

***Electronic Supplementary Information***

**Computational Insights into Ir(III)-Catalyzed Allylic C–H Amination of Terminal Alkene: Mechanism, Regioselectivity, and Catalytic Activity**

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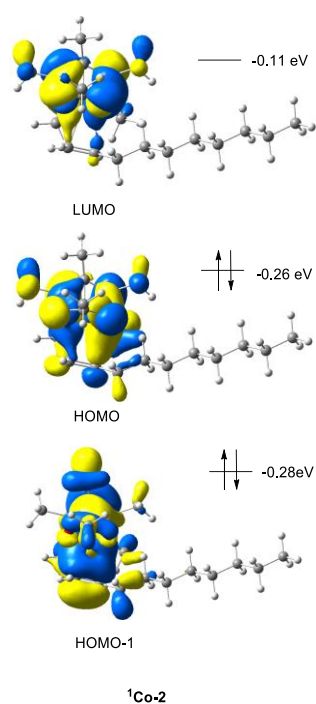
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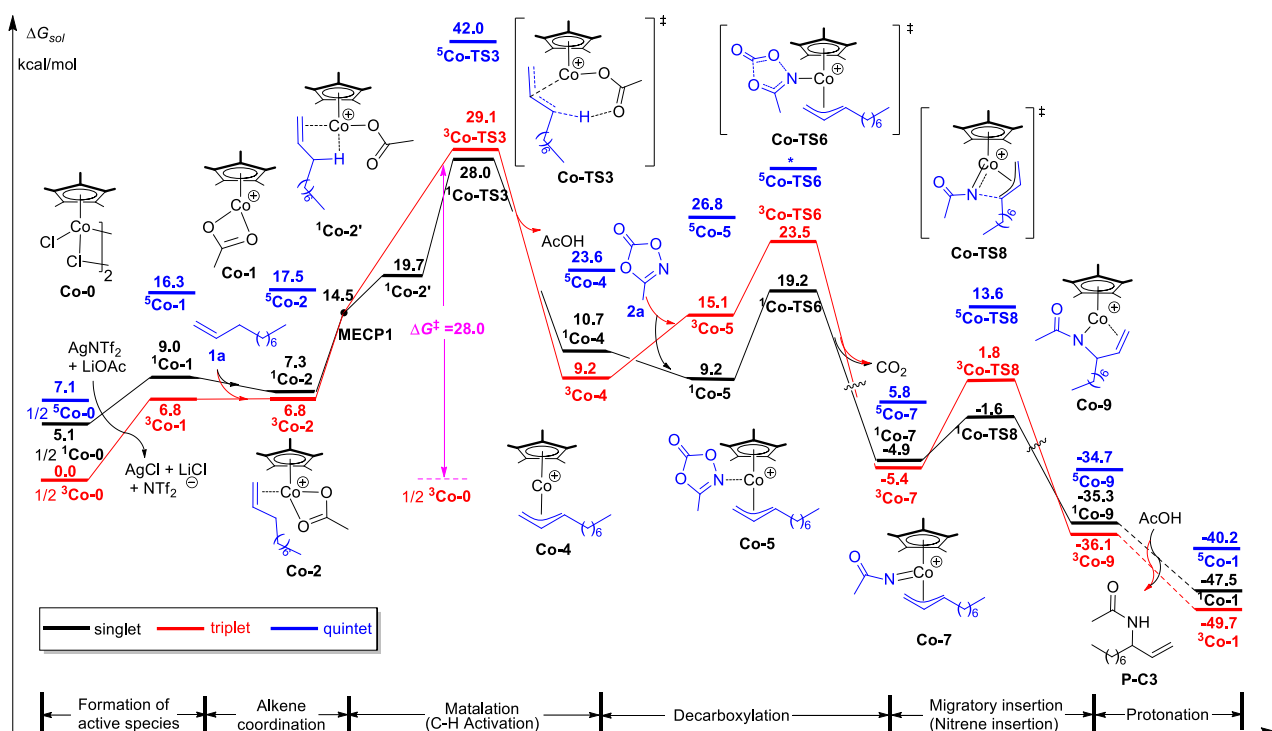
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**Table S1.** Free energy differences (kcal mol<sup>-1</sup>) of several potential Co(III) active species between singlet, triplet, and quintet states (the corresponding singlet states are taken as reference points).

