

The theoretical chemical calculations clarify the mechanism of beta-alkylation of 1-phenylethanol with benzyl alcohol catalyzed by Iron (II) acetylacetonate methods

Wei Feng¹, Junfeng Zhao³, Aiwen Wei¹, Dandan Zhang¹, Huiling Liu^{1*}, Xuri Huang^{1*}, Kai Sun^{2*},

Supporting information

1. The DFT-based single-point energy, thermodynamics and solvation corrections of all optimized compounds studied.

Structure name	solvation correction A.U.	ZPE A.U.	Delta_U(T) A.U.	Delta_H(T) A.U.	Delta_G(T) A.U.	S(T) Cal/Mol-K
IM1_1	-0.04983833	0.373500	0.432073	0.433540	0.259691	235.543
IM1_2	-0.04981007	0.373252	0.432008	0.433475	0.258768	236.706
IM1_3	-0.04980670	0.344036	0.399749	0.401215	0.231514	229.924
IM1_4	-0.04980455	0.344031	0.399749	0.401215	0.231480	229.97
IM1_w1	-0.04813114	0.399287	0.463164	0.464630	0.279249	251.168
IM1_w2	-0.04819571	0.399281	0.463238	0.464705	0.278463	252.335
IM1_w3	-0.04887790	0.370433	0.431228	0.432695	0.252743	243.812
IM1_w4	-0.04901898	0.370163	0.431062	0.432529	0.250498	246.628
IM10_1	-0.05587771	0.479579	0.553316	0.554783	0.342501	287.614
IM10_2	-0.05368033	0.479923	0.553241	0.554708	0.347074	281.319
IM10_w1	-0.05492363	0.504530	0.584281	0.585747	0.358568	307.799
IM10_w2	-0.05640725	0.505362	0.584380	0.585847	0.364017	300.551
IM11_1	-0.05233357	0.484027	0.556141	0.557608	0.352239	278.248
IM11_2	-0.05232857	0.484039	0.556143	0.557609	0.352381	278.059
IM11_w1	-0.05106362	0.509196	0.586617	0.588084	0.372972	291.448
IM11_w2	-0.05133476	0.510112	0.587291	0.588757	0.374785	289.905
IM12	-0.05106147	0.255626	0.287469	0.288936	0.176981	151.685

IM13_1	-0.05071025	0.419391	0.472209	0.473675	0.316019	213.604
IM13_2	-0.05065742	0.392965	0.442188	0.443655	0.294585	201.97
IM14_1	-0.05046314	0.420883	0.473257	0.474724	0.319593	210.183
IM14_2	-0.05106784	0.392826	0.441817	0.443283	0.295254	200.561
IM15	-0.01226832	0.272137	0.304531	0.305997	0.193818	151.989
IM2_1	-0.05116495	0.369129	0.429526	0.430993	0.247857	248.125
IM2_2	-0.05190784	0.369131	0.429541	0.431007	0.247917	248.064
IM2_3	-0.05113656	0.340253	0.397723	0.399190	0.220826	241.66
IM2_4	-0.05246703	0.339964	0.397469	0.398936	0.221381	240.565
IM2_w1	-0.05057372	0.394917	0.460908	0.462375	0.266746	265.052
IM2_w2	-0.05136535	0.394839	0.460654	0.462121	0.269314	261.229
IM2_w3	-0.05163577	0.365756	0.429065	0.430532	0.239637	258.639
IM2_w4	-0.05144713	0.365197	0.428624	0.430091	0.239786	257.84
IM4_1	-0.00603846	0.138340	0.155903	0.157370	0.080745	103.818
IM4_2	-0.00478551	0.109809	0.124124	0.125590	0.056500	93.608
IM5	-0.01365424	0.225482	0.255443	0.256910	0.149738	145.204
IM6_1	-0.05460558	0.456872	0.528920	0.530387	0.324903	278.405
IM6_2	-0.05702196	0.457327	0.529228	0.530695	0.327585	275.189
IM6_w1	-0.05478681	0.481861	0.560155	0.561622	0.340615	299.436
IM6_w2	-0.05496102	0.481720	0.559861	0.561327	0.344091	294.327
IM7_1	-0.05347092	0.461218	0.532574	0.534041	0.329287	277.416
IM7_2	-0.05435516	0.460856	0.532054	0.533521	0.329804	276.01
IM7_w1	-0.05007259	0.487365	0.564115	0.565581	0.350721	291.109
IM7_w2	-0.05007443	0.487377	0.564118	0.565585	0.350734	291.096
IM8	-0.05001470	0.233922	0.264703	0.266170	0.157463	147.284
IM9	-0.01360862	0.249145	0.280068	0.281535	0.172413	147.847
M_1	-0.00870263	0.226308	0.263866	0.265333	0.137411	173.317
M_2	-0.05275740	0.228977	0.269032	0.270499	0.135268	183.221
M_w1	-0.01130206	0.250541	0.294695	0.296162	0.148462	200.115
M_w2	-0.05213351	0.254013	0.300045	0.301511	0.152339	202.109
R1	-0.04903110	0.145530	0.163848	0.165315	0.087508	105.418
R1-H	-0.00506720	0.161801	0.180837	0.182304	0.102699	107.855
R2	-0.05013194	0.117245	0.132279	0.133746	0.063309	95.434

R2-H	-0.00502369	0.133524	0.149580	0.151046	0.077008	100.313
TS1_1	-0.05051980	0.368525	0.427525	0.428991	0.251131	240.978
TS1_2	-0.05022881	0.368519	0.427530	0.428996	0.251126	240.992
TS1_3	-0.05059400	0.339602	0.395649	0.397116	0.224240	234.225
TS1_4	-0.05047252	0.339837	0.395716	0.397183	0.225049	233.22
TS1_w1	-0.04982652	0.394611	0.458823	0.460290	0.270799	256.736
TS1_w2	-0.04960097	0.394118	0.458643	0.460109	0.269496	258.256
TS1_w3	-0.05003321	0.365317	0.426889	0.428356	0.242647	251.612
TS1_w4	-0.04966833	0.365011	0.426740	0.428207	0.241445	253.038
TS2_1	-0.05599559	0.455756	0.527021	0.528488	0.323757	277.384
TS2_2	-0.05235490	0.455323	0.526420	0.527887	0.326136	273.347
TS2_w1	-0.05729535	0.480981	0.557997	0.559464	0.341487	295.331
TS2_w2	-0.05257906	0.480851	0.557414	0.558880	0.344774	290.087
TS3_1	-0.04939990	0.392796	0.444027	0.445494	0.290898	209.458
TS3_2	-0.05049933	0.364573	0.412579	0.414046	0.266470	199.946
TS4_1	-0.05351494	0.478718	0.551351	0.552817	0.342565	284.865
TS4_2	-0.05258398	0.479158	0.551325	0.552792	0.347453	278.209
TS4_w1	-0.05235012	0.505263	0.582543	0.584010	0.368273	292.296
TS4_w2	-0.05194129	0.504792	0.582350	0.583816	0.367360	293.271
TS5_1	-0.05090994	0.415914	0.468102	0.469569	0.312544	212.748
TS5_2	-0.05116286	0.387958	0.436774	0.438241	0.286920	205.02

2. The atomic coordinates of all optimized compounds studied.

IM1_1

O	-1.71197000	-1.24182500	-1.14451100
O	-0.29114600	2.48177500	-0.42122600
O	0.58008800	0.35111500	-2.00729100
C	-4.82296900	0.79537900	1.23853300
C	-3.70914200	0.20730700	0.41272600
C	-3.73607200	-1.15899100	0.09523800
C	-2.73636500	-1.80881300	-0.64490500

C	-2.83361900	-3.29584100	-0.86739200
C	0.95509900	2.71353200	-0.30362900
C	1.72846000	0.86739500	-1.77105700
C	1.34546300	3.83034300	0.61773700
C	1.96162100	1.98077100	-0.96072400
C	2.89487300	0.17240000	-2.41780700
H	-4.41325100	1.17411800	2.18070600
H	-5.25963800	1.65533600	0.72110500
H	-5.61274500	0.07325000	1.46237600
H	-4.56843700	-1.75287900	0.46241900
H	-2.01298000	-3.79513400	-0.33975900
H	-3.77903400	-3.71783100	-0.51587900
H	-2.70709600	-3.52680700	-1.92942300
H	1.34040600	3.39154900	1.62152500
H	2.34378400	4.22435400	0.40616500
H	0.60756500	4.63575000	0.58049600
H	2.99324600	2.27607500	-0.79218500
H	2.69766200	0.02001400	-3.48371800
H	3.83305000	0.72039700	-2.29563900
H	3.01056500	-0.81929100	-1.96598100
C	1.76194100	-0.86323700	1.16363700
C	3.08577900	-0.57915600	1.49850000
C	4.12619600	-1.39222700	1.05675800
C	3.85487200	-2.50730700	0.26420600
C	2.53520900	-2.78848000	-0.09424300
C	1.49947500	-1.96866700	0.34840700
H	3.24352300	0.31315700	2.10186600
H	5.15572700	-1.15811800	1.32627200
H	4.66514600	-3.14577400	-0.08433300
H	2.31640800	-3.64357600	-0.73255600
H	0.47375100	-2.16467600	0.03266300
C	0.65842400	0.06545200	1.70906600
H	0.02464800	0.26411700	0.71585300

O	1.07618200	1.15376100	2.27891900
FE	-1.02191400	0.63915200	-0.81486000
O	-2.78852200	1.01850200	0.07264100
C	-0.37201200	-0.75562500	2.52972700
H	-1.22531800	-0.11106700	2.76663800
H	-0.74458300	-1.64355800	1.99883000
H	0.08689900	-1.07939700	3.47200100

IM1_2

C	1.79915400	-0.85388900	1.13503400
C	3.12970700	-0.55088400	1.42412600
C	4.16545600	-1.35484700	0.95588700
C	3.88280900	-2.48074800	0.18277600
C	2.55594600	-2.78026000	-0.13142600
C	1.52475100	-1.96903300	0.33706100
H	3.29569300	0.34870800	2.01415900
H	5.19999500	-1.10588500	1.19066200
H	4.68927400	-3.11318600	-0.18515600
H	2.32727600	-3.64368100	-0.75480300
H	0.49246500	-2.18089300	0.05596500
C	0.70227500	0.05962600	1.71960800
O	1.12629000	1.14753800	2.28634900
FE	-1.03240900	0.62603800	-0.78203800
O	-2.83316900	1.00674200	0.03704200
O	-1.68805800	-1.27450400	-1.07441000
O	-0.32140200	2.47528200	-0.37933100
O	0.56286700	0.36450200	-1.98560500
C	-4.92622000	0.79863700	1.09778300
C	-3.76178100	0.19575900	0.35623600
C	-3.75711800	-1.18073300	0.08694100
C	-2.72036200	-1.84061400	-0.59133200
C	-2.78826300	-3.33560100	-0.76643900
C	0.92258200	2.72365500	-0.27386800

C	1.70694200	0.89469300	-1.75684600
C	1.30606300	3.84427800	0.64585400
C	1.93256500	2.00705400	-0.94371700
C	2.87597500	0.21666600	-2.41617500
H	-5.34833200	1.62742900	0.52083800
H	-5.71566900	0.07294900	1.31096800
H	-4.57365300	1.22529300	2.04240000
H	-4.59779500	-1.77304200	0.43718500
H	-1.97406500	-3.80335100	-0.20129400
H	-3.73611200	-3.76162400	-0.42653500
H	-2.62961100	-3.59891600	-1.81659900
H	0.56096600	4.64320800	0.61013000
H	1.30881800	3.40674100	1.65000000
H	2.30003600	4.24717000	0.43081200
H	2.96164300	2.31528800	-0.78329300
H	2.67982600	0.08253000	-3.48484900
H	3.81174200	0.76631500	-2.28360900
H	2.99581800	-0.78233600	-1.98201900
H	0.03258300	0.26097000	0.74994000
C	-0.28669400	-0.78292300	2.56905900
H	-0.70352200	-1.64508100	2.02834600
H	0.22345900	-1.14892700	3.46869300
H	-1.11315400	-0.13816000	2.88530300

IM1_3

O	-1.76367200	-1.40354100	-0.74452100
O	-0.31510700	2.36059700	-0.40126600
O	0.50747700	0.08529800	-1.80214700
C	-5.01132700	0.96604200	1.08497700
C	-3.83190700	0.25920000	0.46860500
C	-3.88344400	-1.13133400	0.29028400
C	-2.85485500	-1.88332300	-0.29989800
C	-3.01971400	-3.37507100	-0.44064200

C	0.92732200	2.63257200	-0.40086800
C	1.65425000	0.65070800	-1.70563900
C	1.34688300	3.85619600	0.35914200
C	1.90714100	1.85649800	-1.05101200
C	2.79418800	-0.09839900	-2.33708700
H	-4.69089100	1.49657500	1.98699200
H	-5.39127400	1.72723800	0.39594500
H	-5.82654100	0.28498700	1.34389400
H	-4.77591900	-1.65615000	0.61974200
H	-2.21612100	-3.88647400	0.09944900
H	-3.98105600	-3.73463600	-0.06384500
H	-2.91842100	-3.66399600	-1.49168800
H	0.58130500	4.63295600	0.28789700
H	1.43049600	3.53518400	1.40309900
H	2.31224600	4.24952800	0.02714800
H	2.93882700	2.19053500	-0.98856800
H	2.54225000	-0.36982500	-3.36722500
H	3.72895200	0.46858600	-2.32765100
H	2.95005500	-1.03224800	-1.78459300
C	1.89300000	-0.74606500	1.29477100
C	3.23770500	-0.38169500	1.35122500
C	4.23141400	-1.24868000	0.90352900
C	3.88922300	-2.49720000	0.38476100
C	2.54295400	-2.86121800	0.30465600
C	1.55505500	-1.98936400	0.75494900
H	3.44768600	0.60708500	1.75593900
H	5.27924700	-0.95372200	0.95492300
H	4.66218000	-3.17826800	0.03246000
H	2.26619500	-3.82559000	-0.11961100
H	0.50098400	-2.25937700	0.66970400
C	0.84770600	0.22230100	1.85958400
H	0.02042400	0.24035900	0.98966900
O	1.26378100	1.38643700	2.23460600

FE	-1.04667400	0.48702200	-0.59448800
O	-2.84806800	1.00321500	0.15032700
H	0.24401300	-0.37837300	2.60899900

IM1_4

O	2.84820700	1.00349800	-0.14915800
O	1.76337300	-1.40291500	0.74531900
C	5.01075500	0.96579900	-1.08545800
C	3.83154500	0.25924300	-0.46833300
C	3.88274600	-1.13135400	-0.29036900
C	2.85414500	-1.88306800	0.30017900
C	3.01851000	-3.37490400	0.44065700
H	5.39076100	1.72755000	-0.39708000
H	5.82596200	0.28463900	-1.34413100
H	4.69002500	1.49562500	-1.98779600
H	4.77488400	-1.65639900	-0.62036800
H	2.21497600	-3.88594100	-0.09986500
H	3.97987100	-3.73467600	0.06411400
H	2.91671900	-3.66400700	1.49159500
C	-1.89170300	-0.74646600	-1.29495700
C	-3.23658800	-0.38287600	-1.35218100
C	-4.23001200	-1.25018500	-0.90448600
C	-3.88733500	-2.49824700	-0.38493000
C	-2.54088800	-2.86142300	-0.30395100
C	-1.55327200	-1.98925600	-0.75425500
H	-3.44691400	0.60561400	-1.75742500
H	-5.27799100	-0.95584800	-0.95648800
H	-4.66004400	-3.17957700	-0.03259300
H	-2.26378000	-3.82539200	0.12100700
H	-0.49906600	-2.25853000	-0.66823400
C	-0.84681000	0.22221000	-1.85998400
O	-1.26343200	1.38613700	-2.23510000
FE	1.04631700	0.48771000	0.59501200

O	0.31429400	2.36084600	0.40111300
O	-0.50794600	0.08583500	1.80240300
C	-0.92819500	2.63259900	0.40040700
C	-1.65487100	0.65091100	1.70555700
C	-1.34775100	3.85602200	-0.35988700
C	-1.90794100	1.85651300	1.05064500
C	-2.79469700	-0.09835600	2.33696800
H	-0.58281500	4.63333800	-0.28763800
H	-1.43001600	3.53527400	-1.40401100
H	-2.31376800	4.24862700	-0.02891600
H	-2.93971000	2.19022800	0.98783900
H	-3.72962100	0.46836100	2.32722000
H	-2.95018700	-1.03240100	1.78469900
H	-2.54288000	-0.36945800	3.36722100
H	-0.01935200	0.24072100	-0.99035200
H	-0.24308500	-0.37837800	-2.60947300

IM1_w1

O	-0.53281700	-0.75279300	-1.92881900
O	0.37186800	-2.44608200	0.10827700
O	1.61690800	1.19780900	-1.21256500
O	2.73358100	-0.63928400	0.57263700
C	-2.87110900	-0.56966100	-2.22246000
C	-1.68236600	-1.15533400	-1.51233000
C	-1.89357900	-2.05158900	-0.46522600
C	-0.87616800	-2.63459800	0.31727600
C	-1.22798400	-3.59933400	1.40965200
C	2.52925800	1.95774800	-0.74882400
C	3.53117800	0.31997800	0.81850300
C	2.53330700	3.36733300	-1.28043900
C	3.48153300	1.58512100	0.21040400
C	4.58039900	0.04857500	1.86490700
H	-3.81170700	-1.05024500	-1.94021800

H	-2.94159100	0.49490100	-1.96852600
H	-2.73536100	-0.63510100	-3.30695900
H	-2.92107500	-2.25815500	-0.18146600
H	-0.77745700	-4.57975300	1.21277700
H	-0.82047400	-3.19489600	2.33791000
H	-2.30831000	-3.71355500	1.52525900
H	1.61966900	3.87997400	-0.95845900
H	3.39501500	3.94743900	-0.93957100
H	2.51552000	3.35619100	-2.37435200
H	4.21034400	2.32872900	0.52054100
H	5.27743600	0.88115100	1.99293300
H	4.09319800	-0.15305100	2.82474200
H	5.14331000	-0.85328400	1.60539100
O	1.76404300	-2.20308700	-2.32134200
H	1.48894400	-2.84380100	-1.64844100
H	0.91090400	-1.89698000	-2.67332300
C	-1.93272700	1.02920900	0.99453000
C	-3.26251800	0.73647600	1.29704300
C	-4.30283000	1.46389100	0.72427500
C	-4.02624300	2.49864000	-0.16903700
C	-2.69908800	2.78650800	-0.49366600
C	-1.66345300	2.05279000	0.08082700
H	-3.42115700	-0.09508900	1.98214100
H	-5.33730300	1.22343600	0.96831800
H	-4.83686400	3.06697500	-0.62206700
H	-2.47442000	3.57740800	-1.20823400
H	-0.62934400	2.24986800	-0.20456100
C	-0.82780100	0.19343500	1.67036500
H	-0.16061300	-0.08345900	0.73368800
O	-1.24344600	-0.85079800	2.33120000
C	0.12918100	1.12375000	2.45831000
H	0.53245400	1.94897700	1.85359200
H	-0.40012200	1.54780900	3.32035500

FE	1.10102000	-0.65518700	-0.60772500
H	0.96744800	0.52560700	2.82960400

IM1_w2

C	-1.93795100	1.02464000	0.98972800
C	-3.26729900	0.73526300	1.29705900
C	-4.30756000	1.46844000	0.73185300
C	-4.03143800	2.50517900	-0.15925600
C	-2.70484500	2.78984500	-0.48869000
C	-1.66920200	2.05096400	0.07903200
H	-3.42685000	-0.09911000	1.97856500
H	-5.34171500	1.23052300	0.97963600
H	-4.84220300	3.07741600	-0.60706100
H	-2.48071700	3.58219200	-1.20182300
H	-0.63536800	2.24519400	-0.20979100
C	-0.83160400	0.18264700	1.65442200
O	-1.24319300	-0.87504100	2.29988200
FE	1.11332800	-0.66484400	-0.60807400
O	2.73667900	-0.63103500	0.58607300
O	1.62960200	1.18499600	-1.22511300
O	0.36184500	-2.43266500	0.13066500
O	-0.50671200	-0.76648600	-1.94599800
C	4.56143900	0.07986100	1.89747800
C	3.52433700	0.33567000	0.83514300
C	3.47381000	1.59600100	0.21729000
C	2.53057400	1.95492600	-0.75605600
C	2.53136000	3.36049900	-1.29836000
C	-0.88958200	-2.60521900	0.33409000
C	-1.66448000	-1.14864500	-1.52831700
C	-1.26479800	-3.58285400	1.40712900
C	-1.89390200	-2.02253800	-0.46836100
C	-2.84127100	-0.55921700	-2.25542500
H	5.25256600	0.91728100	2.02601100

H	4.06294500	-0.11432000	2.85306400
H	5.13204000	-0.82167100	1.65441500
H	4.19361100	2.34681100	0.53104200
H	1.61012100	3.86917800	-0.99226400
H	3.38462900	3.94928000	-0.95115700
H	2.52768100	3.34066500	-2.39228000
H	-0.99155300	-4.60284800	1.10510100
H	-0.71555200	-3.31961700	2.31103200
H	-2.33368900	-3.54975000	1.62802900
H	-2.92583600	-2.21081200	-0.18753500
H	-2.70072000	-0.64414500	-3.33801300
H	-3.79001000	-1.02207400	-1.97065000
H	-2.89889400	0.51012900	-2.01902600
H	-0.16351100	-0.07828900	0.71802600
O	1.77677300	-2.24145900	-2.28991600
H	0.92488200	-1.93654800	-2.64730100
H	1.49793300	-2.87389800	-1.61097300
C	0.11792900	1.10505200	2.45966400
H	0.52274400	1.93685800	1.86511700
H	-0.41700800	1.51952000	3.32282800
H	0.95489300	0.50440400	2.82963900

IM1_w3

C	1.90607800	0.98912200	-1.16016900
C	3.24825200	0.68583000	-1.38442300
C	4.25757200	1.50122400	-0.87852300
C	3.93571600	2.63516900	-0.13311600
C	2.59357900	2.93821500	0.10926100
C	1.59013900	2.11912400	-0.40086300
H	3.44368100	-0.21739700	-1.96059000
H	5.30332600	1.25501700	-1.06184400
H	4.72182600	3.27347200	0.26684300
H	2.33328300	3.81084700	0.70700300

H	0.54127200	2.33511700	-0.19093900
C	0.83349700	0.07485200	-1.76101400
O	1.24076500	-1.02883500	-2.31602500
H	0.16919200	0.74480600	-2.38873700
FE	-1.13848300	-0.61574100	0.55918200
O	-2.72820800	-0.64385000	-0.68158400
O	-1.70596000	1.24253200	1.10478400
O	-0.35339900	-2.41329800	-0.04508400
O	0.49007800	-0.56844300	1.88697200
C	-4.38559000	0.05113200	-2.20491300
C	-3.44101900	0.33607700	-1.06631900
C	-3.39879600	1.62839800	-0.51713200
C	-2.55202800	2.00531900	0.53560300
C	-2.61339000	3.41683700	1.06008100
C	0.90117800	-2.58998300	-0.22758000
C	1.65327800	-0.97152500	1.50641000
C	1.29076900	-3.64992200	-1.21416000
C	1.89577100	-1.93512500	0.53065200
C	2.81947900	-0.29678300	2.17380300
H	-5.02381900	-0.80232900	-1.95646700
H	-5.01593400	0.90737800	-2.45937400
H	-3.80871700	-0.23774600	-3.08920800
H	-4.06719300	2.37926900	-0.92882800
H	-1.63321800	3.89321000	0.95307600
H	-3.36152500	4.02794600	0.54802500
H	-2.83714500	3.40564600	2.13161200
H	0.99950900	-4.64138100	-0.84227200
H	0.76579500	-3.45044200	-2.14868800
H	2.36491600	-3.64369300	-1.41137500
H	2.93081100	-2.13753300	0.27197900
H	2.65324200	-0.23194600	3.25390600
H	3.77071500	-0.79897900	1.97689700
H	2.89225900	0.73019400	1.79445800

