

Supporting Information

Mechanism and Origin of Cyclization Selectivity for Ru(II)-Catalyzed *gem*- Hydrogenation of 1,3-Enynes: A DFT Study

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Table of Contents

Benchmark study for the different computational methods.....	S3
Fig. S2 Scan of $r(\text{Ru}\cdots\text{C}_{\text{sp}2})$ vs electronic energy E from complex A7 to intermediate A8	S4
Fig. S3 Scan of $r(\text{Ru}\cdots\text{C}_{\text{sp}2})$ vs electronic energy E from complex B7 to intermediate B8	S5
Fig. S4 Gibbs free energy profile for other possible pathways from A5 to A8 in Reaction A	S6
Fig. S5 Gibbs free energy profile for other possible pathways from B5 to B8 in Reaction B.....	S7
Fig. S6 Calculated the $\text{Ru}\cdots\text{H}^1$ distances in A5 and B5 using B3LYP and B3LYP-D3 methods.....	S8
Table S1 Corrected solution-phase Gibbs free energies in DCE of all species	S9
Cartesian coordinates of all calculated species (in angstrom)	S10

Benchmark study for the different computational methods

- █ PW6B95-D3BJ/def2-TZVPP//PW6B95-D3BJ/def2-SVP
- █ wB97XD-ultrafine/def2-TZVPP//wB97XD-ultrafine/def2-SVP
- █ M06-ultrafine/def2-TZVPP//M06-ultrafine/def2-SVP
- █ M06-D3/6-311++G(d,p)-SDD//B3LYP-D3/6-31G(d,p)-LANL2DZ
- █ M06/6-311++G(d,p)-SDD//B3LYP/6-31G(d,p)-LANL2DZ

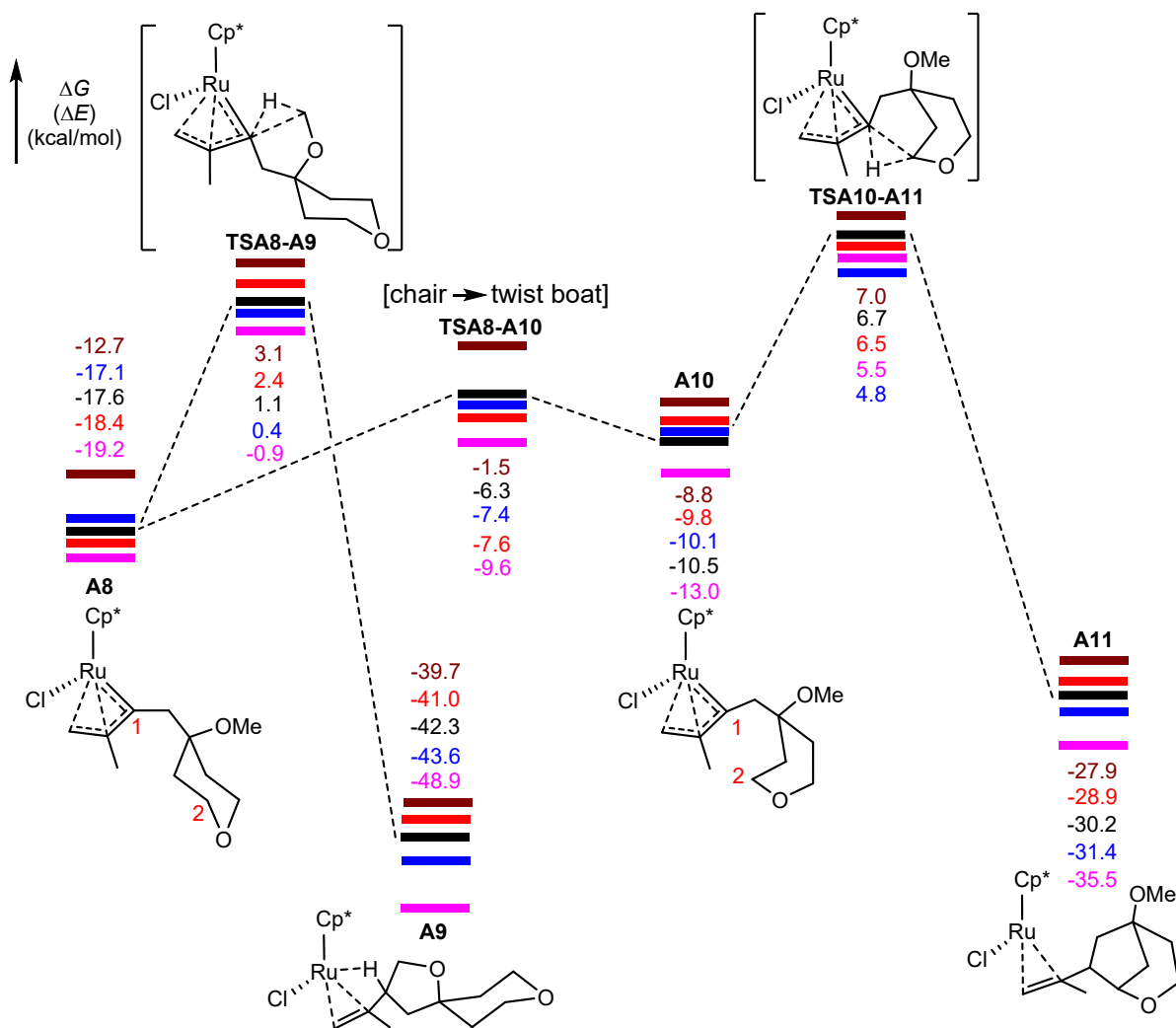


Figure S1. Calculated Gibbs free energy profile for cyclization processes in model reaction A using different computational methods. Full optimizations in dichloroethane solvent have been performed with SMD model.

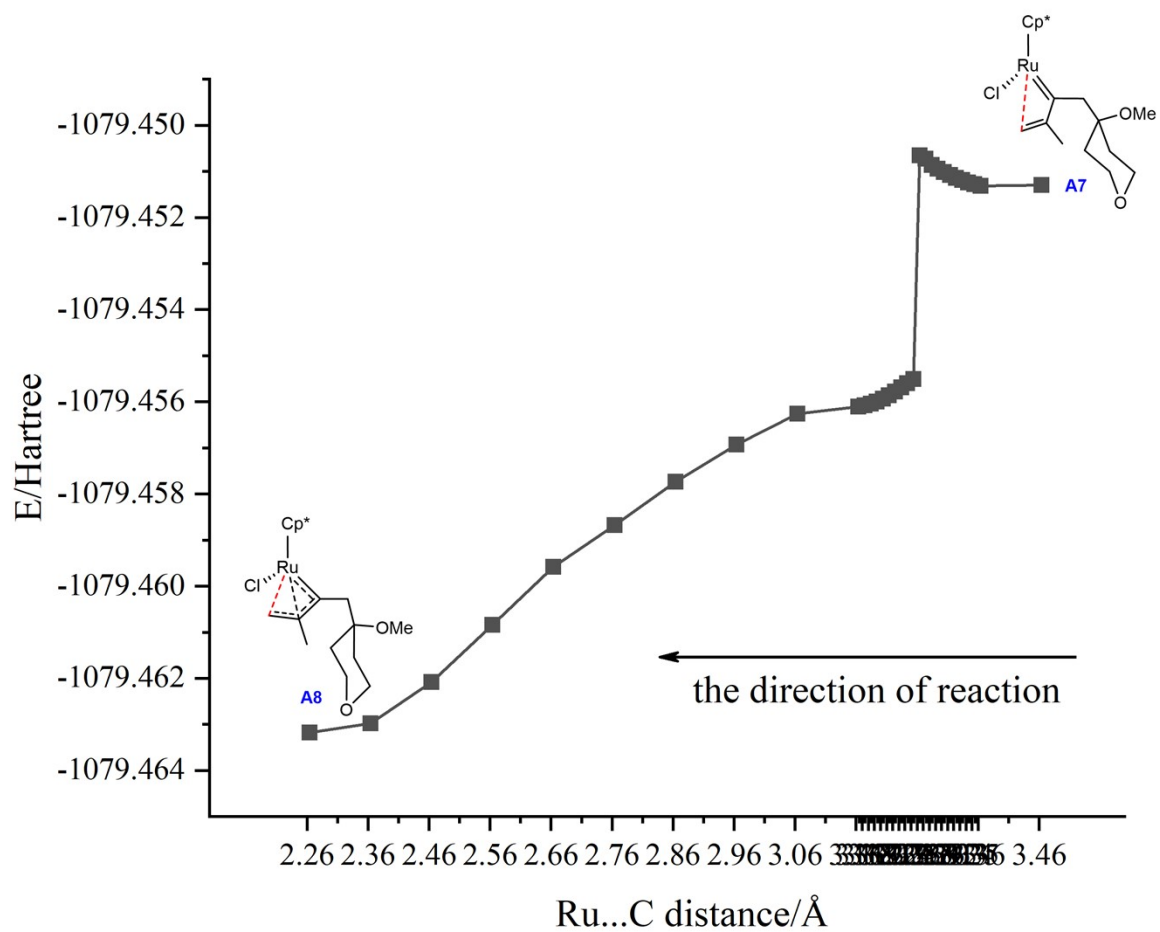


Figure S2. Scan of $r(\text{Ru}\cdots\text{C}_{\text{sp}2})$ vs electronic energy E from complex **A7** to intermediate **A8** in Reaction

A.

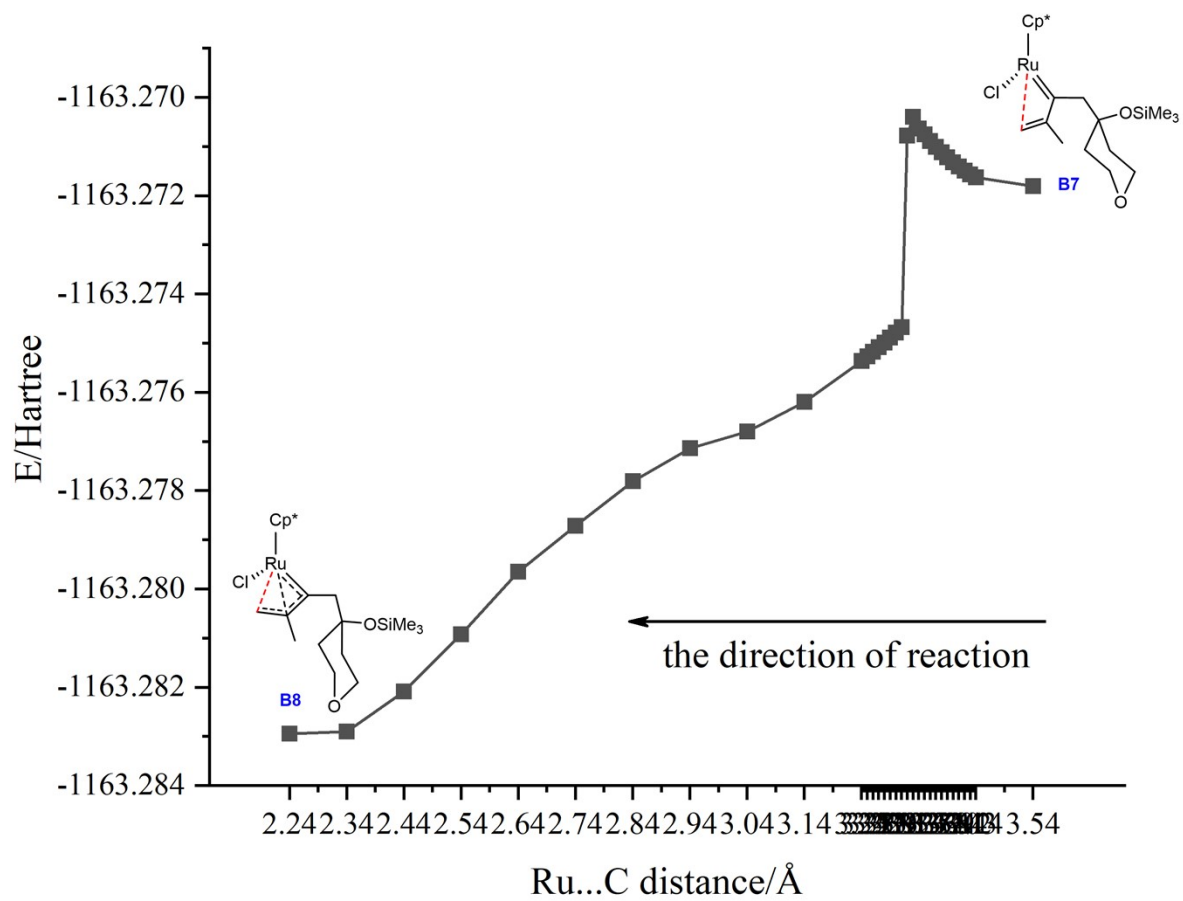


Figure S3. Scan of $r(\text{Ru}\cdots\text{C}_{\text{sp}^2})$ vs electronic energy E from complex **B7** to intermediate **B8** in Reaction

B.

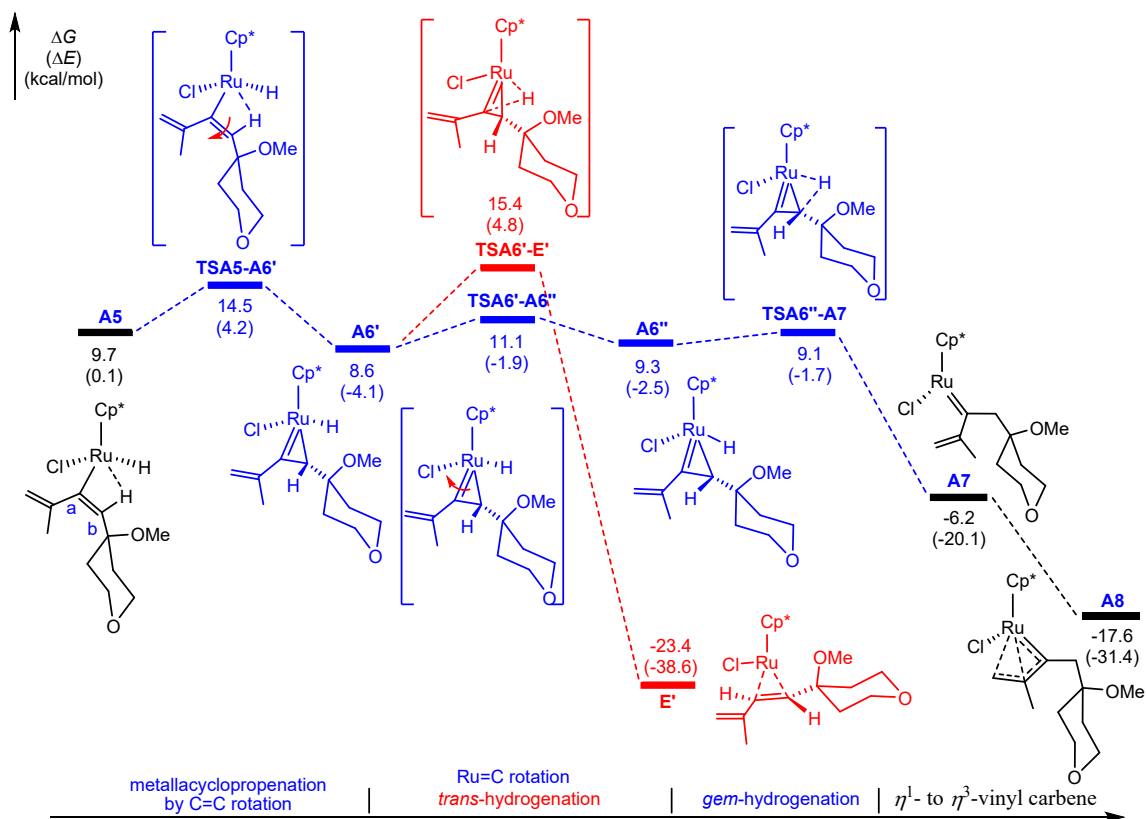


Figure S4. Calculated Gibbs energy profiles for *gem*-hydrogenation and *trans*-hydrogenation of the substrate 1,3-enyne from another metallacyclopropene intermediate **A6'** mediated by $[\text{Cp}^*\text{RuCl}]_4$ in Reaction A.

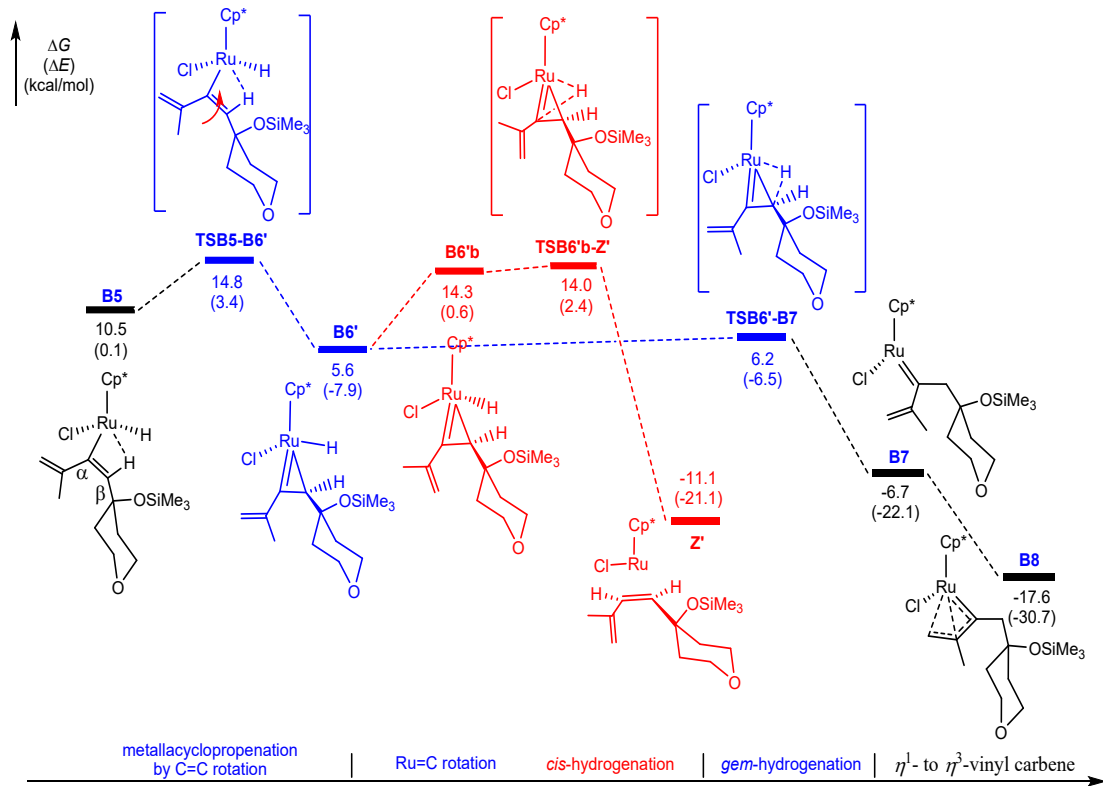


Figure S5. Calculated Gibbs energy profiles for *gem*-hydrogenation and *cis*-hydrogenation of the substrate 1,3-ene from another metallacyclopropane intermediate **B6'** mediated by $[\text{Cp}^*\text{RuCl}]_4$ in Reaction B.

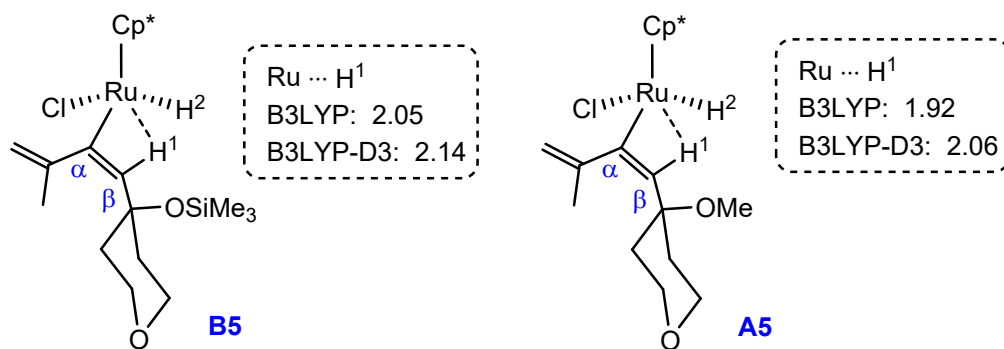


Figure S6. Calculated the Ru...H¹ distances in **A5** and **B5** using B3LYP and B3LYP-D3 methods, respectively.

Table S1. Calculated thermodynamic corrections solution-phase Gibbs free energies in DCE of all the intermediates and transition states (in Hartree).

species	ΔG_{sol}	species	ΔG_{sol}
H₂	-1.171212	B1	-1892.821194
A1	-1523.556811	B2	-1892.821222
A2	-1523.556745	B3	-1893.982529
A3	-1524.719068	TSB3-B4	-1893.967783
TSA3-A4	-1524.709537	B4	-1893.967643
A4	-1524.707847	TSB4-B5	-1893.96758
TSA4-A5	-1524.707109	B5	-1893.975697
A5	-1524.712529	TSB5-B6	-1893.970488
TSA5-A6	-1524.706311	B6	-1893.982923
A6	-1524.718391	TSB6-B7	-1893.980665
TSA6-A7	-1524.716971	B7	-1894.003127
A7	-1524.737863	B8	-1894.020465
A8	-1524.756023	TSB8-B9	-1893.969892
TSA8-A9	-1524.726274	B9	-1894.045234
A9	-1524.795473	TSB8-B10	-1894.001413
TSA8-A10	-1524.737989	B10	-1894.012906
A10	-1524.744759	TSB10-B11	-1893.980259
TSA10-A11	-1524.717287	B11	-1894.041168
A11	-1524.776201	TSB11-B12	-1894.035126
TSA11-A12	-1524.769662	B12	-1894.047646
A12	-1524.78326	B6b	-1893.97744
A6a	-1524.708872	TSB6b-E	-1893.968335
TS6a-Z	-1524.710295	E	-1894.033895
Z	-1524.749511	B8'	-1895.151728
A8'	-1525.898182	TSB5-B6'	-1893.968894
TSA5-A6'	-1524.704963	B6'	-1893.983447
A6'	-1524.714245	TSB6'-B7	-1893.982596
TSA6'-A6''	-1524.710277	B6'b	-1893.969582
A6''	-1524.713237	TSB6'b-Z'	-1893.970168
TSA6''-A7	-1524.713508	Z'	-1894.010052
TSA6'-E'	-1524.703536		
E'	-1524.765338		

**Cartesian coordinates of all calculated species
(in angstrom)**

H₂

H	0.00000000	0.00000000	0.37169200
H	0.00000000	0.00000000	-0.37169200

A1

C	-1.36413600	-1.31866600	-2.24057200
C	-0.56259000	-2.01104100	-1.30704900
C	-0.92455000	-3.37094300	-0.75610300
H	-0.48958900	-4.14689200	-1.39888700
H	-0.53891900	-3.52297700	0.25420000
H	-2.00819000	-3.51323200	-0.75507400
C	0.66709800	-1.41303100	-0.92939200
C	1.48020800	-0.64030200	-0.40790400
C	2.80911500	-0.12204300	0.03228800
O	2.69096900	0.99515200	0.91850100
C	2.34549900	2.25692300	0.34665100
H	2.13923700	2.92129700	1.19017000
H	3.17465400	2.68838900	-0.22875500
H	1.45879800	2.19473000	-0.29290500
C	3.70540500	0.17554600	-1.19724500
C	5.14138000	0.48080500	-0.76496900
C	4.95290600	-0.82228300	1.19006000
C	3.50689200	-1.21495700	0.88229700
H	5.78240700	0.59943400	-1.64385200
H	3.70518000	-0.71155500	-1.83889500
H	3.29564000	1.00022900	-1.78752700
H	5.46122800	-1.63579000	1.71701200
H	4.97217900	0.06893300	1.83479200
H	3.49421300	-2.15818200	0.32755900
H	2.94743200	-1.35688500	1.81264300
H	5.18029900	1.41823800	-0.18852800
O	5.70012700	-0.58515300	-0.00040400
C	-1.40312700	0.41093100	1.86192100
C	-2.13411300	-0.77805400	1.51512400
C	-3.10247100	-0.42132300	0.50635600
C	-2.93955100	0.97542000	0.20303600
C	-1.87526300	1.48799100	1.05269200
C	-1.46682600	2.92635600	1.15244800
H	-1.34871400	3.37208300	0.16151400

H	-2.22682800	3.50375000	1.69526400
H	-0.52163400	3.03623700	1.68972500
C	-0.34952000	0.50446300	2.92386300
H	0.44841100	1.19549100	2.64427000
H	-0.79346000	0.86338000	3.86187800
H	0.10328100	-0.46914300	3.12592800
C	-3.82501200	1.80806300	-0.67332400
H	-3.26066500	2.60873600	-1.15639700
H	-4.29487500	1.20684600	-1.45639900
H	-4.62668000	2.26889500	-0.08042400
C	-4.19109500	-1.30586800	-0.02400200
H	-5.09055000	-1.20172500	0.59721700
H	-4.46702800	-1.03867300	-1.04706800
H	-3.90657300	-2.36071200	-0.01061200
C	-2.05161800	-2.08669400	2.24460100
H	-1.01962500	-2.35547800	2.48763600
H	-2.60368200	-2.02601400	3.19184900
H	-2.48785100	-2.90277000	1.66571700
Ru	-1.11713700	-0.05769900	-0.38631800
Cl	-0.45298500	1.70563200	-2.05395100
H	-0.92770400	-0.66773100	-2.98776700
H	-2.33617900	-1.74364400	-2.47857100

A2

C	-0.17540000	3.42502200	-1.42513300
H	-0.23480000	4.50554800	-1.52525800
H	0.07044700	2.85408900	-2.31504800
C	-0.43400500	2.82598900	-0.25009000
C	-0.79592700	3.60602600	0.99459200
H	-1.83721600	3.41834700	1.27934300
H	-0.17671400	3.30703200	1.84639100
H	-0.66949000	4.68011300	0.83202100
C	-0.44547600	1.37226700	-0.13596000
C	-1.14986100	0.31528200	0.06443800
C	-2.59249600	-0.13269400	0.19538500
O	-2.83660500	-0.62038400	1.52723900
C	-2.24682600	-1.85600000	1.91084500
H	-2.48695400	-1.98762200	2.97028000
H	-2.65371500	-2.70966900	1.35450800
H	-1.15865500	-1.84687400	1.78649600
C	-3.02333900	-1.13869700	-0.89340700
C	-4.52610400	-1.41261500	-0.83208300

