.18595800	-2.21863300
H	-1.45755300	1.62973200	-3.15827100
H	-2.19363400	2.93044900	-2.23777000
C	-0.02564900	2.87863200	-2.12104500
H	-0.05027700	3.74751100	-2.78683600
H	0.13436300	3.28017000	-1.11372200
C	1.15226400	1.98827100	-2.54958800
H	2.01915300	2.60159600	-2.81295100
H	0.86675000	1.41785100	-3.43938600
P	1.67009400	0.78689500	-1.23678800
Pd	-0.20033400	-0.47351200	-0.31537200
C	-3.39683900	0.29598400	-1.41386700
C	-4.47153600	0.14988700	-0.52764100
C	-3.49072400	-0.24088100	-2.70542800
C	-5.62459600	-0.51945700	-0.93184200
H	-4.39679400	0.53075200	0.48372400
C	-4.64925300	-0.90285800	-3.10805700
H	-2.65509300	-0.17162500	-3.39485100
C	-5.71745100	-1.04538500	-2.22117600
H	-6.44672700	-0.63899900	-0.23344600
H	-4.71202600	-1.31605600	-4.10994400
H	-6.61498800	-1.57127400	-2.53142100
C	-2.24420700	2.10880400	0.54239900
C	-3.20288500	3.12149000	0.38221500
C	-1.61475200	1.94984200	1.78275000
C	-3.51250500	3.96747200	1.44488200
H	-3.72155700	3.23877300	-0.56416300
C	-1.92343300	2.80007000	2.84534500
H	-0.88602700	1.15921500	1.91250700
C	-2.87050500	3.81007600	2.67655000
H	-4.25615000	4.74723900	1.31387900
H	-1.42806800	2.66693700	3.80178900
H	-3.11382800	4.47110900	3.50247700
C	2.98800300	-0.20860000	-2.01607000
C	3.24097300	-0.17688500	-3.39497300
C	3.75069900	-1.06128800	-1.19965600
C	4.23810500	-0.98285700	-3.94753600
H	2.67379200	0.47507200	-4.04908300
C	4.74467200	-1.86132900	-1.75628500
H	3.56697900	-1.10701400	-0.13574000
C	4.99049600	-1.82644700	-3.13081500
H	4.42514700	-0.94701800	-5.01652000
H	5.31706800	-2.52063600	-1.11193900
H	5.76294200	-2.45541700	-3.56267300
C	2.55911200	1.88650600	-0.07401900
C	3.90333100	2.23425900	-0.26837600
C	1.85818900	2.43693400	1.00634100

C	4.53082800	3.11928200	0.60745600
H	4.45972500	1.80447700	-1.09458900
C	2.48409500	3.33011600	1.87493600
H	0.82587100	2.15930600	1.17338700
C	3.82313100	3.66989900	1.67878700
H	5.57438300	3.37730300	0.45504400
H	1.92771000	3.74898600	2.70794500
H	4.31644000	4.35633300	2.36006100
C	-1.76272000	-1.59900800	0.37431700
C	-2.30536300	-2.54652500	-0.49890200
C	-2.26451300	-1.49696700	1.67301600
C	-3.34421100	-3.37983400	-0.08093100
H	-1.93645500	-2.62636200	-1.51745400
C	-3.30868000	-2.32921400	2.09035700
H	-1.84555600	-0.78656900	2.37633500
C	-3.85473400	-3.26629600	1.21401200
H	-3.75954800	-4.11030800	-0.76986300
H	-3.68982900	-2.24369400	3.10463400
H	-4.67004400	-3.90699600	1.53746900
S	1.60110600	-2.66994000	1.54851400
O	0.50737700	-3.35983600	2.23919400
O	2.92153400	-3.31535100	1.51582700
C	1.89689700	-1.14796400	2.57629200
F	2.25421700	-1.48661700	3.81831000
F	0.78543500	-0.38099400	2.65950900
F	2.87272800	-0.39081900	2.04446700
O	1.24611600	-2.08805600	0.19674800