H	0.10793800	-0.07649300	-0.84503400
O	-1.75440200	-2.05290100	2.37329700
H	-0.91337800	-1.68574700	2.69701400
H	-1.45417900	-2.73933900	1.75933100

IM1_w4

C	2.03282000	0.91438200	-1.20326200
C	3.37140400	0.53379400	-1.29319300
C	4.38084900	1.35005100	-0.78962000
C	4.06297300	2.56423400	-0.18155400
C	2.72392100	2.94668700	-0.07404100
C	1.72012800	2.12554500	-0.58063800
H	3.56312200	-0.42995600	-1.76281100
H	5.42322000	1.04075200	-0.86461600
H	4.84872700	3.20414800	0.21639100
H	2.46537600	3.88470600	0.41591000
H	0.67129200	2.40945300	-0.47681000
C	0.96263500	-0.00298300	-1.80513000
O	1.35741100	-1.16035100	-2.25097000
H	0.37580900	0.64153200	-2.52673400
FE	-1.10975800	-0.51026100	0.49803700
O	-2.75429800	-0.70536500	-0.65804200
O	-1.71965400	1.36719000	0.90762800
O	-0.32814900	-2.34320600	0.00284400
O	0.48708500	-0.38952000	1.83990500
C	-4.68537800	-0.27297400	-1.93672100
C	-3.61524900	0.17462600	-0.97430200
C	-3.63046400	1.49655800	-0.49963700
C	-2.69345500	2.01604100	0.40604700
C	-2.81388800	3.45251100	0.84584300
C	0.92686800	-2.55697300	-0.11941700
C	1.65370100	-0.85453800	1.54357300
C	1.33118100	-3.68981300	-1.01500500

C	1.90767100	-1.88777900	0.64885600
C	2.80643300	-0.17046600	2.22374400
H	-5.40363800	0.51713200	-2.17203300
H	-4.22141300	-0.61946200	-2.86541900
H	-5.22432600	-1.12975500	-1.51988500
H	-4.41802200	2.15631100	-0.85291400
H	-1.89940500	3.99541800	0.58522600
H	-3.66889000	3.96442600	0.39593200
H	-2.90328100	3.50164500	1.93570400
H	1.08985700	-4.65268300	-0.54373200
H	0.77752200	-3.60234600	-1.94965000
H	2.39934500	-3.66099200	-1.23936800
H	2.94637700	-2.13556600	0.45117800
H	2.60693100	-0.06529800	3.29531300
H	3.75676800	-0.69082800	2.07611700
H	2.90433600	0.84162200	1.81218100
H	0.16232000	-0.05669700	-0.93862000
O	-1.75284600	-1.84990600	2.39610700
H	-0.90942600	-1.46693300	2.69467400
H	-1.45819200	-2.56401300	1.81196100

IM2_1

O	-0.05190400	0.79419300	1.11570300
O	-3.25015800	-0.35611800	-0.85775400
O	-1.07832600	-1.66657700	0.36963300
C	-2.03041000	4.60330600	0.06499700
C	-1.41050200	3.24920700	0.31403700
C	-0.34594700	3.14863400	1.22747200
C	0.25499500	1.93266900	1.59002000
C	1.35680500	1.93355200	2.62136900
C	-3.82054600	-1.47219400	-0.64620200
C	-1.89517500	-2.63226100	0.40484800
C	-5.26992500	-1.55144500	-1.06214100

C	-3.22021900	-2.60040500	-0.06990400
C	-1.38081500	-3.91346800	1.02161200
H	-1.97567100	4.84397100	-1.00161300
H	-3.09434500	4.57885100	0.32310500
H	-1.54839100	5.40388100	0.63337400
H	0.00095200	4.05729100	1.71252300
H	2.26279300	1.49109800	2.19133100
H	1.59347700	2.93463100	2.99332900
H	1.07673700	1.29696600	3.46714400
H	-5.36147900	-1.31432200	-2.12707100
H	-5.71322600	-2.53423900	-0.87824800
H	-5.85230700	-0.79495600	-0.52574500
H	-3.82413100	-3.49741100	0.04060100
H	-0.98654600	-3.71112900	2.02314300
H	-2.14359500	-4.69448100	1.09027800
H	-0.54301500	-4.29624200	0.42787300
C	3.46736900	-0.39584000	-0.64755700
C	4.65441800	-1.09907000	-0.39976700
C	4.62784900	-2.29969700	0.29401500
C	3.40978500	-2.81348700	0.74840200
C	2.22488100	-2.12872100	0.49599300
C	2.24935300	-0.92396300	-0.20305700
H	5.58274500	-0.66871300	-0.76687800
H	5.55295500	-2.83905900	0.48849000
H	3.39059100	-3.75190300	1.30005300
H	1.26260400	-2.50431800	0.83431200
H	1.30602800	-0.42025600	-0.40762500
C	3.55192500	0.90158800	-1.37802600
H	-0.42647800	0.22690200	-1.81957000
O	4.61568000	1.26903100	-1.87100100
FE	-1.36313300	0.29647600	-0.40319600
O	-1.91770000	2.28100300	-0.33010700
C	2.31017500	1.73785700	-1.46435100

H	2.50620900	2.62518100	-2.06780300
H	1.44747700	1.18213600	-1.86620700
H	1.98323300	2.04792200	-0.46405000

IM2_2

C	-2.94698900	0.95297600	-0.77482700
C	-4.15386300	0.64394000	-0.13189000
C	-4.69479200	-0.63064600	-0.22244600
C	-4.02741000	-1.61929200	-0.94898800
C	-2.82021700	-1.32370000	-1.57750100
C	-2.28154200	-0.04274100	-1.50068800
H	-4.64135000	1.43255500	0.44004400
H	-5.63400300	-0.86293400	0.28013500
H	-4.44280600	-2.62604100	-1.00902900
H	-2.27075100	-2.09815900	-2.11213800
H	-1.30324400	0.15309800	-1.94890100
C	-2.39888100	2.33250400	-0.64096400
O	-2.94036900	3.14656600	0.10591400
FE	1.23165200	-0.23611100	-0.38649800
O	2.45456200	1.37068900	0.14527000
O	3.00358500	-1.28110700	-0.58545600
O	-0.13397500	0.65272900	0.91653700
O	0.18524100	-1.97380100	0.00986900
C	4.27845800	2.76972500	0.67089300
C	3.71636000	1.43715700	0.23086600
C	4.60895000	0.38205200	-0.03193000
C	4.20329700	-0.91082600	-0.39753700
C	5.25585500	-1.97941500	-0.58198600
C	-1.01573600	0.12251500	1.66456200
C	-0.76453400	-2.19487700	0.82477800
C	-1.72480900	1.04982900	2.61987600
C	-1.36754400	-1.23730900	1.65313900
C	-1.26168200	-3.62045400	0.88237800

H	3.86417000	3.04427400	1.64901200
H	5.37288400	2.77282500	0.73655900
H	3.96507600	3.55431200	-0.02898300
H	5.67434000	0.56815900	0.09460500
H	5.18230400	-2.40403900	-1.59094000
H	6.27538800	-1.60655100	-0.42878700
H	5.07507300	-2.80658500	0.11624300
H	-0.99022000	1.56906600	3.24815900
H	-2.26487900	1.82664900	2.06267300
H	-2.43721600	0.52296400	3.26572700
H	-2.17009800	-1.56341000	2.31247700
H	-0.44068800	-4.29773900	1.14968000
H	-2.08270000	-3.75614300	1.59624200
H	-1.60981600	-3.92942000	-0.11197600
H	0.76864200	0.13294300	-1.99349300
C	-1.18179500	2.68578200	-1.44165000
H	-0.32940300	2.04262700	-1.16457300
H	-1.34381500	2.51121500	-2.51322400
H	-0.92319200	3.73401400	-1.27211100

IM2_3

O	-0.10822100	0.91072000	-0.94503900
O	3.15210100	-0.45578600	0.72792300
O	0.84040300	-1.59030600	-0.42121900
C	2.05305800	4.60955900	0.12869900
C	1.36635500	3.28792800	-0.12053700
C	0.21876400	3.26250100	-0.93117500
C	-0.44890500	2.08271100	-1.29673300
C	-1.66953800	2.16705400	-2.18010800
C	3.64125500	-1.59144800	0.43345800
C	1.59516500	-2.59565700	-0.54912700
C	5.10781700	-1.76814300	0.74850200
C	2.94426800	-2.65984600	-0.14861500

C	0.97966600	-3.80676400	-1.21438000
H	2.09841500	4.80642800	1.20483100
H	3.08970100	4.56221000	-0.22155600
H	1.55307900	5.44859700	-0.36377500
H	-0.15152300	4.20487400	-1.32618000
H	-2.54402600	1.80079700	-1.62919000
H	-1.87472700	3.18247900	-2.53177000
H	-1.55372600	1.50295800	-3.04327800
H	5.69871200	-1.03762000	0.18576000
H	5.28579000	-1.55884500	1.80819100
H	5.47659100	-2.77170900	0.51718200
H	3.48911500	-3.58201900	-0.33428200
H	0.70653100	-3.56540600	-2.24788600
H	1.64398000	-4.67590300	-1.22419100
H	0.04948000	-4.07345500	-0.70206700
C	-3.34932800	-0.54638600	1.02466200
C	-4.62813300	-0.63595500	0.45390500
C	-4.76798500	-1.06589100	-0.85573000
C	-3.63299700	-1.40803200	-1.60221000
C	-2.36319400	-1.31799900	-1.04085500
C	-2.21882000	-0.88831700	0.27684000
H	-5.48450600	-0.35648000	1.06327700
H	-5.75555300	-1.13591000	-1.30737500
H	-3.74901700	-1.73804400	-2.63327200
H	-1.46692900	-1.55186700	-1.60839900
H	-1.22489900	-0.78692300	0.71669900
C	-3.17824100	-0.08292400	2.40921600
H	0.42286200	0.15503500	1.93288100
O	-4.09910000	0.20202500	3.16066600
FE	1.27129100	0.31463400	0.46772400
O	1.89663200	2.27585600	0.43261900
H	-2.11268000	-0.00410800	2.72911000

IM2_4

O	3.04579000	1.01759400	-0.70999600
O	2.43899900	-1.57820600	0.11577000
C	5.31781400	1.61894600	-0.89950200
C	4.24020700	0.60092800	-0.60900500
C	4.61816900	-0.70086700	-0.24162600
C	3.70075100	-1.70316600	0.11731600
C	4.22895500	-3.04654200	0.56419100
H	5.22500600	2.46430900	-0.20940300
H	6.32778000	1.20631500	-0.81803500
H	5.18119100	2.02621000	-1.90658400
H	5.67896300	-0.93241500	-0.18936100
H	3.81390900	-3.83708800	-0.06964300
H	5.32094900	-3.10726900	0.53526800
H	3.89021100	-3.25815200	1.58400300
C	-3.25188800	0.00562500	-0.94505500
C	-4.60198600	-0.16454800	-0.61189000
C	-5.11800700	-1.43982500	-0.43668900
C	-4.28811400	-2.55345800	-0.59739600
C	-2.94482500	-2.38686400	-0.92885500
C	-2.41989100	-1.10877400	-1.10318300
H	-5.21697600	0.72520000	-0.49751300
H	-6.16512100	-1.57704300	-0.17453900
H	-4.69376900	-3.55350300	-0.45695100
H	-2.29676900	-3.25254900	-1.04033500
H	-1.36291700	-0.95645800	-1.34414900
C	-2.70027800	1.35920000	-1.14177400
O	-3.37038200	2.38134200	-1.08088800
FE	1.25545800	0.07302800	-0.30970000
O	0.42871400	1.90070900	0.22175300
O	-0.12923800	-0.73010300	1.02136200
C	-0.56806400	2.16817700	0.95963800
C	-1.05429000	-0.16054600	1.67899500

C	-0.99301400	3.61358200	1.01489200
C	-1.32274800	1.21867100	1.67484200
C	-1.94265700	-1.06671800	2.49550100
H	-0.11616800	4.26547900	0.99408300
H	-1.59805400	3.83611500	0.12742800
H	-1.60252600	3.84007800	1.89472800
H	-2.16089100	1.57826900	2.26654100
H	-2.62776300	-0.51621700	3.14689700
H	-2.53762400	-1.69288500	1.81976900
H	-1.33264300	-1.74471700	3.10022600
H	0.53198700	-0.24603700	-1.81626100
H	-1.61254300	1.38001800	-1.38038100

IM2_w1

O	-0.96196600	1.66852800	-0.36388200
O	-3.18644900	0.31711500	0.77348500
O	0.03031000	-0.77419700	-1.03191000
O	-1.62339800	-2.31650800	0.60043700
C	-1.13144400	4.00797300	-0.62004900
C	-1.69165500	2.67730600	-0.16975600
C	-2.97552500	2.66293900	0.42117000
C	-3.64409000	1.50736100	0.83233700
C	-5.04124200	1.63304400	1.38697900
C	0.32383600	-1.91042000	-1.53425500
C	-1.16360900	-3.27239200	-0.09648300
C	1.31807000	-1.87459400	-2.66514500
C	-0.19871000	-3.13893900	-1.11203700
C	-1.71674300	-4.64088300	0.21268700
H	-1.83746000	4.83503200	-0.50407400
H	-0.22810400	4.23521500	-0.04353000
H	-0.82677700	3.94362500	-1.66953300
H	-3.49587400	3.61120900	0.52476800
H	-5.73186300	1.03015800	0.78856400

H	-5.06912600	1.22177900	2.40101800
H	-5.40040800	2.66541000	1.41089500
H	2.24088300	-1.38933100	-2.32681200
H	1.55894200	-2.86821200	-3.05303400
H	0.92749300	-1.25992100	-3.48303700
H	0.12316000	-4.03670200	-1.63262100
H	-1.26850700	-5.42827100	-0.39967100
H	-1.55425400	-4.87751800	1.26921500
H	-2.80022900	-4.64624600	0.05500500
O	-2.75703800	-0.19829300	-2.14196400
H	-3.15248600	-0.13532900	-1.26216800
H	-1.85898900	0.12318800	-1.98463100
C	3.53984000	0.40222900	0.63680800
C	4.74951200	1.03369600	0.31652500
C	4.75862400	2.18072600	-0.46375000
C	3.55430800	2.71136900	-0.93445700
C	2.34755800	2.09907800	-0.60958700
C	2.33629000	0.95108700	0.17920000
H	5.66719000	0.59081800	0.69537900
H	5.70131200	2.66361000	-0.71396400
H	3.56245900	3.60516200	-1.55543700
H	1.39611800	2.48807500	-0.96264500
H	1.37776200	0.50405400	0.43545800
C	3.58549700	-0.84845600	1.44916500
H	-0.40313900	0.01900000	1.97697800
O	4.64233400	-1.22645000	1.94739400
C	2.31369100	-1.62812000	1.60719300
H	1.49150700	-1.01848500	2.01319400
H	1.94293500	-1.96901700	0.63204800
FE	-1.21497200	-0.32664400	0.53287400
H	2.49114100	-2.49415400	2.24616400

C	3.50371800	0.22455600	-0.76428100
C	4.67379100	0.57343800	-0.07880100
C	4.94054700	1.89976900	0.23159900
C	4.02761800	2.89344200	-0.12619100
C	2.84938600	2.55077100	-0.78598700
C	2.58649600	1.22323500	-1.11520700
H	5.35439100	-0.22826900	0.19748800
H	5.85467300	2.16442200	0.75884600
H	4.22999800	3.93288000	0.12350600
H	2.11748000	3.31480000	-1.03530400
H	1.63775500	0.96764700	-1.59375400
C	3.28171200	-1.21629900	-1.09375900
O	4.01807800	-2.07987400	-0.62485800
FE	-1.27696100	0.10616500	-0.46989900
O	-3.00123100	-0.97782900	-0.63777200
O	-2.48105300	1.75401300	-0.30903800
O	-0.50873400	-1.90363600	0.01610400
O	-0.01175300	0.68596800	1.09890600
C	-5.24985200	-1.67406100	-0.61257200
C	-4.21101100	-0.58249700	-0.55801800
C	-4.62716700	0.74477500	-0.40133300
C	-3.74547400	1.83044300	-0.25151300
C	-4.31545700	3.20343000	0.00892500
C	0.54378800	-2.18552200	0.64604900
C	1.00005800	0.07596500	1.59039900
C	1.03918800	-3.61342800	0.59285400
C	1.32104400	-1.26782600	1.39526200
C	1.90551800	0.91933700	2.45062800
H	-6.27327300	-1.28833000	-0.60856100
H	-5.10116400	-2.28725600	-1.50709900
H	-5.12449700	-2.34127500	0.24748300
H	-5.69412500	0.93904100	-0.33146700
H	-3.93937700	3.91129800	-0.73663300

H	-5.40900300	3.21938000	-0.00573600
H	-3.97310900	3.56651400	0.98373100
H	0.40466000	-4.20418600	-0.07015600
H	2.07465300	-3.64050400	0.23264500
H	1.03691300	-4.06812900	1.58998100
H	2.22863900	-1.64331800	1.86195800
H	1.33058500	1.36161800	3.27093700
H	2.74592800	0.35527200	2.86386500
H	2.29789300	1.75033400	1.85466700
H	-0.34900900	0.33468400	-1.87377700
O	-2.30258000	-0.82425600	2.31142000
H	-1.59118400	-0.18810500	2.15632900
H	-2.27762700	-1.35014500	1.50051400
C	2.17894700	-1.55032800	-2.05336800
H	1.20682000	-1.13214400	-1.75311400
H	2.39334700	-1.10378300	-3.03186800
H	2.10070600	-2.63303000	-2.16330900

IM2_w3

C	2.99501800	-1.02703200	0.61933500
C	4.26230700	-0.86342100	1.18869300
C	5.14378800	0.07478000	0.66758800
C	4.76419800	0.85026400	-0.43001600
C	3.50383900	0.68331000	-1.00357300
C	2.61761200	-0.25233200	-0.48118300
H	4.52275900	-1.48355200	2.04332200
H	6.12755000	0.20874300	1.11263500
H	5.45381900	1.58778400	-0.83626800
H	3.19934900	1.29195900	-1.85178100
H	1.62061900	-0.37099900	-0.90055100
C	2.06467500	-2.04093600	1.15911900
O	2.34341300	-2.78650700	2.08447000
H	1.09138100	-2.10410800	0.62572400

FE	-0.92754100	0.06869200	0.47800900
O	-2.29711600	-1.34907700	0.96381500
O	-0.50691200	-1.08178500	-1.17065600
O	-2.17538800	1.69499100	0.89897900
O	0.05385100	1.55916900	-0.85146100
C	-3.66568400	-3.26794600	1.03279400
C	-2.56986700	-2.44990600	0.39715800
C	-1.92822800	-2.94430400	-0.75515800
C	-0.94988400	-2.24546500	-1.46708200
C	-0.33544500	-2.87053000	-2.69199400
C	-1.88189900	2.93705900	0.87931900
C	0.06461800	2.80295100	-0.66233600
C	-2.78997000	3.82532400	1.69332100
C	-0.82647100	3.51762500	0.17279800
C	1.13327100	3.58962700	-1.38976100
H	-4.59960900	-2.69642300	1.03604900
H	-3.83750800	-4.21893400	0.52066400
H	-3.41867000	-3.46870100	2.08022900
H	-2.23486600	-3.91620400	-1.13208400
H	0.74907900	-2.95470000	-2.55584000
H	-0.74047100	-3.86182500	-2.91276800
H	-0.48984400	-2.22192900	-3.56090500
H	-3.82435900	3.70510700	1.35538800
H	-2.76672000	3.50610800	2.73995500
H	-2.51792800	4.88280000	1.63713500
H	-0.70218000	4.59483700	0.24388300
H	1.19766700	3.25316300	-2.42863400
H	0.96316100	4.66992600	-1.36776300
H	2.10584800	3.38353000	-0.92821800
H	0.25795800	0.04072200	1.67383400
O	-2.78856400	0.80490100	-1.88171200
H	-1.85742600	0.55559100	-1.95115800
H	-2.82909700	1.18316000	-0.99267700

IM2_w4

C	-3.36974600	-0.08747600	-0.96865600
C	-4.70213400	-0.20134700	-0.55296500
C	-5.23360300	-1.44955300	-0.26344000
C	-4.43749300	-2.59130600	-0.39377600
C	-3.11103100	-2.48017800	-0.80615900
C	-2.57020100	-1.22937900	-1.09276300
H	-5.29173100	0.70862000	-0.46668300
H	-6.26661100	-1.54289400	0.06492300
H	-4.85555600	-3.56981100	-0.16550100
H	-2.48909600	-3.36746600	-0.89272400
H	-1.52418200	-1.11293400	-1.39379300
C	-2.79841900	1.23423100	-1.29457000
O	-3.44439600	2.27219100	-1.29268800
H	-1.71854200	1.20680700	-1.56919800
FE	1.16385800	0.02863000	-0.47253300
O	2.95086900	0.86355000	-1.00890800
O	2.23854800	-1.66133700	-0.01521200
O	0.43694200	1.94336300	0.08509300
O	-0.19533000	-0.62749000	1.04506100
C	5.24666700	1.36188500	-1.19749700
C	4.12737500	0.40184700	-0.87636200
C	4.44746400	-0.89482100	-0.44591300
C	3.49686700	-1.83228500	-0.01157300
C	3.97724200	-3.15605100	0.53303200
C	-0.60914000	2.26358900	0.73143300
C	-1.15610000	-0.00438700	1.59619000
C	-1.03178400	3.70736300	0.65265200
C	-1.41295700	1.37069900	1.46473500
C	-2.08808300	-0.83693800	2.44093300
H	6.23569700	0.89906800	-1.13340700
H	5.10896800	1.77418100	-2.20215600

H	5.21235200	2.21016700	-0.50531900
H	5.49819000	-1.16324700	-0.37457700
H	3.48513900	-3.97789400	0.00320700
H	5.06119800	-3.28021300	0.45489100
H	3.68989600	-3.24725100	1.58605800
H	-0.15376800	4.35673600	0.61843900
H	-1.59521000	3.85452000	-0.27654500
H	-1.68156000	4.00215900	1.48148600
H	-2.28528100	1.77595800	1.97139600
H	-1.51855400	-1.37826200	3.20320800
H	-2.86671900	-0.24316900	2.92789900
H	-2.56814300	-1.59240800	1.80825400
H	0.28654600	-0.27357300	-1.89157200
O	2.23594800	0.75194200	2.22181500
H	1.61891900	0.02017100	2.08693600
H	1.92754300	1.40324200	1.57753900

IM4_1

O	-2.21115300	-1.30889100	0.00001700
C	-1.69192500	-0.20281800	0.00008700
C	-2.53246500	1.05010000	0.00025700
H	-2.32087800	1.66862600	-0.87796000
C	1.81464400	1.27332000	-0.00007900
C	0.42660300	1.19096500	0.00001900
C	-0.20870100	-0.05639100	0.00002100
C	0.57208700	-1.21904300	-0.00006600
C	1.95668300	-1.13760300	-0.00015700
C	2.58062600	0.11017300	-0.00016700
H	2.30051700	2.24504700	-0.00009000
H	-0.16346500	2.10381600	0.00008500
H	0.05472700	-2.17424400	-0.00006300
H	2.55521700	-2.04409500	-0.00022400
H	3.66522000	0.17558200	-0.00024300

H	-2.32086800	1.66839600	0.87863000
H	-3.58654900	0.77577100	0.00023400

IM4_2

C	-0.53313100	0.21212500	-0.00000700
C	-0.04525300	-1.10042200	-0.00001300
C	1.32259000	-1.32835600	0.00000500
C	2.20905600	-0.24898800	0.00001300
C	1.72965400	1.05923900	-0.00000900
C	0.35863200	1.28824100	-0.00000200
H	-0.76328400	-1.91620300	-0.00003800
H	1.70683900	-2.34443600	0.00002300
H	3.28045000	-0.43064400	0.00002400
H	2.42416100	1.89425100	-0.00003000
H	-0.03532200	2.30352200	0.00000000
C	-1.98215400	0.46697400	0.00000700
O	-2.83947500	-0.39397000	0.00000000
H	-2.25341100	1.55239500	0.00005200