C	-4.99593400	0.69795200	0.09204400	C	-2.48097600	-0.19578300	-0.22279400
C	-3.52047200	1.10261000	0.09088200	C	-2.74916900	-1.23691800	0.88483000
H	-4.82632200	-2.06025100	-1.66194600	C	-3.62017400	0.85351500	-0.17858600
H	-2.77588300	-0.70707900	-1.87006800	C	-4.17300000	-1.79123600	0.78816500
H	-2.45819900	-2.06721900	-0.80743300	C	-4.98939600	0.17352800	-0.22564300
H	-5.63046800	1.57482900	-0.07330800	H	-4.38047200	-2.45487800	1.63340000
H	-5.26460900	0.26058800	1.06570100	H	-4.28953300	-2.37129700	-0.13936800
H	-3.29057100	1.64075100	-0.83428900	H	-5.78636700	0.91542800	-0.11464100
H	-3.32452500	1.77288600	0.93354200	H	-5.13125600	-0.33491800	-1.19200400
H	-4.78297200	-1.92781800	0.10735700	O	-2.50098600	-0.95302900	-1.44276900
O	-5.29677700	-0.21894900	-0.95633500	C	-2.41616800	-0.21031400	-2.65946100
C	2.50991200	-0.09141200	1.35118700	H	-3.35663300	0.30346900	-2.89452400
C	2.55594900	1.09786500	0.53243700	H	-1.59805600	0.51920900	-2.63866600
C	2.77770200	0.68801400	-0.82772400	H	-2.21492700	-0.93988300	-3.44864000
C	2.92626300	-0.74689200	-0.84474200	C	-0.22368600	2.88295200	0.55432800
C	2.79768600	-1.21697100	0.50481100	C	0.76116600	3.63210400	0.02930200
C	2.97712200	-2.62819500	0.96796300	C	-1.19651300	3.43703700	1.57672900
H	2.69597900	-3.34320100	0.19363600	H	-2.22444900	3.40601900	1.19770800
H	4.03117300	-2.79763200	1.22623500	H	-1.18006800	2.84880900	2.50164900
H	2.37892800	-2.84086000	1.85734400	H	-0.95199100	4.47439800	1.82218800
C	2.37081500	-0.12458500	2.84173900	H	1.43872300	3.22931000	-0.71539300
H	1.92969300	-1.06455700	3.18187300	H	0.87756800	4.67188100	0.32208900
H	3.35714600	-0.02878000	3.31572300	O	-5.15136700	-0.75468900	0.84379500
H	1.74641400	0.69498600	3.20545500	Ru	0.92540900	-0.21934200	-0.38774300
C	3.27498200	-1.57732200	-2.03971200	C	1.43313200	-0.84459400	1.70663700
H	2.80536500	-2.56178200	-1.98575300	C	2.31654300	0.25244600	1.35683200
H	2.94993900	-1.09783500	-2.96671500	C	1.69709100	-1.92136000	0.80284900
H	4.36194100	-1.72057000	-2.10059700	C	3.13557500	-0.16944600	0.25985100
C	2.97595600	1.59116600	-2.00510000	C	2.73988100	-1.49339900	-0.11730900
H	4.04900300	1.74488800	-2.18125800	C	4.24406000	0.61857600	-0.36562400
H	2.55230000	1.16117000	-2.91666900	H	5.20994300	0.29229900	0.04235700
H	2.52100800	2.56968600	-1.84339100	H	4.27523600	0.47770600	-1.44839000
C	2.59110400	2.50303500	1.04748600	H	4.14227500	1.68716800	-0.16420800
H	2.04819800	2.60473000	1.98931600	C	3.42108400	-2.35104600	-1.14434600
H	3.63454200	2.78668400	1.23858100	H	3.80069900	-1.75168900	-1.97607200
H	2.18149900	3.21737800	0.33135800	H	4.27534800	-2.88003000	-0.70099500
Ru	0.87579900	-0.23799000	-0.11312600	H	2.74484300	-3.10548900	-1.55490100
Cl	0.09879600	-2.50851800	-0.78013200	C	1.11046900	-3.30137800	0.86209400
A3				H	1.74064600	-3.95206100	1.48267000
C	-0.45020000	1.50317000	0.17913200	H	0.10857700	-3.29816200	1.29822500
C	-1.15419500	0.48244400	-0.03294600	H	1.04748600	-3.75605300	-0.12983400

C	0.53338500	-0.87639000	2.90551600
H	1.12239100	-1.04138700	3.81725700
H	-0.00402600	0.06735300	3.03281900
H	-0.20314100	-1.68023100	2.83836200
C	2.52131700	1.49511500	2.17002900
H	1.63148600	1.75480200	2.74760400
H	3.34182000	1.33665500	2.88293200
H	2.78201100	2.35576900	1.55042200
Cl	1.29551300	1.13307200	-2.49510100
H	-2.02342800	-2.05224000	0.79960900
H	-2.61069200	-0.75750400	1.85894800
H	-3.53057700	1.41319700	0.75784400
H	-3.52114200	1.57257400	-0.99727200
H	0.43834700	-1.28477900	-1.71435100
H	-0.25489900	-1.24899200	-1.26516500

TSA3-A4

C	-0.49256900	1.44691700	0.07676000
C	-1.24285400	0.46622700	-0.14013300
C	-2.58618000	-0.18994300	-0.27408800
C	-2.89346600	-1.06922400	0.95943900
C	-3.68034400	0.90643300	-0.36238700
C	-4.33723600	-1.57475400	0.92493500
C	-5.07701100	0.28274500	-0.32344800
H	-4.56854000	-2.12279400	1.84361000
H	-4.47698800	-2.25815100	0.07437000
H	-5.84169100	1.06554400	-0.30234500
H	-5.24489400	-0.33282500	-1.22076700
O	-2.63971800	-1.08883600	-1.38236500
C	-2.44705900	-0.52386700	-2.67712800
H	-3.31858200	0.05368700	-3.01157600
H	-1.55294200	0.10925700	-2.72000700
H	-2.31076100	-1.36710100	-3.35982800
C	-0.19115100	2.82099300	0.42565000
C	0.83412700	3.50312700	-0.11193000
C	-1.14356400	3.44511600	1.42569300
H	-2.16706900	3.46036900	1.03388700
H	-1.16757600	2.87378900	2.36075000
H	-0.84693000	4.47282500	1.65319100
H	1.49097700	3.04897600	-0.84533800
H	1.00349700	4.54206900	0.15671200
O	-5.27251600	-0.50130300	0.85129300

Ru	0.85429200	-0.35344100	-0.31568600
C	1.54680400	-1.07852500	1.70344700
C	2.24523300	0.18010500	1.58476700
C	2.03520300	-1.95287500	0.65326800
C	3.06676700	0.12074900	0.43007400
C	2.93480000	-1.19788100	-0.16621300
C	3.98708800	1.18738800	-0.07604100
H	5.02997800	0.92289300	0.14252000
H	3.89375500	1.30263800	-1.15959900
H	3.78395600	2.15361700	0.39084400
C	3.76058900	-1.70504700	-1.30942400
H	3.83409700	-0.95638400	-2.10223000
H	4.77948200	-1.94111500	-0.97497700
H	3.33275000	-2.61293500	-1.74155400
C	1.75828900	-3.42446800	0.54066100
H	2.48318200	-3.98465900	1.14535200
H	0.75929600	-3.68031100	0.90177300
H	1.84538400	-3.77456800	-0.49040600
C	0.70693800	-1.49685800	2.87484500
H	1.34710200	-1.81342100	3.70910300
H	0.08018300	-0.67807400	3.23800000
H	0.05483200	-2.33628700	2.62327500
C	2.15763500	1.31178500	2.56218300
H	1.19229700	1.32713700	3.07382400
H	2.93233300	1.20151500	3.33267300
H	2.30406300	2.28149200	2.08201800
Cl	1.27450400	0.86106800	-2.49556200
H	-2.20177600	-1.91770200	0.98350900
H	-2.73736200	-0.47536100	1.86574800
H	-3.56315000	1.57981600	0.49269300
H	-3.55676500	1.50653000	-1.26906800
H	0.34917400	-1.36373800	-1.42541500
H	-0.28165900	-1.43357700	-0.18337100

A4

C	-0.54885200	1.43494000	0.06588200
C	-1.28867100	0.43737800	-0.10714700
C	-2.62578800	-0.24046200	-0.19484500
C	-2.88480300	-1.12262000	1.04763900
C	-3.73087900	0.84919700	-0.24141900
C	-4.32653700	-1.63542400	1.06536500
C	-5.12085400	0.21573700	-0.15718300

H	-4.52153400	-2.18401100	1.99207700
H	-4.49213000	-2.32026300	0.22068500
H	-5.88991600	0.99322000	-0.11188200
H	-5.31391200	-0.40219900	-1.04779700
O	-2.71364100	-1.13774000	-1.30106000
C	-2.59163200	-0.56830600	-2.60280800
H	-3.48591700	-0.00209000	-2.89454100
H	-1.70645700	0.07241600	-2.68626700
H	-2.47840800	-1.40969300	-3.29206100
C	-0.25501900	2.82856700	0.33697000
C	0.68841300	3.50780200	-0.33673500
C	-1.11127000	3.47095800	1.40815600
H	-2.17126800	3.44421700	1.13013800
H	-1.01775000	2.93922600	2.36201800
H	-0.82137300	4.51417600	1.56193400
H	1.27909200	3.03141600	-1.11156000
H	0.85881400	4.56177000	-0.13582200
O	-5.27092400	-0.56813300	1.02396900
Ru	0.81946600	-0.34852700	-0.23770300
C	2.50084300	0.43351300	1.35857100
C	3.12709400	0.24337200	0.10513700
C	1.84356400	-0.80155100	1.71584900
C	2.92536500	-1.13969400	-0.31543500
C	2.18460700	-1.79858500	0.71001800
C	3.57958600	-1.76929000	-1.50694300
H	4.64058900	-1.96501000	-1.30272600
H	3.10792600	-2.72027000	-1.76538900
H	3.51912000	-1.11317900	-2.37871200
C	1.93381300	-3.27386200	0.82531400
H	1.85671900	-3.74962700	-0.15480200
H	2.76287100	-3.74986800	1.36501000
H	1.01475900	-3.48550900	1.37677700
C	1.19908200	-1.08513900	3.04097700
H	1.96678400	-1.30036900	3.79585600
H	0.61691100	-0.23183600	3.39883300
H	0.53399900	-1.95013400	2.98712900
C	2.53189500	1.66934400	2.20374600
H	3.38498300	1.63228100	2.89413500
H	2.62996900	2.57614500	1.60329000
H	1.62815700	1.76259100	2.81097800
C	3.93797700	1.23980900	-0.66024700

H	3.88013100	2.23621700	-0.21735500
H	4.99303400	0.93821300	-0.67374400
H	3.59375400	1.29974600	-1.69749600
Cl	1.04670300	0.61569700	-2.57504200
H	-2.19105500	-1.96991600	1.04337000
H	-2.69605100	-0.53033900	1.94908800
H	-3.58981300	1.51951600	0.61239000
H	-3.64233800	1.45409400	-1.14893200
H	0.17365900	-1.48986100	-1.11342600
H	-0.20488700	-1.25981700	0.51497900

TSA4-A5

C	-0.55896300	1.36907800	-0.05826000
C	-1.26854200	0.32353400	-0.11375400
C	-2.60414800	-0.37485600	-0.13429000
C	-2.93237800	-0.95065900	1.26253900
C	-3.71416600	0.63748900	-0.51089000
C	-4.36375300	-1.49073900	1.30886100
C	-5.09617900	-0.00369800	-0.36797600
H	-4.61632900	-1.80921000	2.32490600
H	-4.45987000	-2.36100200	0.64285800
H	-5.87848000	0.73763000	-0.55776200
H	-5.21690900	-0.81954400	-1.09724400
O	-2.59038100	-1.50783900	-1.00153400
C	-2.39040800	-1.24723900	-2.39053400
H	-3.28781700	-0.82899600	-2.86403500
H	-1.54144200	-0.57603200	-2.56385800
H	-2.17476700	-2.21382400	-2.85388300
C	-0.41665700	2.80411700	0.10866700
C	0.53045200	3.51204000	-0.53011800
C	-1.41299400	3.45611800	1.04568300
H	-2.43516500	3.35896900	0.66302700
H	-1.39467300	2.98639800	2.03566500
H	-1.19217600	4.52069000	1.16380000
H	1.22629000	3.03516100	-1.21130400
H	0.59391200	4.58888300	-0.40140200
O	-5.31647300	-0.49139400	0.95323700
Ru	0.90772500	-0.27930300	-0.31723900
C	2.39077600	0.60780900	1.37989900
C	3.15100500	0.32703300	0.21576000
C	1.69840200	-0.60214000	1.76315000
C	2.98204900	-1.07492700	-0.12190400

C	2.12778200	-1.66223700	0.87497000	C	-2.50045700	-2.07691900	-1.82082900
C	3.76658200	-1.80078400	-1.17468000	H	-3.33721000	-1.79653300	-2.47373200
H	4.77712500	-2.02911700	-0.81060800	H	-1.59987700	-1.54441100	-2.14824200
H	3.29080800	-2.74479800	-1.45062600	H	-2.32838800	-3.15191900	-1.92553900
H	3.86959500	-1.19841200	-2.08080900	C	-0.68040100	2.45466200	-0.11756400
C	1.85594800	-3.12736500	1.05838600	C	-0.11051300	3.20623100	-1.07797600
H	1.88099600	-3.66474200	0.10781900	C	-1.47485800	3.07916000	1.01244800
H	2.61888300	-3.56911100	1.71265700	H	-2.50610400	2.71056600	1.03240200
H	0.88148700	-3.30439100	1.51978600	H	-1.03270000	2.83346400	1.98476600
C	0.89178900	-0.77599200	3.01648600	H	-1.50228100	4.16820400	0.91322600
H	1.55402500	-0.86853100	3.88713000	H	0.46832400	2.75014300	-1.87404500
H	0.23180300	0.07706000	3.19640700	H	-0.24452200	4.28460600	-1.09151200
H	0.27553300	-1.67699300	2.97481500	O	-5.50927300	0.10714500	0.64527500
C	2.35912200	1.90031900	2.13612200	Ru	1.08756300	-0.37103300	-0.26734600
H	3.18079000	1.92491700	2.86430800	C	2.32610400	0.83186200	1.34506100
H	2.47324800	2.76457100	1.47809800	C	3.01733300	0.71561600	0.09527900
H	1.42799600	2.01878800	2.69508600	C	2.05551600	-0.49013100	1.83241400
C	4.03123800	1.27684700	-0.53606900	C	3.23893700	-0.69560700	-0.16608600
H	3.93877600	2.29738100	-0.15809800	C	2.65149400	-1.43715000	0.92396500
H	5.08267500	0.97736100	-0.44279400	C	4.09990100	-1.23948400	-1.26611600
H	3.77975800	1.27999800	-1.60103700	H	5.16172600	-1.13480600	-1.00664000
Cl	1.09046100	0.65745300	-2.65755600	H	3.90059300	-2.29872500	-1.44497000
H	-2.22285600	-1.75002100	1.50267200	H	3.92858200	-0.70272200	-2.20208200
H	-2.81763300	-0.15620000	2.00673800	C	2.76889600	-2.91478900	1.16261800
H	-3.64584200	1.49308200	0.16741200	H	2.95950100	-3.45695900	0.23412500
H	-3.57144400	1.01379800	-1.52833900	H	3.60190800	-3.11903000	1.84796400
H	0.55703000	-1.49591900	-1.25904000	H	1.86296200	-3.32810900	1.61337400
H	-0.37653500	-1.12294900	0.09428900	C	1.37200000	-0.82081600	3.12520100
A5				H	2.07370500	-0.73666900	3.96510700
C	-0.51632400	1.00629100	-0.08051800	H	0.53881500	-0.14126000	3.32565800
C	-1.24640700	-0.07462100	0.07285000	H	0.98347300	-1.84207000	3.12242700
C	-2.71867500	-0.49912000	0.02833500	C	2.02291700	2.11174700	2.05987000
C	-3.29855500	-0.55514200	1.45845700	H	2.91190600	2.44034000	2.61434700
C	-3.57931200	0.46088700	-0.81837400	H	1.75626400	2.91261100	1.36642300
C	-4.80105100	-0.84835000	1.43160500	H	1.21359300	1.99216900	2.78343500
C	-5.06317300	0.10226100	-0.70924100	C	3.56817600	1.84356800	-0.72164200
H	-5.22046600	-0.78885800	2.44076800	H	3.01854300	2.77191000	-0.54791400
H	-4.97870300	-1.86332300	1.04546400	H	4.61926300	2.02353000	-0.45899600
H	-5.67280400	0.84207000	-1.23717700	H	3.52275600	1.61734400	-1.78926400
H	-5.25420300	-0.88188500	-1.16476300	Cl	0.89141900	0.15429600	-2.72470100
O	-2.79640700	-1.85201300	-0.44258200	H	-2.77621700	-1.32871000	2.03259200

H	-3.12326100	0.40769000	1.94905900
H	-3.43334400	1.48009800	-0.45109300
H	-3.26121500	0.44865100	-1.86532600
H	1.04088800	-1.80675100	-0.95345400
H	-0.64223200	-1.06021400	0.20667700

TSA5-A6

C	-0.53820600	0.86861400	-0.31106000
C	-1.31736300	-0.19124600	-0.51512700
C	-2.80513400	-0.50629600	-0.31266700
C	-3.11454400	-0.81430500	1.16901800
C	-3.72274600	0.64082000	-0.78759600
C	-4.61518300	-1.01789700	1.39142000
C	-5.18489800	0.33863000	-0.45036000
H	-4.83291100	-1.13125200	2.45829800
H	-4.95227200	-1.92807300	0.87362800
H	-5.82057300	1.19167700	-0.70740400
H	-5.53599600	-0.53277700	-1.02471300
O	-3.11143000	-1.73697800	-0.99201900
C	-3.04299800	-1.72688800	-2.41303300
H	-3.89204800	-1.20372300	-2.87193400
H	-2.11248300	-1.27631100	-2.78188800
H	-3.07127200	-2.77317700	-2.73051000
C	-0.75440500	2.28050100	0.02025300
C	-0.38422700	3.24956900	-0.83587700
C	-1.36161300	2.60617800	1.36987800
H	-2.41155700	2.29907400	1.42181000
H	-0.84092400	2.08080200	2.17642500
H	-1.31160300	3.68084200	1.56828300
H	0.06429300	3.01856800	-1.79734900
H	-0.53998600	4.29777500	-0.59483200
O	-5.36852500	0.10792400	0.94511400
Ru	1.14154400	-0.36000600	-0.22305000
C	2.35615200	0.90067800	1.37932400
C	3.08536500	0.66046200	0.16660300
C	2.02348000	-0.36713100	1.95473200
C	3.28687100	-0.77053600	0.03337000
C	2.61807700	-1.40074900	1.14283400
C	4.17502700	-1.42669400	-0.98074700
H	5.23008500	-1.30930000	-0.70045400
H	3.96636800	-2.49609300	-1.06434300
H	4.03707200	-0.98040900	-1.96836200

C	2.66324100	-2.85759800	1.50166100
H	2.87077700	-3.48033500	0.62892400
H	3.45621800	-3.03858800	2.23909600
H	1.72236200	-3.19707900	1.94257000
C	1.29713000	-0.59570100	3.24575500
H	2.01038600	-0.66614400	4.07744600
H	0.60594000	0.21970600	3.47280700
H	0.72786500	-1.52878200	3.22494700
C	2.10298800	2.25360300	1.96841000
H	3.04615700	2.66851700	2.34684700
H	1.71437500	2.95735300	1.22667800
H	1.40360900	2.21053900	2.80499600
C	3.70483500	1.71102100	-0.70279700
H	3.11319800	2.63039900	-0.70397100
H	4.70976200	1.95945000	-0.33547300
H	3.79730300	1.36564300	-1.73419000
Cl	1.20703200	-0.02259100	-2.70597900
H	-2.56581300	-1.71290100	1.47331300
H	-2.76583400	0.02044300	1.78368400
H	-3.42658600	1.56766100	-0.29097700
H	-3.61039800	0.80772200	-1.86339400
H	1.18430000	-1.83688300	-0.77700000
H	-0.78957400	-1.12268700	-0.84592600

A6

C	0.61843500	3.46130400	-0.61233600
H	0.57506300	4.54721200	-0.61097200
H	1.58825100	2.99952800	-0.75290800
C	-0.50336300	2.71580400	-0.49621500
C	-1.86245600	3.37591900	-0.39008000
H	-2.49599800	3.10359000	-1.24078300
H	-2.39193900	3.07626300	0.51962000
H	-1.76015400	4.46453800	-0.37694000
C	-0.39496600	1.27471100	-0.61018900
C	-1.19482900	0.17087200	-0.95040100
C	-2.45631000	-0.37562500	-0.26023200
O	-2.41352400	-1.81637900	-0.21579400
C	-2.46922700	-2.53490200	-1.44053400
H	-2.29397200	-3.58391100	-1.18500700
H	-3.44831800	-2.45972700	-1.93146400
H	-1.69437100	-2.22344500	-2.15158100
C	-3.70774000	0.12031400	-1.02739300

C	-4.99743800	-0.31402700	-0.32927800
C	-3.95840300	-0.37842700	1.78298400
C	-2.59695500	0.03018800	1.21451500
H	-5.86934700	0.11646000	-0.83198500
H	-3.68093900	1.21319500	-1.06650700
H	-3.69846400	-0.23543000	-2.06328200
H	-4.08213500	0.01231100	2.79794600
H	-4.03045500	-1.47543700	1.82890800
H	-2.47896700	1.11371700	1.30499200
H	-1.80551600	-0.44503500	1.79815500
H	-5.09815000	-1.41049400	-0.35445000
O	-5.04113800	0.14892100	1.01829300
C	1.44681600	-0.63540100	1.79239900
C	1.96944300	0.69761400	1.55606000
C	2.97938600	0.60519000	0.55687400
C	3.10635100	-0.79134200	0.19239900
C	2.20578800	-1.55584500	0.97837100
C	2.12178300	-3.05428700	1.04314800
H	2.36185400	-3.51787400	0.08294500
H	2.83337400	-3.44432000	1.78353800
H	1.12469000	-3.38973300	1.33881500
C	0.56645000	-1.03669200	2.94034700
H	-0.06168200	-1.89655600	2.69247000
H	1.18391400	-1.32147600	3.80367000
H	-0.08281900	-0.21955200	3.26242100
C	4.12203400	-1.32731900	-0.76951900
H	3.86176600	-2.33076700	-1.11377400
H	4.21924800	-0.68447300	-1.64739900
H	5.10601100	-1.38533000	-0.28519200
C	3.89678500	1.69012900	0.07129600
H	4.90345700	1.55863300	0.49033900
H	4.00078600	1.68023200	-1.01839500
H	3.54965700	2.68184000	0.37013000
C	1.60711500	1.90961800	2.36158900
H	0.55057800	1.90937500	2.64111800
H	2.19068300	1.93145300	3.29140900
H	1.81036500	2.83771000	1.82307500
Ru	0.88694300	-0.13085100	-0.35497300
Cl	1.39914800	-0.40234400	-2.76762200
H	0.12212400	-1.48590800	-0.56077600
H	-1.17451500	-0.08641100	-2.01260400

TSA6-A7

C	0.27111900	3.40719500	0.57750200
H	0.14198100	4.38835000	1.02711500
H	1.26833500	3.13158700	0.25208400
C	-0.78152400	2.58165500	0.38435100
C	-2.18227900	3.00494300	0.77280500
H	-2.81509300	3.12455800	-0.11313300
H	-2.66507000	2.26790900	1.42217800
H	-2.15983300	3.96045600	1.30392200
C	-0.54711600	1.32517200	-0.30337400
C	-1.25205400	0.43070300	-1.16022900
C	-2.49990300	-0.42687600	-0.86948600
O	-2.38035100	-1.69720600	-1.54320100
C	-2.40959300	-1.71793700	-2.96548200
H	-2.18511300	-2.74798900	-3.25615200
H	-3.39410100	-1.45193500	-3.37089400
H	-1.65356000	-1.06331000	-3.41660100
C	-3.76843800	0.33203300	-1.32602000
C	-5.03638000	-0.44786900	-0.97052200
C	-4.00139200	-1.50808700	0.85978900
C	-2.66408200	-0.80770600	0.60812700
H	-5.92720600	0.13841000	-1.21716100
H	-3.79825500	1.29834300	-0.81582700
H	-3.73948200	0.53905400	-2.40096200
H	-4.14778900	-1.68094800	1.93060600
H	-4.01366300	-2.48348800	0.35104900
H	-2.60596500	0.09640000	1.22215800
H	-1.84616500	-1.46862500	0.90239100
H	-5.08042700	-1.38940100	-1.53989400
O	-5.10807200	-0.71886800	0.42707200
C	1.32654200	-1.20094200	1.26773600
C	1.94586400	0.09571100	1.45245000
C	2.91492400	0.26297500	0.42713300
C	2.96965700	-0.97977200	-0.33912900
C	2.02115500	-1.87780900	0.19052000
C	1.78189300	-3.29999300	-0.22957100
H	2.07732100	-3.47208600	-1.26751900
H	2.35952800	-3.99133200	0.39860300
H	0.72828200	-3.57533600	-0.13262900
C	0.42390000	-1.87581700	2.25962200
H	-0.17187200	-2.66504900	1.79458100

H	1.02340500	-2.34619200	3.05139000
H	-0.25724200	-1.17144800	2.74308600
C	3.94212300	-1.23930300	-1.44919400
H	3.73756500	-2.18757500	-1.95223900
H	3.90461000	-0.44446100	-2.19967000
H	4.96640700	-1.28410100	-1.05699800
C	3.87436200	1.40348000	0.25537900
H	4.85905000	1.15263500	0.67301700
H	4.02138000	1.64451000	-0.80167700
H	3.52405400	2.30667900	0.76173200
C	1.69926000	1.00473300	2.61962800
H	0.65985300	0.96612500	2.95566600
H	2.32657300	0.69933900	3.46805000
H	1.94104100	2.04532300	2.39196000
Ru	0.82834200	0.04848200	-0.58343800
Cl	1.47887600	0.82429800	-2.84337700
H	-0.16731100	-0.89953900	-1.40106200
H	-1.21809500	0.73152000	-2.21187600

A7

C	-0.35915500	1.19244700	-2.77807800
H	-0.52846100	1.81046700	-3.65697700
H	0.04014500	0.19588600	-2.93495400
C	-0.68693500	1.62703300	-1.54301900
C	-1.26543500	3.01595200	-1.34240800
H	-2.32037300	2.98486600	-1.05239400
H	-0.73277000	3.55868300	-0.55335900
H	-1.18800100	3.59787300	-2.26506700
C	-0.48429900	0.73830000	-0.38510100
C	-1.50521800	0.76789100	0.74467000
C	-2.87582800	0.02805900	0.57176900
O	-3.58928300	0.15798100	1.82135300
C	-4.15740300	1.41579800	2.15110800
H	-4.51303400	1.32926800	3.18226200
H	-3.43140300	2.23889500	2.11055900
H	-5.01423200	1.67728300	1.51594500
C	-2.66433800	-1.48760800	0.42447200
C	-3.98264700	-2.22290700	0.18083300
C	-4.98095000	-0.33045200	-0.79834400
C	-3.72000300	0.52004200	-0.61876100
H	-3.79898000	-3.28276700	-0.02109700
H	-1.97905000	-1.67760300	-0.40646300

H	-2.19251200	-1.87577900	1.33548200
H	-5.51939700	-0.02732700	-1.70198100
H	-5.65978200	-0.19760000	0.05932300
H	-3.11655200	0.44744600	-1.52857800
H	-4.00126500	1.57160500	-0.50068500
H	-4.62845800	-2.15003700	1.06924000
O	-4.66869900	-1.71054600	-0.96107100
C	2.33081300	0.95899700	1.31218600
C	2.51934600	1.35336800	-0.05744400
C	3.05527900	0.20772400	-0.75704700
C	3.41527800	-0.80216500	0.23943000
C	2.94218000	-0.36641000	1.47961200
C	3.00875900	-1.08718200	2.79182300
H	3.24979800	-2.14514000	2.66571900
H	3.77652600	-0.64067600	3.43729300
H	2.05866100	-1.01786300	3.33143000
C	1.89210000	1.83733100	2.44736000
H	1.35755600	1.26698400	3.21310600
H	2.75616500	2.30783000	2.93646000
H	1.23144900	2.63721700	2.10295900
C	4.07612400	-2.10589400	-0.08814300
H	4.20123400	-2.72869800	0.80102700
H	3.48685800	-2.67336900	-0.81651400
H	5.06985900	-1.93835900	-0.52161000
C	3.48825800	0.17984900	-2.19089100
H	4.53287400	0.50964900	-2.28057800
H	3.42453900	-0.82858600	-2.60737500
H	2.87685300	0.84321600	-2.80728800
C	2.34851400	2.72416800	-0.63678200
H	1.67384500	3.33774300	-0.03486000
H	3.31971900	3.23588700	-0.66834600
H	1.96129600	2.69323900	-1.65856200
Ru	1.06998600	-0.27900800	0.01327300
Cl	0.64713400	-2.44059900	-1.10141300
H	-1.71516000	1.81887500	0.98619800
H	-1.06139600	0.32191800	1.64396800