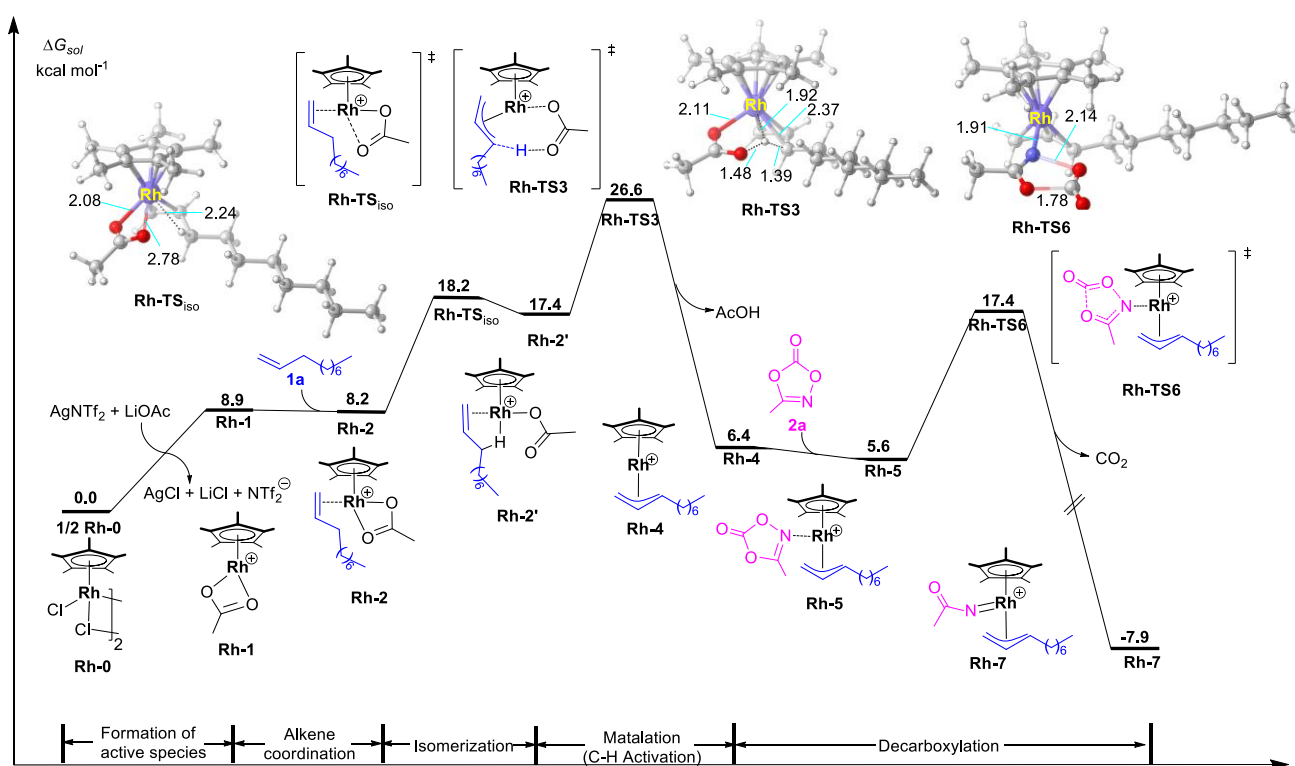
	$G(\text{singlet})$	$G(\text{triplet})$	$G(\text{quintet})$
[Cp*CoCl <sub>2</sub> ] <sub>2</sub>	0.0	-5.1	2.0
Cp*Co(OAc) <sub>2</sub>	0.0	-5.8	0.1
[Cp*Co(OAc)] <sup>+</sup>	0.0	-2.3	7.3
Cp*Co(OAc)(NTf <sub>2</sub> )	0.0	-1.3	7.3
[Cp*Co(NTf <sub>2</sub> )] <sup>+</sup>	0.0	-2.4	9.0