IM5

C	1.26553400	-0.82709900	-0.07831100
O	-1.17240600	-2.18905800	-0.07497400
C	-1.17796300	-0.95863000	-0.04949600
C	0.07892900	-0.18961100	-0.01908100
H	0.03337800	0.89147800	0.08236900
C	-3.83192100	1.77810400	-0.22853400
C	-2.58668100	1.15849700	-0.25061500
C	-2.47405500	-0.21897000	-0.02377400
C	-3.63726700	-0.96026800	0.22288900
C	-4.87760300	-0.34086800	0.25844900
C	-4.97781300	1.03183100	0.03264700
H	-3.90803100	2.84561800	-0.41538000
H	-1.70515700	1.75383400	-0.47042500

H	-3.52919100	-2.02876600	0.38343700
H	-5.77110400	-0.92481300	0.46085200
H	-5.94898000	1.51889000	0.05760800
C	5.00171000	-0.56955300	-0.06742700
C	3.71188300	-1.08232800	-0.12483500
C	2.59155800	-0.24057500	-0.02529600
C	2.81131300	1.13954200	0.13358600
C	4.09805000	1.65107300	0.19216400
C	5.19913900	0.79928000	0.09260000
H	5.85407700	-1.23834100	-0.14489300
H	3.55358700	-2.15156600	-0.24666100
H	1.96282200	1.81370600	0.21584500
H	4.24842800	2.71958700	0.31789000
H	6.20623900	1.20362600	0.14063100
H	1.21430300	-1.91333700	-0.17127400

IM6_1

O	0.50357000	-0.12828100	1.28270800
O	-0.72349300	2.26093600	0.52780800
O	2.89282900	0.39931900	-0.04176700
O	1.96354500	3.02800200	-0.38744900
C	-0.67212200	-1.53235600	2.79405300
C	-0.56162500	-0.27696600	1.96518200
C	-1.62300600	0.64297700	2.01193700
C	-1.63197400	1.86707800	1.32951300
C	-2.78498800	2.81335400	1.54094500
C	4.02149300	0.96502300	-0.07184000
C	3.20825800	3.28956200	-0.35879200
C	5.22708300	0.06088700	0.04789100
C	4.23662100	2.35071500	-0.21734200
C	3.56515000	4.74941000	-0.49351200
H	0.23760600	-2.12758100	2.69714000
H	-0.84076500	-1.29663500	3.85080800

H	-1.52609200	-2.13251700	2.45638100
H	-2.47829700	0.39540800	2.63560000
H	-2.41714800	3.76738500	1.93347000
H	-3.26475800	3.02678800	0.58026500
H	-3.53788800	2.41295100	2.22544100
H	5.05636800	-0.68040900	0.83365000
H	5.36452100	-0.49577800	-0.88666200
H	6.15204200	0.60727400	0.25359600
H	5.26119000	2.71297100	-0.21315100
H	3.08835300	5.32198600	0.30834300
H	4.64344800	4.92882800	-0.46566400
H	3.16406300	5.14063000	-1.43395400
FE	0.94608300	1.27835500	-0.12924200
H	0.43097200	0.65589200	-1.61640400
O	-3.57898300	-2.41971000	0.47828900
C	-2.89083600	-1.61926100	-0.17471800
C	-1.48183500	-1.88607300	-0.47241800
H	-0.85879200	-1.09487100	-0.88919200
C	-3.43744700	1.76800900	-1.84226900
C	-2.78975000	0.62676300	-1.37866000
C	-3.50823100	-0.36292500	-0.69233200
C	-4.88135200	-0.17375100	-0.47685500
C	-5.52501100	0.96367200	-0.94301700
C	-4.80401200	1.94012700	-1.63297800
H	-2.85697700	2.53404800	-2.35105000
H	-1.71327700	0.54519900	-1.52933100
H	-5.41326300	-0.95053200	0.06595700
H	-6.59135100	1.09546100	-0.76978300
H	-5.30518100	2.83570200	-1.99511400
C	-0.94737700	-3.10399800	-0.21821800
C	2.77397900	-2.94090200	-0.75897900
C	1.45425500	-2.53986000	-0.62362800
C	0.43872700	-3.48815800	-0.38815700

C	0.80591200	-4.84298200	-0.28474800
C	2.12931400	-5.24064800	-0.42561600
C	3.12133400	-4.28973700	-0.66383900
H	3.53139100	-2.17854700	-0.91990500
H	1.21184100	-1.48086200	-0.67457000
H	0.02978900	-5.58323300	-0.09514000
H	2.39041800	-6.29393200	-0.34488600
H	4.16018700	-4.59775200	-0.76215900
H	-1.63165900	-3.86698900	0.16026700

IM6_2

O	-0.48637200	-3.28589100	-0.29657900
O	-1.60049000	-0.67581200	-0.30880300
O	2.29196400	-2.17788500	-0.20134500
O	0.71584800	-0.25063100	1.06869400
C	-1.98499300	-5.08402300	-0.52676900
C	-1.70618000	-3.60010800	-0.48140400
C	-2.77539100	-2.71382000	-0.63264600
C	-2.67180400	-1.30771700	-0.51699300
C	-3.93578600	-0.48976600	-0.60688400
C	3.19195500	-1.73042400	0.56948800
C	1.79501500	-0.03518400	1.70839400
C	4.55534200	-2.36246400	0.43434500
C	3.00823900	-0.70734600	1.51523800
C	1.71387600	1.03500400	2.76966300
H	-1.65376300	-5.54893200	0.40738500
H	-3.04193600	-5.31613600	-0.68360300
H	-1.39640300	-5.54278800	-1.32748300
H	-3.76343800	-3.13597800	-0.79466500
H	-4.18257200	-0.08850800	0.38275300
H	-3.77183000	0.37479200	-1.25860200
H	-4.78841400	-1.07391300	-0.96525100
H	4.92344800	-2.21646400	-0.58647900

H	5.28675300	-1.94889600	1.13431100
H	4.48311000	-3.44359700	0.58966300
H	3.86303100	-0.39972200	2.11089500
H	1.36445600	1.97233800	2.32210800
H	0.97039300	0.75610700	3.52509200
H	2.67213400	1.21703200	3.26426600
FE	0.39485400	-1.45024400	-0.58819600
H	0.49244800	-1.20723200	-2.24006800
O	-2.29492000	2.28593300	-1.82776900
C	-1.73894500	2.25560500	-0.71822600
C	-0.30062500	2.16586300	-0.54173300
H	0.09713900	2.38824100	0.44717800
C	-2.94608800	1.80835600	2.85686000
C	-2.13333200	1.75667100	1.72900100
C	-2.55842600	2.33995300	0.52680300
C	-3.81607400	2.95158500	0.47490600
C	-4.62100500	3.01348700	1.60574600
C	-4.18667200	2.44430000	2.80360800
H	-2.61735100	1.33496800	3.78002300
H	-1.19534600	1.20276900	1.74310100
H	-4.14214100	3.35784500	-0.47970400
H	-5.59373800	3.49940100	1.55692200
H	-4.81955000	2.48293700	3.68768500
C	0.53863800	1.69774800	-1.49957300
C	4.06319100	2.25883500	-0.26840400
C	2.68618800	2.37052800	-0.40346700
C	1.98215500	1.61600700	-1.36301200
C	2.72933100	0.76748200	-2.20203600
C	4.10597200	0.65587400	-2.06343000
C	4.78288300	1.39309600	-1.09115800
H	4.57936800	2.84796100	0.48749000
H	2.13679300	3.06509300	0.22887100
H	2.19241400	0.15476700	-2.92192400

H	4.65548200	-0.02570200	-2.70951700
H	5.86033400	1.29545800	-0.97771000
H	0.09841900	1.33802200	-2.42801700

IM6_w1

O	-2.63696100	2.69276000	-2.68454800
H	-0.20076800	0.58879900	1.69245400
C	-2.32818700	2.09838100	-1.64332600
C	-0.97603500	2.17110700	-1.07858300
H	-0.72999000	1.59125700	-0.18901800
C	-4.15942100	-0.04044200	0.93328200
C	-3.14027300	0.68436800	0.32031000
C	-3.36288900	1.30008500	-0.91967000
C	-4.62497800	1.17705100	-1.52109100
C	-5.63448700	0.44605800	-0.91202700
C	-5.40364300	-0.16725800	0.32098600
H	-3.96347600	-0.52512800	1.88637700
H	-2.16851700	0.73687500	0.81231200
H	-4.77183100	1.67068600	-2.47803100
H	-6.60490500	0.35010600	-1.39479300
H	-6.19169200	-0.74493600	0.79956500
C	-0.03514400	2.93506500	-1.67738600
C	3.13458400	2.83706700	0.36097100
C	1.81311100	2.63269600	-0.00847500
C	1.32794300	3.13922700	-1.23092700
C	2.21189700	3.87129500	-2.04463700
C	3.53433900	4.07493700	-1.66994600
C	4.00280400	3.55430400	-0.46489100
H	3.49300400	2.41778900	1.29776700
H	1.15480200	2.05418500	0.64039700
H	1.84282200	4.27082200	-2.98797300
H	4.20156300	4.63841300	-2.31855500
H	5.03821000	3.70692100	-0.16893200

H	-0.33296600	3.44976300	-2.59359500
FE	0.52217600	-0.81942300	1.08624600
O	2.31585900	-0.92156700	2.05569900
O	1.62314500	-0.38523300	-0.60223200
O	-0.29861400	-2.33941400	2.22618200
O	-0.88469500	-1.45524800	-0.37607200
C	4.60183000	-1.15754100	2.57552700
C	3.49701700	-0.87376600	1.58863100
C	3.83022100	-0.57279900	0.25993900
C	2.88604900	-0.34368300	-0.75226600
C	3.36491500	0.00687800	-2.13531600
C	-1.40127600	-2.96728700	2.07639400
C	-1.89457800	-2.20739900	-0.23502000
C	-1.81799500	-3.82776500	3.24184900
C	-2.20941100	-2.92790300	0.93701500
C	-2.80145000	-2.33741600	-1.43109800
H	5.59839900	-1.07650100	2.13306000
H	4.53016400	-0.46692600	3.42233100
H	4.47846500	-2.16527800	2.98496400
H	4.88257900	-0.53192900	-0.00678500
H	3.01993900	1.01661200	-2.38730000
H	4.45400600	-0.02422500	-2.22808400
H	2.91897000	-0.67076300	-2.86971900
H	-1.04845700	-4.58034800	3.44231400
H	-1.89169100	-3.21238700	4.14414700
H	-2.77269100	-4.33436400	3.07663800
H	-3.11667500	-3.52575400	0.93580600
H	-2.23509400	-2.73122300	-2.28126600
H	-3.66162800	-2.98626800	-1.24431500
H	-3.16362800	-1.34608400	-1.72322600
O	1.39087700	-3.49013200	-0.04215000
H	0.99717500	-2.77776400	-0.56320900
H	0.99659000	-3.35654500	0.82977000

IM6_w2

O	2.37929300	-2.15929700	-2.22942400
C	2.03688400	-2.06187000	-1.04228100
C	0.66217200	-2.22051800	-0.58991600
H	0.49435200	-2.35394400	0.47632700
C	3.71620500	-0.81411600	2.13261000
C	2.72666800	-1.15319500	1.21613800
C	3.06273600	-1.77073200	0.00378900
C	4.40814600	-2.03777600	-0.27093300
C	5.39535700	-1.72063800	0.65404400
C	5.05239600	-1.10536400	1.85873500
H	3.44159400	-0.29746700	3.04971800
H	1.68819100	-0.88437200	1.40307900
H	4.64863600	-2.48211300	-1.23399400
H	6.43828400	-1.94051500	0.43461700
H	5.82666000	-0.84072000	2.57580400
C	-0.39187900	-2.06166800	-1.42612300
C	-3.59481300	-2.68397900	0.48167300
C	-2.24131000	-2.60602600	0.18742700
C	-1.79716400	-2.17145300	-1.07563100
C	-2.77339800	-1.82908300	-2.03015400
C	-4.12693200	-1.91289500	-1.73721300
C	-4.54706700	-2.33931000	-0.47772400
H	-3.91154000	-3.00537300	1.47159500
H	-1.51084100	-2.87415600	0.94701300
H	-2.43899100	-1.45153600	-2.99310000
H	-4.85944300	-1.62698700	-2.48852600
H	-5.60751600	-2.39529500	-0.24157700
H	-0.16647100	-1.81994200	-2.46415000
FE	-0.93298100	0.95164200	-0.75065100
O	-0.60651600	0.02316500	1.05645500
O	-2.88065900	1.13423200	-0.08395500

O	1.26160400	0.76414200	-0.76714700
O	-0.42762300	2.94178200	-0.23821200
C	-0.61537400	-0.43385800	3.35778500
C	-1.31995400	0.03055600	2.11244700
C	-2.65709700	0.44091200	2.17488000
C	-3.37284800	0.92424500	1.06337600
C	-4.84664900	1.21030200	1.21140000
C	2.01655000	1.65287300	-1.25380200
C	0.52174200	3.58141400	-0.80440500
C	3.39126600	1.20982600	-1.68184000
C	1.67527300	3.01978900	-1.36131700
C	0.36861400	5.08283900	-0.82038100
H	-1.25904900	-0.44067500	4.24152700
H	-0.20333700	-1.43832000	3.20552400
H	0.23369700	0.24120200	3.52155300
H	-3.17873000	0.34739200	3.12324000
H	-5.40536100	0.55890400	0.53127000
H	-5.21168700	1.05156400	2.22994200
H	-5.06060300	2.24023300	0.90994300
H	3.99185500	0.99843300	-0.78898100
H	3.32246700	0.27050000	-2.23898900
H	3.91327100	1.96493800	-2.27646100
H	2.40761000	3.69412300	-1.79623800
H	0.30402700	5.45503400	0.20752200
H	1.19297200	5.59122700	-1.32733400
H	-0.57324000	5.35124200	-1.30886600
H	-1.10089700	0.69027100	-2.39019800
O	1.32399500	1.98629100	2.05508100
H	0.56479100	2.46954100	1.70375500
H	1.37891000	1.27994500	1.39503100

IM7_1

O	-0.09889100	-2.21737500	1.45743100
---	-------------	-------------	------------

O	0.19988400	-1.87913800	-1.30262700
O	-2.72671900	-0.91453800	1.23792600
O	-2.76016400	-1.69418900	-1.42675100
C	1.86117200	-2.43686100	2.75645400
C	1.17893900	-2.29531900	1.42836600
C	1.95517400	-2.20831700	0.26628100
C	1.44641900	-1.92768500	-1.00549800
C	2.40083100	-1.66546600	-2.13748700
C	-3.90011700	-0.50130700	0.97874500
C	-3.97100100	-1.29698500	-1.36439100
C	-4.58211900	0.27845700	2.06842300
C	-4.56479600	-0.69923000	-0.24533000
C	-4.78004600	-1.47799900	-2.62139300
H	1.25989700	-3.04606100	3.43634000
H	2.86511900	-2.86025600	2.66226300
H	1.96132500	-1.42818300	3.17006500
H	3.03414300	-2.20774400	0.38742600
H	2.15731700	-2.29888600	-2.99692000
H	2.28866200	-0.62394100	-2.45620200
H	3.44474000	-1.81778700	-1.85018500
H	-4.45084700	-0.22224400	3.03117400
H	-4.09872900	1.25856100	2.15090600
H	-5.64675700	0.43512900	1.87580100
H	-5.58646800	-0.34185300	-0.33679500
H	-4.79440400	-2.53545100	-2.90309400
H	-5.80907800	-1.12455500	-2.51796800
H	-4.30112600	-0.94360600	-3.44771900
FE	-1.31387600	-1.65014900	-0.01362500
H	-0.55509400	0.28772700	-0.35226500
O	2.24340600	0.50267300	1.82529200
C	2.37711600	0.91460000	0.63327000
C	1.33248700	1.29569600	-0.20951200
H	1.51605400	1.57747200	-1.24380200

C	5.44868900	1.48322800	-1.60695500
C	4.15727600	1.59472500	-1.10183000
C	3.76753600	0.90334300	0.05413400
C	4.73292900	0.11843800	0.69983400
C	6.02193800	-0.00570700	0.19251700
C	6.38851400	0.67418000	-0.96779900
H	5.72742300	2.03397500	-2.50406700
H	3.43852600	2.23776200	-1.60508100
H	4.41644600	-0.38720400	1.60966600
H	6.74929200	-0.63443700	0.70462600
H	7.39707200	0.58292400	-1.36631400
C	-0.06670300	1.11316400	0.22759100
C	-1.49241300	4.63204800	0.49261300
C	-0.61586300	3.55483100	0.55894400
C	-0.99915600	2.28718700	0.10530300
C	-2.27879600	2.14193300	-0.43872400
C	-3.16225900	3.21673500	-0.50604400
C	-2.77333000	4.46927400	-0.03784700
H	-1.17680000	5.60860700	0.85567000
H	0.39022700	3.67196800	0.95790400
H	-2.58014600	1.16265300	-0.81172400
H	-4.15559300	3.07102900	-0.92843400
H	-3.45700700	5.31398200	-0.09129300
H	-0.02807200	0.77705300	1.27609300

IM7_2

O	1.20848900	3.07868900	-0.11163500
O	-1.03744600	1.66111700	-0.95770500
O	2.90950800	0.92524300	-1.11316000
O	0.64582100	-0.54867300	-1.74239500
C	0.85685500	5.03269700	1.15623200
C	0.31975500	3.83191900	0.42254100
C	-1.05661200	3.61809300	0.37532600

C	-1.67450500	2.54012100	-0.29412600
C	-3.16063700	2.38343900	-0.20562400
C	3.50394700	-0.17891300	-1.35026600
C	1.47843600	-1.50612200	-1.84815900
C	5.00337700	-0.15146400	-1.21787700
C	2.86916600	-1.37450700	-1.70787900
C	0.88601900	-2.86117600	-2.11948300
H	1.49440400	5.62226200	0.48966300
H	0.06598500	5.67379200	1.55351600
H	1.49242900	4.70428000	1.98503900
H	-1.69916700	4.31834300	0.90084800
H	-3.54236300	1.84766500	-1.07735900
H	-3.36867000	1.76861300	0.68392500
H	-3.67175600	3.34426500	-0.09356500
H	5.27476700	0.28467300	-0.25173900
H	5.45117500	-1.14540200	-1.29904300
H	5.43660600	0.49550500	-1.98851100
H	3.48192800	-2.26336100	-1.82519700
H	0.31476700	-3.17686100	-1.23845400
H	0.17653700	-2.80596600	-2.95038300
H	1.64318000	-3.62068200	-2.33084100
FE	0.92879900	1.27268000	-0.93845100
H	0.46621900	0.55288800	1.00876000
O	-2.57334000	0.30874100	2.15932400
C	-2.29334100	-0.55286100	1.26538300
C	-1.01949100	-1.02792500	0.97561900
H	-0.86374400	-1.71512800	0.14928200
C	-4.39995000	-2.03806800	-1.57084100
C	-3.29445800	-1.59880800	-0.84832500
C	-3.43769300	-1.09658800	0.45360500
C	-4.72953800	-1.02008800	0.98982300
C	-5.83451000	-1.46893500	0.27547100
C	-5.67620200	-1.98499300	-1.01084200

H	-4.26846500	-2.41126400	-2.58553600
H	-2.30729600	-1.60037500	-1.30788400
H	-4.82165400	-0.57921800	1.97996000
H	-6.82877800	-1.41009800	0.71694400
H	-6.54063400	-2.32421400	-1.57871400
C	0.16291100	-0.38477900	1.56722700
C	2.52172700	-3.37992900	1.72950200
C	1.36209300	-2.61355600	1.64125700
C	1.41248000	-1.21622400	1.68348800
C	2.66756600	-0.61096500	1.83017400
C	3.82709000	-1.37257800	1.93256400
C	3.76179200	-2.76441200	1.87618400
H	2.45526800	-4.46551000	1.68304100
H	0.38687000	-3.08485600	1.53533800
H	2.72854500	0.47794600	1.83146300
H	4.79039600	-0.87785600	2.04482100
H	4.66969800	-3.36046900	1.94121600
H	-0.12694700	0.04014400	2.54186600

IM7_w1

H	0.97715500	-0.53010000	-2.23900400
O	-1.78565300	0.36503000	-2.55387300
C	-1.43454500	0.87455200	-1.46321000
C	-0.09144900	0.86480700	-0.98242100
H	0.15612300	1.67820000	-0.29871400
C	-3.30094300	2.65866600	1.37860200
C	-2.27895000	2.02251700	0.67938000
C	-2.49892700	1.52835800	-0.61439700
C	-3.77783300	1.66364400	-1.16731200
C	-4.80105600	2.29646600	-0.47015900
C	-4.56509400	2.80591000	0.80582500
H	-3.11324000	3.03109600	2.38371600
H	-1.31060800	1.88073800	1.15574000

H	-3.92525900	1.24984100	-2.16207100
H	-5.78749300	2.39481300	-0.92040500
H	-5.36130300	3.30349900	1.35585000
C	0.96542100	0.54661800	-2.02030700
C	3.93311600	2.58714100	-0.73207300
C	2.63132000	2.20164400	-1.04043300
C	2.36202400	0.97999600	-1.67082200
C	3.45660700	0.16751400	-1.99076200
C	4.76071800	0.54775900	-1.68983200
C	5.00763500	1.76204500	-1.05426000
H	4.10800700	3.53746000	-0.23056300
H	1.80152900	2.85485200	-0.77795200
H	3.26509400	-0.79715100	-2.45893400
H	5.58762200	-0.11546000	-1.93867500
H	6.02454000	2.05801600	-0.80633000
H	0.67554500	1.01232800	-2.98057600
FE	0.03237500	-0.76853900	0.58825600
O	0.84723900	0.50246500	1.94641300
O	1.87455100	-1.57501900	0.33033600
O	-1.83646100	-1.04161600	1.37487600
O	-0.57673200	-2.23071900	-0.83496500
C	2.40672800	1.83662700	3.10492400
C	2.07971400	0.65576500	2.22743000
C	3.12223300	-0.17508000	1.79120600
C	2.96101200	-1.25622100	0.91226800
C	4.14685700	-2.13255800	0.60335800
C	-2.89697200	-1.36859000	0.72268800
C	-1.76300400	-2.33782800	-1.26270000
C	-4.19394900	-1.00878100	1.38991400
C	-2.91664300	-1.98790600	-0.52397900
C	-1.92836500	-2.82944700	-2.67313200
H	3.47019500	1.90077200	3.35040500
H	2.11180800	2.75906700	2.59210400

H	1.82495400	1.79358900	4.03119900
H	4.12551400	0.04236300	2.14653100
H	4.25751100	-2.23351800	-0.48063700
H	5.07987000	-1.74444100	1.02135100
H	3.97371100	-3.13812600	1.00185200
H	-4.21280300	-1.40523700	2.41030400
H	-4.26190300	0.08210800	1.47046200
H	-5.06625000	-1.37544500	0.84260700
H	-3.88399800	-2.14507500	-0.99231900
H	-1.19494900	-3.60866900	-2.89582400
H	-2.93792000	-3.19262600	-2.88496900
H	-1.72467600	-1.96950800	-3.32142200
O	-0.14817200	-3.35509700	1.95749100
H	0.09062000	-3.33250000	1.02125900
H	-0.90326100	-2.75091500	1.98936700

IM8

H	1.74778200	1.83529500	1.85037700
O	-0.59060000	-1.17214200	1.49779000
C	-0.82126300	-0.08309400	0.87308600
C	0.06064000	0.98351500	0.77704800
H	-0.13884800	1.84905400	0.15145800
C	-3.85890100	1.15405400	-1.15431900
C	-2.59545500	1.12854400	-0.57375000
C	-2.17061000	0.04254000	0.20763100
C	-3.07395100	-1.01760900	0.37841800
C	-4.34114000	-0.99451900	-0.19399900
C	-4.74573300	0.09192100	-0.96768300
H	-4.15780500	2.00986500	-1.75882700
H	-1.92413300	1.96880700	-0.73336800
H	-2.71821600	-1.84903400	0.98219500
H	-5.02211200	-1.83178300	-0.03975200
H	-5.73510400	0.11246800	-1.42187200