A8

C	-0.64720500	0.25863800	-0.20260700
C	-1.73154600	0.39649300	0.80511100
C	-3.16888700	-0.10501100	0.43617700
C	-4.13009300	0.32085100	1.56691400

C	-3.69318400	0.49085400	-0.88552500	H	2.15644300	3.36911200	-0.47687800
C	-5.58291300	-0.00454200	1.21877300	H	1.18658400	3.28146300	1.00102400
C	-5.17164800	0.15647700	-1.09657700	C	4.22093500	1.46475400	-1.25316400
H	-6.25887000	0.38588600	1.98615600	H	3.60239000	2.10994000	-1.88425800
H	-5.72192700	-1.09457200	1.16275100	H	5.02631300	2.08870200	-0.84314700
H	-5.55364800	0.66014500	-1.99013600	H	4.68139400	0.71196100	-1.89782900
H	-5.29957100	-0.92819400	-1.23882300	Cl	1.26061900	-2.44673200	-1.13814000
O	-3.23494200	-1.53588800	0.45527300	H	-3.84737300	-0.18976800	2.49460300
C	-2.57686000	-2.25294400	-0.57906800	H	-4.03407700	1.39956700	1.73187000
H	-3.02913200	-2.08710900	-1.56594800	H	-3.57801000	1.57974100	-0.84186700
H	-1.50440400	-2.02182300	-0.63611000	H	-3.11089300	0.14102200	-1.74326200
H	-2.68413100	-3.31291200	-0.32968300	H	-1.44642000	-0.09630700	1.73927500
C	-0.41595900	0.99417000	-1.41155400	H	-1.83252400	1.47226100	1.01645000
C	0.34165900	0.31150600	-2.38614000	TSA8-A9			
C	-0.67118400	2.48410100	-1.51531100	C	-0.82373500	-0.01661700	-0.28101400
H	-1.59001200	2.65303200	-2.08938800	C	-1.83066000	0.39665000	0.75559700
H	-0.79430600	2.96069700	-0.53992500	C	-3.28413300	-0.01437700	0.37821100
H	0.14287500	2.98111800	-2.05176200	C	-4.21014700	-0.05943400	1.59707300
H	0.12474700	-0.71693500	-2.64662200	C	-3.92419500	0.85379300	-0.71703000
H	0.84589700	0.90094200	-3.15065100	C	-5.64933800	-0.40500800	1.20589500
O	-5.97811500	0.60428900	-0.00958700	C	-5.37705100	0.44363600	-0.97389600
Ru	1.21231000	-0.10005700	-0.32814800	H	-6.31274700	-0.31844600	2.07135900
C	2.40014100	1.52850100	0.62936800	H	-5.70237000	-1.44254800	0.84034200
C	3.41880600	0.83705800	-0.15101200	H	-5.84825000	1.13445300	-1.67922400
C	1.95233800	0.64177100	1.68279900	H	-5.41415600	-0.56607200	-1.41348400
C	3.51239000	-0.47150100	0.34104900	O	-3.15112100	-1.40594100	-0.06359900
C	2.55711800	-0.62422200	1.44637900	C	-2.25987100	-1.59386500	-1.04304000
C	4.43149500	-1.55688800	-0.12455800	H	-2.38124000	-1.05638200	-1.98228600
H	5.19092200	-1.76938600	0.63906800	H	-0.94109200	-1.17036500	-0.52760900
H	3.87892200	-2.48221800	-0.31227200	H	-1.94029900	-2.63148200	-1.12425800
H	4.95239100	-1.27992700	-1.04448000	C	-0.32164300	0.79330500	-1.36574600
C	2.45706900	-1.84641000	2.30934500	C	0.48302400	0.12662700	-2.32719900
H	2.42141200	-2.75534800	1.70208000	C	-0.56468100	2.28351500	-1.45549500
H	3.32616000	-1.92618400	2.97632700	H	-1.47598900	2.47367500	-2.03761800
H	1.56122300	-1.82366700	2.93581200	H	-0.69042300	2.76642300	-0.48373700
C	1.10538000	1.02201400	2.86170200	H	0.25894100	2.77770800	-1.97893100
H	1.74225800	1.33108600	3.70136300	H	0.25187300	-0.88402200	-2.65026700
H	0.44147800	1.85913200	2.63317700	H	0.99795800	0.73991700	-3.06464500
H	0.49021800	0.18735100	3.20789000	O	-6.15622300	0.48848500	0.21773500
C	2.14495100	3.00616100	0.55426100	Ru	1.30824800	-0.18886400	-0.28881300
H	2.92913200	3.54992200	1.09840400	C	2.30730900	1.54763600	0.74959100

C	3.23412100	0.99812200	-0.21603100	H	-6.84765600	0.85412900	-0.41257100
C	2.05802700	0.54401000	1.75605800	H	-5.83660500	-0.33242400	-1.26540300
C	3.50534100	-0.34967300	0.15839500	O	-3.15635300	-0.52363400	-1.04561800
C	2.76400000	-0.63463400	1.38287100	C	-2.05013100	0.07391800	-1.70814000
C	4.47318000	-1.29067800	-0.49507900	H	-2.36603300	0.91376500	-2.34814300
H	5.42173600	-1.32555500	0.05873100	H	-0.69897000	-0.34533300	-0.12103400
H	4.07081400	-2.30653600	-0.53116700	H	-1.57189800	-0.68649600	-2.32775900
H	4.70075300	-0.98591400	-1.52026500	C	-0.03389900	1.53957900	-0.97378500
C	2.86370700	-1.90614000	2.17149000	C	0.76134400	1.21085900	-2.07520900
H	2.89712000	-2.77663200	1.51175300	C	0.00612700	2.92792700	-0.38430900
H	3.77320500	-1.91597400	2.78778000	H	-0.78417700	3.54065900	-0.84100100
H	2.00798800	-2.02971800	2.84135600	H	-0.15851500	2.94132600	0.69419000
C	1.26547200	0.74513500	3.01445500	H	0.95840700	3.41646700	-0.60370900
H	1.90939100	1.12448700	3.81975200	H	0.46778100	0.45500900	-2.79356000
H	0.46073900	1.47218100	2.87560200	H	1.49676800	1.93328700	-2.42188200
H	0.81966500	-0.18915300	3.36665300	O	-6.17546500	-0.65698400	0.76075100
C	1.90387900	2.99036600	0.84695000	Ru	1.36374200	-0.08808100	-0.31289200
H	2.65420800	3.55821500	1.41434500	C	2.26330700	0.88203300	1.52021400
H	1.81807900	3.46021000	-0.13575700	C	3.15828800	0.94109300	0.39534700
H	0.94869500	3.11161500	1.36542400	C	2.03591600	-0.50913700	1.83309300
C	3.87462000	1.75917500	-1.34169000	C	3.45787100	-0.41569000	-0.00357800
H	3.20818400	2.52687900	-1.74496800	C	2.77587500	-1.31210700	0.92070000
H	4.78441800	2.26884200	-0.99570600	C	4.46114100	-0.83842000	-1.03347200
H	4.16097300	1.09923600	-2.16495700	H	5.45258700	-0.95782700	-0.57498600
Cl	1.12217700	-2.64884800	-0.86772200	H	4.18446700	-1.79400900	-1.48457300
H	-3.83126400	-0.78938000	2.32064300	H	4.55382700	-0.10049400	-1.83465000
H	-4.19025800	0.92709800	2.07313600	C	2.90970400	-2.80470900	0.93434800
H	-3.89961800	1.89317000	-0.37221700	H	2.86160600	-3.21271000	-0.07827200
H	-3.35645100	0.81127900	-1.65136600	H	3.87022300	-3.10141100	1.37568300
H	-1.59850600	-0.07150500	1.71775300	H	2.11711300	-3.27485400	1.52246600
H	-1.80521900	1.47991200	0.89879200	C	1.18527300	-1.00396200	2.96383100
A9				H	1.78260400	-1.08414800	3.88180900
C	-1.15029300	0.59477200	-0.57386800	H	0.35889200	-0.31913300	3.17266700
C	-2.19718000	1.08805100	0.44608000	H	0.76647100	-1.99158300	2.75495400
C	-3.46191000	0.23456500	0.15674200	C	1.82729000	2.03606000	2.37436500
C	-3.78674500	-0.78395500	1.26101500	H	2.47312600	2.11107700	3.25948600
C	-4.70840400	1.10254900	-0.10150700	H	1.89581700	2.98625100	1.84171400
C	-5.07501100	-1.54648800	0.94606400	H	0.80087600	1.92056700	2.73522400
C	-5.94821300	0.23591900	-0.32874700	C	3.78694400	2.17522800	-0.17907600
H	-5.34960500	-2.20724500	1.77440500	H	3.15099400	3.05432800	-0.05158700
H	-4.93449900	-2.16716100	0.04759400	H	4.73961000	2.38311900	0.32636100

H	4.00032100	2.06068500	-1.24505300
Cl	0.97168500	-1.97283400	-1.90687900
H	-2.95231700	-1.48532500	1.37790800
H	-3.91411000	-0.24876600	2.20971300
H	-4.87409000	1.75465600	0.76513600
H	-4.53796400	1.74748900	-0.97201000
H	-1.86155600	0.97958600	1.48046000
H	-2.41601200	2.14667700	0.27888600

TSA8-A10

C	2.31890700	1.41066600	1.23742900
C	2.56614400	0.31004400	0.17036500
C	3.02459600	0.86779500	-1.21585700
C	2.83967600	2.38632800	-1.49430800
C	2.85637500	2.77560800	0.82737100
H	1.24113300	1.52691600	1.38613400
H	2.73647100	1.08792400	2.19689700
O	2.27889900	3.13808700	-0.42306600
C	1.29951300	-0.58777300	0.03399000
C	0.08435400	0.10546800	-0.46957800
H	3.95652400	2.78812200	0.76097300
H	2.55703500	3.54229800	1.54858200
C	-0.31684900	0.42378600	-1.80901700
C	-0.13982600	-0.54555900	-2.96017900
H	0.07619400	-1.56299900	-2.62567600
H	-1.03244900	-0.56352900	-3.59354900
H	0.69631600	-0.21425800	-3.58810600
C	-1.15295500	1.55266800	-1.91635500
H	-0.92431200	2.46759200	-1.38450900
H	-1.77336700	1.65579300	-2.80529400
H	2.52571600	0.29582400	-2.00217200
H	4.08655300	0.63233400	-1.31431500
H	2.16832900	2.54416800	-2.34288100
H	1.56464600	-1.40449300	-0.65349200
H	1.10697600	-1.02419500	1.01802700
Ru	-1.74801600	0.33482200	-0.08217800
O	3.53498700	-0.66288200	0.62558900
C	-3.93113000	-0.65521600	-0.36784100
C	-3.95138300	-0.04081100	0.88920900
C	-2.82069200	-1.60135200	-0.37740800
C	-2.85307000	-0.59424900	1.69562100
C	-2.23412800	-1.63125000	0.94515300

C	-4.91917200	0.98585400	1.38725000
H	-5.51399800	0.58085500	2.21584000
H	-4.39181400	1.87142200	1.75637200
H	-5.61112200	1.30253000	0.60291400
C	-2.62819300	-0.27011500	3.14161600
H	-3.40268900	-0.73019300	3.76991900
H	-1.65895600	-0.63746500	3.48935300
H	-2.66000300	0.80984000	3.30999000
C	-1.24416200	-2.63938100	1.44916100
H	-1.76906900	-3.51251000	1.85941200
H	-0.58900200	-2.99962000	0.65213100
H	-0.61651800	-2.23181400	2.24573600
C	-2.58641600	-2.61316800	-1.46126700
H	-3.30216000	-3.44062200	-1.36146100
H	-2.72501800	-2.18417200	-2.45709600
H	-1.58204100	-3.04084300	-1.41005600
C	-4.88212900	-0.44543400	-1.50958700
H	-5.65383500	-1.22686000	-1.51989600
H	-5.38864300	0.52058800	-1.44338900
H	-4.36723400	-0.48853600	-2.47373000
Cl	-1.87367300	2.56048500	1.01141000
H	3.81699800	2.81950700	-1.76192100
C	4.80419500	-0.18923000	1.04236800
H	5.39248100	-1.07591800	1.29659500
H	5.34041600	0.35803900	0.25394900
H	4.74992800	0.45066600	1.93300500

A10

C	2.96942000	0.83793300	0.98966200
C	3.09933500	-0.58089700	0.38188100
C	3.66509000	-0.47385800	-1.05446000
C	3.30976900	0.86645700	-1.69562200
C	3.97966300	1.83375700	0.41681600
H	1.96288200	1.21534700	0.78127000
H	3.07074700	0.78534000	2.07918700
O	3.88491600	1.97976200	-1.00566900
C	1.72853300	-1.32604800	0.43456300
C	0.64521600	-0.78720300	-0.43167800
H	5.00638600	1.54400900	0.68082300
H	3.80636100	2.82689200	0.84781500
C	0.15612100	-1.27689100	-1.68549800
C	0.01689300	-2.76042100	-1.96049600

H	0.06134400	-3.36360600	-1.05043900
H	-0.92088500	-2.97524600	-2.48198800
H	0.83549000	-3.08289000	-2.61608300
C	-0.46207700	-0.30861800	-2.50350100
H	0.00195600	0.65367400	-2.67941200
H	-1.15997000	-0.64762400	-3.26789200
H	3.30136900	-1.29880800	-1.67641400
H	4.75653400	-0.55930100	-1.01932100
H	2.21766200	0.98784200	-1.74814200
H	1.94062300	-2.36773700	0.15856900
H	1.41544300	-1.30934800	1.48272000
Ru	-1.04100800	0.06739900	-0.33841400
O	3.90415700	-1.47169600	1.18169000
C	-3.41140000	-0.24414900	-0.04132600
C	-3.10617100	0.96938900	0.58742600
C	-2.57820900	-1.27537900	0.56470600
C	-2.07335500	0.72198700	1.60209100
C	-1.83503300	-0.67959000	1.65410800
C	-3.71709300	2.31035600	0.32794900
H	-4.27271400	2.65362200	1.20994500
H	-2.94513000	3.05498500	0.10960000
H	-4.41290900	2.28270900	-0.51421600
C	-1.57355800	1.75626000	2.56565100
H	-2.32171100	1.96241700	3.34303800
H	-0.65888400	1.42791600	3.06637700
H	-1.35864200	2.69881000	2.05480700
C	-1.06924700	-1.41747500	2.71215800
H	-1.73337900	-1.67306900	3.54875200
H	-0.64668700	-2.35335700	2.33781900
H	-0.25313800	-0.81430900	3.11832400
C	-2.74924600	-2.74640500	0.31706500
H	-3.61861300	-3.12179500	0.87387900
H	-2.92536100	-2.96358900	-0.73993500
H	-1.87929800	-3.32179300	0.64260100
C	-4.43056800	-0.49331000	-1.11459700
H	-5.36319000	-0.88205700	-0.68408500
H	-4.67418600	0.41998200	-1.66306800
H	-4.07812000	-1.23313300	-1.83917100
Cl	-0.50187400	2.41853400	-0.89979900
H	3.69241500	0.91390100	-2.72115800
C	5.19152000	-1.04660000	1.59555200

H	5.15552800	-0.20109100	2.29544800
H	5.63840800	-1.89843300	2.11738700
H	5.84969000	-0.78120900	0.75691100

TSA10-A11

C	3.20969900	-0.70319000	-1.25962600
C	3.27143900	0.57072500	-0.35689700
C	3.63692300	0.14760700	1.09119400
C	2.76471100	-1.02608600	1.40721000
C	3.69639200	-1.96369400	-0.55088400
H	2.18035900	-0.86808200	-1.59078000
H	3.80919300	-0.55063100	-2.16177400
O	3.00205100	-2.15228000	0.71219800
C	1.88149400	1.24363600	-0.27031600
C	0.90842400	0.44967400	0.58491500
H	4.77160000	-1.92493800	-0.34261600
H	3.48741200	-2.86421000	-1.13021600
C	0.17409300	1.02621700	1.68678500
C	0.08332100	2.51905900	1.91942000
H	0.13002700	3.10374700	0.99776700
H	-0.84075000	2.77484400	2.44457700
H	0.91827200	2.84373700	2.55595400
C	-0.57589400	0.11185400	2.47359100
H	-0.17504900	-0.86234200	2.73490000
H	-1.29426300	0.52134500	3.18220500
H	3.46946800	0.96729900	1.79322600
H	4.68580900	-0.16378000	1.16744000
H	1.49219400	-0.58319900	0.94340700
H	2.04227000	2.24518900	0.14139600
H	1.49778500	1.36095300	-1.28810400
Ru	-1.06755600	-0.14686000	0.32604000
O	4.13409200	1.57630800	-0.87970500
C	-3.33139200	-0.14622200	-0.07088400
C	-2.71206600	-0.86428800	-1.14900500
C	-2.79913500	1.18904200	-0.09053200
C	-1.82467900	0.01088500	-1.85817300
C	-1.86827300	1.28794100	-1.19754000
C	-3.02997200	-2.27353600	-1.54853800
H	-3.84562000	-2.27664700	-2.28475700
H	-2.16945800	-2.76874900	-2.00408600
H	-3.34756900	-2.87555500	-0.69508500
C	-1.11144500	-0.30143900	-3.14240400

H	-1.74923700	-0.08766200	-4.01204700
H	-0.20173500	0.29528900	-3.25565000
H	-0.82854700	-1.35642500	-3.20113700
C	-1.25404700	2.55450300	-1.72034600
H	-1.92357400	3.03061700	-2.45003700
H	-1.07135700	3.28305300	-0.92657600
H	-0.30512300	2.36730700	-2.23039600
C	-3.29886200	2.33278900	0.74462700
H	-4.22905700	2.73668400	0.32160200
H	-3.51763800	2.02384400	1.77096300
H	-2.57859500	3.15247800	0.78512600
C	-4.43000600	-0.65353100	0.81919000
H	-5.41771100	-0.51136700	0.35716400
H	-4.32104600	-1.72185800	1.02786600
H	-4.44304800	-0.12983600	1.77960100
Cl	-0.58125300	-2.56941100	0.79944100
H	2.46594900	-1.23667200	2.43271700
C	5.50893100	1.24953400	-1.02734800
H	5.66962400	0.34748000	-1.63234400
H	5.97126400	2.09387800	-1.54583000
H	6.01589300	1.11936100	-0.06175900

A11

C	-4.29075100	-0.85746300	1.14074600
C	-3.69331200	0.46604900	0.56968800
C	-4.01796900	0.54320100	-0.93840500
C	-3.19733900	-0.65137000	-1.43532700
C	-4.73704000	-1.81273600	0.02514500
H	-3.55147400	-1.34175400	1.78749200
H	-5.16216000	-0.63684000	1.76647700
O	-3.80853000	-1.89654400	-1.06235100
C	-2.15160800	0.39664600	0.53381300
C	-1.81656900	-0.51890500	-0.67706900
H	-5.72176300	-1.50287000	-0.35492300
H	-4.84599800	-2.83310600	0.40529300
C	-0.69012800	-0.05410400	-1.58132800
C	-0.79992800	1.30961600	-2.21848300
H	-1.00061600	2.10602600	-1.49797500
H	0.10347600	1.56292100	-2.77724500
H	-1.63727700	1.30760200	-2.93019800
C	0.26411000	-0.93641500	-2.01227100
H	0.20735300	-1.98875500	-1.75060200

H	0.93891700	-0.66505400	-2.81929200
H	-3.63333500	1.47703000	-1.36029300
H	-5.07876100	0.46364100	-1.18958000
H	-1.56365200	-1.52140000	-0.32970200
H	-1.77766600	1.41422100	0.38812000
H	-1.73251200	0.01630300	1.46908300
Ru	1.49241700	-0.34270200	-0.00979500
O	-4.04940500	1.60584800	1.34778400
C	3.61139100	-0.16095100	-0.20977100
C	3.26754400	-0.03939400	1.19319800
C	3.00844700	0.94800900	-0.92076200
C	2.40912000	1.10654200	1.32437300
C	2.26195300	1.72641800	0.02417300
C	3.78842700	-0.89270800	2.30983800
H	4.73243200	-0.48625000	2.69738500
H	3.08224800	-0.94021500	3.14280100
H	3.98081700	-1.91624600	1.97875700
C	1.82217900	1.62875800	2.60035200
H	2.47764400	2.39292900	3.04034700
H	0.84597000	2.09311800	2.43308300
H	1.69779800	0.83387800	3.34026500
C	1.57760400	3.03587600	-0.23272100
H	2.24723200	3.86846800	0.02281500
H	1.29865800	3.15220600	-1.28187600
H	0.67507700	3.15111100	0.37462300
C	3.23451400	1.27241200	-2.36681600
H	4.16674800	1.84079400	-2.48703000
H	3.32483700	0.36867400	-2.97601000
H	2.42587100	1.88014200	-2.77993800
C	4.54983200	-1.16920300	-0.80030500
H	5.58128600	-0.79044700	-0.77929100
H	4.53218400	-2.10936200	-0.24295500
H	4.30113800	-1.38885100	-1.84239600
Cl	0.74251100	-2.49872200	0.94237500
H	-3.07408500	-0.68505100	-2.52190000
C	-5.39785200	2.03463700	1.25129600
H	-6.11745600	1.25048300	1.52623700
H	-5.51446100	2.86412900	1.95472500
H	-5.64977100	2.39578800	0.24467500

TSA11-A12

C	1.43192800	1.37146000	1.77754400
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H	2.08548300	1.12949100	2.61113700
H	1.54825900	2.35559500	1.33588000
C	0.30510500	0.61747700	1.54102200
C	-0.04884300	-0.52454800	2.46380600
H	-0.79888800	-0.18096300	3.19015000
H	-0.48130400	-1.38302200	1.94433000
H	0.82229100	-0.86193100	3.02819200
C	-0.77680300	1.14128000	0.61125300
C	-1.44667300	0.10564400	-0.33138600
C	-2.96030300	0.43239200	-0.26541900
O	-3.79379600	-0.59835100	-0.79679000
C	-3.14341700	0.78598800	1.22134400
C	-1.99669100	1.78568700	1.39194400
C	-3.05002300	3.05024100	-0.41750500
C	-3.30302800	1.68090200	-1.10781900
H	-1.74789000	1.99699400	2.43549200
H	-4.11905100	1.22253400	1.45702900
H	-2.98283800	-0.08689800	1.86165600
H	-4.01452800	3.53469100	-0.22025200
H	-2.49911900	3.70771700	-1.09961500
H	-4.36860500	1.60964300	-1.34520900
H	-2.76093500	1.63099600	-2.05724700
H	-0.33754600	1.95103200	0.02567900
O	-2.32819400	3.04787400	0.82810400
C	2.64583100	-1.76675400	-1.12160300
C	2.52987900	-2.03317200	0.29302700
C	3.50440600	-1.22458200	0.96982500
C	4.22082700	-0.45592100	-0.02672400
C	3.70019200	-0.81644200	-1.33221200
C	4.23598300	-0.34781400	-2.65152700
H	4.57251300	0.69030100	-2.59765100
H	5.09069900	-0.96205300	-2.96489600
H	3.47859100	-0.40946700	-3.43772900
C	1.82449800	-2.42756000	-2.18667300
H	1.78883500	-1.83012900	-3.10110100
H	2.25290200	-3.40528600	-2.44592500
H	0.79747100	-2.60096200	-1.85216500
C	5.40328100	0.42708400	0.23411800
H	6.32812200	-0.16658100	0.24190000
H	5.50993000	1.19421100	-0.53666600
H	5.32605500	0.92861800	1.20283300

C	3.83882400	-1.26571100	2.43048800
H	4.64190500	-1.99284700	2.61200100
H	4.19143800	-0.29627100	2.79210000
H	2.98357400	-1.56630600	3.04075400
C	1.67774700	-3.10764200	0.90109300
H	0.70307900	-3.18558200	0.41034800
H	2.17106400	-4.08357200	0.79584200
H	1.50843400	-2.94190100	1.96670400
Ru	2.16968000	0.13543700	-0.10111200
Cl	2.13087000	2.31205800	-1.31284400
H	-1.28139400	-0.91429900	0.02683900
H	-1.06590300	0.16144000	-1.35522300
C	-3.87385000	-1.81540400	-0.07344600
H	-2.89537200	-2.28924700	0.08369800
H	-4.36239800	-1.69273500	0.90293900
H	-4.48473600	-2.49147400	-0.67881700

A12

C	-0.17868500	-0.85010600	2.06540700
H	-0.83989600	-0.50647000	2.85567300
H	-0.14368300	-1.92052300	1.88519300
C	0.79068200	-0.02290200	1.56260500
C	0.92831700	1.38871300	2.07825300
H	1.77897100	1.44098000	2.77145400
H	1.12274800	2.11375400	1.28374700
H	0.03925700	1.70123000	2.62810400
C	1.89427600	-0.58395900	0.68274300
C	2.21644300	0.20748500	-0.62320200
C	3.75770400	0.42056700	-0.61657800
O	4.19927500	1.47604600	-1.46890300
C	4.05845100	0.55876000	0.88834800
C	3.28564700	-0.65366700	1.42038000
C	4.09559100	-2.08270900	-0.32806600
C	4.50892000	-0.82896700	-1.10903900
H	3.18757800	-0.67518600	2.50869100
H	5.12526600	0.50789900	1.12595500
H	3.64844900	1.48476200	1.30202200
H	4.84005500	-2.87602600	-0.44479400
H	3.14551400	-2.47253800	-0.72036700
H	5.58201100	-0.64124000	-0.99059500
H	4.31357200	-0.98768400	-2.17583500
H	1.60194700	-1.60483800	0.43577000