C	1.40504000	0.87711900	1.42705900
C	3.24934200	-1.43413000	-0.95053500
C	2.30171700	-0.92162900	-0.07432900
C	2.47100800	0.34860900	0.50069100
C	3.60971000	1.08249400	0.15786100
C	4.55591900	0.57511100	-0.73436900
C	4.38224100	-0.68784100	-1.29030700
H	3.10692400	-2.42433900	-1.38057700
H	1.40588300	-1.47888400	0.20057000
H	3.75010800	2.07127000	0.59576400
H	5.43052200	1.16995300	-0.99508200
H	5.11836300	-1.08884500	-1.98450400
H	1.29004800	0.16280300	2.25629100

IM9

C	-1.30370800	-1.01831200	-0.00009100
O	1.18452400	-2.16705900	-0.00019800
C	1.21224900	-0.94444200	-0.00008500
C	-0.07073100	-0.13853900	-0.00004000
H	-0.06246400	0.53295200	-0.87068700
C	3.83592800	1.81358000	0.00016900
C	2.59529200	1.18531300	0.00010600
C	2.51003700	-0.21222600	-0.00000300
C	3.68958400	-0.96719400	-0.00004800
C	4.92713600	-0.34092300	0.00001600
C	5.00196100	1.05163500	0.00012400
H	3.89454400	2.89818600	0.00025200
H	1.69084200	1.78803100	0.00013900
H	3.59698600	-2.04918900	-0.00013500
H	5.83704300	-0.93417700	-0.00001800
H	5.97072000	1.54409400	0.00017500
C	-5.05533100	-0.46683600	0.00017600
C	-3.80397300	-1.06849900	0.00014400

C	-2.62941500	-0.30477400	-0.00002300
C	-2.75290400	1.08623600	-0.00014900
C	-4.00725600	1.69548600	-0.00011500
C	-5.16252400	0.92287600	0.00004300
H	-5.95055300	-1.08276600	0.00030300
H	-3.72527300	-2.15431400	0.00024900
H	-1.86308100	1.71093700	-0.00027000
H	-4.07745200	2.78003900	-0.00021300
H	-6.13994800	1.39738000	0.00006800
H	-1.25158400	-1.69386600	-0.86281000
H	-1.25157100	-1.69400400	0.86251800
H	-0.06248000	0.53288400	0.87066000

IM10_1

C	1.14150300	3.00256200	-0.45371300
C	1.90920900	4.08968700	-0.89404600
C	3.10932500	4.40697900	-0.27129100
C	3.57075100	3.62541500	0.78945000
C	2.82141600	2.53513700	1.22231400
C	1.60859200	2.22902200	0.61365500
H	1.53829300	4.66706500	-1.73701100
H	3.69289900	5.25840900	-0.61558200
H	4.51951600	3.86253500	1.26787300
H	3.18439700	1.89175700	2.01975700
H	1.06805100	1.34727400	0.94156600
C	-0.13530600	2.70738600	-1.16810300
O	-0.33729900	3.18214400	-2.28064700
C	-1.23806400	1.95575800	-0.44287500
H	-0.82918600	1.29739900	0.32935300
H	-1.81673800	2.73625900	0.08150700
C	-2.13119500	1.18911000	-1.40195900
H	-1.56968900	0.28911700	-1.70021900
H	-2.24433300	1.78490600	-2.31577100

C	-3.48596500	0.79013800	-0.89409100
C	-3.84294400	0.83670500	0.45739700
C	-4.44821600	0.32388200	-1.80214100
C	-5.10710100	0.43460800	0.88480400
H	-3.11201700	1.16608600	1.19160100
C	-5.71129300	-0.07724900	-1.38240800
H	-4.18839400	0.27840800	-2.85863400
C	-6.04943800	-0.02289800	-0.03052000
H	-5.34991400	0.47130100	1.94504300
H	-6.43523300	-0.43472000	-2.11169600
H	-7.03483700	-0.33902800	0.30388700
O	2.75221400	-0.73852600	0.58151000
O	1.76599700	-2.80756100	-1.06476600
O	0.24845300	-0.51274000	1.71983500
O	-1.04826000	-2.12636300	-0.15096600
C	5.09070700	-0.48809200	0.74824100
C	3.86886200	-1.19364600	0.20531900
C	4.05412900	-2.29423500	-0.65621900
C	3.00810300	-3.04592600	-1.20609300
C	3.34428500	-4.25748500	-2.04174800
C	-0.84352900	-0.66133800	2.36168100
C	-1.99060200	-2.09428400	0.69696400
C	-0.93505700	0.09106900	3.66636000
C	-1.93765400	-1.41974000	1.93341900
C	-3.26168200	-2.80687400	0.31259300
H	6.03024800	-0.95306300	0.43560800
H	5.08383000	0.55460800	0.41260200
H	5.05183700	-0.46317200	1.84246700
H	5.07251400	-2.60221500	-0.87835400
H	2.90876500	-5.15408900	-1.58794600
H	2.88960800	-4.15997400	-3.03268400
H	4.42114700	-4.40935600	-2.15794900
H	-0.87672600	1.16874500	3.46733700

H	-1.86057100	-0.11142400	4.21361200
H	-0.07922400	-0.15087600	4.30444700
H	-2.81959300	-1.45106000	2.56790400
H	-3.95966100	-2.90979200	1.14859300
H	-3.76663300	-2.24026600	-0.47934800
H	-3.03092400	-3.79490900	-0.09654300
H	0.61656000	-0.03604200	-1.29860800
FE	0.82285200	-1.25667900	-0.13555800

IM10_2

C	0.20165500	2.21975300	0.18846700
H	0.17216400	1.18988900	-0.20534300
H	0.27231200	2.84735400	-0.71372700
C	1.40986300	2.39532800	1.08539500
H	1.33933900	1.63907000	1.88050400
H	1.36677900	3.36312100	1.60085900
C	2.73147200	2.23937400	0.38503200
C	3.87175700	2.87110500	0.89567100
C	2.87724200	1.43055900	-0.75026300
C	5.12263100	2.69269200	0.31080000
H	3.77126400	3.50714500	1.77490300
C	4.12833100	1.25021700	-1.33518800
H	2.01462300	0.90152600	-1.15845000
C	5.25647700	1.87574800	-0.80957200
H	5.99343100	3.19257500	0.73103800
H	4.21730000	0.59890500	-2.20187100
H	6.23217700	1.72834900	-1.26741800
C	-2.35914100	2.19420600	0.12957200
C	-3.58300200	2.55952300	0.70691600
C	-4.78098800	2.26375700	0.07233400
C	-4.77291500	1.58698500	-1.14868100
C	-3.56169500	1.21282100	-1.72499500
C	-2.35793100	1.51979000	-1.09900600

H	-3.55619300	3.06920900	1.66727600
H	-5.72577100	2.55119100	0.52950200
H	-5.71147400	1.33995700	-1.64152400
H	-3.54620800	0.65895600	-2.66107100
H	-1.42393500	1.17338300	-1.54262400
C	-1.10295000	2.49967800	0.87384000
O	-1.15410000	2.96231000	2.01378600
FE	-0.08360600	-1.36095800	-0.55192300
O	1.59802700	-1.03463800	0.68071100
O	0.96507900	-2.97509600	-1.26042600
O	-1.03047700	-0.52635600	1.11322800
O	-1.95506900	-2.04349800	-1.03598200
C	3.76813600	-1.06934100	1.60412900
C	2.73012600	-1.59946100	0.64508600
C	3.07613200	-2.66962700	-0.20420900
C	2.17979400	-3.30225200	-1.07618400
C	2.65818200	-4.49241500	-1.87340100
C	-2.23223500	-0.64001700	1.51473000
C	-3.06824900	-1.91511800	-0.43507400
C	-2.54111200	-0.04106900	2.86253400
C	-3.25947800	-1.27303700	0.79654400
C	-4.26208900	-2.52364000	-1.13022400
H	3.33396000	-0.98711800	2.60534100
H	4.66535700	-1.69341200	1.64908000
H	4.06263600	-0.05678600	1.30528600
H	4.08529900	-3.06747300	-0.13640200
H	3.70732700	-4.73785700	-1.68588700
H	2.04297900	-5.36771300	-1.64045300
H	2.52531800	-4.29611900	-2.94230400
H	-1.94625200	-0.54461800	3.63233600
H	-2.24674400	1.01398200	2.88087900
H	-3.60008200	-0.12327200	3.12478600
H	-4.26178000	-1.25842200	1.21635100

H	-4.08496200	-3.58717600	-1.32043900
H	-5.18832700	-2.41161900	-0.55917200
H	-4.39664000	-2.05112200	-2.10932900
H	0.17436100	-0.21916200	-1.79689600

IM10_w1

C	1.50819500	2.88600300	-0.23203600
C	2.46588700	3.82284800	-0.64257000
C	3.62812700	4.02018900	0.09208500
C	3.85498700	3.27177900	1.24792500
C	2.91741000	2.32453900	1.65270100
C	1.74858700	2.13262500	0.92232700
H	2.26627200	4.38483000	-1.55327200
H	4.36237000	4.75622400	-0.23584400
H	4.77131700	3.41545800	1.82129800
H	3.10348900	1.70120600	2.52622000
H	1.05923300	1.35031600	1.23315200
C	0.26449200	2.76286400	-1.05298500
O	0.21315300	3.27352700	-2.16622700
C	-0.97998900	2.16891700	-0.41978200
H	-0.72025500	1.38635300	0.30325000
H	-1.44088700	2.98608900	0.16623700
C	-1.95612800	1.64816100	-1.45718800
H	-1.51048900	0.73499200	-1.88535200
H	-2.00327700	2.36804500	-2.28559500
C	-3.34303800	1.34607000	-0.96574500
C	-3.66448300	1.24852300	0.39192500
C	-4.37294600	1.13131100	-1.89314200
C	-4.96051400	0.94736400	0.80736300
H	-2.88365100	1.38110700	1.13882400
C	-5.66866000	0.83425400	-1.48519900
H	-4.14165300	1.20052500	-2.95715900
C	-5.97087800	0.74189100	-0.12665300

H	-5.17411400	0.86138600	1.87302100
H	-6.44752800	0.67299700	-2.23066700
H	-6.98359200	0.50479100	0.19801300
O	2.56467000	-0.89506500	0.60250200
O	1.35077200	-2.81135900	-1.11292400
O	0.05881500	-0.61258200	1.68334700
O	-1.45959100	-1.62688400	-0.42828900
C	4.81236500	-0.31579300	0.15801900
C	3.56620500	-1.12251500	-0.12578200
C	3.60891100	-2.05327400	-1.19181800
C	2.53263600	-2.84359300	-1.59991400
C	2.74267500	-3.84253400	-2.71104600
C	-0.98609100	-0.91579900	2.35772200
C	-2.34956400	-1.75882000	0.46755600
C	-0.87987700	-0.68512800	3.84250400
C	-2.16719900	-1.43978400	1.82782200
C	-3.68399100	-2.28243500	0.00557500
H	5.70747600	-0.71481000	-0.33321000
H	4.65098500	0.71206500	-0.19486600
H	4.98446000	-0.25217900	1.23855800
H	4.55204900	-2.17290400	-1.72220200
H	2.45859300	-4.84495200	-2.36773000
H	2.07842000	-3.60054200	-3.54963600
H	3.77614900	-3.87036900	-3.07380900
H	-0.54384600	0.33964900	4.04575800
H	-1.82328000	-0.86407200	4.37050800
H	-0.11588600	-1.35532200	4.25854300
H	-2.99616400	-1.62347400	2.50936100
H	-4.39658600	-2.41285600	0.82797600
H	-4.12017500	-1.58253400	-0.72003200
H	-3.55259000	-3.24074500	-0.51182200
O	1.29629900	-3.37821100	1.75780200
H	1.28381900	-3.49274300	0.79226800

H	1.57340200	-2.44921300	1.82617000
H	0.73696000	0.13694400	-1.41640000
FE	0.50038500	-1.09275300	-0.26123000

IM10_w2

C	-2.59985900	2.05141500	-0.42314200
C	-3.87385200	1.79331500	0.09841300
C	-4.97718400	1.68391100	-0.73707000
C	-4.82819800	1.84145100	-2.11450600
C	-3.56544600	2.10294900	-2.64533900
C	-2.46096900	2.20455300	-1.80743400
H	-3.95800600	1.66858600	1.17468400
H	-5.95775000	1.47017600	-0.31632100
H	-5.69002000	1.75502800	-2.77255900
H	-3.43989200	2.21561000	-3.71957400
H	-1.47771800	2.37700500	-2.23495800
C	-1.47016600	2.19711100	0.54551400
O	-1.68050300	2.06520900	1.74804300
FE	0.09571700	-1.35904000	-0.03059300
O	1.85842800	-1.07081500	0.94204100
O	1.17073600	-2.08949800	-1.59412900
O	-0.82725300	-1.32361600	1.96487900
O	-1.72023300	-2.39563000	-0.49161500
C	4.14215100	-1.02365600	1.51758900
C	3.03431200	-1.37124400	0.55741100
C	3.35871000	-1.96711300	-0.67196700
C	2.41990700	-2.31517000	-1.65726300
C	2.89813200	-3.00999800	-2.90876900
C	-2.06269100	-1.09914500	2.12944200
C	-2.83810900	-1.94542000	-0.07847600
C	-2.46756400	-0.51026700	3.45727300
C	-3.06387100	-1.34745800	1.16833500
C	-3.99089400	-2.06050500	-1.04328900

H	3.96428200	-1.50283500	2.48577400
H	5.12991800	-1.31546700	1.14939200
H	4.14041400	0.05811000	1.69445200
H	4.40480200	-2.18937900	-0.86600600
H	2.58839700	-2.44337300	-3.79313100
H	3.98371600	-3.14153400	-2.93402900
H	2.42385600	-3.99392800	-2.98810300
H	-2.02370400	-1.09085800	4.27177200
H	-2.06639900	0.50537500	3.51733500
H	-3.55271900	-0.46877500	3.59154200
H	-4.08137000	-1.04873300	1.40733200
H	-3.98031200	-3.03916600	-1.53176100
H	-4.96430900	-1.89107500	-0.57372300
H	-3.85774700	-1.30745200	-1.82910500
H	-0.50033200	0.13203900	-0.57690100
O	0.20587400	-3.84076300	1.06460200
H	-0.56732800	-3.74223000	0.48953100
H	0.03301300	-3.17304900	1.74388800
C	-0.11566300	2.66683400	0.06210500
H	0.08869200	2.27411300	-0.93609600
H	-0.14964100	3.76631300	-0.02591500
C	0.99447500	2.24158700	1.01959700
H	0.82388300	1.18433600	1.26492400
H	0.91386400	2.80173300	1.95723700
C	2.36307000	2.38563800	0.42545800
C	3.30715900	3.27820800	0.93972000
C	2.72862200	1.59194900	-0.67111400
C	4.58155000	3.37834100	0.38356300
H	3.03694000	3.89605100	1.79534700
C	4.00086900	1.68304100	-1.22378700
H	2.00371200	0.87715300	-1.06337100
C	4.93327700	2.57935200	-0.70061900
H	5.30187900	4.07859700	0.80184400

H	4.26878700	1.03641300	-2.05641100
H	5.92944200	2.64909400	-1.13211300
IM11_1			
O	0.22894200	-1.90372700	1.71661200
O	1.33582200	-1.45861200	-2.14582200
O	2.77911900	-1.54849000	0.24960100
C	-3.24515500	-3.09790200	-0.73322900
C	-1.99228800	-2.70372700	0.00274800
C	-2.05610400	-2.45265700	1.38224000
C	-0.95597500	-2.04973400	2.15758600
C	-1.15629200	-1.73695900	3.61682300
C	2.24099400	-0.63592200	-2.49588500
C	3.56066000	-0.75793500	-0.39608800
C	2.10138100	-0.03500700	-3.86366500
C	3.34897800	-0.29375100	-1.69259500
C	4.77286500	-0.29868600	0.36431800
H	-3.50789400	-2.30742500	-1.44523300
H	-3.06712000	-4.00335100	-1.32088000
H	-4.09619100	-3.26026400	-0.06605700
H	-3.01795100	-2.56101900	1.87588800
H	-0.40201600	-2.25289900	4.21801100
H	-1.00551800	-0.66362700	3.77912000
H	-2.15329200	-2.00397500	3.97700300
H	1.28057500	0.68493100	-3.80027800
H	3.00535000	0.48864800	-4.18622300
H	1.84139100	-0.80693800	-4.59439600
H	4.05775500	0.42505400	-2.09232600
H	5.28694100	-1.15660300	0.80934400
H	5.47358100	0.26434300	-0.25787400
H	4.44593800	0.34535000	1.18902900
O	-0.94365800	-2.58928700	-0.71159200
C	1.60533600	1.79723100	0.52371700

C	2.47572300	2.81266900	0.12728400
C	3.41397900	3.33428000	1.01409400
C	3.49941500	2.83971000	2.31517500
C	2.64745100	1.80866900	2.71385300
C	1.71026800	1.29118600	1.82236900
H	2.38729300	3.14652700	-0.90477000
H	4.08741900	4.12796900	0.69195700
H	4.23376500	3.24311100	3.01012600
H	2.72441600	1.39836600	3.71967600
H	1.07414700	0.45657700	2.11908800
C	0.56962400	1.28689100	-0.48898900
H	0.62345700	0.10693000	-0.33294400
O	0.75997600	1.65436100	-1.72212700
C	-0.87102500	1.55350200	0.05047000
H	-1.01211600	1.12907500	1.05813200
H	-1.01349700	2.64168900	0.13258700
C	-1.88622700	0.97251500	-0.92611700
H	-1.76962200	-0.12064000	-0.94139300
H	-1.58374400	1.33033200	-1.91836300
C	-3.30121000	1.34407200	-0.61164600
C	-3.84691100	2.54664800	-1.07984000
C	-4.11120900	0.52916200	0.18981200
C	-5.14925200	2.92080800	-0.76457700
H	-3.22825500	3.19183300	-1.70168100
C	-5.41574600	0.89753200	0.50670700
H	-3.69500300	-0.40322900	0.57211900
C	-5.94314100	2.09602700	0.03043900
H	-5.54942900	3.85896700	-1.14406900
H	-6.02493300	0.24513200	1.12940100
H	-6.96294400	2.38420900	0.27543300
FE	0.85342500	-1.80672200	-0.21284000

C	1.60445900	1.79712300	0.52382400
C	2.47485700	2.81248400	0.12722700
C	3.41300800	3.33434800	1.01400500
C	3.49830100	2.84014600	2.31523600
C	2.64633300	1.80917300	2.71409100
C	1.70929500	1.29142300	1.82262000
H	2.38647900	3.14612200	-0.90490100
H	4.08646500	4.12796500	0.69173000
H	4.23255700	3.24376500	3.01016000
H	2.72319600	1.39913700	3.72002600
H	1.07319300	0.45686700	2.11948600
C	0.56875600	1.28660800	-0.48878600
O	0.75898600	1.65416200	-1.72191500
FE	0.85450400	-1.80672300	-0.21291700
O	-0.94275800	-2.58906600	-0.71169700
O	0.23036500	-1.90496800	1.71668700
O	1.33678500	-1.45883400	-2.14582100
O	2.77989100	-1.54679000	0.24984000
C	-3.24460600	-3.09626100	-0.73331900
C	-1.99140500	-2.70315300	0.00266400
C	-2.05501800	-2.45242300	1.38223200
C	-0.95463300	-2.05037000	2.15765000
C	-1.15473800	-1.73791200	3.61698400
C	2.24162300	-0.63587300	-2.49614700
C	3.56121800	-0.75634400	-0.39621700
C	2.10154900	-0.03512400	-3.86392700
C	3.34949200	-0.29301300	-1.69303200
C	4.77307400	-0.29603900	0.36408800
H	-3.06641500	-4.00001500	-1.32349100
H	-4.09500500	-3.26083300	-0.06587400
H	-3.50857100	-2.30407400	-1.44300300
H	-3.01690300	-2.56043100	1.87589100
H	-1.00420500	-0.66457700	3.77949100

H	-2.15161700	-2.00520500	3.97730100
H	-0.40022300	-2.25379700	4.21791400
H	1.84036700	-0.80692800	-4.59436200
H	1.28132500	0.68544200	-3.79999400
H	3.00569000	0.48778300	-4.18722700
H	4.05807400	0.42580700	-2.09309500
H	5.28694100	-1.15330900	0.81057600
H	5.47406800	0.26613300	-0.25857400
H	4.44576300	0.34918900	1.18771600
H	0.62265600	0.10661400	-0.33264000
C	-0.87194800	1.55299600	0.05072800
H	-1.01308000	1.12815300	1.05821600
H	-1.01444600	2.64114800	0.13327900
C	-1.88702800	0.97241400	-0.92619800
H	-1.77016600	-0.12070200	-0.94223600
H	-1.58463500	1.33092900	-1.91821000
C	-3.30212100	1.34345400	-0.61159200
C	-3.84821000	2.54596600	-1.07945000
C	-4.11191400	0.52801900	0.18955700
C	-5.15072200	2.91957100	-0.76419700
H	-3.22974400	3.19157300	-1.70104300
C	-5.41662500	0.89580700	0.50641700
H	-3.69542300	-0.40436600	0.57157600
C	-5.94440500	2.09426300	0.03046500
H	-5.55118800	3.85770700	-1.14344400
H	-6.02563600	0.24298300	1.12884200
H	-6.96433500	2.38201000	0.27543000

IM11_w1

C	1.69391500	1.97485900	-0.23742200
C	2.60563700	2.73426200	-0.97096600
C	3.55054100	3.53137200	-0.32964100
C	3.59884100	3.57867000	1.06334400

C	2.70482500	2.80515300	1.80602000
C	1.76489700	2.00648900	1.15898300
H	2.53548800	2.64782200	-2.05373500
H	4.25695700	4.11951800	-0.91494600
H	4.33677800	4.20021700	1.56791100
H	2.75136500	2.81540500	2.89417200
H	1.10046700	1.36646500	1.73992800
C	0.64691000	1.15016400	-1.00423600
O	0.83067400	1.06565600	-2.29199900
C	-0.78437200	1.60435400	-0.57640900
H	-0.91266500	1.46328400	0.50800000
H	-0.89864400	2.68086500	-0.77713300
C	-1.81248400	0.81451400	-1.36102800
H	-1.59844700	-0.25869200	-1.22529200
H	-1.61269800	0.98760700	-2.42539900
C	-3.26183300	1.05647100	-1.04682600
C	-3.69208500	1.62388800	0.15856000
C	-4.24894100	0.67028800	-1.96513900
C	-5.04661900	1.78390500	0.44081000
H	-2.94955300	1.93226000	0.89090500
C	-5.60326900	0.82322500	-1.68861500
H	-3.93401600	0.23379400	-2.91241600
C	-6.01142200	1.38091900	-0.47812100
H	-5.34953500	2.22484400	1.38871600
H	-6.34398800	0.50889200	-2.42139100
H	-7.06935500	1.50380300	-0.25710700
O	2.71359800	-1.29098100	0.82320400
O	1.24694100	-2.15859800	-1.40232100
O	0.04453100	-0.75769600	2.22633800
O	-1.22524400	-2.26294900	0.24148400
C	4.69147100	-0.06764100	0.41226800
C	3.47992100	-0.80278600	-0.08647900
C	3.25546600	-0.89627500	-1.46050500