O	3.98422300	-1.85706900	1.08236800	H	-2.35600700	2.51003000	-2.38592900
C	-2.47930400	0.85331900	-1.42642800	H	-1.94418500	4.19911500	-2.01569400
C	-2.14383100	1.68621400	-0.28525300	C	-0.57507400	1.40410900	-0.53561100
C	-2.78525200	1.13394300	0.87158900	C	-1.07056300	0.13917600	-0.91336300
C	-3.47164300	-0.07256300	0.46340300	C	-2.28550100	-0.45923900	-0.16991200
C	-3.31392800	-0.21874000	-0.97359900	O	-2.31590000	-1.89828900	-0.28794200
C	-3.98286000	-1.25616000	-1.82329900	C	-2.71416900	-2.45823100	-1.53308500
H	-4.08711100	-2.20479000	-1.29038900	H	-2.51161100	-3.53096900	-1.46775500
H	-4.99033400	-0.92420700	-2.10816700	H	-3.78579000	-2.32869900	-1.72874000
H	-3.42544200	-1.44862100	-2.74315200	H	-2.15349600	-2.05419500	-2.38488400
C	-2.05485500	1.11550400	-2.83950400	C	-3.58388100	0.17567900	-0.73767600
H	-2.07833900	0.20392600	-3.44194400	C	-4.82282400	-0.27903500	0.04154700
H	-2.72332900	1.84723900	-3.31324300	C	-3.57652200	-0.61790200	2.01044200
H	-1.04083000	1.52376600	-2.88388200	C	-2.27512300	-0.17379500	1.34241900
C	-4.34599700	-0.91918400	1.33825200	H	-5.71152300	0.24974200	-0.31793200
H	-5.37724300	-0.53918800	1.33257700	H	-3.49643700	1.26235700	-0.64533100
H	-4.37614400	-1.95658800	0.99411300	H	-3.70584100	-0.04776800	-1.80271600
H	-4.00019800	-0.91604600	2.37565800	H	-3.57687000	-0.33969300	3.06901400
C	-2.85159800	1.74333700	2.24001800	H	-3.68349900	-1.71125500	1.94429700
H	-3.79649800	2.28944800	2.36389800	H	-2.15191100	0.90347500	1.49141300
H	-2.81227100	0.98610600	3.02826900	H	-1.42521900	-0.66765600	1.81832400
H	-2.04141200	2.45565800	2.41070800	H	-4.99398700	-1.35805100	-0.09635600
C	-1.39222100	2.98155600	-0.36018100	O	-4.71258100	0.02068200	1.42962400
H	-0.59953200	2.94587100	-1.11321400	C	1.50142200	-1.82231600	-0.60837300
H	-2.06938900	3.79974300	-0.64135400	C	1.35667200	-1.74579700	0.84308800
H	-0.93987700	3.24655000	0.59800000	C	2.35643100	-0.87742100	1.32553300
Ru	-1.39782800	-0.35447100	0.03877200	C	3.18516400	-0.47374300	0.19168900
Cl	-0.63675200	-2.53195000	-0.85168600	C	2.68795100	-1.10332800	-0.97491600
H	1.71835400	1.18112500	-0.63065000	C	3.30527700	-1.08237900	-2.34248800
H	1.88563100	-0.33507700	-1.51337900	H	3.87736700	-0.16820800	-2.51725300
C	3.91103000	2.80535500	-1.07003500	H	3.99211000	-1.93107000	-2.45918400
H	2.84040400	2.98049200	-0.89532800	H	2.54880800	-1.16353700	-3.12691900
H	4.46344300	3.10372700	-0.16834900	C	0.79554400	-2.80015500	-1.49644100
H	4.22821200	3.45003400	-1.89506000	H	0.67783800	-2.41550500	-2.51312200
A6a				H	1.37934000	-3.72845100	-1.56601100
C	-1.16456500	3.59039200	0.40936600	H	-0.18838400	-3.05079900	-1.10407100
H	-1.62059800	4.57274600	0.31399300	C	4.45562000	0.30534500	0.31000700
H	-0.80069100	3.29919800	1.38720700	H	4.78422300	0.69396300	-0.65711400
C	-1.07429800	2.76971400	-0.65038000	H	4.33784600	1.14859800	0.99350900
C	-1.56203200	3.17442300	-2.02785900	H	5.25261200	-0.34254200	0.69909200
H	-0.74532200	3.12293300	-2.75807400	C	2.64178400	-0.50229400	2.74753700

H	3.52596700	-1.03619100	3.12010200
H	2.84254000	0.56965300	2.83418100
H	1.80426000	-0.74657900	3.40557600
C	0.41429200	-2.58615300	1.64970300
H	-0.55135600	-2.70135600	1.15391300
H	0.84406900	-3.58966600	1.77815000
H	0.24889900	-2.17390900	2.64816300
Ru	0.98950000	0.39240200	-0.19634000
Cl	1.98482700	2.47439000	0.74836800
H	1.31269000	0.91549800	-1.64281000
H	-1.05167100	-0.13299500	-1.97113500

TSA6a-Z

C	-1.30558800	3.50385200	0.16436900
H	-1.79733500	4.45989800	0.00104500
H	-0.99538600	3.26292300	1.17326000
C	-1.10390100	2.65741000	-0.85662700
C	-1.50949500	2.99148800	-2.27828100
H	-0.63964000	2.96459800	-2.94627200
H	-2.23435700	2.26804300	-2.66816700
H	-1.94989000	3.99115200	-2.33183600
C	-0.54964500	1.31209300	-0.67604100
C	-1.05223600	0.01413500	-0.87210100
C	-2.30296100	-0.49049500	-0.12729000
O	-2.35087000	-1.93479800	-0.18485300
C	-2.75218800	-2.54622200	-1.40398200
H	-2.53682700	-3.61328900	-1.29849100
H	-3.82686800	-2.43465700	-1.59590200
H	-2.20395300	-2.16958000	-2.27653400
C	-3.58079700	0.14439000	-0.73521800
C	-4.83563600	-0.23775300	0.05704400
C	-3.61242100	-0.52616000	2.04715000
C	-2.29116400	-0.15410500	1.37410100
H	-5.70747200	0.29792800	-0.33226400
H	-3.46536600	1.23190300	-0.69762100
H	-3.70137800	-0.13214600	-1.78792500
H	-3.61217700	-0.20529500	3.09355300
H	-3.75552500	-1.61724900	2.02392900
H	-2.11966100	0.92047300	1.48953300
H	-1.46345600	-0.67317900	1.86532000
H	-5.03691600	-1.31689300	-0.03040400
O	-4.72214300	0.12454200	1.42964000

C	1.59733900	-1.75991000	-0.70852500
C	1.46306100	-1.75856400	0.74251200
C	2.43396300	-0.87327100	1.26638200
C	3.22317800	-0.36035800	0.15088800
C	2.72860200	-0.94289300	-1.04655400
C	3.29737300	-0.77358200	-2.42431200
H	3.78897500	0.19463500	-2.54462600
H	4.04547800	-1.55262000	-2.62097800
H	2.52425600	-0.86003600	-3.19191600
C	0.89941700	-2.69210900	-1.65038400
H	0.71494400	-2.22658800	-2.62333900
H	1.51867100	-3.58172700	-1.82783900
H	-0.05491700	-3.02646500	-1.24377400
C	4.43794100	0.50144000	0.29287100
H	4.73767000	0.93651700	-0.66393800
H	4.25902700	1.31877300	0.99566500
H	5.28107600	-0.09318300	0.66877300
C	2.72105000	-0.58316700	2.70733100
H	3.62456700	-1.11469200	3.03406400
H	2.88589300	0.48646700	2.86283700
H	1.89816600	-0.89707000	3.35419800
C	0.53635300	-2.64200400	1.52108200
H	-0.43491600	-2.73976300	1.03161200
H	0.97340200	-3.64659100	1.60772100
H	0.37664900	-2.26712400	2.53499800
Ru	1.02336200	0.35843000	-0.12630600
Cl	1.74313700	2.42860400	1.09307700
H	0.98648800	1.19299700	-1.51518900
H	-0.90561400	-0.47854300	-1.83326200

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C	-1.56287300	3.00739900	0.81742000
H	-2.04238300	3.94151400	1.09994200
H	-1.25654900	2.35498000	1.62545900
C	-1.32270700	2.72160700	-0.46831700
C	-1.66867000	3.71143900	-1.56232600
H	-0.76709400	4.00780800	-2.11460100
H	-2.35750800	3.27601500	-2.29734500
H	-2.12891400	4.61503700	-1.15269700
C	-0.70318700	1.47623200	-1.00163200
C	-1.12826600	0.16584100	-0.91611000
C	-2.34629000	-0.44199600	-0.20786900

O	-2.45596500	-1.82321100	-0.63509100	H	0.91092000	-4.01371500	0.26239700
C	-2.89220500	-2.07772000	-1.96373100	H	0.16502900	-3.04811900	1.53567200
H	-2.69558300	-3.13664200	-2.15453900	Ru	1.16841600	0.26960600	0.08135500
H	-3.96716800	-1.89966700	-2.09414300	Cl	1.79628900	2.50816200	0.95467200
H	-2.35169400	-1.48649400	-2.71469600	H	-0.02364100	1.67113900	-1.83418800
C	-3.64894700	0.33403700	-0.52817200	H	-0.74940600	-0.49010000	-1.68958700
C	-4.84880300	-0.25291300	0.21987800	A8'			
C	-3.49950600	-1.07253500	1.96656200	C	-0.23593300	0.99272600	-2.51311000
C	-2.21701600	-0.53798100	1.32611500	H	-0.32724000	1.56098400	-3.43646700
H	-5.73676500	0.36569100	0.05455000	H	0.10729500	-0.03397200	-2.58191000
H	-3.51293900	1.37140400	-0.21529300	C	-0.60286100	1.52713300	-1.32916300
H	-3.84421000	0.34338900	-1.60559400	C	-1.13693400	2.94844200	-1.26563900
H	-3.41973400	-1.04583500	3.05794700	H	-2.22174900	2.97065800	-1.11829200
H	-3.66828000	-2.11608900	1.66119200	H	-0.69002100	3.51151300	-0.43955400
H	-2.00848500	0.45744600	1.72330200	H	-0.91751400	3.47952200	-2.19642500
H	-1.37522100	-1.18683800	1.58274100	C	-0.53683700	0.70255700	-0.10034200
H	-5.07443100	-1.26914000	-0.13994300	C	-1.72036900	0.85887100	0.84689700
O	-4.63253800	-0.27483600	1.62860600	C	-3.04621400	0.07823300	0.52990400
C	1.76207400	-1.45785400	-1.13304500	O	-3.91973300	0.25115200	1.66696000
C	1.40709000	-1.93579800	0.17207600	C	-4.53028400	1.51596400	1.86878700
C	2.28983300	-1.30265200	1.13141300	H	-5.02520900	1.46265100	2.84315200
C	3.20565600	-0.46433100	0.41680100	H	-3.80772100	2.34238200	1.89888900
C	2.84942300	-0.51360600	-0.98507000	H	-5.29170100	1.74663400	1.11213100
C	3.58596700	0.15586600	-2.10534800	C	-2.80780500	-1.44121800	0.47786500
H	4.05121700	1.08903600	-1.77780300	C	-4.08105700	-2.20087300	0.10031100
H	4.38314400	-0.49777300	-2.48563900	C	-4.95974200	-0.36276300	-1.07675600
H	2.92025100	0.38401100	-2.94263000	C	-3.73467300	0.50609500	-0.78096400
C	1.21738800	-1.95032600	-2.44002700	H	-3.86518200	-3.26566500	-0.03283400
H	1.12935300	-1.14516200	-3.17609700	H	-2.02315100	-1.65683900	-0.25369100
H	1.89129300	-2.70535400	-2.86660900	H	-2.45553500	-1.78713700	1.45701700
H	0.23759800	-2.41900900	-2.32219200	H	-5.38275000	-0.10424000	-2.05274100
C	4.37048000	0.27728900	0.99548600	H	-5.74005200	-0.19963100	-0.31632600
H	4.54452400	1.22237600	0.47760200	H	-3.02121600	0.39646500	-1.60287500
H	4.22347500	0.50063700	2.05425100	H	-4.03028200	1.56031600	-0.74935700
H	5.28057600	-0.33096400	0.90529000	H	-4.83354000	-2.10153200	0.89775000
C	2.30011800	-1.56864000	2.60598600	O	-4.62301000	-1.74535400	-1.13857000
H	2.88032300	-2.47454300	2.82770800	C	2.50273200	0.91113400	1.37811500
H	2.75073300	-0.74250300	3.16116200	C	2.56667700	1.35272200	0.00304200
H	1.28957200	-1.72535500	2.99363600	C	3.00496700	0.25116100	-0.77732400
C	0.44334400	-3.04317900	0.47843600	C	3.41326700	-0.82262300	0.13841100
H	-0.47461400	-2.96530300	-0.10758600	C	3.12616500	-0.41607500	1.44406900

C	3.38758300	-1.16772400	2.71692200	H	-2.84191300	-1.98501600	-2.53824400
H	3.52043300	-2.23742900	2.53712700	H	-1.17513900	-1.89770000	-1.90590500
H	4.29830900	-0.79683200	3.20533300	C	-3.18465800	0.35834600	-1.10262400
H	2.56853600	-1.04732100	3.43225600	C	-4.67077800	0.11707100	-1.37817800
C	2.25013700	1.79029100	2.57065200	C	-5.05621600	-0.77358300	0.76554400
H	1.88755500	1.21288400	3.42566300	C	-3.60164100	-0.58016300	1.19960900
H	3.17372900	2.29561900	2.88539300	H	-5.05902900	0.87843200	-2.06189500
H	1.50953400	2.56469100	2.35278100	H	-3.05214100	1.38858500	-0.76206200
C	4.03485700	-2.11021600	-0.30840500	H	-2.60883000	0.25885100	-2.02818300
H	4.21570600	-2.78400900	0.53282800	H	-5.72906400	-0.66123700	1.62170700
H	3.38908500	-2.62818400	-1.02516000	H	-5.19481800	-1.78253800	0.34916200
H	4.99794300	-1.92493800	-0.80094600	H	-3.50684000	0.37007300	1.72875500
C	3.27478500	0.23991300	-2.25198200	H	-3.30813200	-1.38044300	1.88826800
H	4.33919500	0.42656100	-2.45071300	H	-4.82177800	-0.86704600	-1.84900500
H	3.02462000	-0.72874500	-2.69403400	O	-5.45221300	0.20877100	-0.18877600
H	2.70049600	1.00844500	-2.77494000	C	1.89386900	-1.13974500	1.52484400
C	2.33054600	2.75069000	-0.47951400	C	2.36660700	0.21883100	1.58294000
H	1.61254300	3.28366400	0.14809700	C	3.13465000	0.46623600	0.40318500
H	3.27327300	3.31346900	-0.44849700	C	3.19166000	-0.75929000	-0.36954400
H	1.96876000	2.77445300	-1.50961200	C	2.43441500	-1.75664200	0.33714500
Ru	1.02440400	-0.34965000	0.29156500	C	2.33374000	-3.21318600	-0.01019900
Cl	0.60237400	-2.31845900	-1.19532500	H	2.48436100	-3.38209800	-1.07855400
H	-1.98101800	1.92262100	0.91000000	H	3.09924700	-3.78533400	0.53037500
H	-1.44071900	0.54266200	1.85355000	H	1.36014900	-3.62749800	0.26369900
H	0.24383700	-0.78912800	1.79661500	C	1.11694000	-1.83189800	2.60385300
H	-0.00808100	-1.38919600	1.28893500	H	0.63877800	-2.74372700	2.23668200
TSA5-A6'				H	1.77983300	-2.11711200	3.43069100
C	-0.01916400	3.28476100	0.25771000	H	0.33974400	-1.18445600	3.02211600
H	-0.22533800	4.32140900	0.51219700	C	4.03473700	-0.96624200	-1.59321300
H	0.82732400	3.07384600	-0.38436000	H	3.70763500	-1.83928100	-2.16331900
C	-0.83184300	2.29612200	0.69207900	H	3.99140300	-0.09861200	-2.25626200
C	-2.00413000	2.62272300	1.59859000	H	5.08607100	-1.12197000	-1.31673200
H	-2.96595400	2.41939800	1.11837600	C	3.87514000	1.72701000	0.08144200
H	-1.96840000	2.02788400	2.51767500	H	4.91626500	1.64927500	0.42257400
H	-1.98808800	3.68045100	1.87597600	H	3.88769000	1.91759400	-0.99371500
C	-0.50532000	0.90065700	0.41671700	H	3.42924000	2.59365800	0.57629800
C	-1.21717500	-0.27393500	0.44745400	C	2.15117100	1.18809700	2.70551000
C	-2.64640700	-0.59513900	-0.01922600	H	1.29415000	0.90965900	3.32340400
O	-2.68384300	-1.97456200	-0.44034500	H	3.03433400	1.21411600	3.35735300
C	-2.17488600	-2.30792000	-1.72837200	H	1.98826200	2.20505000	2.33730600
H	-2.11300200	-3.40012300	-1.75275000	Ru	1.06197700	-0.08714400	-0.34940300

Cl	1.15828300	1.49943200	-2.30589500
H	-0.76503800	-1.15696000	0.89859100
H	0.85792800	-1.01093300	-1.63667300

A6'

C	0.20851800	3.62487700	0.16969800
H	0.03783300	4.68960500	0.30923000
H	1.17478100	3.30883400	-0.20240300
C	-0.76454900	2.72691400	0.45079000
C	-2.10824000	3.18633600	0.97751100
H	-2.92888800	2.87009100	0.32628100
H	-2.30276200	2.77491100	1.97372900
H	-2.13731400	4.27714300	1.04840800
C	-0.47147000	1.31329900	0.33470600
C	-1.07610800	0.07971800	0.67854500
C	-2.42178600	-0.47875600	0.17076800
O	-2.39132900	-1.92500700	0.20863500
C	-1.93286900	-2.65519200	-0.92182300
H	-1.86438500	-3.69771400	-0.59622900
H	-2.63823400	-2.61296800	-1.76246100
H	-0.95020400	-2.32724600	-1.27264900
C	-2.85764900	0.07950600	-1.19547600
C	-4.31062300	-0.27027900	-1.53197200
C	-4.90624800	-0.51626400	0.72681700
C	-3.50980400	-0.13980300	1.22076400
H	-4.62308900	0.25378900	-2.44064200
H	-2.76015000	1.16995100	-1.16577500
H	-2.19380600	-0.26920200	-1.99268600
H	-5.66789800	-0.19501400	1.44455800
H	-4.98469300	-1.60758900	0.60767800
H	-3.48892100	0.92930800	1.44145600
H	-3.28364000	-0.67886200	2.14796600
H	-4.41916700	-1.35079300	-1.71465900
O	-5.21200300	0.13437000	-0.50448500
C	1.59302500	-1.46055600	1.25801400
C	2.22711500	-0.21044500	1.62314800
C	3.05842100	0.17762400	0.54329500
C	2.99449900	-0.86999400	-0.47619600
C	2.12946600	-1.89009800	-0.00973300
C	1.88118200	-3.22558500	-0.64718100
H	1.98183600	-3.18336100	-1.73442400
H	2.60610700	-3.96210400	-0.27541900

H	0.88407900	-3.60508000	-0.41318200
C	0.76174200	-2.31381300	2.16940900
H	-0.03428800	-2.83163900	1.62967400
H	1.39507500	-3.07354100	2.64630000
H	0.30285400	-1.72817900	2.96964900
C	3.84920100	-0.90638200	-1.70651000
H	3.48950900	-1.64757800	-2.42493100
H	3.86393800	0.06651500	-2.20461300
H	4.88319400	-1.16903500	-1.44618400
C	3.96756000	1.36608800	0.47490500
H	5.00612100	1.06729500	0.67025500
H	3.93476800	1.82651100	-0.51674000
H	3.69788900	2.12506000	1.21385500
C	2.05815100	0.49830100	2.93483100
H	1.03601600	0.41561900	3.31591600
H	2.72028400	0.06256600	3.69468900
H	2.30260600	1.56030300	2.85376400
Ru	0.87645800	0.11398300	-0.29103900
Cl	1.51852900	1.64527400	-2.15402300
H	-0.89165500	-0.27422900	1.69442900
H	0.08249600	-0.53616700	-1.49981200

TSA6'-A6''

C	-0.73428600	3.59918200	0.25773800
H	-1.08322100	4.56780000	0.60698800
H	-0.31139200	3.53054500	-0.73731800
C	-0.86162600	2.50862400	1.03978600
C	-1.41402400	2.59476000	2.45116600
H	-2.32900800	2.00666900	2.56819100
H	-0.68831300	2.20798000	3.17606800
H	-1.63054000	3.63460000	2.71079700
C	-0.49430400	1.17895100	0.58478200
C	-1.07235800	-0.10730600	0.67371600
C	-2.40513200	-0.49623300	-0.00934400
O	-2.39138000	-1.90080400	-0.33186800
C	-2.56193500	-2.83673500	0.72229200
H	-2.29411100	-3.81470700	0.31187700
H	-1.91495300	-2.63769900	1.58464800
H	-3.60037200	-2.88860200	1.07594500
C	-2.63579800	0.20444000	-1.35916600
C	-4.03740900	-0.06621300	-1.90747100
C	-4.94281100	-0.39399300	0.23747600

C	-3.59412400	-0.13110200	0.91501800	H	-0.03804400	3.88779200	-2.16033300
H	-4.20812000	0.51613600	-2.81819900	H	0.48767400	2.12308100	-2.39787700
H	-2.49754600	1.28365700	-1.23229600	C	-0.49579900	2.55895900	-0.56276300
H	-1.88833800	-0.14032100	-2.08007900	C	-1.18012100	3.58853700	0.31207500
H	-5.76157600	-0.04725400	0.87632100	H	-2.25939900	3.41104000	0.36387100
H	-5.08670900	-1.47138100	0.06000300	H	-0.80015200	3.55302600	1.33881200
H	-3.53063400	0.93736900	1.14108200	H	-1.01972600	4.59679100	-0.07978300
H	-3.53765600	-0.66809100	1.86806400	C	-0.44384900	1.18306300	-0.11304800
H	-4.14357500	-1.13261100	-2.15812600	C	-1.14434700	0.32678000	0.76320600
O	-5.05850000	0.32042100	-0.98820500	C	-2.53482600	-0.28730400	0.47937400
C	2.08161300	-1.84243700	-0.38530400	O	-2.68097800	-1.53966800	1.17936900
C	1.73713600	-1.57074700	0.99124500	C	-2.33088200	-2.75662400	0.52951800
C	2.45201800	-0.38953600	1.41929500	H	-2.31651400	-3.52220600	1.31159800
C	3.15107600	0.11614000	0.29557100	H	-3.06961100	-3.05466900	-0.22603700
C	2.92152700	-0.78744600	-0.83035600	H	-1.34383600	-2.72305900	0.05750900
C	3.60666100	-0.67582100	-2.15836400	C	-2.89365500	-0.37139800	-1.01545300
H	3.60717800	0.35776600	-2.51312300	C	-4.37492500	-0.68974700	-1.23914700
H	4.65075100	-1.00725200	-2.08227200	C	-5.00668600	0.21445000	0.83490900
H	3.11646800	-1.29208600	-2.91631600	C	-3.57530300	0.62934000	1.17391200
C	1.68548300	-3.07077200	-1.15135200	H	-4.61782400	-0.62099900	-2.30433600
H	1.71726600	-2.89988200	-2.22976300	H	-2.67710300	0.60290600	-1.46789900
H	2.36798700	-3.90027400	-0.92351500	H	-2.26361000	-1.09962500	-1.53176900
H	0.67433500	-3.39461500	-0.89260700	H	-5.72415900	0.91558100	1.27341900
C	4.07908900	1.29046400	0.26043000	H	-5.21339400	-0.78774500	1.24058100
H	3.86332300	1.93246200	-0.59869800	H	-3.42065000	1.66241300	0.84835600
H	4.00072000	1.89363600	1.16831700	H	-3.42219400	0.59034400	2.25853900
H	5.11923500	0.95014000	0.17396900	H	-4.60777200	-1.71427600	-0.90957100
C	2.48471900	0.14528500	2.82138800	O	-5.23390500	0.23235100	-0.57191100
H	3.26968700	-0.35450400	3.40473400	C	2.23383300	0.31558800	1.55942000
H	2.69278800	1.21786100	2.84123400	C	2.65344700	1.16822600	0.45632900
H	1.53914700	-0.02524500	3.34354800	C	3.08611400	0.33458500	-0.59646600
C	1.03571700	-2.52137600	1.91252500	C	3.02345700	-1.04550800	-0.12742200
H	0.35316300	-3.18122300	1.37435600	C	2.56455900	-1.04891900	1.21355500
H	1.77726500	-3.15343900	2.41949600	C	2.48968000	-2.22928900	2.13987600
H	0.47369800	-2.00231100	2.69438200	H	2.34450700	-3.16477800	1.59409500
Ru	0.87158000	0.16076400	-0.28033800	H	3.42155600	-2.32315800	2.71339100
Cl	1.38805400	2.02572300	-1.87015500	H	1.67287400	-2.12947900	2.85925500
H	-0.90788800	-0.66784500	1.59548400	C	1.84308600	0.79211800	2.92819500
H	0.07607600	-0.35552800	-1.54552300	H	1.24352300	0.04623000	3.45676700
A6''				H	2.73445900	0.98821900	3.53914000
C	0.02485200	2.87588600	-1.76847300	H	1.26709600	1.72059900	2.88693000

C	3.51677200	-2.22452800	-0.90973900	H	-5.28449900	-0.83731000	1.13303500
H	3.15715900	-3.16708400	-0.48945700	H	-3.50770600	1.60871800	0.65447400
H	3.18953100	-2.17483700	-1.95113200	H	-3.51519400	0.59476100	2.10717400
H	4.61465300	-2.25319300	-0.90332000	H	-4.64585000	-1.84955700	-0.97304300
C	3.63868900	0.75290900	-1.92650700	O	-5.29710600	0.10283000	-0.72205300
H	4.73040500	0.63650400	-1.95262800	C	2.16182600	0.32171300	1.48714000
H	3.22861100	0.14311600	-2.73754100	C	2.58473900	1.13122900	0.35547100
H	3.41433400	1.80010100	-2.14432200	C	3.02935400	0.25578000	-0.66244700
C	2.70710600	2.66494100	0.50247400	C	2.99068300	-1.10222800	-0.12710500
H	1.92067200	3.08326700	1.13572200	C	2.50944700	-1.05727300	1.19975200
H	3.66784000	2.98859200	0.92507900	C	2.41204900	-2.20288800	2.16696900
H	2.61495900	3.11274800	-0.48980700	H	2.25977700	-3.15541000	1.65287500
Ru	0.79050000	-0.25344200	-0.08776800	H	3.33458300	-2.29079100	2.75645800
Cl	0.34398200	-1.47616000	-2.19163600	H	1.58764800	-2.06760100	2.87197300
H	-1.03172400	0.50349900	1.83774300	C	1.75550000	0.84428800	2.83490900
H	-0.00199100	-1.43843100	0.56199800	H	1.11579500	0.13306800	3.36495900
TSA6"-A7				H	2.63819000	1.02117700	3.46390100
C	-0.07984000	2.80751300	-1.92664800	H	1.21516500	1.79151300	2.75743100
H	-0.15133900	3.81347600	-2.33214700	C	3.49426700	-2.30771400	-0.85969900
H	0.39111100	2.04935700	-2.54412100	H	3.16990300	-3.23620000	-0.38349500
C	-0.59452100	2.50108100	-0.71627300	H	3.14286100	-2.31971800	-1.89443500
C	-1.28759500	3.53628200	0.14519000	H	4.59236800	-2.30729100	-0.87781400
H	-2.36555300	3.35179200	0.20088100	C	3.61135400	0.62738600	-1.99451800
H	-0.90653400	3.51911300	1.17207500	H	4.70925800	0.59627100	-1.96708400
H	-1.13652400	4.54045400	-0.26075500	H	3.28870600	-0.06307300	-2.77945500
C	-0.51039600	1.13164900	-0.24595400	H	3.31975200	1.63709300	-2.29478100
C	-1.22071800	0.28715400	0.65549700	C	2.63679000	2.62853900	0.33552600
C	-2.60638900	-0.34819600	0.37334600	H	1.85882800	3.07443700	0.96001100
O	-2.74807400	-1.57181400	1.11948400	H	3.60377500	2.96999900	0.72877700
C	-2.34680500	-2.80417400	0.52646000	H	2.53066500	3.03109400	-0.67451000
H	-2.31285700	-3.53361100	1.34162200	Ru	0.74905000	-0.26810900	-0.14800600
H	-3.06889200	-3.16031200	-0.22000800	Cl	0.28193100	-1.73271100	-2.09281200
H	-1.35892800	-2.75478700	0.05791600	H	-1.14450200	0.52232600	1.72188900
C	-2.94693800	-0.49215600	-1.12047900	H	-0.25722500	-1.20234300	0.65740500
C	-4.42246500	-0.83671100	-1.34310100	TSA6'-E'			
C	-5.08232900	0.14791200	0.68580200	Ru	1.00523900	0.27221800	0.00964900
C	-3.65763500	0.58884700	1.02050600	Cl	2.47686100	2.27006800	-0.21463800
H	-4.65659100	-0.81458100	-2.41213400	O	-2.14147500	-0.70157300	-1.29375400
H	-2.73752500	0.46723900	-1.60670400	C	-0.42429000	1.51608500	0.22679200
H	-2.30416400	-1.23271600	-1.60205100	C	-1.09081200	0.36994100	0.70980400
H	-5.80868600	0.86154100	1.08789200	C	-2.25752600	0.22418400	-2.36890500