C	2.14477600	-1.52637700	-2.05470500
C	1.97207100	-1.47195200	-3.54237400
C	-1.15738300	-0.46243600	2.53937900
C	-2.28179000	-1.84548600	0.81544900
C	-1.31391200	0.54725400	3.64555300
C	-2.30342800	-0.97640100	1.91869000
C	-3.58370500	-2.30476400	0.21660600
H	5.37547900	0.21606500	-0.39179500
H	4.36444000	0.84337300	0.92700100
H	5.22508200	-0.67786400	1.14852800
H	3.94667800	-0.37905900	-2.11916400
H	1.62033400	-2.43423800	-3.92555400
H	1.20656900	-0.70951600	-3.72020400
H	2.88686200	-1.17388100	-4.06139700
H	-0.92367300	1.51481900	3.30689900
H	-2.35533100	0.68261000	3.94999900
H	-0.71592000	0.25589800	4.51405500
H	-3.27128400	-0.64803600	2.28555500
H	-4.45658900	-1.92964700	0.75750700
H	-3.64624300	-1.95449800	-0.81949800
H	-3.61795900	-3.39836200	0.18568200
O	1.60411900	-3.81081900	0.86955800
H	1.54657100	-3.84716500	-0.09637700
H	2.39813200	-3.27042900	1.01399700
H	0.70311400	0.10135000	-0.44798000
FE	0.67832500	-1.62632400	0.52004800

IM11_w2

C	1.34505100	2.04794800	0.47243900
C	2.10536400	3.13956900	0.05201200
C	2.95003600	3.80400900	0.93773100
C	3.05162300	3.37963900	2.26238000
C	2.31262100	2.27355600	2.68570500

C	1.47050900	1.61233800	1.79514700
H	2.00785200	3.41901800	-0.99562600
H	3.53760300	4.65595700	0.59705500
H	3.71356900	3.89513300	2.95607800
H	2.40539000	1.91809700	3.71100600
H	0.92683000	0.72259900	2.11381600
C	0.39282700	1.38170600	-0.53181700
O	0.57403400	1.70158300	-1.78429800
FE	0.92708500	-1.70048100	-0.10608100
O	-0.90123100	-2.46570700	-0.51996600
O	0.39157300	-1.70649200	1.83865100
O	1.40406700	-1.34268800	-2.07610700
O	2.90975200	-1.18492200	0.28561100
C	-3.19639600	-2.99160100	-0.40619000
C	-1.90679300	-2.57785500	0.25150700
C	-1.89878100	-2.30114200	1.62919600
C	-0.76964900	-1.86292000	2.33854600
C	-0.90305700	-1.51410400	3.79694000
C	2.15683800	-0.37903400	-2.44985000
C	3.52790000	-0.26959900	-0.37805100
C	1.91490800	0.14821800	-3.83236500
C	3.22126900	0.12924800	-1.67670000
C	4.64158600	0.42298300	0.35557100
H	-3.03493500	-3.87812800	-1.02600500
H	-3.99533500	-3.18997900	0.31364700
H	-3.53060800	-2.19021300	-1.07578200
H	-2.83195700	-2.41315000	2.17472100
H	-0.77551200	-0.43260400	3.92225000
H	-1.87212800	-1.79766000	4.21564700
H	-0.10461300	-1.99227500	4.37139900
H	2.05170200	-0.64908200	-4.57299200
H	0.88095400	0.49491100	-3.86907700
H	2.57155200	0.98612700	-4.07647800

H	3.78004500	0.96317100	-2.09072100
H	5.26938600	-0.30960000	0.87255600
H	5.26060100	1.03951100	-0.30165400
H	4.20501100	1.07429100	1.12302700
H	0.55718400	0.23079500	-0.30869500
O	2.19552700	-3.66162800	-0.65406500
H	2.90029700	-3.08773800	-0.30895800
H	2.07280100	-3.32488700	-1.55380600
C	-1.07593800	1.56260600	-0.03293200
H	-1.21057900	1.15386000	0.98232800
H	-1.29310300	2.64023600	0.01997400
C	-2.03307300	0.89469900	-1.01244200
H	-1.82623700	-0.18517000	-1.01594700
H	-1.75865800	1.26402500	-2.00745000
C	-3.47566700	1.15492800	-0.70767200
C	-4.18762000	2.15301400	-1.38408000
C	-4.14904000	0.43840500	0.29147100
C	-5.51894700	2.42523000	-1.08112700
H	-3.67793300	2.72075900	-2.16090200
C	-5.48044000	0.70368800	0.59633800
H	-3.60497800	-0.33523900	0.83414700
C	-6.17417000	1.70013000	-0.08900600
H	-6.04853800	3.20585300	-1.62378500
H	-5.98049600	0.13028000	1.37467500
H	-7.21491400	1.90850200	0.14852000

IM12

C	2.45477000	0.21036000	-0.29762800
C	3.24591400	0.77269000	0.70457900
C	4.39694100	0.13036200	1.15403400
C	4.78245300	-1.09116300	0.60204500
C	4.00218500	-1.66136400	-0.40587100
C	2.85214600	-1.01167900	-0.84763300

H	2.89761400	1.73442500	1.08021800
H	5.00672600	0.58290800	1.93689300
H	5.68616700	-1.59282200	0.94587200
H	4.29746900	-2.61374100	-0.84696800
H	2.24891600	-1.45211000	-1.64427300
C	1.19847400	0.98279400	-0.74666700
H	1.26058600	0.93159300	-1.89308200
O	1.07496800	2.18371700	-0.22726200
C	-0.04101400	0.06260600	-0.42710900
H	0.00223200	-0.92291300	-0.92097200
H	-0.04767200	-0.11906800	0.65882000
C	-1.29971400	0.82531600	-0.81547400
H	-1.35898800	0.89649500	-1.91168200
H	-1.09569900	1.84418100	-0.44121300
C	-2.57179500	0.26390700	-0.27537000
C	-2.82540900	0.25719200	1.10661600
C	-3.55860500	-0.27848700	-1.11058800
C	-4.00362100	-0.26515300	1.62452800
H	-2.07345300	0.67671100	1.77291000
C	-4.74095100	-0.80518700	-0.59747900
H	-3.38436700	-0.28317000	-2.18608900
C	-4.97277600	-0.80331100	0.77563300
H	-4.17232000	-0.25202200	2.70000400
H	-5.48595500	-1.21969700	-1.27476300
H	-5.89499800	-1.21381100	1.18071400

IM13_1

C	-1.93139400	2.51862800	0.00492900
C	-0.86396800	2.29378200	1.06612300
H	-1.33473600	2.12652200	2.04223000
H	-0.26700900	3.21138100	1.16097300
C	-3.90364800	-0.72309300	0.48565200
C	-2.93629900	0.26766100	0.65159300

C	-2.97426800	1.43345400	-0.12038500
C	-4.01545200	1.58234000	-1.04577500
C	-4.98933100	0.60226000	-1.20182800
C	-4.93475500	-0.56134300	-0.43457000
H	-3.81626600	-1.63389000	1.07420400
H	-2.12394900	0.10649800	1.36144200
H	-4.05397200	2.48452300	-1.65721300
H	-5.78821700	0.74147400	-1.92817300
H	-5.68700300	-1.33697900	-0.56307200
O	0.09043600	0.22277000	1.90320000
C	0.06294800	1.03809700	0.83222200
C	2.94632800	2.67149700	-1.13682600
C	1.66621600	2.27883300	-0.75669500
C	1.45690100	1.50454200	0.38967000
C	2.56686500	1.12701900	1.14324800
C	3.85088000	1.51608500	0.77023000
C	4.04895300	2.29128100	-0.37039600
H	3.08930900	3.26987600	-2.03624000
H	0.80825300	2.56517900	-1.36781200
H	2.36082100	0.50244700	2.00989000
H	4.70853000	1.20457700	1.36627800
H	5.05267300	2.59081400	-0.66759900
H	-0.35385800	0.55752300	-0.10352100
C	3.18517100	-2.31214200	0.27197300
C	1.84079400	-2.44142600	0.60068800
C	0.84679800	-2.03298500	-0.29099800
C	1.23180900	-1.47136300	-1.50856200
C	2.57737200	-1.33147600	-1.83981900
C	3.55972900	-1.75912600	-0.95228900
H	3.94958100	-2.61957800	0.98375700
H	1.52770700	-2.82803900	1.56772300
H	0.45941100	-1.11172000	-2.18929600
H	2.85987500	-0.86430800	-2.78120100

H	4.61190600	-1.62829400	-1.19654100
C	-0.61958700	-2.22318100	0.05580300
H	-1.18858500	-1.47754900	-0.54125800
O	-0.87707200	-2.08620000	1.41803100
H	-0.48131000	-1.16616300	1.67517000
H	-2.44888900	3.47610200	0.17739700
H	-1.44979400	2.64117400	-0.97890100
C	-1.09039200	-3.60746400	-0.37431200
H	-2.15724000	-3.72187000	-0.15522300
H	-0.93028900	-3.77736300	-1.44499400
H	-0.54387300	-4.37617900	0.18406800

IM14_1

C	-2.17196200	2.11162200	0.42579800
C	-1.15579700	1.71706900	1.49498700
H	-1.61961200	1.02867900	2.20973200
H	-0.85254200	2.59646800	2.07923800
C	-3.80778100	-1.29379100	-0.18564100
C	-2.91279000	-0.33077500	0.28130500
C	-3.11069200	1.01838700	-0.03254900
C	-4.22315600	1.36556800	-0.81149400
C	-5.11407600	0.40343100	-1.27330900
C	-4.90693000	-0.93958200	-0.96104200
H	-3.62311800	-2.33565000	0.06849200
H	-2.06623400	-0.68072800	0.88648200
H	-4.38888700	2.41563500	-1.05578700
H	-5.97102100	0.70131500	-1.87467000
H	-5.59776600	-1.69885400	-1.32198700
O	0.70845800	0.23978600	1.95158600
C	0.09795100	1.00967300	0.96048200
C	1.94318900	4.08075900	-0.46392000
C	0.94500100	3.30252400	0.12501900
C	1.13460500	1.93685400	0.35029800

C	2.36345800	1.37322600	-0.01970300
C	3.35424900	2.14136400	-0.61531100
C	3.14997000	3.50359800	-0.84242300
H	1.77272400	5.14387500	-0.62497300
H	0.00970600	3.77666000	0.41609700
H	2.52366800	0.31737000	0.18358900
H	4.29460000	1.67349500	-0.90221000
H	3.92688300	4.10830000	-1.30613300
H	-0.24023800	0.34864000	0.13168100
C	3.56890000	-2.22469100	0.52349300
C	2.21806000	-2.32995700	0.83747000
C	1.23854700	-2.20514300	-0.15183000
C	1.65123500	-1.95459800	-1.46218300
C	3.00182800	-1.83712000	-1.78481400
C	3.96883300	-1.97654200	-0.79100200
H	4.31873500	-2.31941800	1.30743100
H	1.87235900	-2.48027300	1.85832800
H	0.89032200	-1.83312800	-2.23450700
H	3.30158400	-1.62299400	-2.80969800
H	5.02503700	-1.87537100	-1.03447900
C	-0.23905600	-2.35676400	0.22468300
H	-0.79532000	-1.78887000	-0.58018900
O	-0.53815600	-1.95111000	1.47903400
H	0.24893200	-0.67578100	1.86571200
H	-2.78016900	2.96014400	0.77224600
H	-1.63764200	2.49661600	-0.45701600
C	-0.62523600	-3.83771500	0.01160000
H	-1.68922900	-3.96846500	0.23922400
H	-0.43712300	-4.19561900	-1.01081600
H	-0.05816600	-4.46584600	0.70977400

IM15

C	1.23699100	-1.70482100	0.65869000
---	------------	-------------	------------

C	-0.12078600	-1.02460100	0.85933900
H	-0.08064600	-0.31580700	1.69712800
H	-0.85343000	-1.79243300	1.13598300
C	3.89927600	1.00270900	0.93047000
C	2.88852900	0.10877900	1.26358100
C	2.36360500	-0.77158000	0.30902600
C	2.88299500	-0.72708300	-0.98943800
C	3.89457400	0.16987400	-1.32790600
C	4.40518000	1.03802500	-0.36806400
H	4.29363200	1.67731200	1.68541300
H	2.49181600	0.08980500	2.27710600
H	2.48379300	-1.40551300	-1.74176300
H	4.28250900	0.18901000	-2.34267300
H	5.19355400	1.73855700	-0.62789900
O	0.01598800	0.98299200	-0.54024500
C	-0.64228100	-0.25817300	-0.36641900
C	-4.39776400	-0.81884100	-0.26901800
C	-3.03251900	-1.03013500	-0.42412200
C	-2.12111800	0.01227000	-0.23713000
C	-2.60138200	1.27635700	0.10491400
C	-3.96922000	1.48908900	0.26138400
C	-4.87076300	0.44531000	0.07685400
H	-5.09433800	-1.63846500	-0.42449500
H	-2.66453800	-2.01756800	-0.70192800
H	-1.89260400	2.08752400	0.23528500
H	-4.33207700	2.47876700	0.52718100
H	-5.93736900	0.61498900	0.19634300
H	-0.49032900	-0.90281100	-1.25531100
H	0.95342100	0.80365200	-0.67485100
H	1.48816200	-2.25331400	1.57511400
H	1.13864000	-2.46071700	-0.13164300

R1-H

H	1.87575200	-1.15945300	-1.54491100
C	-2.07452100	1.08083400	-0.21214800
C	-0.69824000	1.21927200	-0.36388700
C	0.15357400	0.13116700	-0.16551100
C	-0.39708600	-1.10373100	0.18388200
C	-1.77367100	-1.24603700	0.33220300
C	-2.61596800	-0.15449400	0.13535700
H	-2.72628500	1.93545300	-0.37340300
H	-0.27435100	2.18309100	-0.64379400
H	0.27009200	-1.94941200	0.33290400
H	-2.19114500	-2.21261800	0.60240900
H	-3.69068400	-0.26635600	0.24841800
C	1.65240700	0.29694000	-0.28733800
H	1.84800500	1.11832800	-1.00108600
O	2.29535300	-0.89380800	-0.71993900
C	2.28573800	0.65616700	1.04400100
H	3.36785800	0.76212600	0.93399600
H	1.87591800	1.59253000	1.43110300
H	2.08861900	-0.13393100	1.77452400

R1

C	0.19349500	0.04256900	-0.19169500
C	-0.45576000	-1.15836500	0.09696700
C	-1.83743500	-1.20685700	0.26688500
C	-2.60217600	-0.04639100	0.14553600
C	-1.96640300	1.16169700	-0.15097200
C	-0.58318900	1.19794400	-0.31801200
H	0.20808600	-2.02193400	0.15966100
H	-2.33188200	-2.15396600	0.49052300
H	-3.68407200	-0.08038500	0.27194900
H	-2.55648200	2.07385700	-0.25229900
H	-0.09004700	2.14216800	-0.56169500
C	1.73552800	-0.01072000	-0.37309200

H	1.87152600	0.56827000	-1.36132700
O	2.24644500	-1.21516200	-0.32563200
C	2.35351200	0.96216600	0.68704600
H	3.43962700	0.98200200	0.53810800
H	1.97914000	1.99942100	0.65235500
H	2.16711900	0.55960200	1.69180000

R2-H

H	-3.59833000	-0.28507800	-0.00001800
C	1.87607200	0.99642300	-0.00017400
C	0.51916700	1.29793300	-0.00006100
C	-0.43665400	0.27809100	0.00015900
C	-0.01175700	-1.04906600	0.00024100
C	1.34846800	-1.35104100	0.00010100
C	2.29568500	-0.33254900	-0.00010200
H	2.60761600	1.80025800	-0.00036000
H	0.19480500	2.33763100	-0.00015300
H	-0.75647100	-1.83741700	0.00037800
H	1.66799400	-2.38977000	0.00014600
H	3.35591600	-0.56973900	-0.00022100
C	-1.89731900	0.62902900	0.00040400
H	-2.11737900	1.25614600	0.88272600
O	-2.67485700	-0.54782900	-0.00063200
H	-2.11726100	1.25767700	-0.88085600

R2

C	0.00000000	0.56796700	0.00000000
C	-0.93955400	-0.46338600	0.00000000
C	-0.53901100	-1.79822200	0.00000000
C	0.81658800	-2.12609400	0.00000000
C	1.76806100	-1.10032400	0.00000000
C	1.35595500	0.22976500	0.00000000
H	-1.97793000	-0.12910100	0.00000000

H	-1.28306900	-2.59721000	0.00000000
H	1.13447900	-3.16843400	0.00000000
H	2.83083100	-1.34780600	0.00000000
H	2.09666200	1.03476500	0.00000000
C	-0.52415400	2.01910500	0.00000000
H	0.06149800	2.48375600	0.87928400
H	0.06149800	2.48375600	-0.87928400
O	-1.81891100	2.15842700	0.00000000

TS1_1

O	-1.44720200	-0.87345900	-1.31680500
O	-0.46722300	2.62833900	0.44222200
O	0.77163900	0.90970900	-1.38541100
C	-5.02583500	0.30040400	0.99977900
C	-3.73696300	-0.01737200	0.28340500
C	-3.69297700	-1.12200900	-0.58242700
C	-2.56267300	-1.48416900	-1.33176500
C	-2.63332500	-2.69231700	-2.23195800
C	0.59542700	3.30554400	0.27269600
C	1.70928600	1.76148400	-1.31437900
C	0.65477100	4.62005700	1.01102500
C	1.68021300	2.92942700	-0.53160800
C	2.93500200	1.46457600	-2.13868100
H	-4.86391200	0.26231600	2.08191300
H	-5.33715100	1.32431300	0.76893000
H	-5.83777700	-0.38472600	0.74003600
H	-4.59365500	-1.71972100	-0.69408100
H	-1.89884600	-3.43553600	-1.90123300
H	-3.62233000	-3.15909500	-2.24379200
H	-2.35602900	-2.41574200	-3.25418100
H	0.59720600	4.43685500	2.08873400
H	1.56467700	5.18816200	0.79799000
H	-0.21573600	5.23128300	0.75230000

H	2.53914000	3.59336900	-0.57402300
H	2.64198200	1.13557800	-3.14016800
H	3.61256700	2.31968700	-2.21727600
H	3.47616500	0.62863300	-1.68035100
C	1.81444400	-1.60997700	1.00697500
C	3.10565500	-1.45651900	1.51861700
C	4.22351900	-1.61458900	0.70463000
C	4.06700200	-1.93854000	-0.64157500
C	2.78061300	-2.08142100	-1.16520900
C	1.66567800	-1.91461700	-0.35150400
H	3.18998000	-1.20728500	2.57350600
H	5.22196000	-1.49053300	1.12166700
H	4.93783800	-2.06610700	-1.28265100
H	2.64562400	-2.29989600	-2.22328800
H	0.66859000	-1.96340800	-0.78543600
C	0.65511900	-1.47988700	1.97748800
H	-0.03424300	-0.17648200	1.13189300
O	0.89975300	-1.15187600	3.15366800
FE	-0.84043400	0.70332500	-0.13786300
O	-2.76413900	0.76313700	0.52824600
C	-0.54828300	-2.37924700	1.70683200
H	-1.40532400	-2.00637500	2.27200500
H	-0.82608000	-2.44238600	0.65207500
H	-0.31603600	-3.39112300	2.07047900

TS1_2

C	2.20266400	-0.55830100	1.34687800
C	3.41835900	-0.05564500	0.87472400
C	4.32558100	-0.87726400	0.21336400
C	4.03103100	-2.22432100	0.01397800
C	2.81060000	-2.73279300	0.46258500
C	1.90564200	-1.90612300	1.11819000
H	3.61327300	1.00158900	1.03865100

H	5.26526700	-0.46609500	-0.15215400
H	4.73669700	-2.87115300	-0.50412100
H	2.55837500	-3.77619600	0.28414400
H	0.93353800	-2.29117400	1.41966800
C	1.31761200	0.37983400	2.13523900
O	1.58173000	1.59258500	2.13822100
FE	-1.03272300	0.30033500	-0.34344400
O	-2.82133500	1.08210400	0.24330700
O	-2.05313100	-1.47118700	-0.58862300
O	-0.19476100	2.16031700	-0.54280400
O	0.32239900	-0.31652100	-1.74257900
C	-5.09221900	1.43562900	0.76726500
C	-3.96255100	0.52900900	0.34380700
C	-4.23537500	-0.82314400	0.08829100
C	-3.27428900	-1.73966000	-0.37337100
C	-3.69656400	-3.16135700	-0.65701300
C	0.99195500	2.41126100	-0.90979900
C	1.41739800	0.25342000	-2.05558100
C	1.57260400	3.71899300	-0.44344100
C	1.79600100	1.54730700	-1.67837000
C	2.36525700	-0.57773000	-2.88295500
H	-5.21152600	2.24613000	0.04051500
H	-6.04605700	0.90949600	0.86712900
H	-4.84687800	1.91103200	1.72248200
H	-5.25615000	-1.17308900	0.21899500
H	-3.11948900	-3.85005300	-0.03095400
H	-4.76206700	-3.33378100	-0.47877700
H	-3.46337500	-3.41873700	-1.69529700
H	0.81639600	4.50769900	-0.47884100
H	1.86261000	3.58110100	0.60454200
H	2.45386100	4.02304300	-1.01662300
H	2.79077900	1.88689900	-1.95564100
H	1.85435900	-0.94618900	-3.77866400

H	3.26342100	-0.02850800	-3.18075000
H	2.66975400	-1.45480200	-2.30153200
H	-0.14808900	0.00467000	1.11082100
C	0.59499200	-0.21872900	3.33364700
H	0.18897000	-1.21614800	3.15119300
H	1.30493800	-0.28033100	4.17278000
H	-0.21922300	0.44516600	3.62716900

TS1_3

O	1.37264100	-0.91225400	1.30113100
O	0.48744900	2.56300800	-0.59009200
O	-0.77056500	0.95017600	1.31517900
C	5.00040800	0.06389900	-1.03230600
C	3.69702500	-0.18036200	-0.31357500
C	3.56836000	-1.32121000	0.49314600
C	2.42448400	-1.62205100	1.25105000
C	2.40464400	-2.88156600	2.08042100
C	-0.53746000	3.29370200	-0.41081000
C	-1.67153300	1.84204200	1.24704000
C	-0.56089000	4.58745300	-1.18667900
C	-1.61330700	2.98877900	0.43609500
C	-2.88698300	1.61671200	2.10924900
H	4.82132300	0.10039700	-2.11156200
H	5.40237300	1.04248800	-0.75037200
H	5.75238500	-0.70218000	-0.82430500
H	4.41297800	-2.00221600	0.55070000
H	1.61914300	-3.54735400	1.70515700
H	3.35628200	-3.42008900	2.06298000
H	2.14418000	-2.64488800	3.11675000
H	0.33275800	5.17623300	-0.95597500
H	-0.52316200	4.37294700	-2.25950200
H	-1.44785700	5.19234100	-0.97854200
H	-2.44094500	3.69114100	0.48480900

H	-2.58160100	1.33295500	3.12100700
H	-3.54326000	2.49036500	2.15818900
H	-3.45635500	0.77172400	1.70434100
C	-1.67127700	-1.83238700	-0.98437100
C	-2.83298700	-1.83957000	-1.75866100
C	-4.08642700	-1.85399000	-1.15375400
C	-4.19123800	-1.87592400	0.23616100
C	-3.03080300	-1.87730600	1.01452700
C	-1.78020000	-1.85298900	0.40891500
H	-2.70930700	-1.83757200	-2.83931600
H	-4.98746000	-1.85568400	-1.76543600
H	-5.17018700	-1.89244500	0.71258600
H	-3.10484300	-1.88117400	2.10107800
H	-0.87073300	-1.80878000	1.00706300
C	-0.33486900	-1.88497700	-1.66751400
H	0.10805700	-0.31697300	-1.15089500
O	-0.24665200	-2.00779800	-2.89861300
FE	0.84386300	0.67199400	0.08772200
O	2.79404500	0.69475300	-0.50200000
H	0.46878300	-2.25769700	-0.98796000

TS1_4

O	2.80022300	1.02714300	-0.41302300
O	2.03912600	-1.49208900	0.51106000
C	5.06930300	1.37125700	-0.94993700
C	3.94379000	0.47667400	-0.49100500
C	4.22245600	-0.86285800	-0.17974100
C	3.26338400	-1.76302600	0.31557600
C	3.69101300	-3.16818300	0.66526500
H	5.18248000	2.21201100	-0.25740100
H	6.02631800	0.84698300	-1.02664100
H	4.82263300	1.80511700	-1.92435200
H	5.24530700	-1.21313200	-0.29186300

H	3.11602600	-3.88792100	0.07321000
H	4.75719200	-3.34431000	0.49477400
H	3.45993500	-3.37721500	1.71490400
C	-2.26375100	-0.54897800	-1.50782400
C	-3.42547000	-0.04289400	-0.91940900
C	-4.33597600	-0.89494600	-0.30242900
C	-4.09993600	-2.26845000	-0.27219300
C	-2.93979100	-2.78144700	-0.85745000
C	-2.03172300	-1.92654200	-1.46904400
H	-3.57941000	1.03303300	-0.96132100
H	-5.23346300	-0.48802200	0.16144700
H	-4.81046200	-2.93703600	0.21009300
H	-2.74299000	-3.85129700	-0.82569000
H	-1.10829700	-2.31074700	-1.90070900
C	-1.35925800	0.38252900	-2.25060800
O	-1.58017000	1.59722600	-2.30652300
FE	1.01296800	0.26128100	0.20037300
O	0.21571600	2.14057100	0.38287500
O	-0.36944300	-0.31596400	1.59047400
C	-0.95392200	2.43483000	0.77121900
C	-1.44733500	0.28421500	1.90333600
C	-1.48053200	3.77565800	0.33517100
C	-1.78327900	1.59411200	1.53784800
C	-2.42314500	-0.52439300	2.71984300
H	-0.70244300	4.53860900	0.42486100
H	-1.73949600	3.69101600	-0.72574800
H	-2.36962500	4.08691900	0.89189200
H	-2.76327700	1.96673600	1.82509000
H	-3.31544400	0.04253000	3.00177900
H	-2.73357500	-1.39820700	2.13695900
H	-1.93362700	-0.89910000	3.62491900
H	0.11424600	-0.05796400	-1.24180000
H	-0.74778300	-0.13174200	-3.02471700

TS1_w1			
O	0.66113100	0.95969600	-1.57182300
O	-0.64354300	2.63805500	0.27612400
O	-1.38833400	-1.14768100	-1.14601400
O	-2.70483800	0.43872900	0.78296500
C	2.97030700	1.33231400	-1.93518900
C	1.66741400	1.66887300	-1.25928600
C	1.65590400	2.71979700	-0.32247700
C	0.52130100	3.14376900	0.38133100
C	0.65232500	4.28880900	1.35265600
C	-2.45048800	-1.84568200	-1.04822400
C	-3.61312500	-0.43877200	0.63805300
C	-2.49246600	-3.08300100	-1.90813900
C	-3.53710300	-1.55665100	-0.21054100
C	-4.85626100	-0.23461000	1.46687400
H	3.65434700	2.18505000	-1.97896800
H	3.46409400	0.53085000	-1.37297000
H	2.78519900	0.94890700	-2.94169900
H	2.59146700	3.24051200	-0.13739100
H	-0.12748200	5.03258600	1.16216600
H	0.48573800	3.91079500	2.36642800
H	1.63207600	4.77258800	1.31611300
H	-1.66924000	-3.75075100	-1.62889900
H	-3.43392100	-3.63210700	-1.81948200
H	-2.33292700	-2.81523900	-2.95759800
H	-4.38559100	-2.23523800	-0.23000300
H	-5.61623100	-1.00086600	1.29054800
H	-4.59450200	-0.23571100	2.53012800
H	-5.28718500	0.74887400	1.25348400
O	-1.96351600	1.90815000	-2.10415800
H	-1.74143800	2.55782400	-1.42035500
H	-1.08838600	1.63340700	-2.41488000

C	2.08760100	-1.39256400	0.98460900
C	3.42844600	-1.17553400	1.31489800
C	4.44813300	-1.49504000	0.42189100
C	4.14130900	-2.04256100	-0.82244000
C	2.80372600	-2.24158500	-1.17049400
C	1.78727500	-1.91616200	-0.27945700
H	3.63095800	-0.75625700	2.29732600
H	5.48743200	-1.32283800	0.69863700
H	4.93484900	-2.29654800	-1.52306200
H	2.55105300	-2.63644400	-2.15291200
H	0.74760500	-2.02096300	-0.58390300
C	1.04808100	-1.11288700	2.05175000
H	0.20279800	0.04527700	1.04940600
O	1.41430000	-0.58094800	3.11403500
C	-0.16043900	-2.04281600	2.07146800
H	-0.55808800	-2.27532800	1.07991600
H	0.13177800	-2.98367200	2.56116400
FE	-0.92785200	0.56756100	-0.16464600
H	-0.95346700	-1.58347100	2.66489200

TS1_w2

C	2.57089100	-0.62208000	1.17279200
C	3.80350300	-0.14499500	0.71551800
C	4.67242200	-0.96918900	0.00698400
C	4.31870600	-2.28965400	-0.26306900
C	3.07930600	-2.76863800	0.16619000
C	2.21463800	-1.94265200	0.87512600
H	4.04602300	0.89114400	0.93871700
H	5.62866100	-0.58086200	-0.33965100
H	4.99296500	-2.93689200	-0.82031400
H	2.78126800	-3.78888700	-0.06629300
H	1.22833800	-2.30001300	1.16418400
C	1.74709100	0.29699800	2.03935200

O	2.01877500	1.50417100	2.06604800
FE	-1.06682300	0.20774000	-0.15399400
O	-2.74741500	0.75897700	0.83647100
O	-1.94139700	-1.59827000	-0.47488200
O	-0.44140900	2.24192300	-0.37164600
O	0.23885500	-0.07540000	-1.82330900
C	-5.00405100	0.92774800	1.49576200
C	-3.86627500	0.15563700	0.87463900
C	-4.11009100	-1.13728300	0.38485600
C	-3.15184600	-1.92788800	-0.26972800
C	-3.56001700	-3.28281000	-0.79451800
C	0.78037300	2.53019000	-0.56994200
C	1.37393800	0.50325600	-1.88200800
C	1.26517100	3.82596500	0.02100700
C	1.68919700	1.73172700	-1.28859600
C	2.43551700	-0.22191800	-2.66725800
H	-5.93320000	0.35251500	1.54205300
H	-4.73203400	1.24653100	2.50723300
H	-5.18520600	1.84170200	0.92010900
H	-5.11590200	-1.53682800	0.48449300
H	-2.91245600	-4.05774300	-0.37116600
H	-4.60134800	-3.53029400	-0.56939700
H	-3.41661700	-3.31721800	-1.87964800
H	0.52814900	4.61699700	-0.14495100
H	1.36517300	3.67588600	1.09983600
H	2.23649300	4.13588500	-0.37477600
H	2.71101300	2.08963900	-1.37973200
H	2.06500900	-0.44383300	-3.67372400
H	3.37208300	0.33781100	-2.74028100
H	2.64183700	-1.18233500	-2.18332400
H	0.16122800	-0.06294900	1.01291700
O	-2.26396700	1.16881800	-2.32635800
H	-1.46513500	0.68637900	-2.58752700

H	-1.89604400	1.90482100	-1.81585900
C	1.03117600	-0.33401400	3.22096600
H	0.61273100	-1.31912100	3.00608100
H	1.75171000	-0.43382300	4.04762200
H	0.22723300	0.32609700	3.54821900

TS1_w3

C	2.00775200	-1.53072600	1.02508700
C	3.27341300	-1.31420200	1.57534400
C	4.41897600	-1.46445700	0.79870500
C	4.31291900	-1.84665800	-0.53843400
C	3.04879000	-2.05945300	-1.09467100
C	1.90590100	-1.89936400	-0.32094200
H	3.31769900	-1.04195300	2.62739900
H	5.40128100	-1.29560200	1.23773600
H	5.20734200	-1.97130700	-1.14634300
H	2.95758500	-2.33768700	-2.14332200
H	0.91509700	-2.02499400	-0.75624300
C	0.80295900	-1.47453700	1.91807000
O	0.91565000	-1.30599500	3.13950200
H	-0.07409500	-2.00720900	1.48008400
FE	-0.92596900	0.49983300	-0.14667100
O	-2.75544800	0.32882700	0.69774000
O	-1.25704400	-1.28379800	-1.06140900
O	-0.80425200	2.57914200	0.32656900
O	0.72220600	0.98005100	-1.42279600
C	-4.84936100	-0.48429400	1.40796200
C	-3.56614500	-0.64715400	0.63233200
C	-3.35707300	-1.83274500	-0.09267500
C	-2.23384500	-2.08339100	-0.89399300
C	-2.13077000	-3.39697700	-1.62625900
C	0.29905000	3.20131800	0.44795100
C	1.65292200	1.77236400	-1.07179400

C	0.27800500	4.40388000	1.35797600
C	1.50081300	2.85454100	-0.18556800
C	3.01912000	1.49935600	-1.64134700
H	-5.38504900	0.40351700	1.05612200
H	-5.51005200	-1.35166300	1.32444800
H	-4.62169300	-0.31271000	2.46484000
H	-4.12838400	-2.59683200	-0.04775300
H	-1.25413300	-3.94731200	-1.26562200
H	-3.01537200	-4.02679300	-1.49822700
H	-1.96978700	-3.21917600	-2.69435800
H	-0.54503500	5.06903800	1.07888000
H	0.07766000	4.07276600	2.38204300
H	1.21565600	4.96610100	1.34771700
H	2.37639700	3.46367700	0.02169600
H	2.93565400	1.13944200	-2.67044300
H	3.67579700	2.37332200	-1.60438500
H	3.48630800	0.69258900	-1.06316500
H	0.13781400	-0.05090900	1.12371000
O	-1.90175500	1.79923900	-2.15492000
H	-0.98285800	1.59954400	-2.38582700
H	-1.79805400	2.44377100	-1.43949600

TS1_w4

C	-2.61535800	-0.54498200	-1.41310100
C	-3.77288800	-0.01085800	-0.83934000
C	-4.68459500	-0.83468400	-0.18741700
C	-4.45194700	-2.20675000	-0.10169000
C	-3.29341400	-2.74637400	-0.66657900
C	-2.38499600	-1.92040000	-1.31604000
H	-3.92558700	1.06265800	-0.92740300
H	-5.58197600	-0.40812800	0.25811700
H	-5.16305500	-2.85283200	0.40921500
H	-3.09854100	-3.81415900	-0.58985900

H	-1.46301200	-2.32274400	-1.73325500
C	-1.72279700	0.34356700	-2.21545100
O	-1.91716800	1.55861000	-2.30622800
H	-1.11676100	-0.20576300	-2.96652500
FE	1.01870700	0.14379100	0.00677900
O	2.69853400	0.78229800	-0.93436200
O	1.96476200	-1.62690000	0.32219600
O	0.34786600	2.14067000	0.30494400
O	-0.29826400	-0.26129000	1.63911800
C	4.96452100	1.07080300	-1.51256800
C	3.84634100	0.23627300	-0.93845000
C	4.13762200	-1.04752200	-0.45074600
C	3.19753400	-1.89155000	0.16126700
C	3.65485600	-3.22793000	0.69289000
C	-0.85435300	2.43396600	0.59403500
C	-1.41310500	0.33300100	1.80392400
C	-1.36483100	3.75196700	0.07968800
C	-1.72926400	1.61290100	1.32811700
C	-2.45803400	-0.43874100	2.56752700
H	5.92357200	0.54500100	-1.52756500
H	4.71308200	1.38191700	-2.53163800
H	5.07545600	1.98865200	-0.92568900
H	5.16584200	-1.39378400	-0.51436600
H	3.06801000	-4.03182500	0.23650900
H	4.71652600	-3.41750500	0.51035200
H	3.46764400	-3.27978700	1.77054300
H	-0.58807400	4.51744400	0.15544100
H	-1.59974300	3.61206500	-0.98021900
H	-2.26977800	4.08709800	0.59485900
H	-2.73433100	1.98377800	1.51094900
H	-2.02815000	-0.83141800	3.49437100
H	-3.34533700	0.15689200	2.80013400
H	-2.77105900	-1.30018000	1.96705000

H	-0.17672700	-0.12431700	-1.20165400
O	2.17155100	1.04926600	2.25802800
H	1.39557400	0.50868100	2.46731200
H	1.78002500	1.78233900	1.76110300

TS2_1

O	0.43820400	-1.67386200	1.33040300
O	0.35309100	-1.96675000	-1.45202100
O	-2.38660200	-1.10247400	1.47794600
O	-2.57713500	-1.97371100	-1.18455200
C	2.53419900	-1.86501400	2.39605200
C	1.68608100	-1.86355000	1.15551200
C	2.30337500	-2.03833100	-0.09487000
C	1.61272800	-2.08778800	-1.31288500
C	2.39381900	-2.32009400	-2.58306200
C	-3.65086500	-1.07482500	1.38981500
C	-3.82368700	-1.89183200	-0.94479200
C	-4.39057600	-0.60717300	2.62045700
C	-4.39472400	-1.43625800	0.25149900
C	-4.73167800	-2.33338900	-2.06576600
H	2.03809100	-2.43293100	3.18806500
H	3.53494600	-2.27095300	2.22090700
H	2.62833700	-0.82772300	2.74186200
H	3.38513900	-2.14140900	-0.11540100
H	2.05481500	-3.24123900	-3.06931300
H	2.19809400	-1.50573300	-3.28899700
H	3.47172800	-2.38375500	-2.40934500
H	-4.04378600	-1.16039600	3.49831700
H	-4.16067400	0.44804600	2.80933900
H	-5.47548000	-0.71324600	2.53214600
H	-5.47861800	-1.39399200	0.31530200
H	-4.52094300	-3.37610600	-2.32463900
H	-5.79248600	-2.23842700	-1.81758500

H	-4.52165500	-1.74247300	-2.96284300
FE	-0.99828200	-1.34518100	-0.05283400
H	-0.88519700	0.27987500	-0.40387600
O	2.15670500	1.30156900	2.18590200
C	2.27210800	1.52487300	0.96598500
C	1.21499100	2.10269600	0.17079100
H	1.46099600	2.53290500	-0.79891300
C	4.85939900	0.57657700	-1.67250100
C	3.66728800	1.00546500	-1.09808200
C	3.55785200	1.16555100	0.28921100
C	4.67252200	0.87330900	1.08498500
C	5.86508100	0.44814900	0.51444900
C	5.96415300	0.29821200	-0.86928600
H	4.92035700	0.43698100	-2.74992400
H	2.79327500	1.17229100	-1.72353200
H	4.55688000	0.97435300	2.16117100
H	6.72198500	0.22425300	1.14666100
H	6.89414900	-0.04471300	-1.31758000
C	-0.09202300	1.99839900	0.56097800
C	-2.18825400	4.47238300	-1.38600400
C	-1.07773400	3.79130400	-0.89488000
C	-1.22752300	2.71864200	-0.00320000
C	-2.53105000	2.37173400	0.39511900
C	-3.63592800	3.05217700	-0.08787600
C	-3.47221800	4.10895900	-0.98879400
H	-2.04831600	5.29829700	-2.08092600
H	-0.07752000	4.09695200	-1.19416400
H	-2.64549600	1.51990500	1.06160800
H	-4.63292800	2.74854800	0.22639800
H	-4.33796100	4.64211900	-1.37528100
H	-0.28052400	1.45403700	1.48563300

O	0.32960400	3.38840100	-0.03006200
O	-1.47296700	1.25376900	-0.31423900
O	2.55328400	1.60187600	-0.77953800
O	0.63244200	-0.31706500	-1.45905300
C	-0.55875100	5.49129300	0.55181700
C	-0.73449200	4.01685700	0.28454900
C	-2.00972000	3.45379700	0.39492100
C	-2.31330000	2.10728900	0.10677300
C	-3.71954400	1.61885600	0.31726400
C	3.35068600	0.74600200	-1.27598100
C	1.65086900	-0.95086900	-1.88391800
C	4.80999500	1.12738000	-1.26825700
C	2.97484600	-0.49265100	-1.81915900
C	1.36892000	-2.29503100	-2.50691200
H	-0.15141100	5.98431900	-0.33733200
H	-1.49241500	5.98630000	0.83292000
H	0.17527800	5.63697800	1.35081500
H	-2.82534400	4.10033900	0.70695200
H	-4.04219800	1.00558300	-0.52937400
H	-3.72892300	0.96439200	1.19848300
H	-4.42940400	2.43624800	0.47373200
H	5.12874200	1.31942100	-0.23855300
H	5.45346900	0.35382600	-1.69715400
H	4.95732700	2.06096900	-1.82151700
H	3.75785000	-1.14472000	-2.19625800
H	0.82089500	-2.91943100	-1.79206000
H	0.71787200	-2.17656800	-3.38010900
H	2.27815200	-2.82256000	-2.80869900
FE	0.56918400	1.39863600	-0.33410000
H	0.74196400	0.72723500	1.22473600
O	-2.37757200	-0.70943200	2.43385400
C	-1.99539900	-1.29078800	1.39881800
C	-0.63180300	-1.61986700	1.10492800

H	-0.42885900	-2.16400300	0.18607600
C	-3.71469000	-2.04822200	-1.91545800
C	-2.71933000	-1.74270600	-0.99157000
C	-3.01890600	-1.68448800	0.37586500
C	-4.33493800	-1.91599700	0.78957600
C	-5.32563200	-2.23497800	-0.13121700
C	-5.01720500	-2.30442700	-1.49017100
H	-3.47623500	-2.07076400	-2.97686500
H	-1.71573100	-1.48592000	-1.32647200
H	-4.55220000	-1.81966700	1.85120800
H	-6.34362000	-2.42333600	0.20529600
H	-5.79264900	-2.54339800	-2.21537900
C	0.42398700	-1.08202500	1.80197500
C	3.42924100	-3.14256700	0.77887100
C	2.11268000	-2.73961400	0.98475400
C	1.81326300	-1.51570500	1.60290700
C	2.89110400	-0.72709600	2.03883400
C	4.20343900	-1.13295700	1.84650700
C	4.48365300	-2.34054800	1.20352200
H	3.62902000	-4.09085600	0.28300200
H	1.29388300	-3.38488500	0.67512100
H	2.67117700	0.24181400	2.48162500
H	5.01850200	-0.49486000	2.18235600
H	5.51343700	-2.64949700	1.03738000
H	0.19047900	-0.53751500	2.71352600

TS2_w1

H	-0.43034600	0.31609800	-0.57881000
O	2.31588200	1.15833300	2.37721400
C	2.45188600	1.55301400	1.20645100
C	1.42560500	2.29053300	0.49977400
H	1.71370700	2.88340700	-0.36756800
C	4.92764000	0.76296900	-1.57902800

C	3.76797100	1.17779300	-0.93137100
C	3.70644400	1.21230400	0.46831900
C	4.82769200	0.80173100	1.20026100
C	5.98849300	0.39565900	0.55584000
C	6.04354600	0.37733700	-0.83853000
H	4.95461800	0.72217400	-2.66577500
H	2.88205400	1.42759300	-1.51073800
H	4.74474600	0.79929700	2.28429000
H	6.85414200	0.08528000	1.13712200
H	6.94893600	0.05091600	-1.34562100
C	0.10645500	2.09750500	0.77597700
C	-1.89937500	4.74829400	-1.01589300
C	-0.82171300	4.06490300	-0.46097900
C	-1.00394500	2.82954100	0.17967800
C	-2.30993500	2.31640300	0.26702400
C	-3.38369500	2.99676200	-0.28620200
C	-3.18456900	4.21801900	-0.93506400
H	-1.73540700	5.70479500	-1.50826100
H	0.17673700	4.49474800	-0.50898000
H	-2.45301500	1.34648500	0.73825000
H	-4.37958600	2.56322300	-0.21988400
H	-4.02541700	4.75123400	-1.37317300
H	-0.14227700	1.37694300	1.55437400
FE	-1.07575200	-1.18316400	-0.23608000
O	-2.80407200	-1.02839800	-1.28244000
O	-2.20213800	-1.02868200	1.47415700
O	0.12428400	-2.16961500	-1.68801600
O	0.45725100	-1.90547700	1.09158500
C	-5.06450100	-0.80244700	-1.90514000
C	-3.99389000	-0.92702100	-0.85018300
C	-4.36934200	-0.89978800	0.50384800
C	-3.46880500	-0.98328500	1.57810300
C	-4.01046400	-1.00244400	2.98563800

C	1.39980600	-2.10984200	-1.66948100
C	1.68849400	-1.98766500	0.79484800
C	2.07541200	-2.13163900	-3.01739600
C	2.19469800	-2.03167400	-0.52139900
C	2.65759400	-2.02781300	1.94437400
H	-6.07561100	-0.80965500	-1.48800500
H	-4.92130800	0.13292100	-2.45788400
H	-4.97029800	-1.61406100	-2.63286800
H	-5.42974300	-0.83883400	0.73392000
H	-3.59815300	-0.16073400	3.55194900
H	-5.10228900	-0.95408600	3.02331800
H	-3.67815500	-1.91199600	3.49619700
H	1.70478600	-2.97089200	-3.61444800
H	1.80617400	-1.21903600	-3.56096600
H	3.16540300	-2.18739500	-2.94716300
H	3.27425700	-2.02413300	-0.64794100
H	2.29644400	-2.72284100	2.70798800
H	3.66820600	-2.31048400	1.63536900
H	2.69589200	-1.03145300	2.40288400
O	-1.47629900	-3.73683000	0.08762500
H	-0.89741600	-3.45608800	0.81093800
H	-0.90580900	-3.63071200	-0.68823500

TS2_w2

O	2.40928600	-0.71347000	-2.49758200
C	2.02349300	-1.33020100	-1.48262100
C	0.65975900	-1.67161600	-1.21059100
H	0.45300300	-2.26084500	-0.32133300
C	3.70798800	-2.12330200	1.83944200
C	2.71968900	-1.82285600	0.90625700
C	3.03909700	-1.73028200	-0.45534200
C	4.36696800	-1.92220600	-0.85235900
C	5.35033800	-2.23596500	0.07783400

C	5.02258800	-2.33970600	1.43022400
H	3.45306900	-2.17234600	2.89616600
H	1.70589900	-1.59459900	1.23227100
H	4.59927300	-1.79926100	-1.90809200
H	6.37768500	-2.39315800	-0.24595100
H	5.79240800	-2.57412400	2.16279400
C	-0.39212400	-1.08914200	-1.87686700
C	-3.42522200	-3.14856400	-0.94097500
C	-2.10318600	-2.75766100	-1.13053100
C	-1.78532700	-1.50983600	-1.69030400
C	-2.85106800	-0.68301900	-2.08302400
C	-4.16923300	-1.07536100	-1.90424300
C	-4.46738400	-2.30870200	-1.32034500
H	-3.63950100	-4.11627800	-0.49083200
H	-1.29500100	-3.43039200	-0.85248600
H	-2.61685200	0.30222800	-2.48015100
H	-4.97472600	-0.40723700	-2.20291200
H	-5.50185700	-2.60714300	-1.16362700
H	-0.15665900	-0.49202400	-2.75383700
FE	-0.61517000	1.29584900	0.41716300
O	-0.55029400	-0.48216500	1.41739300
O	-2.60592200	1.33778300	0.75859400
O	1.50634800	1.30909600	0.44243700
O	-0.39866300	3.33261100	-0.05171600
C	-1.17803300	-2.53522400	2.38677200
C	-1.53333000	-1.18855700	1.80836400
C	-2.88326900	-0.81408400	1.73342600
C	-3.34199200	0.40762700	1.21926200
C	-4.82412400	0.68441300	1.21037500
C	2.26071200	2.06918200	-0.24269000
C	0.58268900	3.85581900	-0.68002200
C	3.67097600	1.60330300	-0.47262700
C	1.85898100	3.29885100	-0.80569800