H	-1.79040600	-0.25616200	-3.23372300	C	-4.17430300	-2.00328800	0.41152300
H	-3.30386300	0.44066600	-2.62052800	H	-2.82978200	-1.25293300	1.90703200
H	-1.74197100	1.17214400	-2.18572800	H	-2.06617400	-2.30861300	0.71629800
C	2.68204900	-0.86461300	1.07808100	C	-4.87947100	0.14825100	-0.20470900
C	1.48174600	-1.62024800	1.17058700	H	-3.57047100	1.11434600	1.19455800
C	1.10446300	-2.02052400	-0.17810600	H	-3.33502100	1.64398200	-0.46630700
C	2.11525900	-1.54377400	-1.08004900	H	-4.48466700	-2.85550200	1.02444500
C	3.08452100	-0.84735800	-0.32229900	H	-4.14597200	-2.33143100	-0.63925800
C	3.50220700	-0.31047600	2.20304800	H	-5.68226600	0.86781200	-0.01361700
H	3.86587700	0.69290900	1.96331500	H	-4.91420900	-0.11611300	-1.27298600
H	2.92402000	-0.25047500	3.12879600	O	-5.17280300	-1.00012400	0.58377300
H	4.37704000	-0.94561300	2.39629000	E'			
C	0.80385900	-2.04639700	2.43739400	Ru	-0.97848100	0.05128500	0.24190000
H	0.90132400	-1.28995200	3.22092100	Cl	-1.74871200	1.18581500	2.34456900
H	-0.25943000	-2.23945000	2.28304900	O	2.19127000	-1.19432500	0.84664300
H	1.25848300	-2.97159400	2.81646100	C	0.58624400	1.78165100	0.23700600
C	0.08357800	-3.05313200	-0.56084300	C	1.14984600	0.72040100	-0.46856700
H	-0.67819800	-2.65711800	-1.23555100	C	1.71360600	-0.98113800	2.16609300
H	0.58523600	-3.88757800	-1.06667800	H	1.64494000	-1.96883500	2.63131300
H	-0.41566600	-3.46257000	0.31922500	H	2.39034400	-0.36594300	2.77273700
C	2.15530800	-1.82207000	-2.55342300	H	0.71556800	-0.52339700	2.18542000
H	2.68401700	-1.03641000	-3.09919500	C	-2.57705900	-0.24485900	-1.18263000
H	2.67484200	-2.76868100	-2.75313100	C	-1.39408400	-0.88483400	-1.71351500
H	1.14856200	-1.90571300	-2.97103200	C	-0.99733900	-1.90656800	-0.78760000
C	4.38087500	-0.30439900	-0.82984000	C	-1.96731700	-1.93452500	0.29222300
H	4.65562900	0.61953300	-0.31880400	C	-2.95617200	-0.94475300	0.02769300
H	5.17572400	-1.04228800	-0.65362400	C	-3.40377900	0.79971600	-1.86716100
H	4.34697000	-0.10388200	-1.90348100	H	-3.87673700	1.47383300	-1.14798900
H	0.17071700	0.89779400	-1.25905400	H	-2.80649900	1.40182300	-2.55521700
H	-1.16087500	0.30129700	1.79852600	H	-4.20399900	0.32430300	-2.45135800
C	-0.73785800	2.93281200	0.13101800	C	-0.79996200	-0.63351300	-3.06585000
C	-1.34573900	3.53240300	1.38407800	H	-0.93858500	0.40164000	-3.38677600
H	-2.27770800	3.02978000	1.66198400	H	0.26880000	-0.85777300	-3.09543100
H	-0.65959500	3.43343200	2.23352700	H	-1.29105900	-1.27286100	-3.81168300
H	-1.55378300	4.59518100	1.23531000	C	0.08269500	-2.92817900	-0.97679300
C	-0.54532300	3.65597300	-0.98555700	H	0.74230100	-2.98660900	-0.10844600
H	-0.84352800	4.69978700	-1.02904200	H	-0.36564600	-3.91745500	-1.13724100
H	-0.10077300	3.22431000	-1.87544000	H	0.69862200	-2.70144600	-1.84935900
C	-2.35566800	-0.25475200	0.05238100	C	-1.94655300	-2.90446900	1.43299800
C	-2.79534900	-1.50748600	0.84157000	H	-2.46479100	-2.51076500	2.31055000
C	-3.52309400	0.76508200	0.15733500	H	-2.44303200	-3.84125400	1.14601800

H	-0.92180000	-3.15383500	1.72189200
C	-4.19558700	-0.68395200	0.82557800
H	-4.44718200	0.37863100	0.84500100
H	-5.04273100	-1.22068300	0.37754700
H	-4.09205800	-1.02362400	1.85770900
H	0.84320500	1.89417900	1.28636000
H	1.06155600	0.74608400	-1.55053300
C	-0.00147100	2.99947600	-0.36439100
C	-0.10812700	3.11339600	-1.86671800
H	0.87168100	2.99524200	-2.34568000
H	-0.76315900	2.34607900	-2.28912500
H	-0.50788500	4.09009400	-2.15252400
C	-0.33833800	4.03766100	0.42521500
H	-0.71506900	4.96707700	0.00661700
H	-0.25675600	3.98019400	1.50648100
C	2.41803800	-0.04934900	0.00326100
C	3.12262800	-0.64481600	-1.23639000
C	3.42685600	0.92940700	0.66043500
C	4.48981100	-1.23389500	-0.88836500
H	3.25614700	0.14953100	-1.97929800
H	2.49028600	-1.41792500	-1.68406300
C	4.77786900	0.25692000	0.91295400
H	3.57310100	1.77545900	-0.02002200
H	3.03928200	1.34257300	1.59643100
H	5.00202000	-1.57328100	-1.79442300
H	4.36736000	-2.09880600	-0.21936700
H	5.49760500	0.98418500	1.30252800
H	4.67236300	-0.54632700	1.65896100
O	5.34526000	-0.26419600	-0.28678800

B1

C	-0.37830700	-0.60290400	-2.90394600
C	0.62947200	-1.42723900	-2.36733200
C	1.01690400	-2.75132300	-2.99312400
H	1.84303500	-2.58478500	-3.69666400
H	1.35689700	-3.47861200	-2.25290500
H	0.18378600	-3.17310900	-3.55930500
C	1.50635400	-0.90249200	-1.36940300
C	2.19499100	-0.51041100	-0.43837100
C	3.12545400	-0.05047900	0.61011600
O	3.10365800	1.36755000	0.74451400
C	4.55226800	-0.57989600	0.29200900
C	5.50823000	-0.32521900	1.45860000
C	3.76954100	-0.35906000	3.04492800
C	2.69882400	-0.62444300	1.98724600
H	6.47998600	-0.78493000	1.25364100
H	4.49011200	-1.65834300	0.11071800
H	4.93074900	-0.11307000	-0.62304100
H	3.49479400	-0.83629400	3.99052700
H	3.86597300	0.72255300	3.22291400
H	2.54559300	-1.70417900	1.88946400
H	1.74962900	-0.16656300	2.28232100
H	5.66637100	0.75392200	1.60003800
O	5.03006300	-0.91008900	2.66677700
C	-1.51375900	-2.55466700	0.95012900
C	-1.35278000	-3.30716400	-0.27244300
C	-2.30367100	-2.80514200	-1.22904200
C	-3.00614700	-1.69862000	-0.61572000
C	-2.51848300	-1.57009000	0.75135600
C	-3.05663400	-0.61786600	1.77521800
H	-3.27777100	0.35463700	1.33009300
H	-3.98335700	-1.00981700	2.21474900
H	-2.34493600	-0.45776500	2.58934300
C	-0.75436700	-2.81210700	2.21555400
H	-0.68087700	-1.91683900	2.83754600
H	-1.26318900	-3.58493100	2.80748500
H	0.25600900	-3.17508200	2.01098500
C	-4.18565500	-0.97191800	-1.18740500
H	-4.25150100	0.04703300	-0.79895300
H	-4.13427300	-0.91503800	-2.27791000
H	-5.11794600	-1.49101000	-0.92507800

C	-2.64454900	-3.41088500	-2.55737100
H	-3.45376500	-4.14328100	-2.43462200
H	-2.99429500	-2.65665700	-3.26684000
H	-1.79702600	-3.93347100	-3.00613800
C	-0.50528700	-4.53898900	-0.40557800
H	0.50372400	-4.38935800	-0.00907000
H	-0.95434000	-5.36842800	0.15661000
H	-0.41674100	-4.86116800	-1.44440800
Ru	-0.93722900	-1.15746900	-0.80158500
Cl	-1.14934800	1.30951900	-0.48209900
H	-0.32480900	0.47676700	-2.83804300
H	-0.97949100	-1.00742800	-3.71422400
Si	3.46297600	2.66348000	-0.29035700
C	2.92537000	2.38102400	-2.06511500
H	3.15448600	3.28091800	-2.65064300
H	3.44542000	1.54420300	-2.54300500
H	1.84879400	2.20324000	-2.14114500
C	2.50659900	4.08732700	0.46132000
H	1.42922400	3.88879100	0.44581300
H	2.79954600	4.26429900	1.50237900
H	2.68303300	5.01584300	-0.09468100
C	5.30425300	3.04317100	-0.26158500
H	5.50034700	3.96676900	-0.82105300
H	5.67478000	3.19674900	0.75792600
H	5.90478700	2.25253800	-0.72468300

B2

C	-0.57594200	3.44555900	0.76762800
H	-0.64708600	4.36206900	1.34740500
H	-0.61085500	3.53521200	-0.31406700
C	-0.47238500	2.25156800	1.37734000
C	-0.41251600	2.12549200	2.88213800
H	-1.29172400	1.60065900	3.26825900
H	0.46453200	1.55169200	3.19913300
H	-0.36557500	3.11218600	3.35167700
C	-0.45352100	1.02958100	0.58291800
C	-1.06896100	-0.00144000	0.11781500
C	-2.47249400	-0.55379500	-0.04398200
O	-3.20676700	-0.31561300	1.16746600
C	-2.51635700	-2.04427500	-0.43871800
C	-3.92034500	-2.48157300	-0.86455400
C	-4.54109700	-0.31154100	-1.50965800

C	-3.17634600	0.27261000	-1.15108800	H	-3.93966800	-3.44430500	2.09720300
H	-3.89347500	-3.50691800	-1.24737300	C	-1.53440600	-1.60870100	3.27083300
H	-1.82930300	-2.19067900	-1.27443800	H	-1.62399200	-2.07388700	4.26083200
H	-2.16457500	-2.66755200	0.39131200	H	-1.08034500	-2.35126600	2.60528600
H	-4.98124300	0.23461000	-2.35023200	H	-0.84147800	-0.76797900	3.36258100
H	-5.22903500	-0.22958800	-0.65310300	C	-4.01463100	0.18949700	3.80437700
H	-2.53909000	0.26989200	-2.04035400	H	-4.07498500	-0.18635800	4.83285400
H	-3.28367900	1.30613600	-0.80516400	H	-3.44956300	1.12715900	3.82574200
H	-4.61855200	-2.45830200	-0.01596500	H	-5.03531200	0.42745500	3.48293800
O	-4.43267300	-1.67160400	-1.92156800	B3			
C	2.54733900	-0.27635400	0.70221900	C	0.87981500	-2.98595600	-2.01409500
C	2.65396900	1.07546800	0.21377000	H	0.90782700	-3.74659900	-2.78944200
C	2.87146100	1.02171300	-1.21122400	H	1.52198000	-3.11019400	-1.14966200
C	2.94284400	-0.34610100	-1.59954200	C	0.03532700	-1.94493700	-2.11261700
C	2.69992200	-1.16098800	-0.43474700	C	-0.89751400	-1.77959700	-3.29659300
C	2.77146800	-2.65575400	-0.37263500	H	-1.94289000	-1.74950200	-2.96919200
H	2.43097100	-3.11283400	-1.30437000	H	-0.70123100	-0.84191500	-3.82975900
H	3.80664800	-2.98037800	-0.19932900	H	-0.78090600	-2.60723000	-4.00222700
H	2.15974500	-3.05084700	0.44238800	C	-0.07767000	-0.91024500	-1.10497500
C	2.48825100	-0.71696300	2.13267800	C	-0.69657600	0.01211700	-0.50991200
H	1.86694400	-1.60814000	2.25305500	C	-1.97074700	0.80400300	-0.34362300
H	3.49681500	-0.96627100	2.48884100	O	-3.09381400	-0.06503500	-0.17822400
H	2.09021600	0.06521200	2.78207100	C	-2.23495300	1.57745400	-1.66428200
C	3.26831600	-0.85271900	-2.96903300	C	-3.45196300	2.49373000	-1.53611000
H	2.79622100	-1.81635400	-3.16490000	C	-3.15747300	2.74612500	0.78521300
H	2.94852400	-0.15653700	-3.74773900	C	-1.92696600	1.83765900	0.80270500
H	4.35491600	-0.98187200	-3.06176100	H	-3.57541100	3.09142100	-2.44487900
C	3.08072800	2.21158000	-2.09494000	H	-1.35411100	2.17986600	-1.90596400
H	4.13834900	2.50789800	-2.08664400	H	-2.38946000	0.85810200	-2.47427600
H	2.80553300	1.99864600	-3.13058900	H	-3.06315900	3.52572900	1.54775700
H	2.49665000	3.07037800	-1.75381200	H	-4.06628500	2.16595800	1.00638400
C	2.77956300	2.32058400	1.03459900	H	-1.02953700	2.45406900	0.68577900
H	2.40932400	2.18381000	2.05154400	H	-1.85755900	1.32984300	1.76985700
H	3.83994300	2.59723400	1.10196700	H	-4.36370200	1.89425500	-1.39427800
H	2.24616800	3.16325000	0.58908000	O	-3.30095600	3.42037500	-0.46267600
Ru	0.87497800	-0.00333600	-0.65285200	C	2.27057100	1.53962100	-0.82441200
Cl	-0.01584800	-1.17335300	-2.64145000	C	2.94186100	0.29479200	-1.13984700
Si	-3.23952500	-1.09030400	2.67247900	C	3.59713100	-0.16955000	0.04617100
C	-4.34152200	-2.61674300	2.69072900	C	3.30575100	0.74526200	1.11203200
H	-4.43264700	-2.97542500	3.72442100	C	2.50103600	1.82158200	0.55917300
H	-5.35441700	-2.40159000	2.33347900	C	2.10803800	3.07211300	1.28933400

H	1.90124500	2.87747200	2.34482500	C	0.47590900	4.12321900	-0.84921100
H	2.92475100	3.80468800	1.24500700	H	-0.58213700	4.26641800	-1.09492300
H	1.22390500	3.53961100	0.84916300	H	0.56497500	4.19852400	0.24056200
C	1.61530600	2.44305800	-1.82459000	H	1.04733000	4.93850100	-1.30185300
H	0.93026600	3.14668300	-1.34606300	C	0.31322800	1.62725400	-0.76748700
H	2.37517300	3.03065600	-2.35666100	C	-0.65725400	0.99186200	-0.29072200
H	1.05702900	1.87801700	-2.57502500	C	-2.11772200	0.86440200	0.04697700
C	3.90496700	0.70761800	2.48879300	O	-2.72392300	-0.18287300	-0.69301700
H	3.27132600	1.21770500	3.21905000	C	-2.81661700	2.17684700	-0.40308900
H	4.05544600	-0.31894600	2.83292700	C	-4.26401200	2.22418700	0.08460600
H	4.88353200	1.20593400	2.49701000	C	-3.79918600	0.88218100	1.96160700
C	4.47475100	-1.37682800	0.15731400	C	-2.32728000	0.72294000	1.57323600
H	5.52943200	-1.07649500	0.10096500	H	-4.72187300	3.18258700	-0.17876400
H	4.32456400	-1.89389800	1.10790000	H	-2.27330400	3.03030800	0.01382500
H	4.28757600	-2.08833300	-0.64990500	H	-2.78050800	2.24475600	-1.49490800
C	3.10975700	-0.26893600	-2.51833900	H	-3.90117600	0.88296800	3.05122200
H	2.25106400	-0.04481600	-3.15470500	H	-4.39745700	0.04522900	1.57083600
H	3.99555400	0.17333700	-2.99412400	H	-1.74555300	1.50722800	2.06981000
H	3.24547300	-1.35195400	-2.50562700	H	-1.94711900	-0.24087200	1.92378900
Ru	1.33137300	-0.06039100	0.45160500	H	-4.85228300	1.42374200	-0.38876100
Cl	1.21455100	-2.38201700	1.45817300	O	-4.34004500	2.11822000	1.50493200
H	0.16129200	0.51924400	1.65864300	C	2.14015500	0.08041300	1.91825500
H	0.72927300	0.12292200	2.10770700	C	3.03798500	0.71910200	0.98383000
Si	-3.51597600	-1.32714600	0.86680600	C	3.52079400	-0.27213800	0.09067400
C	-5.38991500	-1.34282300	0.76564600	C	2.97674300	-1.55875800	0.48346000
H	-5.80631300	-2.15678100	1.37102900	C	2.16563300	-1.34384000	1.64467800
H	-5.82319600	-0.40448900	1.12987200	C	1.57427200	-2.41362800	2.51654500
H	-5.73448400	-1.48969700	-0.26442400	H	1.31381600	-3.30639800	1.94353400
C	-2.97309700	-1.05248900	2.64433100	H	2.30432100	-2.71035300	3.28075700
H	-1.88362700	-1.04319800	2.75296300	H	0.67727900	-2.06805100	3.03563200
H	-3.37189800	-0.12576600	3.07059000	C	1.54537900	0.73148700	3.13296100
H	-3.34789600	-1.88052400	3.25998900	H	0.68477200	0.17375200	3.50890600
C	-2.83718400	-2.96850900	0.26297700	H	2.28677900	0.77998800	3.94164400
H	-3.07543800	-3.14581700	-0.79167200	H	1.22152300	1.75487100	2.92636800
H	-1.75210600	-3.03443000	0.38691600	C	3.38374200	-2.87464300	-0.10836500
H	-3.28496200	-3.78767700	0.84015500	H	2.69619200	-3.67436000	0.17815200
TSB3-B4				H	3.40614700	-2.82473000	-1.20015400
C	1.94228500	2.67738000	-2.27297100	H	4.38732200	-3.15903400	0.23490600
H	2.38995300	3.56914500	-2.70264700	C	4.49350400	-0.07776500	-1.03085800
H	2.27563900	1.70938300	-2.62955800	H	5.45711300	-0.53928100	-0.77938900
C	0.97332000	2.78158100	-1.34815100	H	4.12976200	-0.54779400	-1.94939400

H	4.67319900	0.98006500	-1.23432700
C	3.44925900	2.15892300	1.02259100
H	2.68773700	2.78446700	1.49438600
H	4.36942200	2.26505300	1.61243900
H	3.64715200	2.55686800	0.02530700
Ru	1.14397600	-0.36483200	-0.05840100
Cl	1.27592700	-0.80335600	-2.54486900
H	-0.12549800	-0.85043500	0.74188400
H	0.17375600	-1.60818800	-0.26373700
Si	-3.14065400	-1.81558300	-0.64942500
C	-5.00277500	-1.88998900	-0.89823700
H	-5.33042900	-2.92807300	-1.03590900
H	-5.55328400	-1.48568500	-0.04133600
H	-5.31057400	-1.32991800	-1.78864900
C	-2.70938600	-2.71403600	0.94478100
H	-1.63511700	-2.71700300	1.15340000
H	-3.22973100	-2.30245400	1.81590200
H	-3.02503900	-3.76095500	0.84779700
C	-2.29935900	-2.63930800	-2.10767500
H	-2.62500100	-2.18941400	-3.05270900
H	-1.20953400	-2.54593300	-2.05819200
H	-2.54958100	-3.70660600	-2.14735500

B4

C	0.03346900	1.06009800	-1.21779500
C	-0.79539100	0.69243800	-0.35356900
C	-2.15665800	0.74919600	0.28136400
C	-2.08443300	1.51828300	1.62526400
C	-3.09791800	1.54841100	-0.66135300
C	-3.48256600	1.81948500	2.16635700
C	-4.43576700	1.85376600	0.01505600
H	-3.41472400	2.42865900	3.07301900
H	-3.99817100	0.88181900	2.42309700
H	-5.04655200	2.49139500	-0.63188600
H	-4.99577800	0.92476400	0.20005700
O	-2.68566600	-0.53021300	0.58602100
C	0.53253900	1.79830500	-2.36075900
C	1.20213200	1.20454200	-3.36348400
C	0.22310800	3.28072400	-2.35245700
H	-0.85892400	3.45532000	-2.33706400
H	0.63735000	3.76488900	-1.46064500
H	0.63931900	3.76868600	-3.23820800

H	1.41183200	0.14020700	-3.34668500
H	1.53289500	1.78156600	-4.22247000
O	-4.25949200	2.56894400	1.23484200
Ru	1.16260900	-0.27216800	0.24889200
C	3.24642800	1.01922500	0.12370900
C	3.52435600	-0.32323800	-0.22112300
C	2.59645600	1.01983700	1.41278500
C	3.11558500	-1.18643900	0.88143000
C	2.59814500	-0.34836300	1.91540500
C	3.40558400	-2.65436100	0.96314900
H	4.47143600	-2.82510100	1.16439000
H	2.83439600	-3.13164900	1.76286400
H	3.15592500	-3.15492400	0.02405300
C	2.26879500	-0.76604000	3.31922300
H	1.91007700	-1.79684200	3.35911200
H	3.16688300	-0.69822900	3.94679800
H	1.50381200	-0.12586700	3.76476600
C	2.26827600	2.24778600	2.21039400
H	3.17639200	2.65186100	2.67660300
H	1.84469800	3.03465200	1.58057900
H	1.55350200	2.03163100	3.00737700
C	3.59291500	2.23326400	-0.68205200
H	4.64420500	2.50538800	-0.52092600
H	3.45752100	2.06396900	-1.75317100
H	2.98639300	3.09476600	-0.39337200
C	4.20211300	-0.80641100	-1.46358400
H	4.31102300	-0.00745800	-2.20028100
H	5.20460200	-1.18383900	-1.22439600
H	3.63678000	-1.62421800	-1.92062300
Cl	0.90215200	-1.97396700	-1.60878700
H	-1.52643800	0.92051800	2.35320000
H	-1.54613100	2.45942700	1.46944400
H	-2.61011800	2.49443800	-0.91829700
H	-3.25953400	0.99496200	-1.59050600
H	0.24849300	-1.34874300	0.95104500
H	0.28382300	0.27298800	1.42169500
Si	-3.19305400	-1.89696100	-0.27959700
C	-2.21022900	-3.34538100	0.39184200
H	-2.63073600	-4.29759300	0.04551600
H	-1.17001000	-3.29317700	0.05449300
H	-2.21794200	-3.35957500	1.48797300

C	-5.01400300	-2.13601400	0.12423800
H	-5.19405500	-2.11194200	1.20523700
H	-5.64114800	-1.36450500	-0.33646600
H	-5.36785600	-3.10698600	-0.24408500
C	-2.96635400	-1.75986900	-2.13716100
H	-3.64528200	-1.03473800	-2.59792300
H	-1.93697500	-1.49557200	-2.39720100
H	-3.17782600	-2.73594900	-2.59278900

TSB4-B5

C	-0.64101500	1.42007800	-0.27984100
C	-1.41582200	0.42720300	-0.15406500
C	-2.78870500	-0.18042000	0.00288200
C	-2.95469200	-0.71865000	1.44762600
C	-3.85726800	0.92018400	-0.21351800
C	-4.40232200	-1.12485000	1.72380000
C	-5.25360400	0.42237300	0.16902500
H	-4.51918700	-1.42822900	2.76869300
H	-4.68496300	-1.97689300	1.08709800
H	-5.97533900	1.24183300	0.09596300
H	-5.58064900	-0.37781300	-0.51088400
O	-2.97862400	-1.29116900	-0.85810100
C	-0.40641100	2.85252600	-0.34319100
C	0.58253600	3.38630200	-1.08067000
C	-1.35060600	3.71275000	0.47164800
H	-2.37378900	3.64964900	0.08520700
H	-1.38058200	3.38926500	1.51820000
H	-1.03886000	4.76052100	0.44162300
H	1.23928300	2.76337200	-1.67752900
H	0.71842400	4.46351200	-1.12090100
O	-5.29990200	-0.03637400	1.51719700
Ru	0.73507300	-0.32353600	-0.27896800
C	2.26323700	0.67528800	1.31837100
C	2.99154600	0.26897600	0.17211900
C	1.55424100	-0.47413600	1.82808500
C	2.78581600	-1.15709200	-0.02588600
C	1.93654500	-1.62370800	1.03403400
C	3.53160400	-1.99295800	-1.02297600
H	4.55948300	-2.17264800	-0.68090400
H	3.05501800	-2.96511400	-1.16960300
H	3.58610300	-1.49357100	-1.99359700
C	1.62436400	-3.05628400	1.35854800

H	1.65076100	-3.68592400	0.46632700
H	2.36412500	-3.44956400	2.06813800
H	0.63811400	-3.16389500	1.81634500
C	0.78419200	-0.51604900	3.11553600
H	1.47394500	-0.61168000	3.96442100
H	0.20062400	0.39502700	3.27182200
H	0.10109200	-1.36765900	3.14972300
C	2.26917400	2.03967900	1.93710400
H	3.13348700	2.14429100	2.60619600
H	2.33660000	2.82966200	1.18530400
H	1.37271100	2.21516600	2.53629600
C	3.89268800	1.11974200	-0.66753000
H	3.76484300	2.18235700	-0.44922400
H	4.94267900	0.86353100	-0.47529800
H	3.70101900	0.96174000	-1.73259700
Cl	1.01210300	0.24593900	-2.72612900
H	-2.29241300	-1.57917100	1.59065200
H	-2.65887400	0.06329000	2.15495200
H	-3.60751000	1.77441400	0.42249300
H	-3.84436400	1.26359500	-1.25191100
H	0.27584700	-1.63116300	-1.02905000
H	-0.58879400	-1.00111900	0.28227900
Si	-3.17207300	-1.55980500	-2.52251300
C	-1.99663300	-2.95721400	-2.95005200
H	-2.17868800	-3.31751000	-3.96987100
H	-0.95323800	-2.63008700	-2.89370800
H	-2.12411100	-3.80866800	-2.27162300
C	-4.93853700	-2.14174200	-2.79919300
H	-5.21849100	-2.92612200	-2.08672200
H	-5.66676400	-1.32846600	-2.70672300
H	-5.04696300	-2.56120400	-3.80725700
C	-2.81239800	-0.05930300	-3.58586700
H	-3.55244100	0.73889700	-3.46669900
H	-1.81729400	0.34805700	-3.38069200
H	-2.83070100	-0.36090800	-4.64132000

B5

C	-0.11599600	-1.32464600	-0.29091300
C	0.82246700	-0.56724100	0.25761900
C	2.35655600	-0.59965000	0.35720300
C	2.78024200	-1.41670600	1.60457800
C	2.99917600	-1.23352400	-0.89534400

C	4.29700000	-1.61197900	1.64242300	H	-4.12853500	-0.66325200	-2.16804800
C	4.49956600	-1.46016800	-0.69981200	Cl	-1.13095500	0.45084000	-2.65525400
H	4.57904700	-2.26272400	2.47623500	H	2.44607800	-0.89071000	2.50568600
H	4.79976300	-0.64264500	1.77961700	H	2.29242000	-2.39491700	1.58255400
H	4.91478200	-2.00871500	-1.55110400	H	2.51710300	-2.19538500	-1.09260100
H	5.02748700	-0.49644900	-0.62993400	H	2.82225300	-0.59749600	-1.76737600
O	2.85818400	0.71274600	0.58340400	H	-1.06304400	1.87098800	-0.46210900
C	-0.22819800	-2.68766800	-0.80872800	H	0.45677600	0.40871500	0.71562300
C	-0.88142800	-2.95746100	-1.95535900	Si	2.97940600	2.20119300	-0.20680000
C	0.36566600	-3.80573200	0.02661800	C	1.85168800	3.41055100	0.68600000
H	1.45927600	-3.75502300	0.05306400	H	2.04286500	4.43695200	0.34933500
H	0.01851300	-3.75255800	1.06421600	H	0.79422600	3.19299000	0.49914800
H	0.08418400	-4.78144300	-0.38036200	H	2.01737500	3.38387100	1.76946400
H	-1.30964400	-2.16152700	-2.55417600	C	4.76169300	2.74483500	0.02422200
H	-0.96029900	-3.97831600	-2.32024500	H	5.04862100	2.74580300	1.08208900
O	4.77138800	-2.24808200	0.45729000	H	5.45982200	2.09045600	-0.50992600
Ru	-1.40317500	0.34253600	-0.15490200	H	4.90898700	3.76256700	-0.35752600
C	-2.93559400	-0.96901600	1.07100200	C	2.55639300	2.15334600	-2.03453800
C	-3.50210700	-0.41427800	-0.12538300	H	3.29569100	1.59372500	-2.61790200
C	-2.48184200	0.11276200	1.89306600	H	1.56806500	1.72376200	-2.23081200
C	-3.46045300	1.03409100	-0.01341900	H	2.54862000	3.18025300	-2.42274300
C	-2.82915300	1.35328900	1.24343600	TSB5-B6			
C	-4.13529600	1.98927100	-0.95145100	C	1.32089000	3.25384400	-1.18549300
H	-5.21309200	2.02661900	-0.74495600	H	1.46036000	4.31008600	-1.40224400
H	-3.73766800	3.00166000	-0.84838500	H	1.90725500	2.53413500	-1.74353900
H	-4.00312000	1.68151000	-1.99117500	C	0.40241100	2.85524500	-0.27809900
C	-2.70336300	2.71610400	1.86032200	C	-0.40438400	3.88540700	0.49014400
H	-2.69978000	3.50261800	1.10301600	H	-1.46408900	3.86327400	0.21756700
H	-3.55004500	2.90211000	2.53413000	H	-0.34253200	3.71029900	1.56943100
H	-1.78793000	2.81107700	2.44980900	H	-0.02987700	4.89229800	0.28512200
C	-1.85027800	-0.01524700	3.24630200	C	0.27070400	1.44417700	0.06920200
H	-2.62158200	-0.05834400	4.02640000	C	-0.70882500	0.68390400	0.65736700
H	-1.25004700	-0.92516800	3.32842800	C	-2.23226100	0.69341800	0.43270000
H	-1.20585400	0.83868300	3.47077300	O	-2.70706000	-0.63863600	0.60935000
C	-2.91182300	-2.42330200	1.42604600	C	-2.64756300	1.27647600	-0.93101100
H	-3.89191300	-2.71938500	1.82273200	C	-4.16232200	1.46808600	-1.02940800
H	-2.70959700	-3.04966200	0.55399500	C	-4.41087700	1.66793900	1.30408200
H	-2.16725300	-2.64264400	2.19431700	C	-2.91063100	1.51580200	1.56007300
C	-4.18657300	-1.18574600	-1.21119500	H	-4.41886000	1.99047800	-1.95630700
H	-3.74631400	-2.17802300	-1.33687400	H	-2.16779800	2.25085000	-1.05885300
H	-5.24864300	-1.32115600	-0.96588300	H	-2.28985500	0.63437900	-1.74017400

H	-4.86229600	2.32502200	2.05427300
H	-4.90972900	0.68856400	1.36435900
H	-2.45898900	2.50870700	1.61424100
H	-2.74166000	1.01274800	2.51859400
H	-4.68064500	0.49672800	-1.03915400
O	-4.66469200	2.27129600	0.03687000
C	2.21831800	-0.78150100	1.79169700
C	2.89874900	0.40587100	1.34338500
C	3.52461900	0.11148200	0.09112100
C	3.27527500	-1.28818400	-0.21573700
C	2.49139000	-1.83883400	0.85127100
C	2.14288400	-3.28547700	1.04334600
H	2.06418000	-3.81312100	0.09060100
H	2.92410000	-3.78076000	1.63531000
H	1.19933900	-3.40888600	1.57983500
C	1.49694600	-0.93289300	3.09738700
H	0.78124000	-1.75858500	3.06711500
H	2.20632300	-1.14040200	3.90900500
H	0.95314700	-0.02348600	3.36996100
C	3.89746200	-2.03877000	-1.35509700
H	3.37608900	-2.97971800	-1.54780700
H	3.87587100	-1.44973100	-2.27529000
H	4.94599500	-2.27625000	-1.13120200
C	4.41590900	1.01880700	-0.69983800
H	5.46935500	0.82387800	-0.45786400
H	4.28517900	0.86093800	-1.77303900
H	4.21690400	2.07152000	-0.48412400
C	3.00708000	1.69534200	2.10112700
H	2.16119800	1.84415800	2.77666800
H	3.91876400	1.69208000	2.71302900
H	3.06551900	2.55764800	1.43235300
Ru	1.32275100	-0.21963700	-0.27885000
Cl	1.40052900	0.29927400	-2.74815500
H	-0.44042100	-0.03236600	1.43355100
H	0.61142800	-1.49187000	-0.94764300
Si	-2.98431400	-2.08169200	-0.21485500
C	-4.79412600	-2.50244700	0.07118200
H	-5.46723500	-1.80720300	-0.44277900
H	-5.01764800	-3.50942800	-0.30255000
H	-5.04627500	-2.48536300	1.13773800
C	-2.63321500	-2.04170000	-2.05851200

H	-2.78251100	-3.05043600	-2.46554100
H	-3.30460100	-1.37078000	-2.60421800
H	-1.60118500	-1.75066100	-2.27893300
C	-1.91942000	-3.39510800	0.60009900
H	-2.04145900	-3.39161000	1.68952900
H	-2.19009000	-4.39540800	0.24071800
H	-0.85968000	-3.23626900	0.37646400

B6

C	-1.58414700	3.32955300	1.02630500
H	-1.89053100	4.35817900	1.19836600
H	-1.84952100	2.58998600	1.77478500
C	-0.84821000	2.98845100	-0.05579700
C	-0.42389900	4.00169200	-1.09727300
H	0.65279100	4.19521500	-1.04795000
H	-0.63947500	3.64378700	-2.10974300
H	-0.94679400	4.95055400	-0.94833300
C	-0.41894500	1.61369900	-0.18379500
C	0.57934300	0.84198600	-0.81335600
C	2.05789500	0.79817800	-0.37393000
O	2.62833300	-0.44932800	-0.75941800
C	2.26072100	1.11999100	1.11709400
C	3.73472500	1.33381600	1.46561300
C	4.26901800	2.00810000	-0.72613000
C	2.82155300	1.87003800	-1.19847700
H	3.83217200	1.67087300	2.50241500
H	1.72111300	2.04780900	1.34012800
H	1.82010800	0.34196200	1.74357300
H	4.77391200	2.81672000	-1.26445300
H	4.82130500	1.07529300	-0.91722100
H	2.32340700	2.83793000	-1.08569700
H	2.79703800	1.59642800	-2.25934100
H	4.30313500	0.39631200	1.36766800
O	4.33574500	2.34483100	0.65772700
C	-2.43793800	-0.48854100	-1.62712100
C	-3.29141600	0.35183000	-0.80012400
C	-3.52864900	-0.33692300	0.40480800
C	-2.89273600	-1.65050500	0.31185700
C	-2.29079500	-1.76521600	-0.96767000
C	-1.70084300	-3.00008900	-1.58345800
H	-1.33102300	-3.69488800	-0.82586600
H	-2.46395800	-3.52910500	-2.17047000

H	-0.87674000	-2.76364000	-2.26076000	H	-0.67761200	3.27353200	1.69469500
C	-2.05212200	-0.19746400	-3.04820400	H	-1.20708700	4.45738500	0.48434600
H	-1.14032000	-0.72787100	-3.33636200	C	-0.60542300	1.09259600	-0.10692200
H	-2.84650400	-0.51462700	-3.73703100	C	-1.28585200	0.11092800	0.67078100
H	-1.88823200	0.87118000	-3.21429700	C	-2.67599000	-0.47319600	0.32587800
C	-3.02688300	-2.72688800	1.34753200	O	-2.86885300	-1.69193900	1.03446100
H	-2.29008100	-3.52106400	1.20098500	C	-2.95497200	-0.60801600	-1.18032100
H	-2.89075200	-2.32476300	2.35517800	C	-4.41992100	-0.95285000	-1.45618600
H	-4.02345800	-3.18635300	1.30352900	C	-5.14955300	0.06725400	0.53786100
C	-4.35322200	0.11634900	1.57108100	C	-3.73232900	0.50508500	0.90830200
H	-5.29884200	-0.43928200	1.62018900	H	-4.61456000	-0.93832100	-2.53317200
H	-3.82424800	-0.05381800	2.51403600	H	-2.72783100	0.35320500	-1.65546100
H	-4.59732400	1.17967800	1.50605700	H	-2.29255400	-1.34672600	-1.63418800
C	-3.85743400	1.67706100	-1.21347100	H	-5.88199700	0.79712000	0.89758300
H	-3.17148900	2.22920300	-1.86115200	H	-5.37812400	-0.90399900	1.00278200
H	-4.78742300	1.53142100	-1.77934000	H	-3.56056000	1.50574400	0.50140700
H	-4.09059300	2.31050300	-0.35396900	H	-3.62760300	0.55376800	1.99801800
Ru	-1.11839300	-0.10516900	0.19448200	H	-4.65699000	-1.96343300	-1.08903600
Cl	-0.78101000	-0.20677300	2.63774800	O	-5.31770200	-0.00799700	-0.87536800
H	0.49557500	0.68023200	-1.89262700	C	2.16749000	0.23942000	1.32326800
H	0.14572500	-1.04091600	0.18280000	C	2.56344800	1.05928800	0.19052900
Si	3.07499900	-1.96625600	-0.19106300	C	2.92304600	0.18760600	-0.86101200
C	4.92638200	-2.13658300	-0.48287500	C	2.88063100	-1.18270400	-0.34739700
H	5.51434200	-1.46318600	0.15073000	C	2.46320400	-1.14382700	0.99860400
H	5.25530700	-3.15976100	-0.26182700	C	2.40172400	-2.29104200	1.96421600
H	5.18927200	-1.92740800	-1.52629700	H	2.26307500	-3.24637100	1.45246500
C	2.70012400	-2.30333500	1.61903500	H	3.33687800	-2.35678800	2.53673500
H	2.92033500	-3.35773100	1.83140000	H	1.58944300	-2.17249400	2.68559600
H	3.31562200	-1.70205000	2.29615700	C	1.84058200	0.74712900	2.69786100
H	1.64897800	-2.12796800	1.86831000	H	1.21933500	0.03811600	3.25222100
C	2.19261700	-3.23711300	-1.25492300	H	2.75814400	0.90136100	3.28150300
H	2.27043200	-2.99425100	-2.32100800	H	1.31193200	1.70359800	2.66257500
H	2.62955600	-4.23307500	-1.11139200	C	3.31668400	-2.38648900	-1.12563200
H	1.13022800	-3.30389300	-1.00196800	H	3.06150900	-3.31450000	-0.60772200
TSB6-B7				H	2.84487000	-2.41033600	-2.11195500
C	-0.33438500	3.02021000	-1.53031400	H	4.40452800	-2.37528900	-1.27405100
H	-0.43721900	4.07794900	-1.75859100	C	3.42354500	0.55897600	-2.22392100
H	0.05187500	2.37223300	-2.31064200	H	4.50990100	0.41600400	-2.29481200
C	-0.70935700	2.52247100	-0.33345900	H	2.95895800	-0.06357100	-2.99469500
C	-1.25393200	3.40324900	0.77139700	H	3.21077800	1.60487100	-2.45924500
H	-2.29324800	3.15687300	1.01007600	C	2.65720000	2.55525500	0.19326800

H	1.91567100	3.01125100	0.85324800
H	3.64694100	2.86490300	0.55549800
H	2.52477200	2.97919500	-0.80517300
Ru	0.66446500	-0.28894100	-0.27911300
Cl	0.23524200	-1.41019400	-2.44725200
H	-1.18355400	0.17467400	1.75919400
H	-0.35031500	-1.35791900	0.34542000
Si	-2.64164400	-3.35667300	0.94514900
C	-4.26321100	-4.09976400	1.53714000
H	-5.07834900	-3.92245500	0.82651500
H	-4.17172600	-5.18526500	1.66580700
H	-4.56639800	-3.67931600	2.50293400
C	-2.22407200	-4.02335300	-0.75811000
H	-2.03241300	-5.10154200	-0.67757400
H	-3.04319500	-3.89345100	-1.47353000
H	-1.32726600	-3.55900000	-1.18021400
C	-1.27775500	-3.82292900	2.14848900
H	-1.42280600	-3.34679300	3.12523400
H	-1.25637600	-4.90763800	2.31080500
H	-0.29307000	-3.52714000	1.77237500

B7

C	-0.87605200	3.29925600	-0.79123700
H	-0.96186500	4.25055800	-1.31128400
H	-1.23361200	3.25614000	0.23238100
C	-0.30013000	2.23090200	-1.37944500
C	0.20574800	2.31143700	-2.80872000
H	1.29726600	2.26573200	-2.86284200
H	-0.17834500	1.48117400	-3.41140500
H	-0.11667500	3.24647500	-3.27552900
C	-0.16437400	0.96727800	-0.63481700
C	1.12257600	0.16079400	-0.77364200
C	2.43552400	0.66315300	-0.08106000
O	3.47889700	-0.28382200	-0.34614500
C	2.25596700	0.82958400	1.43891800
C	3.51179500	1.40317600	2.09584300
C	4.17171700	2.50074400	0.11814900
C	2.94744600	1.99973900	-0.65235900
H	3.32813300	1.60884500	3.15515500
H	1.41212800	1.50043600	1.62394100
H	2.00320100	-0.13069500	1.89897800
H	4.47091900	3.49089800	-0.24079300

H	5.01880400	1.81400700	-0.03158400
H	2.15691400	2.75288500	-0.58340200
H	3.21062100	1.87100200	-1.70817300
H	4.34271200	0.68311200	2.02999100
O	3.89706200	2.64600200	1.50949000
C	-2.53773300	-1.29444200	-1.15239100
C	-3.04006300	0.04497200	-1.28616100
C	-3.63654100	0.39716000	-0.01916600
C	-3.73041600	-0.82467600	0.78807000
C	-3.03811800	-1.83506400	0.12176500
C	-2.79887100	-3.24233800	0.57811400
H	-3.05266500	-3.37804900	1.63187800
H	-3.40366600	-3.94709500	-0.00722300
H	-1.75154900	-3.53287400	0.44349700
C	-1.90528900	-2.12794500	-2.22811200
H	-1.20586200	-2.85714500	-1.80826800
H	-2.66605100	-2.69083500	-2.78617800
H	-1.35718900	-1.51046700	-2.94425500
C	-4.39491900	-0.89115500	2.12799100
H	-4.27997700	-1.87509400	2.58917100
H	-3.97827900	-0.14759200	2.81500600
H	-5.46920700	-0.68918000	2.03260100
C	-4.36957900	1.67033300	0.27721100
H	-5.42153800	1.58682400	-0.03062600
H	-4.35650000	1.90018400	1.34598800
H	-3.93397600	2.51740100	-0.25861100
C	-3.09114900	0.87046300	-2.53427900
H	-2.34720600	0.54647000	-3.26552800
H	-4.07944500	0.76677900	-3.00204000
H	-2.93328100	1.93268300	-2.33270600
Ru	-1.51201400	0.00276400	0.28392500
Cl	-1.11205500	0.49775100	2.64648300
H	1.35242800	0.03395600	-1.84131300
H	0.93955000	-0.84459800	-0.36970900
Si	3.64628500	-1.95952900	-0.32701300
C	5.50033300	-2.22391300	-0.21829900
H	5.90998500	-1.82577900	0.71690400
H	5.74398900	-3.29234900	-0.25653400
H	6.02598700	-1.73532800	-1.04645500
C	2.79702900	-2.78829200	1.13221700
H	2.98891600	-3.86855900	1.09901500

H	3.17377700	-2.42108800	2.09300100
H	1.70979200	-2.65334300	1.12185300
C	3.00200900	-2.70861800	-1.92853900
H	3.39349300	-2.17955200	-2.80504400
H	3.31623200	-3.75654600	-2.01174500
H	1.90848800	-2.69207500	-1.98990500

B8

C	0.17677700	-0.61134300	-0.24888800
C	1.17904800	-1.03857900	0.76967700
C	2.70317600	-0.86238900	0.47781800
C	3.47957000	-1.68998200	1.53289500
C	3.12044100	-1.37095600	-0.91609600
C	4.97931200	-1.69044900	1.24583800
C	4.64273600	-1.41824200	-1.07018200
H	5.50845600	-2.33671400	1.95337100
H	5.38395600	-0.67164300	1.34556100
H	4.91378400	-1.88013100	-2.02482700
H	5.06267000	-0.40035800	-1.05964500
O	3.10370200	0.48582300	0.69085300
C	-0.16370500	-1.23282200	-1.49670900
C	-0.80838600	-0.38174300	-2.41796000
C	-0.15643400	-2.73550300	-1.69766400
H	0.69275300	-3.00994400	-2.33437900
H	-0.06584000	-3.28985600	-0.76081300
H	-1.06604100	-3.06214200	-2.21186500
H	-0.43741500	0.61641400	-2.61340000
H	-1.39823700	-0.83334000	-3.21451700
O	5.25942500	-2.20631200	-0.05498300
Ru	-1.61037400	0.02757100	-0.33776500
C	-2.90480200	-1.48716800	0.66900800
C	-3.86962200	-0.75139100	-0.14247300
C	-2.41333700	-0.60610000	1.70416600
C	-3.88863300	0.57081900	0.31733600
C	-2.93041600	0.68825900	1.42456900
C	-4.74183000	1.69738700	-0.17403000
H	-5.48580300	1.97120000	0.58538400
H	-4.13645400	2.58464400	-0.38285300
H	-5.28041800	1.42980000	-1.08657200
C	-2.75140600	1.92395400	2.25285600
H	-2.64884900	2.80883700	1.61886600
H	-3.61901200	2.07998800	2.90795900

H	-1.86375300	1.85731100	2.88725500
C	-1.61182800	-1.00312200	2.90839600
H	-2.28196100	-1.23964400	3.74581700
H	-1.00265100	-1.88979700	2.72024700
H	-0.94915900	-0.19887400	3.23845700
C	-2.75143800	-2.98017200	0.64117200
H	-3.57277500	-3.45052900	1.19868400
H	-2.78490200	-3.37390600	-0.37750900
H	-1.81613900	-3.30645600	1.10261100
C	-4.70217900	-1.35779900	-1.23316900
H	-4.12179600	-2.06139000	-1.83729700
H	-5.54891400	-1.91545100	-0.81115400
H	-5.10777300	-0.59677100	-1.90432700
Cl	-1.49124100	2.39534500	-1.07444600
H	3.28844600	-1.27637500	2.52976800
H	3.11749000	-2.72430900	1.52055500
H	2.72515300	-2.38460500	-1.04740600
H	2.68920400	-0.74625700	-1.70315100
H	0.98002600	-0.54367400	1.72408200
H	1.01634700	-2.11602800	0.92479500
Si	3.08591300	2.01844600	0.00234700
C	4.79908200	2.71933000	0.32825300
H	4.86357700	3.75919400	-0.01488400
H	5.04025700	2.71107900	1.39754200
H	5.57910600	2.15256100	-0.19277500
C	1.81426100	3.05856400	0.90722800
H	1.90207900	4.11348100	0.61846100
H	0.79151800	2.74113500	0.67683000
H	1.95838800	3.00196900	1.99261000
C	2.75307200	2.03685700	-1.84666800
H	1.78914100	1.58800700	-2.10611100
H	3.53602500	1.52251700	-2.41462600
H	2.72855000	3.07726600	-2.19555300

TSB8-B9

C	0.45863400	0.02919100	-0.42297400
C	1.36585800	-0.57537600	0.62512600
C	2.89775600	-0.73754800	0.41914900
C	3.46225200	-1.56097000	1.59823800
C	3.28600200	-1.45691500	-0.88785300
C	4.95315300	-1.84549200	1.41497500
C	4.78838600	-1.74567300	-0.93479500

H	5.32191100	-2.50211100	2.20933600	H	3.29943200	-1.01785900	2.53644600
H	5.52273200	-0.90484600	1.45757600	H	2.92228800	-2.51307900	1.66117200
H	5.03898100	-2.33091800	-1.82521100	H	2.74480200	-2.40703000	-0.94422200
H	5.35364900	-0.80212800	-0.97742700	H	2.99949300	-0.85866000	-1.75928700
O	3.57475200	0.53066100	0.47211400	H	1.23445100	-0.01487500	1.55795100
C	-0.16651100	-0.64539000	-1.53811100	H	0.95820300	-1.57361600	0.81590600
C	-1.04058300	0.13929800	-2.34258600	Si	3.03948400	2.02682400	-0.06105300
C	0.01876800	-2.11833600	-1.82360200	C	4.43062200	2.82914000	-1.02330900
H	0.83558300	-2.25542500	-2.54317400	H	4.14970700	3.83487500	-1.35655700
H	0.25629400	-2.70783000	-0.93626500	H	5.32717400	2.92719200	-0.39938900
H	-0.88534000	-2.53108600	-2.28011100	H	4.70118100	2.24455700	-1.90911000
H	-0.80911400	1.17018400	-2.58976900	C	2.52243700	3.09836000	1.38283800
H	-1.63120100	-0.38498900	-3.09204900	H	2.15951300	4.07277000	1.03455200
O	5.21160600	-2.52093500	0.18492900	H	1.72019900	2.63460800	1.96744500
Ru	-1.68790300	0.20863500	-0.24462800	H	3.36506600	3.28256600	2.05905100
C	-2.47750800	-1.63726700	0.80109600	C	1.58579500	1.71631600	-1.20328000
C	-3.45199900	-1.17041100	-0.16133100	H	0.50724000	1.23128800	-0.49843800
C	-2.34672100	-0.63695000	1.83335100	H	1.80359800	1.16407300	-2.11377000
C	-3.87089500	0.13427600	0.24121300	H	0.95087400	2.57594400	-1.43231900
C	-3.17601400	0.46037400	1.48083000	B9			
C	-4.95108900	0.96605400	-0.38460500	C	0.76585400	0.20456400	-0.38538200
H	-5.90860600	0.82387900	0.13601300	C	1.66583600	-0.63710500	0.57505300
H	-4.70622900	2.03083300	-0.34240800	C	3.19764400	-0.65110800	0.35041300
H	-5.10468000	0.70050000	-1.43435700	C	3.85305300	-1.49221200	1.46840400
C	-3.42493600	1.69160900	2.29913500	C	3.63000000	-1.25419800	-1.00370900
H	-3.47687900	2.58217400	1.66818200	C	5.35973200	-1.63125200	1.25338400
H	-4.37681000	1.60487500	2.84026300	C	5.15048300	-1.40704900	-1.08344600
H	-2.63759400	1.85136800	3.04097800	H	5.79806300	-2.29787100	2.00297800
C	-1.53678200	-0.78182000	3.08799100	H	5.84455200	-0.64747100	1.34623800
H	-2.12645700	-1.27255700	3.87436200	H	5.43889400	-1.91302700	-2.01040700
H	-0.64510500	-1.39302800	2.92577800	H	5.63008200	-0.41616000	-1.07310500
H	-1.21419700	0.18769600	3.47708200	O	3.75357900	0.67459000	0.47344700
C	-1.92486700	-3.03107800	0.88346300	C	-0.07654500	-0.57509100	-1.39926100
H	-2.56285100	-3.65198800	1.52736800	C	-0.90228200	0.14820500	-2.27348800
H	-1.88556300	-3.51475300	-0.09440200	C	0.16884800	-2.04074900	-1.67689900
H	-0.91932400	-3.05056700	1.31403200	H	1.09070200	-2.14936900	-2.26328800
C	-4.01910600	-1.96833700	-1.29959600	H	0.27730500	-2.65897200	-0.78542500
H	-3.29369900	-2.67945700	-1.70399300	H	-0.64458100	-2.44982700	-2.28038100
H	-4.89038600	-2.54820200	-0.96555600	H	-0.76127800	1.20441100	-2.46493500
H	-4.34989200	-1.32364900	-2.11818800	H	-1.43950500	-0.39812900	-3.04532200
Cl	-1.66276500	2.71118900	-0.54037900	O	5.65871600	-2.20713900	-0.01759100

Ru	-1.83164100	0.15044900	-0.23257300
C	-2.50822000	-1.76364600	0.75259100
C	-3.30200700	-1.46554600	-0.40867400
C	-2.71859400	-0.70665300	1.71927000
C	-3.95033900	-0.19376500	-0.18448400
C	-3.61179700	0.24464000	1.16475400
C	-4.98878200	0.43520600	-1.06441600
H	-5.99261100	0.08576700	-0.78535600
H	-4.97996400	1.52425700	-0.97548800
H	-4.83056400	0.18124000	-2.11604800
C	-4.18300000	1.45067200	1.84576700
H	-4.21927400	2.30748000	1.16921300
H	-5.20619600	1.24418500	2.18647800
H	-3.59538000	1.73926700	2.72127300
C	-2.10552700	-0.67394100	3.08712800
H	-2.69265500	-1.28818800	3.78266800
H	-1.08902000	-1.07750500	3.07961900
H	-2.06650200	0.34016500	3.49192600
C	-1.79786200	-3.05259900	1.04754000
H	-2.42547000	-3.68818000	1.68678900
H	-1.58326700	-3.61904700	0.13976800
H	-0.85656900	-2.89165000	1.58104500
C	-3.55041700	-2.36197200	-1.58490100
H	-2.76118100	-3.10634900	-1.70903200
H	-4.49492100	-2.90557800	-1.44855500
H	-3.63354800	-1.79432900	-2.51559600
Cl	-1.87921400	2.63523500	-0.52418100
H	3.65925300	-1.02163600	2.43937800
H	3.40078700	-2.49118400	1.48110300
H	3.17034400	-2.24295700	-1.11488100
H	3.28350500	-0.63232300	-1.83568100
H	1.52529300	-0.24466500	1.58931000
H	1.31724200	-1.67077100	0.61075700
Si	2.89549900	2.07039500	0.07085200
C	4.04711200	3.20646800	-0.87251000
H	3.53696800	4.13579200	-1.15327900
H	4.91798300	3.48295700	-0.26673400
H	4.41421500	2.73717100	-1.79190600
C	2.29704500	2.93262100	1.62718700
H	1.74710500	3.84842600	1.37803600
H	1.62902800	2.29843700	2.22080000

H	3.13735800	3.21927600	2.27075900
C	1.47679200	1.45201400	-0.99490200
H	0.02639200	0.67584300	0.35007300
H	1.88738200	1.18842900	-1.97693100
H	0.74135000	2.24315100	-1.16687800