C	0.30451400	5.19349900	-1.31863600
H	-2.05525600	-3.11265200	2.69156600
H	-0.61833200	-3.11525400	1.64331600
H	-0.51374500	-2.41131400	3.24897500
H	-3.62546200	-1.53001700	2.07526900
H	-5.12635800	1.00890000	0.21016600
H	-5.41871200	-0.18838300	1.49492500
H	-5.05640600	1.50817400	1.89449100
H	4.04363900	1.05579300	0.39776100
H	3.66260200	0.89783900	-1.31422500
H	4.34804500	2.42736300	-0.71637900
H	2.60062800	3.85751400	-1.36992700
H	-0.09274500	5.88924400	-0.57265100
H	1.18867600	5.63573100	-1.78546200
H	-0.47445200	5.07686200	-2.07913800
H	-0.66619600	0.71887600	-1.18962300
O	0.03577300	2.46379200	2.61947400
H	-0.09478300	3.16495000	1.96432700
H	0.84330600	2.02982000	2.30907500

TS3_2

O	-3.11869800	1.78311200	1.55836000
C	-2.62575600	1.03486900	0.69426600
C	-1.24852800	1.09567000	0.26169000
H	-1.13193800	0.90122900	-0.81288800
H	-0.63655800	-0.01567400	0.74445200
C	-3.86395100	-2.05279900	-1.20003900
C	-3.00149600	-1.10411100	-0.65862200
C	-3.50152600	-0.03169200	0.09027800
C	-4.88326700	0.05319700	0.29464200
C	-5.74718500	-0.88869400	-0.25105900
C	-5.23982800	-1.94680700	-1.00444100
H	-3.45845500	-2.88593700	-1.77090900

H	-1.92897300	-1.20658800	-0.79535300
H	-5.24060400	0.88258000	0.90024700
H	-6.82051000	-0.80301800	-0.08937100
H	-5.91244500	-2.68868800	-1.43040300
C	-0.52328600	2.35287900	0.71220500
C	3.08777400	1.62495700	-0.23547100
C	1.82221400	1.51549200	0.32995200
C	0.84718700	2.49921700	0.11639600
C	1.18701400	3.59867500	-0.67708400
C	2.45652700	3.71742000	-1.24131200
C	3.41273800	2.72959300	-1.02359000
H	3.81855900	0.83669700	-0.06229200
H	1.55551100	0.64626400	0.92979900
H	0.43792000	4.36944000	-0.85602300
H	2.69682000	4.58269500	-1.85674900
H	4.40217200	2.81653600	-1.46795800
H	-0.45105900	2.33307200	1.80916500
C	4.13607100	-2.62449300	-0.92062500
C	2.78547300	-2.31822900	-1.04813500
C	2.03382200	-1.89952800	0.05407200
C	2.66735700	-1.80290400	1.29347700
C	4.02039900	-2.10784000	1.42745800
C	4.76201400	-2.51890800	0.32227200
H	4.70772800	-2.93981500	-1.79178100
H	2.29990900	-2.39335800	-2.02171800
H	2.05765300	-1.47377700	2.13162400
H	4.50132100	-2.02251300	2.40057800
H	5.81942400	-2.75415400	0.42513000
C	0.56130200	-1.55540200	-0.07672100
H	0.48418400	-0.83557100	-0.93265000
O	-0.00773500	-1.07637300	1.06259000
H	-1.12036900	3.25200200	0.49125200
H	0.06077000	-2.47869600	-0.46940400

TS4_1

O	0.46467600	0.74435600	1.54603300
O	-2.09304300	2.03964600	-1.43153800
O	-2.37130600	0.81590100	1.06960900
C	2.32960800	4.25366700	-0.37670200
C	1.61768900	3.04462800	0.17637000
C	2.03716700	2.51428300	1.40437700
C	1.47708800	1.35975300	1.98907800
C	2.14031000	0.76687400	3.20693400
C	-3.35625300	1.91822900	-1.45599800
C	-3.60309200	0.80933200	0.74745800
C	-4.04764900	2.49010300	-2.66863700
C	-4.12940700	1.31485900	-0.45111600
C	-4.54116600	0.19555500	1.75285900
H	2.81319900	3.99173000	-1.32376500
H	1.60298000	5.03912700	-0.60548100
H	3.08520100	4.65246800	0.30556300
H	2.88247000	2.98294600	1.90144400
H	1.39078700	0.52104100	3.96439300
H	2.62472100	-0.17444900	2.92092400
H	2.90013300	1.42235800	3.64208300
H	-3.68628300	1.98337400	-3.56907200
H	-5.13595700	2.39499200	-2.62264800
H	-3.78702500	3.54756500	-2.77998000
H	-5.20488800	1.26273000	-0.59563700
H	-4.28003900	0.52931100	2.76139300
H	-5.59035700	0.42775900	1.54963200
H	-4.41545400	-0.89336000	1.73746800
O	0.69389400	2.56707600	-0.55812600
C	-1.34290600	-2.43018500	-0.22858400
C	-2.36987500	-3.22337700	-0.74545600
C	-3.36224200	-3.73787900	0.08364600

C	-3.33438200	-3.47311000	1.45122100
C	-2.31922000	-2.66974800	1.97381500
C	-1.33637700	-2.14525100	1.14174300
H	-2.35224700	-3.41565600	-1.81530400
H	-4.15672500	-4.35383100	-0.33520700
H	-4.10439000	-3.87802000	2.10580900
H	-2.30921100	-2.42940300	3.03547700
H	-0.58789700	-1.46668600	1.54657500
C	-0.26115700	-1.97311100	-1.18513300
H	-0.50800100	-0.32286400	-0.90812300
O	-0.38903500	-2.22364600	-2.39944400
C	1.15308300	-1.90546500	-0.59952300
H	1.16599100	-1.39949900	0.37226600
H	1.48960500	-2.94255200	-0.42875400
C	2.10742000	-1.21313400	-1.56322500
H	1.71233200	-0.20280300	-1.74258700
H	2.06837400	-1.74230700	-2.52178900
C	3.50195700	-1.13818400	-1.02335400
C	4.43504800	-2.16045100	-1.23052200
C	3.88816500	-0.04903600	-0.23406600
C	5.70696700	-2.09803600	-0.66632800
H	4.15224900	-3.01621600	-1.84222300
C	5.15419500	0.01581400	0.33825000
H	3.17286400	0.75337800	-0.06435200
C	6.07283500	-1.00988900	0.12383700
H	6.41733600	-2.90327300	-0.84370300
H	5.42004400	0.87338500	0.95451400
H	7.06549100	-0.96267700	0.56625200
FE	-0.76898600	1.20912700	-0.11319600

TS4_2

C	0.18183800	2.51602500	0.08568000
H	0.43630200	2.22666700	-0.93869400

H	0.01814600	3.60671300	0.06713300
C	1.32880100	2.16818400	1.03808300
H	1.08795900	1.19165200	1.48157100
H	1.36782900	2.88067200	1.86939400
C	2.66549000	2.07468300	0.36510300
C	3.75452100	2.86646700	0.74062500
C	2.85627700	1.13569900	-0.65818100
C	4.99533500	2.72754500	0.11999800
H	3.62377700	3.59848600	1.53679400
C	4.09279200	0.98781000	-1.27523500
H	2.01851800	0.49731900	-0.94345700
C	5.17020000	1.78520500	-0.89004800
H	5.82887500	3.35497100	0.43000000
H	4.21674700	0.22956900	-2.04609200
H	6.13950700	1.66911600	-1.36979900
C	-2.25498500	1.81450400	-0.45955900
C	-3.55215400	1.99187300	0.03094800
C	-4.64712400	2.01086400	-0.82616500
C	-4.46300200	1.85763000	-2.19880500
C	-3.17396700	1.66713400	-2.69945700
C	-2.08316200	1.64113900	-1.83727300
H	-3.66445600	2.09709500	1.10731800
H	-5.64969600	2.14443000	-0.42324500
H	-5.31667700	1.87018000	-2.87342800
H	-3.02182100	1.52237700	-3.76722600
H	-1.08739100	1.44149500	-2.22751600
C	-1.12063400	1.85845000	0.53635500
O	-1.38750500	1.84561500	1.75078700
FE	-0.13965000	-1.39682800	0.26112500
O	1.67397800	-1.35126900	1.21456000
O	0.89246400	-2.11872900	-1.34511300
O	-1.14877700	-1.36688700	2.02758700
O	-1.91638300	-1.98421500	-0.60252400

C	3.97103500	-1.42174500	1.74476800
C	2.82614100	-1.69323300	0.80478100
C	3.09525000	-2.24843700	-0.45980300
C	2.12608000	-2.41864000	-1.45739600
C	2.54577000	-2.96658900	-2.79880100
C	-2.38788300	-1.11411800	2.15777900
C	-3.07180900	-1.70247600	-0.15515300
C	-2.81351800	-0.57873800	3.49735300
C	-3.35422500	-1.27637700	1.15158300
C	-4.20516800	-1.82497300	-1.14262900
H	3.73009600	-1.77714400	2.75087300
H	4.91070000	-1.87191800	1.41195500
H	4.11728400	-0.33692400	1.81491100
H	4.12384500	-2.50928300	-0.69453300
H	3.59725500	-3.26643300	-2.82458800
H	1.92139400	-3.82469800	-3.06637300
H	2.37966800	-2.20917300	-3.57307300
H	-2.32285700	-1.13279200	4.30241200
H	-2.47177200	0.46002300	3.55189400
H	-3.89796300	-0.60343300	3.64011500
H	-4.38426900	-1.02777300	1.39277400
H	-4.17118200	-2.80253800	-1.63390600
H	-5.18761100	-1.68232000	-0.68342800
H	-4.07729500	-1.06762900	-1.92408500
H	-0.43564000	0.29540900	-0.00662400

TS4_w1

C	1.66704700	2.28159800	-0.36271500
C	2.70769800	2.98013800	-0.98453800
C	3.73677500	3.54685800	-0.23797800
C	3.74298700	3.42308000	1.15008200
C	2.72190700	2.70626900	1.77760400
C	1.69661500	2.13809200	1.03030100

H	2.67157100	3.06196600	-2.06785900
H	4.53626000	4.08977100	-0.73931000
H	4.54474500	3.86546200	1.73821600
H	2.73537700	2.57270500	2.85738700
H	0.94362900	1.52870200	1.52511600
C	0.54144000	1.78884600	-1.23678100
O	0.67051500	1.83669600	-2.46918400
C	-0.86455700	1.80282300	-0.63320300
H	-0.85067000	1.43622700	0.39964200
H	-1.19117800	2.85736600	-0.59444100
C	-1.82083100	0.99807300	-1.49099900
H	-1.49216000	-0.05297900	-1.44109700
H	-1.66834800	1.29401900	-2.53558500
C	-3.27682000	1.07708600	-1.13610800
C	-3.72436100	1.43319400	0.14155000
C	-4.24761500	0.73996600	-2.09003100
C	-5.08041900	1.43333000	0.45856300
H	-2.99570700	1.69131700	0.90627900
C	-5.60370300	0.73890400	-1.78005500
H	-3.92006900	0.46692600	-3.09230900
C	-6.02881800	1.08341900	-0.49827800
H	-5.39522200	1.70431800	1.46457400
H	-6.33248600	0.46922100	-2.54194100
H	-7.08756400	1.08120200	-0.24988300
O	2.70367700	-1.20403800	0.87646600
O	1.41445700	-2.61546100	-1.18502100
O	-0.02605700	-0.50714100	2.10393300
O	-1.28407200	-2.01775800	0.08414300
C	4.75349000	-0.14885700	0.35895200
C	3.55231200	-0.96308800	-0.04100200
C	3.43788000	-1.38372500	-1.37647400
C	2.38791600	-2.17219200	-1.87322600
C	2.37748600	-2.52459600	-3.33850700

C	-1.21849900	-0.42922700	2.55115400
C	-2.32425100	-1.77083300	0.77454100
C	-1.39554800	0.41669400	3.78624800
C	-2.34357400	-1.02519200	1.96692200
C	-3.62201400	-2.30384700	0.22748700
H	5.53801700	-0.14538500	-0.40270600
H	4.43737900	0.88532200	0.53682300
H	5.16095000	-0.52217700	1.30313800
H	4.21571100	-1.07897800	-2.07098000
H	2.13017600	-3.58199900	-3.47081700
H	1.58363100	-1.94852400	-3.82600800
H	3.32256100	-2.30187400	-3.84119800
H	-1.14542700	1.45912200	3.55269500
H	-2.41558700	0.38632700	4.17951400
H	-0.69878600	0.09706400	4.56742000
H	-3.30673400	-0.86571800	2.44417700
H	-4.46176800	-2.15767000	0.91243400
H	-3.85795200	-1.78933300	-0.71162900
H	-3.52289700	-3.36828300	-0.00632200
O	1.26564400	-3.51636300	1.46762700
H	1.33898700	-3.72590100	0.52447200
H	2.04938700	-2.96513500	1.61305900
H	0.72310900	0.02637000	-0.65365600
FE	0.60855700	-1.36453100	0.37830900

TS4_w2

C	-2.32252000	1.88426200	-0.62316000
C	-3.62794000	2.20460200	-0.23514800
C	-4.67294400	2.18863000	-1.15338700
C	-4.43004600	1.84993800	-2.48281700
C	-3.13511200	1.50521300	-2.87629600
C	-2.09432700	1.51790100	-1.95530300
H	-3.78536000	2.45741100	0.81061500

H	-5.68239200	2.44011600	-0.83239100
H	-5.24427100	1.83494000	-3.20438800
H	-2.94043100	1.20942000	-3.90498200
H	-1.10004500	1.19164400	-2.25268500
C	-1.23532800	2.01437200	0.41000900
O	-1.54608300	2.14377400	1.60305200
FE	-0.07796000	-1.37494900	0.22305600
O	1.83339300	-1.28444500	0.90783300
O	0.67362300	-1.95720600	-1.56642200
O	-0.86179800	-1.31019200	2.22406900
O	-2.07761800	-2.04057500	-0.21978500
C	4.16934300	-1.50418400	1.12485000
C	2.90184900	-1.65297800	0.32462600
C	2.97431300	-2.14650000	-0.99038700
C	1.87191600	-2.28444400	-1.84758600
C	2.08441400	-2.85624000	-3.22733900
C	-1.99015000	-0.75992700	2.43302700
C	-3.06804100	-1.41785000	0.28778000
C	-2.13821900	-0.02665300	3.73789100
C	-3.07565400	-0.78579400	1.53887300
C	-4.31208800	-1.36404600	-0.56045100
H	4.07464700	-2.02966900	2.08037700
H	5.05171600	-1.87545300	0.59539200
H	4.32439100	-0.44394100	1.35702600
H	3.94999400	-2.44311700	-1.36671500
H	1.73341200	-2.14665200	-3.98390200
H	3.13073100	-3.10115300	-3.43038500
H	1.48051500	-3.76163500	-3.34784300
H	-1.74767800	-0.63354000	4.56047600
H	-1.53595200	0.88404300	3.66937600
H	-3.17137800	0.26219200	3.94926600
H	-3.98035900	-0.25939400	1.83071000
H	-4.54201800	-2.36068800	-0.95005400

H	-5.18064200	-0.96909600	-0.02598900
H	-4.12065000	-0.71708100	-1.42420900
H	-0.59203000	0.25639600	0.01493900
O	-0.23500800	-3.75512900	0.97539200
H	-1.06884900	-3.61756100	0.49961000
H	-0.38808700	-3.26093500	1.79467800
C	0.13309600	2.49597500	-0.05081400
H	0.39175500	2.07178700	-1.02524400
H	0.07240300	3.58886300	-0.19274800
C	1.21052100	2.16367500	0.97765900
H	1.00505100	1.14339500	1.33444000
H	1.11226900	2.82297200	1.84666700
C	2.60323700	2.21277000	0.42652700
C	3.58773100	3.04624300	0.96407300
C	2.95994000	1.37962500	-0.64323500
C	4.88614300	3.05126400	0.45697200
H	3.32805600	3.69511000	1.79956100
C	4.25499000	1.37398500	-1.14773700
H	2.21100200	0.70319600	-1.05481800
C	5.22573200	2.21412100	-0.60182500
H	5.63491600	3.70962400	0.89324900
H	4.50895700	0.69413000	-1.95858800
H	6.24007700	2.20978000	-0.99482400

TS5_1

C	-2.28865600	2.30244400	0.25150500
C	-1.19989800	2.04920000	1.28762900
H	-1.64347400	1.60430900	2.18566800
H	-0.77170600	3.01114300	1.60174100
C	-3.82598900	-1.19942900	0.18358900
C	-2.98085100	-0.13729900	0.49991000
C	-3.19692500	1.13204400	-0.04411000
C	-4.29365300	1.30681800	-0.89811500

C	-5.14497000	0.25121900	-1.20640200
C	-4.91189300	-1.01305700	-0.66555800
H	-3.60438300	-2.17567400	0.60929200
H	-2.13316200	-0.33470500	1.15215100
H	-4.47577600	2.29163400	-1.32951900
H	-5.99065800	0.41360000	-1.87247600
H	-5.57004100	-1.84378600	-0.91200700
O	0.24974800	0.17722200	1.82504500
C	-0.06332900	1.07022100	0.84692400
C	2.25928000	3.67409900	-0.81293800
C	1.10617400	3.04993900	-0.34045100
C	1.16956700	1.83220400	0.34657300
C	2.42811900	1.26004500	0.54942700
C	3.58144600	1.87159400	0.06978500
C	3.50590700	3.08476500	-0.61295000
H	2.18394100	4.62507500	-1.33897900
H	0.14014900	3.52560100	-0.50721600
H	2.45432200	0.32029300	1.09503200
H	4.54794200	1.39425200	0.22706800
H	4.40795500	3.56741300	-0.98537800
H	-0.45318300	0.56880100	-0.08248800
C	3.52144900	-2.28171600	0.57258600
C	2.15149700	-2.39744400	0.78025700
C	1.24582100	-2.09670300	-0.24010900
C	1.74574600	-1.66250500	-1.46823300
C	3.11689500	-1.53533300	-1.68030700
C	4.01125300	-1.85003100	-0.66058900
H	4.21490700	-2.51081600	1.38022500
H	1.73906500	-2.68662000	1.74410800
H	1.04227100	-1.39744800	-2.25842400
H	3.48833500	-1.16986600	-2.63575500
H	5.08243900	-1.73909300	-0.81797800
C	-0.24763300	-2.27426500	0.00581300

H	-0.76622800	-1.58584500	-0.70583200
O	-0.60637900	-2.04295900	1.31556400
H	-0.20717400	-0.99981600	1.58173900
H	-2.91555100	3.15488900	0.55654900
H	-1.83005100	2.62243600	-0.69792800
C	-0.65602600	-3.69657400	-0.38319100
H	-1.73597400	-3.82048400	-0.25010400
H	-0.40049000	-3.93556200	-1.42306200
H	-0.15040600	-4.41525200	0.27241800

M_1

FE	0.00000000	0.00000000	0.00009400
O	0.99341100	1.37282700	-0.99418500
O	-0.99375000	1.37283800	0.99391900
O	0.99375000	-1.37283800	0.99391900
O	-0.99341100	-1.37282700	-0.99418500
C	1.77102200	3.45475800	-1.77157700
C	0.87930000	2.64288600	-0.87983400
C	0.00000000	3.28982800	0.00002500
C	-0.87947200	2.64290800	0.87970700
C	-1.77093400	3.45477800	1.77170700
C	0.87947200	-2.64290800	0.87970700
C	-0.87930000	-2.64288600	-0.87983400
C	1.77093400	-3.45477800	1.77170700
C	0.00000000	-3.28982800	0.00002500
C	-1.77102200	-3.45475800	-1.77157700
H	2.81726400	3.20044700	-1.57835800
H	1.57792600	3.20029200	-2.81779700
H	1.63639800	4.52937400	-1.63705900
H	0.00014400	4.37470300	0.00016100
H	-2.81724200	3.20072000	1.57852000
H	-1.57780800	3.20006300	2.81786400
H	-1.63609700	4.52939400	1.63739900

H	1.63609700	-4.52939400	1.63739900
H	2.81724200	-3.20072000	1.57852000
H	1.57780800	-3.20006300	2.81786400
H	-0.00014400	-4.37470300	0.00016100
H	-1.57792600	-3.20029200	-2.81779700
H	-1.63639800	-4.52937400	-1.63705900
H	-2.81726400	-3.20044700	-1.57835800

M_2

O	1.43550300	1.39692800	0.30161100
O	-1.43573800	-1.39703500	0.30050400
O	-1.43668300	1.39718700	0.30139700
C	3.31958200	-2.50323100	-0.59219900
C	2.58565800	-1.23732400	-0.21141500
C	3.20218800	0.00107400	-0.45984700
C	2.58389300	1.23854000	-0.21139800
C	3.31642900	2.50546100	-0.59156600
C	-2.58442800	-1.23821200	-0.21172600
C	-2.58509800	1.23767600	-0.21105300
C	-3.31742300	-2.50474300	-0.59213800
C	-3.20249000	-0.00041300	-0.45892100
C	-3.31877200	2.50382300	-0.59176100
H	3.43081100	-3.14618700	0.28725800
H	2.72823000	-3.07221600	-1.31782400
H	4.30963100	-2.31211800	-1.01765100
H	4.19123300	0.00189800	-0.91184000
H	3.42678800	3.14820700	0.28815400
H	4.30675100	2.31562400	-1.01693000
H	2.72450600	3.07404700	-1.31704700
H	-2.72515100	-3.07389300	-1.31686800
H	-3.42902600	-3.14718600	0.28766300
H	-4.30727800	-2.31445600	-1.01839200
H	-4.19171800	-0.00054000	-0.91051900

H	-2.72800300	3.07182400	-1.31865100
H	-4.30951500	2.31310600	-1.01576100
H	-3.42832900	3.14753400	0.28734800
H	-0.00162700	-0.00187600	2.55765200
FE	-0.00003400	-0.00078400	0.86927800
O	1.43771100	-1.39699200	0.30203000

M_w1

O	1.46630500	1.38908800	-0.06877100
O	1.46579100	-1.38883900	-0.06945800
O	-1.44132500	1.38718400	-0.00093000
O	-1.44136100	-1.38674300	-0.00034300
C	3.52462400	2.50544400	-0.33320800
C	2.72395800	1.23868200	-0.22656600
C	3.37554600	-0.00017400	-0.30583900
C	2.72346000	-1.23883700	-0.22739400
C	3.52360500	-2.50583500	-0.33513200
C	-2.68427300	1.23929100	-0.25137900
C	-2.68429500	-1.23895200	-0.25092800
C	-3.47226300	2.50558100	-0.43590900
C	-3.33159000	0.00014600	-0.36653000
C	-3.47227200	-2.50529700	-0.43513200
H	3.36475300	3.11960200	0.55782000
H	4.59440400	2.32161800	-0.45094200
H	3.17027800	3.09558100	-1.18374700
H	4.45229700	-0.00033400	-0.44030400
H	3.36354800	-3.12067900	0.55538700
H	3.16895500	-3.09510800	-1.18614300
H	4.59344900	-2.32234600	-0.45281000
H	-4.53661400	2.32353200	-0.59734700
H	-3.34814600	3.15444000	0.43606200
H	-3.07552600	3.06121800	-1.29105300
H	-4.39468900	0.00012300	-0.58449100

H	-4.53664100	-2.32330400	-0.59653000
H	-3.07560000	-3.06107500	-1.29021900
H	-3.34807100	-3.15401000	0.43693300
O	-0.19888600	-0.00147800	2.31251800
H	-0.75894900	0.76621900	2.47630700
H	-0.75940300	-0.76959800	2.47290600
FE	0.03702900	0.00038900	0.10623600

M_w2

FE	0.04329100	0.00242400	-0.93221200
O	1.47478000	1.40071900	-0.45727600
O	1.46982400	-1.40046500	-0.45294900
O	-1.39838200	1.40865900	-0.24029200
O	-1.39863200	-1.40698100	-0.24625500
C	3.37453100	2.49932000	0.40528000
C	2.63973600	1.23709000	0.02170700
C	3.26504200	-0.00183300	0.23428800
C	2.63620500	-1.23915000	0.02389500
C	3.36822900	-2.50291500	0.40773400
C	-2.62353500	1.24025200	0.04580600
C	-2.62308500	-1.23985400	0.04167300
C	-3.41539800	2.49934100	0.31000400
C	-3.27366900	0.00010700	0.15566800
C	-3.41460100	-2.49977100	0.30345700
H	2.82808700	3.01664400	1.20137300
H	4.39547300	2.30941400	0.74985700
H	3.40743800	3.18591700	-0.44690800
H	4.26508700	-0.00293200	0.66066500
H	3.40044700	-3.18931600	-0.44465600
H	4.38933100	-2.31507500	0.75296500
H	2.82029700	-3.01957900	1.20324600
H	-2.96571200	3.05177300	1.14183900
H	-3.36212900	3.15675700	-0.56375900

H	-4.46575600	2.30326500	0.54414200
H	-4.32729800	-0.00042300	0.42234000
H	-2.96481400	-3.05342300	1.13443200
H	-4.46506700	-2.30458100	0.53788300
H	-3.36093000	-3.15562600	-0.57143800
H	-0.17327500	0.00368200	-2.60333600
O	-0.08957000	-0.00118400	2.11325900
H	-0.29446000	-0.75698100	1.54649800
H	-0.31718300	0.74593000	1.54341400

M_3-H

FE	-0.00002400	0.59606000	-1.41478400
O	-1.38412900	-0.88265100	-1.42872200
O	-1.41568600	1.70537200	-0.50470000
O	1.38424100	-0.88252600	-1.42900500
O	1.41551200	1.70531100	-0.50445600
C	-3.35061400	-2.12242600	-1.30455300
C	-2.62446400	-0.86731200	-1.09566900
C	-3.31492200	0.23904400	-0.55186900
C	-2.64854000	1.45477700	-0.26479400
C	-3.41927600	2.54684600	0.33595600
C	2.62453400	-0.86717600	-1.09581400
C	2.64832700	1.45470300	-0.26433900
C	3.35088700	-2.12208700	-1.30521800
C	3.31485400	0.23911600	-0.55168800
C	3.41893000	2.54672400	0.33666600
C	4.73196000	0.04782500	-0.00932100
C	-4.73196500	0.04770700	-0.00937200
C	-4.76239000	2.53618100	0.39229200
H	-5.31014500	3.39815800	0.77064800
H	-2.83825100	3.40655300	0.66130900
C	-5.52637700	1.36004200	-0.12102400
H	-6.48405400	1.24953300	0.41031400

C	-4.68341300	-2.22143800	-1.16773100
H	-5.19831200	-3.15660100	-1.38415500
C	-5.49521100	-1.02102000	-0.81219000
H	-2.74169300	-2.96651500	-1.62142800
H	-6.40359700	-1.30497000	-0.26031800
C	4.68370400	-2.22094000	-1.16845200
H	5.19874200	-3.15594800	-1.38521600
C	4.76204400	2.53619900	0.39303600
C	5.52619100	1.36029700	-0.12059100
C	5.49533400	-1.02052200	-0.81251700
H	6.40378000	-1.30452400	-0.26076900
H	2.83779900	3.40629000	0.66220300
H	2.74209300	-2.96615300	-1.62239500
H	6.48387700	1.24977000	0.41072800
H	5.30968500	3.39814300	0.77163400
H	5.85890700	-0.56245200	-1.75000800
H	-5.79164500	1.53189700	-1.17870400
H	5.79145300	1.53247300	-1.17822100
H	-5.85887900	-0.56333200	-1.74983000
C	-4.71191300	-0.32654300	1.50428600
C	-3.65298300	-1.31990900	2.00400300
C	-2.33960100	-0.69715300	2.34971200
C	-1.16657600	-1.07894700	1.84272200
C	4.71204900	-0.32690600	1.50421900
C	3.65304000	-1.32029200	2.00372600
C	2.33973900	-0.69744700	2.34954300
C	1.16667300	-1.07888800	1.84238000
H	5.71623700	-0.70138300	1.75834100
H	-4.58768300	0.60196700	2.07802900
H	-5.71611400	-0.70084700	1.75861600
H	4.58795900	0.60144500	2.07824700
O	0.00008700	-0.48152700	2.22935100
H	-4.06011100	-1.79760700	2.90945500

H	-3.50719200	-2.13080200	1.28247100
H	3.50714900	-2.13098400	1.28199900
H	4.06012900	-1.79826300	2.90905600
H	-1.06392600	-1.85833100	1.08479300
H	-2.34335400	0.12048200	3.07128200
H	1.06389600	-1.85799200	1.08417400
H	2.34357300	0.11992700	3.07140900
H	-0.00004500	1.16796700	-2.99940800

M_3

FE	-0.47222600	-0.80962200	0.00000000
O	0.86984100	-1.32325400	1.38828500
O	-1.71889800	-0.49051500	1.49811000
O	0.86984100	-1.32325400	-1.38828500
O	-1.71889800	-0.49051500	-1.49811000
C	2.15820000	-1.24640300	3.32263900
C	0.87548600	-1.06014700	2.64270100
C	-0.23700200	-0.59759600	3.37822000
C	-1.48373200	-0.36785600	2.75528600
C	-2.62246500	0.03685900	3.58246400
C	0.87548600	-1.06014700	-2.64270100
C	-1.48373200	-0.36785600	-2.75528600
C	2.15820000	-1.24640300	-3.32263900
C	-0.23700200	-0.59759600	-3.37822000
C	-2.62246500	0.03685900	-3.58246400
C	-0.03539900	-0.06383000	-4.79471900
C	-0.03539900	-0.06383000	4.79471900
C	-2.55664000	0.06096300	4.92269300
H	-3.44046700	0.30414900	5.50923800
H	-3.54076100	0.26233500	3.04731000
C	-1.29901600	-0.28965500	5.64079700
H	-1.21609700	0.27872900	6.57791000
C	2.29622200	-1.09155100	4.64709900

H	3.25995000	-1.26575900	5.12264200
C	1.13159100	-0.76339600	5.51353700
H	2.99067900	-1.53650900	2.68691700
H	1.44352900	-0.15446400	6.37308800
C	2.29622200	-1.09155100	-4.64709900
H	3.25995000	-1.26575900	-5.12264200
C	-2.55664000	0.06096300	-4.92269300
C	-1.29901600	-0.28965500	-5.64079700
C	1.13159100	-0.76339600	-5.51353700
H	1.44352900	-0.15446400	-6.37308800
H	-3.54076100	0.26233500	-3.04731000
H	2.99067900	-1.53650900	-2.68691700
H	-1.21609700	0.27872900	-6.57791000
H	-3.44046700	0.30414900	-5.50923800
H	0.77154600	-1.70888300	-5.95510100
H	-1.35358400	-1.34800700	5.94735100
H	-1.35358400	-1.34800700	-5.94735100
H	0.77154600	-1.70888300	5.95510100
C	0.20221400	1.47676000	4.73963800
C	1.14593200	2.04914500	3.67139300
C	0.53797200	2.09017100	2.30557000
C	1.12931700	1.69215700	1.18123600
C	0.20221400	1.47676000	-4.73963800
C	1.14593200	2.04914500	-3.67139300
C	0.53797200	2.09017100	-2.30557000
C	1.12931700	1.69215700	-1.18123600
H	0.54887200	1.79205800	-5.73431400
H	-0.77467500	1.95871600	4.59849000
H	0.54887200	1.79205800	5.73431400
H	-0.77467500	1.95871600	-4.59849000
O	0.41141100	1.64306800	0.00000000
H	1.38686200	3.07572600	3.98383000
H	2.10052000	1.51049800	3.65330200

H	2.10052000	1.51049800	-3.65330200
H	1.38686200	3.07572600	-3.98383000
H	2.14674600	1.30257800	1.11770500
H	-0.49342700	2.43807500	2.23251200
H	2.14674600	1.30257800	-1.11770500
H	-0.49342700	2.43807500	-2.23251200

M_4-H

FE	0.47359700	0.00027900	-1.93777700
O	-0.97637300	-1.35813700	-1.57044500
O	-0.97596800	1.35905000	-1.56942500
O	1.79194600	-1.37585700	-1.24239800
O	1.79192000	1.37641500	-1.24192300
C	-2.91086000	-2.46291500	-0.89417400
C	-2.13866200	-1.22838500	-1.03965100
C	-2.73844600	0.00037300	-0.67252600
C	-2.13833800	1.22923300	-1.03885300
C	-2.91024400	2.46384600	-0.89257200
C	2.85702700	-1.22896100	-0.54603000
C	2.85702000	1.22933000	-0.54566000
C	3.43420700	-2.45130500	0.02184900
C	3.48747300	0.00013400	-0.25433600
C	3.43422400	2.45149100	0.02259000
C	4.63445200	-0.00003500	0.73903400
C	-3.94963100	0.00020600	0.26159900
C	-4.16364000	2.48731900	-0.41053000
H	-4.73080100	3.41734600	-0.38118600
H	-2.41558500	3.36660100	-1.24465500
C	-4.85155400	1.24419600	0.04248600
H	-5.41959100	1.43674800	0.96739000
C	-4.16430500	-2.48637800	-0.41224800
H	-4.73172800	-3.41626700	-0.38358700
C	-4.85190500	-1.24337000	0.04155000

H	-2.41640500	-3.36556000	-1.24683300
H	-5.42006300	-1.43639100	0.96628500
C	4.66005100	-2.49026700	0.57175000
H	5.07742200	-3.42974400	0.93200400
C	4.66005300	2.49026100	0.57253100
C	5.49557800	1.25360800	0.62851600
C	5.49559000	-1.25363100	0.62804400
H	6.21027400	-1.29268100	1.46173900
H	2.82184800	3.34605600	-0.07300500
H	2.82178500	-3.34581600	-0.07398800
H	6.21018000	1.29240700	1.46229400
H	5.07744700	3.42963200	0.93303700
H	6.11208100	-1.18325900	-0.28761600
H	6.11217500	1.18354200	-0.28709600
H	4.18780600	-0.00023900	1.75410400
H	-5.62491900	1.00093900	-0.70635000
H	-5.62513900	-0.99936600	-0.70717800
C	-3.48408500	-0.00043100	1.76948500
H	-4.41830200	-0.00045900	2.35531700
C	-2.60252600	-1.21961400	2.16864100
H	-2.81340100	-1.50989700	3.21149700
H	-2.78922200	-2.10692400	1.56178300
C	-2.60211400	1.21817500	2.16946700
H	-2.78854000	2.10596600	1.56322800
H	-2.81287400	1.50779700	3.21252900
C	-1.22113600	0.66491400	2.03790400
C	-1.22136100	-0.66673600	2.03747100
C	0.14675300	-1.18252000	1.79166300
H	0.54651500	-1.82240200	2.59918400
H	0.21809800	-1.75697600	0.85191200
C	0.14714000	1.18039300	1.79237600
H	0.21861600	1.75536200	0.85294900
H	0.54715500	1.81965700	2.60025400

O	0.95528800	-0.00117700	1.69304100
H	0.67257700	0.00073100	-3.60487400
M_4			
FE	0.57661200	-0.00087100	-0.63841700
O	-0.83322900	-1.35472700	-1.12141900
O	-0.83270600	1.35381000	-1.12142700
O	1.99103100	-1.38125700	-0.44528000
O	1.99037700	1.38042800	-0.44526100
C	-2.89293000	-2.44741300	-1.21751500
C	-2.10724600	-1.22433000	-1.04107300
C	-2.78986700	-0.00009500	-0.86791000
C	-2.10673500	1.22386000	-1.04125900
C	-2.89198200	2.44717200	-1.21817400
C	3.24319600	-1.23470100	-0.20251400
C	3.24258600	1.23448000	-0.20254400
C	4.00130600	-2.46980100	0.01165100
C	3.92251800	0.00004300	-0.12049000
C	4.00012700	2.46994800	0.01158200
C	5.38685500	0.00041900	0.29660800
C	-4.20804900	0.00030300	-0.30373600
C	-4.22607900	2.46281500	-1.09452300
H	-4.78279200	3.38017300	-1.28002200
H	-2.32763400	3.33838500	-1.47926600
C	-5.01464500	1.24999800	-0.74412200
H	-5.74757400	1.49822200	0.03873500
C	-4.22702300	-2.46249700	-1.09371900
H	-4.78411500	-3.37968300	-1.27892900
C	-5.01511600	-1.24932300	-0.74350700
H	-2.32896900	-3.33891500	-1.47844700
H	-5.74786600	-1.49711800	0.03965900
C	5.34222600	-2.49435500	0.03303200
H	5.87113400	-3.43942300	0.14200600

C	5.34103300	2.49515500	0.03291600
C	6.13130200	1.24849900	-0.17078700
C	6.13189700	-1.24732700	-0.17071700
H	7.10556900	-1.30894100	0.33045300
H	3.40828700	3.37712300	0.09959400
H	3.40990600	-3.37725800	0.09970200
H	7.10494800	1.31060000	0.33037500
H	5.86948500	3.44048600	0.14182600
H	6.36446200	-1.14725700	-1.24602500
H	6.36390600	1.14849800	-1.24609100
H	5.41178800	0.00046500	1.40283400
H	-5.63529300	1.00130400	-1.62056000
H	-5.63599700	-1.00073700	-1.61980800
C	-4.12507100	0.00061600	1.27570500
H	-5.17045800	0.00090600	1.62021300
C	-3.35827700	-1.21739000	1.87014800
H	-3.78436700	-1.48834900	2.84794900
H	-3.41559400	-2.11634200	1.25214600
C	-3.35773500	1.21847700	1.86976800
H	-3.41464100	2.11726700	1.25151300
H	-3.78372700	1.48990000	2.84748600
C	-1.97555700	0.66688400	2.01276700
C	-1.97585100	-0.66637500	2.01294400
C	-0.58062600	-1.17878900	1.99667800
H	-0.22168000	-1.53285200	2.97660800
H	-0.37738800	-1.95616100	1.25232000
C	-0.58010000	1.17868300	1.99642700
H	-0.37649300	1.95580600	1.25191800
H	-0.22103100	1.53277700	2.97630300
O	0.18368700	-0.00024800	1.61095300

TS3_1

O	-3.08945500	1.98744500	1.53271600
---	-------------	------------	------------

C	-2.67894300	1.17525700	0.68330700
C	-1.33675600	1.17817800	0.13321500
H	-1.33549400	0.94805900	-0.94249700
H	-0.67276200	0.03611100	0.51287900
C	-4.12169400	-2.09174600	-0.66749700
C	-3.19944000	-1.14288800	-0.23404300
C	-3.63174200	0.11291900	0.20717600
C	-5.00366300	0.38577100	0.22970800
C	-5.92322100	-0.55513000	-0.21954200
C	-5.48421800	-1.79849500	-0.67540800
H	-3.77237300	-3.07020300	-0.99388800
H	-2.13859400	-1.38120800	-0.16984400
H	-5.31836000	1.35327300	0.61382500
H	-6.98729100	-0.32455500	-0.21179100
H	-6.20285900	-2.53826600	-1.02328400
C	-0.58517400	2.45648300	0.47177300
C	3.11779000	1.61075100	0.22275500
C	1.78093000	1.59071400	0.60385500
C	0.85524400	2.48606200	0.05118400
C	1.32106800	3.40562300	-0.89384300
C	2.66093700	3.43404600	-1.27772700
C	3.56635800	2.53598500	-0.71959400
H	3.80586500	0.88378900	0.65040300
H	1.42270300	0.83544300	1.30155800
H	0.61378900	4.10755700	-1.33474000
H	2.99684700	4.15835400	-2.01801300
H	4.61136300	2.54956200	-1.02158800
H	-0.65524500	2.59133600	1.55947600
C	4.49486700	-1.99752800	-0.63830000
C	3.18550500	-1.70044500	-1.00198100
C	2.17014800	-1.61630100	-0.04350100
C	2.50101200	-1.84041600	1.29322100
C	3.81025800	-2.14122900	1.66405000

C	4.81388100	-2.22213700	0.70085900
H	5.27277500	-2.04684900	-1.39839500
H	2.94531600	-1.50389400	-2.04708000
H	1.69682700	-1.74949500	2.01928100
H	4.05164100	-2.30994400	2.71235200
H	5.83764700	-2.45141800	0.98941300
C	0.73370900	-1.27774100	-0.42871400
H	0.80374700	-0.36528400	-1.07075900
O	-0.06163900	-1.05989700	0.67046500
C	0.16841000	-2.39489100	-1.32495500
H	-0.80540400	-2.09536100	-1.72671600
H	0.82392500	-2.64151700	-2.17044700
H	0.02223100	-3.30131400	-0.72621700
H	-1.09914000	3.33839300	0.05464100

TS5_2

C	2.46148700	1.99063100	-0.25372200
C	1.35915100	1.78720200	-1.28699100
H	1.77008700	1.28391200	-2.16942500
H	1.00393800	2.76789200	-1.63252800
C	3.77387300	-1.59962600	-0.10296900
C	2.99143400	-0.49555100	-0.43689300
C	3.30017100	0.77390300	0.06075200
C	4.42530300	0.90402200	0.88574600
C	5.21535600	-0.19384700	1.20988400
C	4.88914700	-1.45706600	0.71675100
H	3.48205500	-2.57327000	-0.49002800
H	2.12234800	-0.65690100	-1.07070200
H	4.68045800	1.88829500	1.27967500
H	6.08565000	-0.06483600	1.85085600
H	5.49935600	-2.31991500	0.97544600
O	-0.24034300	0.02665700	-1.77869200
C	0.15153800	0.90885800	-0.82215500

C	-1.95080700	3.72306100	0.79173500
C	-0.85235400	3.00018400	0.32916700
C	-1.01407300	1.77519600	-0.32860300
C	-2.31498900	1.29885000	-0.51176100
C	-3.41466600	2.00855500	-0.04088300
C	-3.24071300	3.22797500	0.61263400
H	-1.79851600	4.67766000	1.29377500
H	0.14774600	3.40520800	0.48020900
H	-2.41765900	0.35450700	-1.03929900
H	-4.41599000	1.60369700	-0.18300200
H	-4.09969300	3.78794200	0.97796200
H	0.50956700	0.39994700	0.11699500
C	-3.65695600	-2.21300200	-0.60021200
C	-2.28907100	-2.35427000	-0.81115200
C	-1.38951800	-2.27123000	0.25419400
C	-1.89415600	-2.02880100	1.53366300
C	-3.26195300	-1.88218800	1.75048800
C	-4.15150400	-1.97703100	0.68223700
H	-4.34370900	-2.27001200	-1.44312600
H	-1.87329500	-2.49711700	-1.80486100
H	-1.19738100	-1.93355200	2.36693600
H	-3.63468500	-1.67728800	2.75242800
H	-5.21981800	-1.85019800	0.84555700
C	0.09568100	-2.45895700	0.00580100
H	0.63660200	-1.82393000	0.74738300
O	0.49059500	-2.24688200	-1.29201300
H	0.16325000	-1.19204500	-1.54523200
H	3.13770400	2.80058300	-0.56850600
H	2.02118500	2.34903600	0.69059000
H	0.34449200	-3.49901900	0.30828600

IM13_2

C	1.94137900	2.30687000	0.67403300
---	------------	------------	------------

C	0.90913500	2.44572900	-0.43605900
H	1.40969300	2.54204400	-1.40704600
H	0.35360000	3.38034900	-0.27847400
C	3.86701000	-0.67972600	-0.73225500
C	2.91051600	0.32542100	-0.59339000
C	2.97296100	1.22216600	0.47797200
C	4.02800000	1.09234700	1.39124600
C	4.99042000	0.09943900	1.24547400
C	4.91082900	-0.79683400	0.17970800
H	3.76301800	-1.38379500	-1.55492300
H	2.09159100	0.38740300	-1.31261100
H	4.08868200	1.78424600	2.23212700
H	5.80106600	0.01973900	1.96778700
H	5.65544600	-1.58250800	0.06927700
O	-0.04489300	0.70010300	-1.83901700
C	-0.07979500	1.22314300	-0.59664700
C	-3.11138700	2.34310900	1.49858300
C	-1.82469200	1.94008700	1.15194400
C	-1.48567100	1.67158900	-0.17723700
C	-2.47096000	1.81790200	-1.15477200
C	-3.75807800	2.22785200	-0.81722500
C	-4.08618900	2.49181100	0.51199300
H	-3.36121600	2.53307400	2.54158600
H	-1.06876500	1.80689200	1.92748200
H	-2.17528200	1.57084100	-2.17256500
H	-4.51635500	2.33609600	-1.59209300
H	-5.09533100	2.79947400	0.78021300
H	0.22758700	0.50082700	0.21766600
C	-3.00286700	-1.90215100	0.03049600
C	-1.74297600	-1.73006300	-0.53703500
C	-0.67909300	-2.55206000	-0.15559600
C	-0.91218900	-3.55884100	0.78563400
C	-2.17410200	-3.74046400	1.34478400

C	-3.22645600	-2.90763000	0.96948200
H	-3.81316300	-1.23466200	-0.25736700
H	-1.55050600	-0.93660300	-1.26081100
H	-0.08775300	-4.20819700	1.08302800
H	-2.33750700	-4.53323200	2.07314200
H	-4.21306100	-3.04028900	1.40892700
C	0.71276500	-2.31871600	-0.70299400
H	1.26153700	-1.71252400	0.04868800
O	0.77681700	-1.75723100	-1.97038600
H	0.44567100	-0.79371800	-1.91950600
H	2.46963700	3.26127400	0.82762600
H	1.42286100	2.12217900	1.62932300
H	1.24179100	-3.28776600	-0.72508400

IM14_2

C	2.31044500	1.82186700	-0.40825400
C	1.27627900	1.48902200	-1.48177600
H	1.70548600	0.78360000	-2.20160200
H	1.01884300	2.38735200	-2.05939400
C	3.75484900	-1.67286100	0.18260800
C	2.91196000	-0.65869300	-0.27215900
C	3.19038900	0.67657800	0.04035400
C	4.32914600	0.95831900	0.80762200
C	5.16900100	-0.05451600	1.25655500
C	4.88192700	-1.38309600	0.94453000
H	3.50376900	-2.70120600	-0.06967000
H	2.04226500	-0.96106500	-0.87055500
H	4.55747200	1.99641900	1.05205800
H	6.04866600	0.19272100	1.84808400
H	5.53330700	-2.18108000	1.29573800
O	-0.65791100	0.10564600	-1.94624000
C	-0.01108400	0.84131900	-0.95159600
C	-1.70662500	3.99239100	0.48210100

C	-0.74677300	3.16855300	-0.10859600
C	-1.00213900	1.81417900	-0.33703500
C	-2.25531800	1.30800500	0.03447600
C	-3.20846700	2.12174800	0.63130700
C	-2.93937600	3.47263700	0.85971800
H	-1.48562700	5.04580900	0.64556000
H	0.21013500	3.59797200	-0.39885000
H	-2.46413700	0.26054900	-0.16913100
H	-4.16962300	1.69862400	0.91865400
H	-3.68666100	4.11340700	1.32367900
H	0.29451300	0.16303700	-0.12549300
C	-3.66055400	-2.23587700	-0.57198500
C	-2.30774500	-2.37515400	-0.86575400
C	-1.34410100	-2.32849100	0.14522100
C	-1.77481800	-2.12260000	1.45833100
C	-3.12630100	-1.97341000	1.76084000
C	-4.07845900	-2.03301700	0.74398700
H	-4.39714000	-2.26892900	-1.37366600
H	-1.94602400	-2.49355500	-1.88481800
H	-1.02672200	-2.05518000	2.24962700
H	-3.43880600	-1.79301900	2.78856900
H	-5.13511700	-1.90525000	0.97256500
C	0.13070600	-2.49711500	-0.20930000
H	0.69321600	-1.94806300	0.60317700
O	0.47203300	-2.15210800	-1.46504500
H	-0.24621800	-0.83147100	-1.86265700
H	2.96223300	2.64058400	-0.74699200
H	1.79491700	2.22699700	0.47694500
H	0.36063900	-3.57528700	0.03129100