TSB8-B10

C	2.22253200	1.45743000	1.28792300
C	2.53920800	0.38466200	0.21247100
C	2.98552600	0.99586400	-1.15911000
C	2.86389600	2.53594300	-1.36545700
C	2.83168400	2.81227400	0.96755500
H	1.14018900	1.60476400	1.35801500
H	2.57342900	1.07823500	2.25285900
O	2.30544800	3.26105500	-0.27801400
C	1.29864000	-0.55820600	0.04384800
C	0.06937400	0.10873300	-0.45939800
H	3.93306200	2.77179100	0.93175500
H	2.54713100	3.55566500	1.71831100
C	-0.32860000	0.41513800	-1.80329400
C	-0.13353500	-0.56324000	-2.94393200
H	0.05083100	-1.58327800	-2.59823000
H	-1.00545900	-0.56708800	-3.60561400
H	0.72912600	-0.25213100	-3.54616700
C	-1.17427600	1.53478800	-1.92625000
H	-0.95965100	2.45616700	-1.39970700
H	-1.78932400	1.62411800	-2.82036100
H	2.45118700	0.49016100	-1.96718700
H	4.03800600	0.74028700	-1.28507800
H	2.22454800	2.75578700	-2.22490400
H	1.58568300	-1.35203500	-0.65927900
H	1.11282600	-1.01584100	1.01969200
Ru	-1.76832900	0.32598200	-0.08453000
O	3.58489900	-0.42079200	0.76907300
Si	4.69275800	-1.55505200	0.19329900
C	5.10191300	-2.58142500	1.70886700
H	4.21107500	-3.07823200	2.10938500
H	5.83614100	-3.35963700	1.46887400
H	5.52597900	-1.96301600	2.50791800
C	6.25606700	-0.71147900	-0.42521500
H	6.11847300	-0.21579200	-1.39261100
H	6.61632100	0.04001700	0.28675300

H	7.05704700	-1.45063800	-0.55315300	C	1.30283700	-0.60182400	0.04271300
C	4.00674500	-2.65799300	-1.16670500	C	0.04833100	-0.12953800	-0.59905300
H	3.13889300	-3.23683800	-0.83251300	H	3.90790100	2.62430200	1.08136900
H	3.71813600	-2.09826200	-2.06303900	H	2.56010100	3.65992900	1.57770600
H	4.77867900	-3.37614700	-1.47148000	C	-0.36916900	-0.20534100	-1.96745700
C	-3.93663000	-0.68523500	-0.38227500	C	-0.12619100	-1.44279600	-2.80789800
C	-3.97646400	-0.05007600	0.86422800	H	0.13423300	-2.31746200	-2.20662400
C	-2.82123100	-1.62544000	-0.36208900	H	-1.00377300	-1.68045600	-3.41698200
C	-2.88584500	-0.58432000	1.69334300	H	0.70550300	-1.25113700	-3.49731200
C	-2.24993500	-1.62865800	0.96724700	C	-1.27017600	0.80073200	-2.37396200
C	-4.95527000	0.98012600	1.33295900	H	-1.09267100	1.84188300	-2.13511100
H	-5.56382300	0.58401700	2.15590700	H	-1.89375500	0.61023500	-3.24640000
H	-4.43680200	1.87160000	1.70054600	H	2.59086600	0.40747800	-2.02831000
H	-5.63435300	1.28541700	0.53293300	H	3.95340200	1.17029600	-1.20754500
C	-2.68362300	-0.23551300	3.13686300	H	1.17541200	2.41846600	-1.43515800
H	-3.46126300	-0.69524200	3.76152600	H	1.71556700	-1.43604400	-0.54058700
H	-1.71497500	-0.58531500	3.50364900	H	1.09972200	-0.95831700	1.05675400
H	-2.73052600	0.84641200	3.28744000	Ru	-1.79359400	0.13783500	-0.26110600
C	-1.25401900	-2.61633200	1.49948200	O	3.52829900	-0.17589700	0.83118900
H	-1.77170800	-3.49310200	1.91111300	Si	4.81597200	-1.16541600	0.37561600
H	-0.57924700	-2.97504500	0.71820600	C	5.33261800	-1.97168400	1.98756300
H	-0.64724300	-2.18857300	2.30161300	H	4.52678600	-2.58234400	2.41000200
C	-2.56604500	-2.65331500	-1.42616500	H	6.20151800	-2.62355400	1.83843300
H	-3.27450500	-3.48615000	-1.31946600	H	5.60803000	-1.22079600	2.73685300
H	-2.69796200	-2.24344500	-2.43095400	C	6.24998200	-0.15430800	-0.30120000
H	-1.55820200	-3.07048600	-1.35745600	H	6.07023700	0.21065900	-1.31821400
C	-4.87350900	-0.49841000	-1.53954100	H	6.46220300	0.71356600	0.33356300
H	-5.64280900	-1.28223100	-1.54603800	H	7.16044600	-0.76602200	-0.33325300
H	-5.38342500	0.46709100	-1.49642000	C	4.33102000	-2.47362000	-0.88444000
H	-4.34648600	-0.55657500	-2.49631200	H	3.53482900	-3.13069100	-0.51801000
Cl	-1.89717400	2.56051700	0.99211700	H	4.00337700	-2.03856500	-1.83511600
H	3.86476400	2.93973700	-1.58758700	H	5.19929000	-3.10799300	-1.10445800
B10				C	-3.99724300	-0.82556200	-0.19800400
C	1.99414400	1.62127800	1.10127000	C	-3.93104000	0.05946600	0.88562000
C	2.43890500	0.46986700	0.17099300	C	-2.90530800	-1.78021600	-0.05226800
C	2.86453400	1.06851100	-1.19896100	C	-2.80060800	-0.32848900	1.73938000
C	2.27426500	2.46026100	-1.42196700	C	-2.24211900	-1.52494600	1.20981400
C	2.85138200	2.86292700	0.88425800	C	-4.85350000	1.19701700	1.19105200
H	0.94379400	1.87068100	0.91754700	H	-5.47338800	0.95908600	2.06543200
H	2.07882400	1.28423800	2.13936000	H	-4.29082700	2.10698500	1.41883900
O	2.72180200	3.39931400	-0.44152500	H	-5.52427900	1.41209900	0.35542200

C	-2.48576900	0.30315000	3.06218700	H	0.49642000	-1.20649600	0.72112000
H	-3.20335700	-0.01583500	3.83018600	H	1.52288500	1.60147400	0.82352500
H	-1.48618000	0.02743700	3.40877900	H	1.02028000	1.24949700	-0.83223100
H	-2.53233900	1.39383500	2.99877800	Ru	-1.90321900	-0.20339100	0.15042400
C	-1.24004000	-2.41659500	1.88209400	O	3.61386700	0.89241300	-0.23171700
H	-1.75288500	-3.14047100	2.52951900	Si	5.29914900	0.83966900	-0.13020400
H	-0.64955000	-2.98938400	1.16233400	C	5.81923500	2.51345800	-0.79184700
H	-0.55049700	-1.84834300	2.51182000	H	5.40326700	3.32883300	-0.18934800
C	-2.74629400	-3.01231100	-0.89558900	H	6.91064400	2.61671700	-0.77937400
H	-3.45650700	-3.78475600	-0.57077800	H	5.48440400	2.65856000	-1.82511000
H	-2.94768400	-2.81250300	-1.95165000	C	6.03530100	-0.53513900	-1.17702500
H	-1.74302600	-3.43754700	-0.81556200	H	5.73608700	-1.53204900	-0.83496500
C	-5.00953900	-0.84848100	-1.30535500	H	5.75719600	-0.44275700	-2.23276100
H	-5.78839300	-1.59711600	-1.10724400	H	7.13069000	-0.49314000	-1.12488000
H	-5.50422800	0.11904500	-1.42166400	C	5.86822200	0.65294000	1.65162500
H	-4.55136200	-1.10694400	-2.26453700	H	5.36448300	1.36878500	2.31112300
Cl	-1.85616500	2.57988300	0.18712300	H	5.69684100	-0.35161300	2.05296100
H	2.59508400	2.85682300	-2.39128700	H	6.94589600	0.84828000	1.72036500
TSB10-B11				C	-4.09449800	0.46707000	-0.17038100
C	2.42728200	-0.98955500	-1.29524000	C	-3.68195000	-0.22141000	-1.34740000
C	2.56380300	-0.03977200	-0.06028100	C	-3.20780500	1.59374000	-0.00196000
C	2.70270300	-0.90565400	1.21825400	C	-2.55867700	0.47004800	-1.93838200
C	1.64445100	-1.96089800	1.12544100	C	-2.27890300	1.61003900	-1.11226300
C	2.64872300	-2.45965700	-0.94966700	C	-4.35281400	-1.41882800	-1.94900300
H	1.43223200	-0.88467000	-1.73828900	H	-5.01051500	-1.10635300	-2.77174100
H	3.15169100	-0.69489600	-2.05864100	H	-3.62421900	-2.12652300	-2.35018700
O	1.79537600	-2.87344500	0.15178800	H	-4.96566100	-1.95099400	-1.21784500
C	1.26920800	0.79364800	0.12998900	C	-1.94951200	0.15437300	-3.27446700
C	0.11197500	-0.03457600	0.65891700	H	-2.50953400	0.63122600	-4.09179600
H	3.68743000	-2.65832800	-0.66257800	H	-0.91527300	0.50393100	-3.34258000
H	2.38645800	-3.11698400	-1.77974800	H	-1.94888000	-0.92203500	-3.46927100
C	-0.62847300	0.31744100	1.84841500	C	-1.33279500	2.72808900	-1.44357100
C	-0.52552500	1.67813400	2.50254200	H	-1.85660500	3.52401100	-1.99066100
H	-0.30696300	2.48310900	1.79636100	H	-0.90139200	3.18078800	-0.54638700
H	-1.45014900	1.92548100	3.03066100	H	-0.50965700	2.38875400	-2.07829000
H	0.28113400	1.66794400	3.24883600	C	-3.41203200	2.70197200	0.99050200
C	-1.56805200	-0.64498400	2.30297900	H	-4.19169300	3.38971300	0.63474200
H	-1.34105300	-1.70605400	2.28295900	H	-3.73562200	2.32427600	1.96490700
H	-2.27843700	-0.33821800	3.06927600	H	-2.50431100	3.29015000	1.13946900
H	2.58243300	-0.30192000	2.12029500	C	-5.29717900	0.16423900	0.67663400
H	3.68227400	-1.39754200	1.25802000	H	-6.18390900	0.70331700	0.31356600

H	-5.53975000	-0.90208800	0.67044100
H	-5.14172700	0.46160900	1.71786200
Cl	-1.79123400	-2.71260800	-0.09651900
H	1.20631600	-2.39142700	2.02406600

B11

C	3.27153100	1.54804700	1.24860100
C	2.94706500	0.38280700	0.25993700
C	3.11373700	0.90571200	-1.18326800
C	2.00593300	1.96348600	-1.20579400
C	3.39648600	2.89839800	0.53011100
H	2.49939200	1.59962600	2.02391800
H	4.21944000	1.34296900	1.75450600
O	2.37559500	3.12478900	-0.44778500
C	1.43096800	0.07446900	0.27106700
C	0.77858800	1.25600000	-0.49635900
H	4.38499700	2.97371800	0.05297400
H	3.32195400	3.72548100	1.24274600
C	-0.33556400	0.91322800	-1.47075800
C	-0.04088800	-0.08914200	-2.56098000
H	0.35162400	-1.03559500	-2.18170300
H	-0.92738100	-0.29330200	-3.16379300
H	0.72332300	0.32485400	-3.23400200
C	-1.44706800	1.71755800	-1.55350300
H	-1.52647700	2.61764900	-0.95183200
H	-2.13138000	1.62584700	-2.39238600
H	2.89652200	0.10773600	-1.89954700
H	4.10098000	1.31637100	-1.41205100
H	0.38093900	1.98662000	0.20987100
H	1.28247600	-0.87708500	-0.24760800
H	1.04119600	-0.03356700	1.28718400
Ru	-2.24321500	0.21952800	0.11615700
O	3.66016100	-0.79757100	0.59637100
Si	5.23233300	-1.30001600	0.25155700
C	5.44561100	-2.82098300	1.32473800
H	4.71657400	-3.59827200	1.06888000
H	6.44532100	-3.25405600	1.20161300
H	5.31683000	-2.58182400	2.38639900
C	6.52041200	-0.00520900	0.69797000
H	6.40198300	0.92153600	0.12530400
H	6.49738300	0.25086100	1.76302800
H	7.52352500	-0.39230500	0.47829900

C	5.43050000	-1.76118500	-1.56121800
H	4.64163800	-2.44442600	-1.89603100
H	5.42084500	-0.88676800	-2.22064000
H	6.39050000	-2.27069700	-1.71315600
C	-4.28792000	-0.31970100	-0.17603900
C	-3.88675700	-0.77713500	1.14341100
C	-3.51045200	-1.04586800	-1.15841700
C	-2.82946500	-1.72471100	0.96412600
C	-2.59524200	-1.89632500	-0.45624100
C	-4.53142400	-0.38832000	2.43933200
H	-5.40428100	-1.02474700	2.63763700
H	-3.84348800	-0.49805900	3.28138500
H	-4.87388000	0.64912400	2.42209000
C	-2.10151500	-2.45670600	2.04977900
H	-2.56047900	-3.43877200	2.22749400
H	-1.05472400	-2.62890700	1.78312400
H	-2.12489100	-1.90386800	2.99220300
C	-1.68359800	-2.92500700	-1.05662400
H	-2.17515300	-3.90742900	-1.06145500
H	-1.42259700	-2.68639500	-2.08928800
H	-0.75577900	-3.03271500	-0.48680300
C	-3.74006500	-0.99645400	-2.63948300
H	-4.60982700	-1.61219400	-2.90565000
H	-3.94576400	0.02029100	-2.98688200
H	-2.88505700	-1.38133500	-3.19987600
C	-5.43156100	0.60097200	-0.47596600
H	-6.36922700	0.03387300	-0.56108300
H	-5.56677600	1.34515700	0.31340500
H	-5.28121000	1.13181500	-1.42007000
Cl	-1.95324600	2.06390100	1.73832400
H	1.75301200	2.32212400	-2.20764100

TSB11-B12

C	1.45815200	1.40681500	1.79787800
H	2.11977800	1.18534100	2.63091400
H	1.56704500	2.38136000	1.33367900
C	0.33148800	0.64433100	1.58868800
C	-0.00951300	-0.47538300	2.54274600
H	-0.75006400	-0.11474200	3.27069300
H	-0.44818100	-1.34631700	2.05037600
H	0.86963700	-0.79817300	3.10348100
C	-0.75804400	1.14977500	0.65676000

C	-1.48438900	0.08719900	-0.20860200	Ru	2.18420200	0.13927900	-0.06521000
C	-2.99340600	0.41991300	-0.09753800	Cl	2.15763400	2.30647500	-1.29826900
O	-3.72472600	-0.75197000	-0.42351300	H	-1.34495900	-0.92172600	0.18944100
C	-3.10133400	0.87264900	1.36911200	H	-1.14336600	0.08300100	-1.24817100
C	-1.93756100	1.86340200	1.43200000	Si	-5.36560200	-1.12180700	-0.53366300
C	-3.07479800	3.02160200	-0.40523900	C	-5.99976800	-0.80453300	-2.27493300
C	-3.37329700	1.61582300	-1.00404900	H	-7.01733300	-1.19883500	-2.38898900
H	-1.64777300	2.14545900	2.44813600	H	-6.03399700	0.26300700	-2.51898100
H	-4.05576900	1.34056700	1.62618800	H	-5.37157000	-1.29666800	-3.02625600
H	-2.93140300	0.02227400	2.03764800	C	-6.42142700	-0.17494800	0.69992600
H	-4.02613200	3.51754100	-0.17366500	H	-6.09261900	-0.33153000	1.73281400
H	-2.57050000	3.63916000	-1.15681600	H	-6.43477300	0.90335000	0.50723400
H	-4.44925600	1.57166100	-1.19598000	H	-7.45923900	-0.52600800	0.63296800
H	-2.87729300	1.50161700	-1.97310000	C	-5.43876800	-2.95857900	-0.15970900
H	-0.31061500	1.91762200	0.02250700	H	-6.46107400	-3.34274000	-0.25887900
O	-2.27250400	3.08749900	0.78724400	H	-4.80305600	-3.53421700	-0.84210600
C	2.62143000	-1.79021600	-1.04472800	H	-5.10403300	-3.16937000	0.86246300
C	2.54378100	-2.02101900	0.37784300	B12			
C	3.53810600	-1.19787500	1.00762200	C	-1.58893400	-1.84651800	1.44207600
C	4.23388900	-0.46203600	-0.02777400	H	-2.29183400	-1.77178600	2.26703400
C	3.67697600	-0.85269900	-1.30852200	H	-1.69822600	-2.70343400	0.78501800
C	4.18296900	-0.42970300	-2.65462500	C	-0.42656600	-1.10848200	1.45066900
H	4.53527600	0.60444100	-2.64112500	C	-0.10495200	-0.21169400	2.62325400
H	5.02026400	-1.06538800	-2.97250800	H	0.59545500	-0.73041600	3.29270200
H	3.40405000	-0.50405900	-3.41849900	H	0.37454500	0.72578300	2.33035100
C	1.76894800	-2.47315900	-2.07077600	H	-0.99832500	0.01839200	3.20661700
H	1.70353400	-1.89286800	-2.99459800	C	0.69159200	-1.44981400	0.47564400
H	2.19174900	-3.45455300	-2.32544300	C	1.37886100	-0.24390200	-0.23538800
H	0.75339700	-2.64187800	-1.70082000	C	2.90796700	-0.44075500	-0.04644100
C	5.42410700	0.42514700	0.17812000	O	3.53877600	0.83012300	-0.11395300
H	6.34769600	-0.17040100	0.18549800	C	2.96492800	-1.11439500	1.33680700
H	5.51496800	1.16604900	-0.61971400	C	1.89869300	-2.19992600	1.15407500
H	5.36884100	0.95886700	1.13098800	C	2.71012800	-2.77471700	-1.03114800
C	3.90697900	-1.20028400	2.46045500	C	3.48303300	-1.44624100	-1.06375800
H	4.70728900	-1.92985100	2.64449000	H	1.61575000	-2.71281200	2.07661800
H	4.27665600	-0.22423900	2.78542600	H	3.94302700	-1.53897300	1.58039100
H	3.06339400	-1.47425600	3.09875900	H	2.68009000	-0.40191900	2.11757200
C	1.70355300	-3.07595500	1.03448000	H	3.29510500	-3.57508500	-1.49418400
H	0.71418300	-3.15707800	0.57476900	H	1.78251200	-2.67648300	-1.61228900
H	2.18773500	-4.05702600	0.93479600	H	4.53633100	-1.62755400	-0.82021500
H	1.56739500	-2.88703400	2.10092100	H	3.43712200	-1.03377000	-2.07812000

H	0.25953600	-2.12624600	-0.26258100
O	2.41160100	-3.22629300	0.29426200
C	-2.63692500	1.86638900	-0.81804400
C	-2.48492900	1.88128500	0.62295200
C	-3.46547700	0.99519700	1.17705300
C	-4.19486600	0.39386800	0.07956900
C	-3.70046400	0.97458900	-1.15871900
C	-4.26918700	0.73453900	-2.52450800
H	-4.63726500	-0.28868400	-2.63017000
H	-5.11139500	1.41343300	-2.71406600
H	-3.52551000	0.90232900	-3.30764800
C	-1.82454200	2.69069900	-1.76943800
H	-1.86626900	2.29439800	-2.78688100
H	-2.20135900	3.72208500	-1.79728600
H	-0.77479000	2.73749500	-1.46397900
C	-5.37782000	-0.51728900	0.20979300
H	-6.30609500	0.06466000	0.29677000
H	-5.47800000	-1.17040800	-0.66098900
H	-5.30068300	-1.14900000	1.09892100
C	-3.79422100	0.81235800	2.62824300
H	-4.64651200	1.44942000	2.90061100
H	-4.07624900	-0.21927700	2.85649700
H	-2.96057800	1.08900700	3.27748400
C	-1.58333700	2.81199300	1.37900000
H	-0.61963400	2.94104900	0.87752100
H	-2.04293900	3.80673600	1.45732900
H	-1.39221300	2.46075200	2.39509400
Ru	-2.15313800	-0.18433400	-0.13273600
Cl	-1.92744300	-1.94776300	-1.86144100
H	1.11389000	0.70655600	0.23588800
H	1.10284400	-0.17939400	-1.29239800
Si	5.14778600	1.32305800	-0.21275200
C	5.85475800	1.05214900	-1.93423600
H	6.81929400	1.56668600	-2.02957200
H	6.02761000	-0.00642000	-2.15463400
H	5.19301700	1.45381300	-2.71018900
C	6.23901100	0.46309700	1.05320000
H	5.86286900	0.58995000	2.07430900
H	6.33513900	-0.61088700	0.85954400
H	7.25105900	0.88642300	1.02124100
C	5.05829300	3.16172700	0.14486700

H	6.04892600	3.62554900	0.06937400
H	4.40049600	3.67392800	-0.56653300
H	4.67558700	3.35839000	1.15264300

B6b

C	1.24051000	3.21291600	-0.47370200
H	1.50596900	4.26667500	-0.44566700
H	1.64194700	2.62458500	-1.29040600
C	0.38341700	2.68882300	0.43297500
C	-0.16173900	3.53510700	1.55543100
H	-1.24690500	3.63264000	1.49340000
H	0.05371400	3.07657300	2.52620100
H	0.30003400	4.52637200	1.53244100
C	-0.04625700	1.31908600	0.18999800
C	0.60988200	0.13303000	-0.20495200
C	1.78604300	-0.51952800	0.57134600
O	2.89013300	-0.68107900	-0.32758300
C	1.43975900	-1.95822100	1.02304700
C	2.55509300	-2.56280700	1.87551500
C	3.25614400	-0.45718900	2.65083300
C	2.20061200	0.27974700	1.82439000
H	2.25905100	-3.54836300	2.24920900
H	0.51436200	-1.93383300	1.60396000
H	1.27221000	-2.58094100	0.13875900
H	3.45147000	0.08234000	3.58308700
H	4.20512900	-0.51978500	2.09503900
H	1.31095800	0.43126400	2.44603800
H	2.57752900	1.26689300	1.54381200
H	3.46983800	-2.68573400	1.27490300
O	2.82925700	-1.76408900	3.02508200
C	-2.21278700	-0.26217900	-1.93512100
C	-3.33319900	0.18683000	-1.18373800
C	-3.65044100	-0.84227400	-0.19662200
C	-2.71581600	-1.89646000	-0.33319700
C	-1.79219100	-1.53009300	-1.37803900
C	-0.78840300	-2.44959600	-2.00510400
H	-0.37687000	-3.16226500	-1.28764300
H	-1.27768200	-3.02899500	-2.79993800
H	0.04042000	-1.90821300	-2.46723900
C	-1.61016000	0.38934400	-3.14321700
H	-0.52048600	0.28939700	-3.16061500
H	-1.98747800	-0.08290700	-4.05983800

H	-1.85366300	1.45306900	-3.19210900	C	1.79354200	0.48808700	0.30958100
C	-2.71840800	-3.20428900	0.40315700	O	2.48811700	-0.74489200	0.07164500
H	-1.70746500	-3.60200500	0.52176800	C	1.49039700	0.55050900	1.82043300
H	-3.16006100	-3.10843500	1.39762800	C	2.76434100	0.72076300	2.64872400
H	-3.30174300	-3.95235300	-0.14977100	C	3.88038100	1.85734300	0.91838300
C	-4.85470000	-0.81766800	0.69149000	C	2.67927700	1.72032300	-0.02012300
H	-5.76203300	-0.99889800	0.10061700	H	2.51680200	0.82776000	3.70956900
H	-4.80224100	-1.58685300	1.46592300	H	0.83081600	1.40051300	2.01940800
H	-4.95838400	0.15290400	1.18336700	H	0.96737500	-0.35457500	2.13468800
C	-4.16320600	1.40938300	-1.42879200	H	4.40326100	2.79898600	0.72109200
H	-3.63027400	2.14125900	-2.04114600	H	4.60194000	1.04175600	0.76618200
H	-5.09190400	1.14726300	-1.95268900	H	2.06490900	2.61726800	0.09216400
H	-4.43584400	1.88979800	-0.48498000	H	3.01190100	1.69247100	-1.06138400
Ru	-1.52720300	0.11474200	0.25884600	H	3.41065400	-0.16359900	2.53914600
Cl	-2.75647200	1.55125000	1.88144500	O	3.48020700	1.89956800	2.28488300
H	0.64562200	-0.13183900	-1.25995400	C	-1.66879200	-1.92743000	-0.75312800
H	-1.13646600	-0.64173600	1.60014400	C	-2.98986800	-1.41311200	-0.79052500
Si	4.01557900	0.18213400	-1.22745200	C	-3.40285700	-1.14245800	0.58575000
C	4.69379400	1.70579300	-0.36126300	C	-2.32834600	-1.45963800	1.44502900
H	5.14988000	1.45518000	0.60270100	C	-1.23365800	-1.92215400	0.63334500
H	5.47812500	2.15399200	-0.98482700	C	-0.02371900	-2.63934700	1.15264700
H	3.93633500	2.47704400	-0.18864000	H	0.15323500	-2.41984400	2.20790500
C	5.40396300	-1.05368900	-1.48928600	H	-0.19147500	-3.72233700	1.07071500
H	6.20330700	-0.62403200	-2.10492300	H	0.88005700	-2.39066600	0.59641400
H	5.85036500	-1.36318700	-0.53753000	C	-0.89350300	-2.49007800	-1.90307600
H	5.04472200	-1.95590300	-1.99729500	H	0.18179000	-2.40107900	-1.73897600
C	3.30093200	0.64679400	-2.90407200	H	-1.11813800	-3.55795800	-2.02929700
H	2.51180000	1.40399500	-2.84712100	H	-1.13917400	-1.98844800	-2.84306900
H	4.08882600	1.05137800	-3.55204100	C	-2.32711500	-1.38762300	2.94335900
H	2.88457100	-0.23190800	-3.41051900	H	-1.34790600	-1.09489200	3.33087500
TSB6b-E				H	-3.06346200	-0.67001800	3.31303800
C	0.28341900	3.34563200	-2.18759600	H	-2.57248000	-2.36637200	3.37581400
H	0.30203400	4.37679400	-2.52856200	C	-4.77928900	-0.72386900	0.99212300
H	0.73782500	2.60153000	-2.83526700	H	-5.45338300	-1.59061600	0.96844700
C	-0.32009100	3.01509300	-1.02826800	H	-4.79751500	-0.31716500	2.00632500
C	-0.90622400	4.05920300	-0.10898300	H	-5.17860300	0.03319500	0.31396600
H	-1.95445000	3.84512500	0.10771800	C	-3.89258600	-1.32258100	-1.98243900
H	-0.36557500	4.07143400	0.84566800	H	-3.32822600	-1.36190800	-2.91774400
H	-0.82395700	5.05265400	-0.55863900	H	-4.60523700	-2.15806600	-1.98710800
C	-0.37293900	1.60200800	-0.65179100	H	-4.46664300	-0.39261200	-1.97021900
C	0.54228100	0.52217700	-0.61276400	Ru	-1.58390500	0.24019700	-0.09124200

Cl	-3.41774300	1.85455500	-0.59235100	O	2.22633200	3.55866500	-0.83641000
H	0.77182000	0.05902700	-1.57502000	C	-2.03841700	-0.65062700	1.76949800
H	-1.01664900	1.43637800	0.90824900	C	-2.91516800	-1.14101800	0.72973100
Si	3.73412700	-1.38668400	-0.86688800	C	-3.62948600	-0.00681600	0.17879600
C	4.30092600	-0.29523300	-2.28940600	C	-3.14089000	1.17435600	0.80453600
H	4.82201900	0.60970500	-1.96208400	C	-2.15162800	0.77512000	1.79826300
H	5.00417200	-0.86682900	-2.90892200	C	-1.54501300	1.69877100	2.81013500
H	3.47055600	0.00271000	-2.93929800	H	-1.30843800	2.67597000	2.38124600
C	5.19076800	-1.79230500	0.25169700	H	-2.25728100	1.86718900	3.62953500
H	5.93004100	-2.38704400	-0.29955100	H	-0.63361500	1.28603700	3.24837100
H	5.70552300	-0.90197700	0.62702400	C	-1.27226300	-1.50210400	2.73629000
H	4.87639200	-2.38726700	1.11705500	H	-0.40193600	-0.97914500	3.14129300
C	3.09639100	-3.00074600	-1.58667800	H	-1.91400500	-1.77496800	3.58479500
H	2.32208100	-2.83819100	-2.34386700	H	-0.92931100	-2.42996700	2.27311100
H	3.91871400	-3.53872400	-2.07492300	C	-3.62526200	2.57649900	0.58696700
H	2.68635800	-3.66474300	-0.81784000	H	-2.80655900	3.29927000	0.65570600
E				H	-4.09769400	2.69389400	-0.39126100
C	0.41546700	-3.49498400	-0.01473300	H	-4.36689100	2.85043500	1.34920100
H	0.18316900	-4.55553800	-0.06364100	C	-4.71372600	-0.08713300	-0.85051200
H	0.99540100	-3.16311100	0.84006400	H	-5.67753700	-0.26999600	-0.35639800
C	0.01250600	-2.65076900	-0.98255400	H	-4.80150200	0.83869500	-1.42217900
C	-0.72514900	-3.15971100	-2.19952400	H	-4.54506200	-0.90569600	-1.55416600
H	-1.69258300	-2.66128500	-2.31993500	C	-3.23109800	-2.58062500	0.46033300
H	-0.15090500	-2.95212400	-3.11166700	H	-2.34424800	-3.21194300	0.54576200
H	-0.89493100	-4.23850800	-2.14439100	H	-3.96933300	-2.94348700	1.18885800
C	0.34672000	-1.20681000	-0.99055300	H	-3.65773500	-2.72130900	-0.53564500
C	0.80133400	-0.44621500	0.07665800	Ru	-1.44175500	0.17710300	-0.20394400
C	1.74382000	0.76323000	-0.06810100	Cl	-1.67011500	0.81477100	-2.59314700
O	3.00690700	0.42214300	0.53113200	H	0.86247400	-0.89802200	1.06368000
C	1.23790000	1.97532700	0.73929300	H	0.46062500	-0.79582500	-1.98876100
C	2.12144100	3.20644500	0.54086500	Si	4.13458600	-0.82752400	0.45579500
C	2.80386100	2.49722700	-1.59491900	C	4.09910400	-1.80132700	-1.14919200
C	1.96739500	1.21796100	-1.52526500	H	4.27391700	-1.16531100	-2.02350800
H	1.69049500	4.07436100	1.05027600	H	4.89623400	-2.55570400	-1.13054700
H	0.21605200	2.21090800	0.41759700	H	3.15335400	-2.33313100	-1.29500300
H	1.19911600	1.71232700	1.80115800	C	5.79486300	0.02720000	0.65022700
H	2.86320600	2.85547000	-2.62737200	H	6.60714900	-0.70751000	0.70802400
H	3.82956100	2.30414400	-1.24397200	H	6.01266100	0.69314800	-0.19234600
H	0.99530900	1.40256600	-1.99463900	H	5.83067200	0.62792300	1.56641700
H	2.46524500	0.42808700	-2.09699600	C	3.87503800	-1.98375900	1.91481100
H	3.12209500	3.02584600	0.96289500	H	2.93487400	-2.54031900	1.84157900

H	4.68647600	-2.71955700	1.97382200
H	3.86245900	-1.43002700	2.86083900

B8'

C	0.10277200	-1.23954700	-3.29387400
H	0.22983900	-1.08357500	-4.36248700
H	-0.12555500	-2.25102800	-2.96777400
C	0.25393500	-0.22541500	-2.42323600
C	0.56495400	1.17807100	-2.89399500
H	-0.26739500	1.85641000	-2.68217700
H	1.43367600	1.58797400	-2.37592000
H	0.75287100	1.19546300	-3.97139100
C	0.11721700	-0.45208800	-0.96107800
C	-1.29524100	-0.72259100	-0.47715700
C	-2.43167900	0.35340000	-0.55254700
O	-1.92861300	1.51950700	0.10153400
C	-3.60923200	-0.24276800	0.26479900
C	-4.93716700	0.48499900	0.07016500
C	-4.30435800	1.30748600	-2.03109900
C	-2.93278600	0.62620700	-1.98771600
H	-5.74546600	-0.06667300	0.56089400
H	-3.74432700	-1.28540700	-0.04599400
H	-3.33666200	-0.24834700	1.32600400
H	-4.65810200	1.36752300	-3.06534100
H	-4.25159700	2.33605100	-1.64237900
H	-3.01966300	-0.33605900	-2.50359400
H	-2.21251100	1.22762500	-2.54603600
H	-4.90454000	1.49011900	0.51383500
O	-5.28887300	0.57458000	-1.30938100
C	3.44439900	0.66815800	-0.10691100
C	3.44633600	-0.36827000	-1.10293000
C	3.51235300	-1.61919800	-0.41186700
C	3.77483000	-1.34362600	1.00154600
C	3.71837700	0.04465700	1.18653000
C	3.92237900	0.80463200	2.46472000
H	3.76265600	0.17561400	3.34389600
H	4.94552400	1.19942400	2.51977500
H	3.24479800	1.66056300	2.53474200
C	3.55183300	2.14669700	-0.35831500
H	3.06627700	2.72769700	0.43097700
H	4.60584600	2.45551000	-0.38665400
H	3.10228100	2.43505800	-1.31137800

C	4.07952700	-2.39427300	2.02433500
H	4.10818200	-1.98055000	3.03561800
H	3.32991000	-3.19030400	2.00389900
H	5.05847700	-2.84866300	1.82295800
C	3.61712100	-2.97101100	-1.05367200
H	4.66653900	-3.22916300	-1.25242200
H	3.19942000	-3.74827300	-0.40887800
H	3.08145500	-2.99986000	-2.00645400
C	3.58288600	-0.20811600	-2.58802900
H	3.44179900	0.82692100	-2.90283300
H	4.59582800	-0.50469600	-2.89084800
H	2.88096000	-0.83553700	-3.14414800
Ru	1.59927300	-0.61770900	0.26291800
Cl	0.69532900	-2.72958400	1.26798400
H	0.65142800	0.61106500	1.11598800
H	0.61599000	-0.04809800	1.61712500
Si	-1.99452600	3.18457500	0.27037100
C	-1.83238800	4.12114300	-1.35239800
H	-1.81818500	5.19858800	-1.14259600
H	-0.90119600	3.88174800	-1.87639800
H	-2.66593200	3.93910900	-2.03848300
C	-0.51062400	3.57352700	1.35452800
H	-0.56519400	3.04230500	2.31168600
H	0.42828200	3.29143400	0.86533900
H	-0.45920200	4.64661500	1.57525200
C	-3.54359100	3.77472600	1.15968200
H	-4.43946500	3.74886000	0.53102900
H	-3.74509500	3.18878500	2.06328100
H	-3.40169900	4.81690100	1.47396800
H	-1.25107300	-1.04775800	0.56257400
H	-1.64131600	-1.58787400	-1.06323500

TSB5-B6'

C	0.01733100	1.00761600	-0.38927600
C	-0.98572800	0.21870100	-0.01071500
C	-2.47059800	0.44169100	0.30875800
C	-2.63266700	0.96325300	1.75822600
C	-3.13593500	1.44663500	-0.65737000
C	-4.08868800	1.32287300	2.05750800
C	-4.55931800	1.78306100	-0.20583300
H	-4.17690800	1.77765600	3.04944000
H	-4.71298400	0.41692600	2.04012000

H	-4.98278500	2.56949500	-0.83851900	H	-2.54918700	2.36707900	-0.68892200
H	-5.20626600	0.89639900	-0.28900000	H	-3.15118700	1.03623500	-1.67120400
O	-3.18178200	-0.79754400	0.27062600	H	1.20209400	-1.96444800	0.29707800
C	0.13969800	2.40627300	-0.81495100	H	-0.72146100	-0.84754400	0.19057100
C	0.54878600	2.70876200	-2.06031800	Si	-3.32246800	-2.08968000	-0.81009300
C	-0.15970100	3.48836200	0.20329500	C	-2.06307900	-3.41910500	-0.38576500
H	-1.22596200	3.52526000	0.44999000	H	-2.30828000	-4.35263900	-0.90778100
H	0.37303000	3.30862800	1.14200600	H	-1.05053500	-3.13225400	-0.68887400
H	0.13496900	4.47094700	-0.17706700	H	-2.05020600	-3.63684300	0.68858000
H	0.77901000	1.93240700	-2.78359500	C	-5.05224300	-2.74588700	-0.49598800
H	0.64768200	3.74226600	-2.38201700	H	-5.20388300	-2.98289000	0.56330200
O	-4.58889500	2.28389700	1.12938300	H	-5.81919200	-2.01896700	-0.78622400
Ru	1.45313600	-0.41319900	0.16726000	H	-5.23321600	-3.66341600	-1.06842300
C	3.08829700	1.13446000	0.93047400	C	-3.11855000	-1.60444900	-2.61262600
C	3.56614600	0.23975300	-0.08535000	H	-3.87868500	-0.89157100	-2.94933700
C	2.63866100	0.34716600	2.03703300	H	-2.13012600	-1.17752900	-2.81201800
C	3.51258700	-1.11313700	0.43850400	H	-3.21465300	-2.50221200	-3.23689000
C	2.92441900	-1.03912200	1.75210000				
C	4.12273500	-2.31464700	-0.21731800	B6'			
H	5.21291100	-2.30836900	-0.08671800	C	1.95637100	3.08212600	-1.62701800
H	3.73851200	-3.24427400	0.20959000	H	2.23502700	4.07560600	-1.96845700
H	3.91243900	-2.32479700	-1.28931800	H	2.72282700	2.31672300	-1.63490600
C	2.77922100	-2.16646100	2.73280200	C	0.68672300	2.79958400	-1.25729800
H	2.76867400	-3.13593000	2.23032100	C	-0.39545400	3.85565700	-1.34705300
H	3.61797400	-2.16334300	3.44115800	H	-1.16191200	3.56189600	-2.07177200
H	1.85866600	-2.07761300	3.31597000	H	-0.89740500	4.01413300	-0.38761500
C	2.08458600	0.86365600	3.33049300	H	0.02753800	4.81123200	-1.66880600
H	2.89419800	1.02959500	4.05322800	C	0.35343600	1.43238800	-0.90880000
H	1.55990600	1.81308500	3.19790900	C	-0.76779500	0.58618300	-0.85416800
H	1.38891400	0.14948600	3.77911800	C	-2.03571400	0.70567100	0.01263200
C	3.16052100	2.62700000	0.85122000	O	-2.46179900	-0.59182200	0.43637300
H	4.20908900	2.94376800	0.92218400	C	-3.14633000	1.39297900	-0.82358200
H	2.77325200	3.00371100	-0.09975200	C	-4.38263400	1.71202900	0.02040400
H	2.61569600	3.10778900	1.66534200	C	-3.13893300	1.83074600	2.00747000
C	4.20107700	0.64948200	-1.37809400	C	-1.81937400	1.51899200	1.30186900
H	3.75603900	1.56872000	-1.76821800	H	-5.10581400	2.28658900	-0.56730900
H	5.27362300	0.83429100	-1.22989100	H	-2.75628000	2.33044400	-1.23008600
H	4.09325100	-0.12797100	-2.13632900	H	-3.42124700	0.75958000	-1.67438900
Cl	1.15610100	-1.19695900	-2.19739400	H	-2.96899500	2.48887500	2.86549600
H	-2.28218500	0.19621300	2.45821100	H	-3.59714700	0.90064400	2.37792200
H	-2.00823100	1.85232400	1.88884500	H	-1.31462700	2.45931000	1.05907500
				H	-1.17267100	0.95575400	1.97702300

H	-4.87444000	0.78665600	0.35350600
O	-4.05084800	2.51492100	1.15039800
C	1.86591700	-0.16379300	1.90613000
C	2.73047500	0.79057500	1.23699500
C	3.52301600	0.08044900	0.29259400
C	3.17442600	-1.32300700	0.39590500
C	2.19906700	-1.48014600	1.41352300
C	1.67352900	-2.77511000	1.96411800
H	1.65717000	-3.56223000	1.20620000
H	2.30991700	-3.12590100	2.78787000
H	0.66043400	-2.66461400	2.35834400
C	1.07124700	0.10579500	3.15064700
H	0.19082100	-0.53825700	3.22209200
H	1.69015700	-0.08819700	4.03769000
H	0.74144300	1.14540700	3.20645100
C	3.84970800	-2.42044600	-0.36887300
H	3.25600300	-3.33747600	-0.37288300
H	4.03189400	-2.13199000	-1.40660800
H	4.82039100	-2.65571700	0.08784800
C	4.65432900	0.61054600	-0.53953900
H	5.61962600	0.28874200	-0.12618300
H	4.61160700	0.24481800	-1.57050000
H	4.66134500	1.70260700	-0.56644300
C	2.85609200	2.23612100	1.61622800
H	1.89260600	2.66251300	1.90739600
H	3.53348600	2.34216800	2.47395200
H	3.25824700	2.84246400	0.80168900
Ru	1.20562000	-0.16537400	-0.27335000
Cl	1.30953800	-1.25401500	-2.49922800
H	0.06050200	-1.20801000	-0.02440400
H	-0.97047400	0.03566600	-1.77550800
Si	-3.06509300	-1.99791800	-0.27686200
C	-2.27720900	-3.40216700	0.68661700
H	-2.70888600	-4.36751200	0.39575400
H	-1.19859300	-3.45269100	0.50330000
H	-2.43214200	-3.28419800	1.76531600
C	-2.68059700	-2.17534700	-2.10684800
H	-1.60537900	-2.16545800	-2.31331600
H	-3.07456400	-3.13738600	-2.45991100
H	-3.15272700	-1.39464100	-2.71338600
C	-4.93073600	-2.06981200	-0.03733800

H	-5.30858800	-3.05610600	-0.33555600
H	-5.21316500	-1.91622300	1.01038700
H	-5.46029600	-1.32451100	-0.64080500

TSB6'-B7

C	0.21238500	3.37277300	0.47473600
H	0.06327500	4.35721200	0.91086000
H	1.21756300	3.10642900	0.16747400
C	-0.82581400	2.52998300	0.27630300
C	-2.23772500	2.94262900	0.63541300
H	-2.84737500	3.07303000	-0.26525200
H	-2.73550400	2.19616800	1.26181300
H	-2.23222900	3.89166500	1.17858500
C	-0.56260000	1.26532700	-0.38532700
C	-1.24308400	0.32736100	-1.21443200
C	-2.47452000	-0.54608800	-0.88944500
O	-2.36841500	-1.79074900	-1.58632500
C	-3.75841500	0.21155900	-1.31084900
C	-5.02678700	-0.50233400	-0.83426700
C	-3.91548100	-1.54680000	0.94941600
C	-2.57439000	-0.90111900	0.60374700
H	-5.90812700	0.11119200	-1.04651700
H	-3.74161100	1.21203000	-0.87108600
H	-3.78360200	0.33648100	-2.39919200
H	-3.99962000	-1.70251800	2.02954700
H	-4.00240300	-2.52795100	0.45700900
H	-2.45352100	0.00902400	1.20067400
H	-1.76135300	-1.58245700	0.86056600
H	-5.15054000	-1.46355300	-1.35354500
O	-5.01191800	-0.71506000	0.57487000
C	1.38468600	-1.20673700	1.22392800
C	1.91501200	0.12551400	1.43594100
C	2.90177600	0.36368000	0.44206000
C	3.04661800	-0.86023600	-0.33899300
C	2.14436900	-1.82458600	0.15687200
C	2.01837200	-3.25783400	-0.27445700
H	2.33633000	-3.40099200	-1.31034500
H	2.64340100	-3.90614400	0.35464200
H	0.98890800	-3.61503000	-0.18714800
C	0.51204800	-1.95277500	2.19116300
H	-0.04184500	-2.75811400	1.70251900
H	1.13229600	-2.41380100	2.97241600

H	-0.20516800	-1.29729100	2.69047700	C	-1.83920800	0.57708100	0.35160200
C	4.06311500	-1.04821900	-1.42330100	O	-2.53931300	-0.67392700	0.33975000
H	3.84161300	-1.92214200	-2.04071600	C	-2.79135900	1.73454800	-0.05895500
H	4.10704000	-0.17570600	-2.07977200	C	-3.90864500	1.95329100	0.96566800
H	5.06059700	-1.19233400	-0.98714800	C	-2.60561700	1.09368500	2.72202800
C	3.79674300	1.56104400	0.31285000	C	-1.40976200	0.83415100	1.80729300
H	4.79932100	1.34329600	0.70527600	H	-4.49818600	2.83655700	0.69841600
H	3.91576000	1.86241400	-0.73246100	H	-2.20684100	2.65747500	-0.12482200
H	3.40636800	2.41757900	0.86837100	H	-3.21907800	1.54639700	-1.04997200
C	1.57588400	1.00802900	2.59995200	H	-2.26847800	1.34942900	3.73154800
H	0.53558000	0.88837900	2.91337800	H	-3.23328100	0.19144200	2.79143800
H	2.20666100	0.74943300	3.46114800	H	-0.74945400	1.70766000	1.83070700
H	1.74055300	2.06519100	2.37890900	H	-0.83916200	-0.02112100	2.17503500
Ru	0.85144700	0.02257500	-0.62908700	H	-4.58897600	1.09076700	0.99514400
Cl	1.49276800	0.78198400	-2.89714300	O	-3.38509000	2.19844900	2.26838700
H	-0.10879500	-0.96506000	-1.44449400	C	1.16371100	-1.98597200	0.53147400
H	-1.22298500	0.58951500	-2.27580600	C	1.87411300	-1.35081700	1.62315300
Si	-2.43613200	-2.31102800	-3.19455200	C	3.12833100	-0.94027700	1.13310700
C	-1.25014500	-3.76320900	-3.25348700	C	3.23645100	-1.34936600	-0.26355800
H	-1.29868900	-4.27407700	-4.22245500	C	2.04098200	-2.04023300	-0.60848700
H	-0.21564700	-3.43703900	-3.09899100	C	1.76981500	-2.78667300	-1.88197000
H	-1.48827100	-4.50119900	-2.47883500	H	2.38327000	-2.41355800	-2.70521200
C	-1.93247500	-1.00658000	-4.44855900	H	1.99668300	-3.85332300	-1.75387900
H	-0.91115000	-0.64516800	-4.28981000	H	0.72192700	-2.70891400	-2.18306600
H	-1.97357900	-1.44622500	-5.45366900	C	-0.08994700	-2.79059000	0.68468000
H	-2.60420300	-0.14118200	-4.45248600	H	-0.51720500	-3.04947000	-0.28483800
C	-4.17098900	-2.91164700	-3.60321500	H	0.14984600	-3.73044400	1.20137700
H	-4.17009300	-3.42044800	-4.57550400	H	-0.85469600	-2.27144400	1.26176400
H	-4.54055900	-3.62929600	-2.86208200	C	4.48386700	-1.23808200	-1.08454700
H	-4.89395900	-2.09115400	-3.66812300	H	4.28674300	-1.42358400	-2.14346600
B6'b				H	4.92463100	-0.24230000	-0.98979100
C	0.63285400	4.01257800	-0.41292300	H	5.22914300	-1.97204900	-0.75093500
H	0.50487400	5.03493300	-0.75991900	C	4.23048200	-0.31402900	1.92583900
H	1.07236700	3.86850100	0.56732500	H	5.02722700	-1.04731600	2.10768600
C	0.24036000	2.97339700	-1.16867900	H	4.66833400	0.53088500	1.38715600
C	-0.36729400	3.15706000	-2.54486800	H	3.87500100	0.04094200	2.89658200
H	0.21033100	2.60892700	-3.29888000	C	1.41668700	-1.27420900	3.05091900
H	-1.39236100	2.77302200	-2.58379700	H	0.35214400	-1.49635600	3.14744600
H	-0.37983100	4.21406800	-2.82537700	H	1.95637800	-2.01180300	3.65990600
C	0.28855700	1.60450700	-0.66776500	H	1.60218000	-0.29180200	3.49462700
C	-0.64614500	0.54772500	-0.63356700	Ru	1.51062100	0.20980900	-0.26101800

Cl	3.30104500	1.93786100	-0.44047500	O	-3.41358100	2.43765800	2.00994000
H	1.59991500	0.13060100	-1.82135300	C	1.38454400	-2.06270800	0.15727300
H	-0.92094300	0.07649500	-1.57803000	C	1.83964800	-1.52330300	1.43198500
Si	-3.51280100	-1.51752900	-0.75402600	C	3.10787100	-0.94042000	1.22762800
C	-3.77476100	-3.17677700	0.08173500	C	3.46629900	-1.10600200	-0.17422000
H	-4.48575900	-3.78587100	-0.48935600	C	2.42250900	-1.85491700	-0.80694400
H	-2.84595200	-3.74904200	0.16962400	C	2.43597400	-2.38289300	-2.21089600
H	-4.18646600	-3.05154800	1.08985300	H	3.03407400	-1.75304600	-2.87343200
C	-2.70859100	-1.75332300	-2.43884400	H	2.86939100	-3.39137700	-2.22882100
H	-1.72275400	-2.22543900	-2.37096700	H	1.42774600	-2.45180800	-2.62691900
H	-3.34259200	-2.40607700	-3.05278300	C	0.18639600	-2.94244700	-0.01987000
H	-2.59680700	-0.81024600	-2.98538500	H	-0.11489500	-3.00533300	-1.06825500
C	-5.20130800	-0.73166100	-1.02914200	H	0.41950700	-3.96254100	0.31480900
H	-5.79550900	-1.39190300	-1.67436700	H	-0.66478400	-2.58317700	0.55989900
H	-5.75837600	-0.60895200	-0.09417700	C	4.79061300	-0.73187500	-0.76501600
H	-5.15040000	0.24236900	-1.52626800	H	4.75931800	-0.73934300	-1.85783900
TSB6'b-Z'				H	5.09236700	0.26778500	-0.44202300
C	0.30080200	3.83551100	-0.70649100	H	5.56823300	-1.44023100	-0.44982200
H	0.12031500	4.82197900	-1.12702200	C	3.99883400	-0.33394600	2.26511700
H	0.62907200	3.78142900	0.32401500	H	4.84515500	-1.00282700	2.46945400
C	0.11336100	2.73301500	-1.44589300	H	4.39845600	0.62421700	1.92283500
C	-0.32631200	2.79349500	-2.89399200	H	3.46932300	-0.16908400	3.20663900
H	0.40891200	2.30203600	-3.54321300	C	1.13533600	-1.69488100	2.74396400
H	-1.28036300	2.27398900	-3.04107700	H	0.05842200	-1.81794100	2.61238900
H	-0.43779800	3.82994500	-3.22509200	H	1.50399800	-2.59785500	3.24992100
C	0.24194600	1.37505800	-0.90203300	H	1.30770200	-0.85093200	3.41626300
C	-0.66911300	0.35804900	-0.60065100	Ru	1.58843500	0.18827800	-0.18540200
C	-1.89279200	0.55434300	0.32639400	Cl	3.06248400	2.19485200	0.14286100
O	-2.57283800	-0.70366800	0.46975400	H	1.52665200	0.50286700	-1.76677300
C	-2.84683400	1.63995300	-0.23745600	H	-0.77727500	-0.49121100	-1.26856100
C	-3.95003500	2.02052000	0.75751800	Si	-3.61462600	-1.59671400	-0.52319900
C	-2.65752400	1.38757400	2.61009200	C	-3.58688300	-3.32125100	0.21609500
C	-1.46509300	0.99583600	1.74131700	H	-4.36246600	-3.94468200	-0.24481900
H	-4.52714200	2.86647600	0.37008600	H	-2.62724600	-3.82516400	0.06511800
H	-2.26192900	2.53792800	-0.45378200	H	-3.78458700	-3.29506600	1.29383000
H	-3.29151000	1.30608400	-1.18168000	C	-3.06579100	-1.64178600	-2.32278100
H	-2.31885000	1.76523600	3.58014100	H	-2.07656500	-2.09345200	-2.45263100
H	-3.30245000	0.51327100	2.79136800	H	-3.77669400	-2.24537000	-2.90147000
H	-0.79726000	1.85842400	1.64828900	H	-3.04354900	-0.64638500	-2.77948200
H	-0.90079300	0.18943600	2.21741300	C	-5.39244500	-0.98079300	-0.47575600
H	-4.64366300	1.18398900	0.91630500	H	-6.02514400	-1.69711600	-1.01594300

H	-5.78155400	-0.91510600	0.54622700	C	5.59284400	-0.19754000	-0.98750700
H	-5.52983300	-0.00634500	-0.95541700	H	5.42360200	0.13465900	-2.01530600
Z'				H	6.01395900	0.64144600	-0.42780900
C	-1.90584300	3.94952900	0.18335100	H	6.35144400	-0.99160800	-1.01580100
H	-2.27010200	4.96443900	0.32465500	C	4.90857200	-0.18580000	2.15495200
H	-1.41603000	3.48150900	1.03180900	H	5.57535900	-0.98140200	2.51498200
C	-2.04029300	3.32040500	-0.99331600	H	5.53503600	0.64162900	1.81191900
C	-2.66581800	3.99442100	-2.19322400	H	4.32355000	0.16562200	3.00976900
H	-1.96399100	4.01823200	-3.03669700	C	2.10175200	-1.65226800	2.56108300
H	-3.54962600	3.44286800	-2.53764300	H	1.02268200	-1.79107200	2.45209700
H	-2.96575100	5.02148500	-1.96684400	H	2.50586200	-2.56474900	3.01997900
C	-1.49470900	1.96392400	-1.25010100	H	2.26856000	-0.83117400	3.26430800
C	-1.72612300	0.77147200	-0.67263100	Ru	2.52485500	0.35154100	-0.01332400
C	-2.65637500	0.31078500	0.44099500	Cl	2.95727700	2.73676700	-0.43174100
O	-2.92331200	-1.09111900	0.23532200	H	-0.79496100	1.94438400	-2.08949400
C	-3.98064600	1.09287300	0.56329400	H	-1.14467700	-0.06208900	-1.06365700
C	-4.78018000	0.65611600	1.79370500	Si	-3.70360700	-1.97681300	-0.97365700
C	-2.84517200	-0.02072800	2.95570600	C	-3.19991000	-3.74504300	-0.60188200
C	-1.92405500	0.38722300	1.80608300	H	-3.66098200	-4.44154400	-1.31229800
H	-5.66042100	1.29490500	1.91859400	H	-2.11422600	-3.87977800	-0.66451300
H	-3.75709300	2.15751400	0.65351200	H	-3.51400000	-4.04553200	0.40419500
H	-4.58191400	0.96132200	-0.34283200	C	-3.16005400	-1.49597300	-2.70827700
H	-2.34296600	0.11865800	3.91851400	H	-2.08670400	-1.64693000	-2.86634600
H	-3.11823300	-1.08297900	2.86328600	H	-3.68844200	-2.12004800	-3.44028800
H	-1.58411000	1.41517600	1.96655500	H	-3.39027800	-0.45190200	-2.94462200
H	-1.03998000	-0.26004400	1.78303500	C	-5.57811800	-1.84253800	-0.87693900
H	-5.12859600	-0.38164000	1.68598900	H	-6.02855300	-2.54434600	-1.59070000
O	-4.01852300	0.78796500	2.99346300	H	-5.95748100	-2.10360300	0.11709800
C	2.28929200	-1.81524200	-0.04536800	H	-5.94912800	-0.84351500	-1.12933600
C	2.76246400	-1.38948800	1.24168000				
C	4.02588400	-0.70110500	1.05915300				
C	4.33242000	-0.70534800	-0.35550900				
C	3.24473700	-1.37677000	-1.03809800				
C	3.17136600	-1.65081400	-2.50943200				
H	3.68949800	-0.88060700	-3.08721800				
H	3.64200800	-2.61526500	-2.74465400				
H	2.13656000	-1.69645600	-2.86042500				
C	1.04274800	-2.60425900	-0.31424100				
H	0.64608900	-2.40029800	-1.31280700				
H	1.24552300	-3.68232500	-0.25790800				
H	0.25765600	-2.38016300	0.41279800				

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