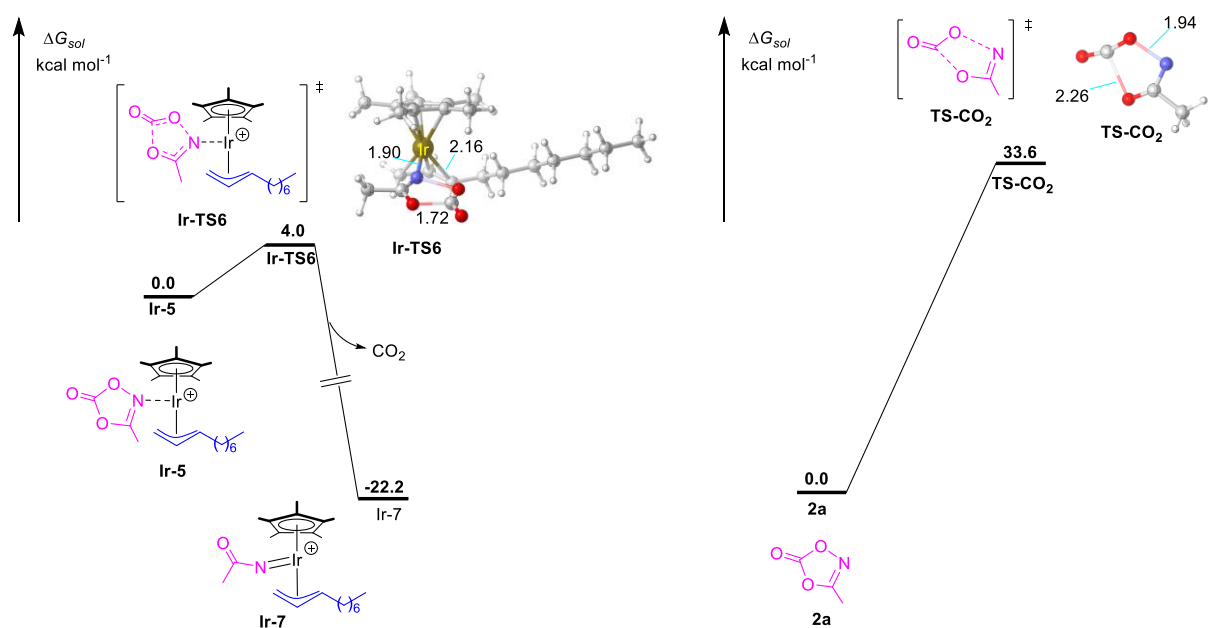
**Fig. S1** Frontier molecular orbital analysis of alkene-coordinating  $\pi$ -complexes <sup>1</sup>Co-2.



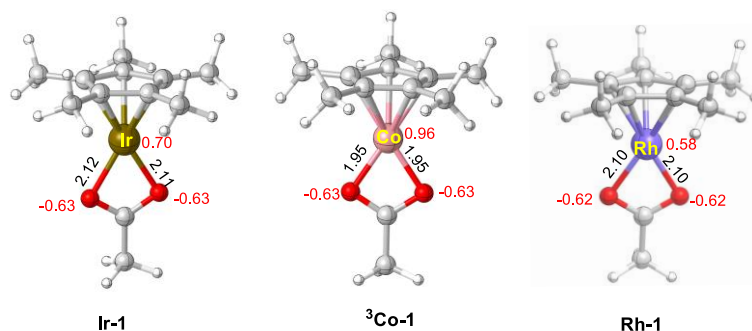
**Fig. S2** Calculated free energy profiles for intermolecular allylic C–H amidation of 1-decene by the Co catalyst.



**Fig. S3** Calculated free energy profiles for allylic C–H activation by the Rh(III) catalyst. Bond distances shown in the structures are given in angstroms.



**Fig. S4** Calculated free energy profiles for CO<sub>2</sub> extrusion by the Ir(III) catalyst and the uncoordinated organic molecule. Bond distances shown in the structures are given in angstroms.



**Fig. S5** Optimized structures of **Ir-1**, **Rh-1** and **<sup>3</sup>Co-1**. Bond distances shown in the structures are given in angstroms (Å). Red number represents the NPA charge.

### Cartesian coordinates for all of the stationary points

#### [Cp\*IrCl<sub>2</sub>]<sub>2</sub>

Ir	-1.84986100	0.21493800	-0.00004900
Ir	1.84985800	-0.21493200	0.00005300
Cl	0.00004900	0.00009600	-1.68234700
Cl	-0.00004900	-0.00008600	1.68235500
Cl	-1.50062100	2.61062800	0.00006700
Cl	1.50060700	-2.61062200	-0.00009800
C	2.83286400	1.59652100	0.71551800
C	2.83285300	1.59665500	-0.71509100
C	3.54560300	0.40109600	-1.17278800

C	3.54561300	0.40087500	1.17298300
C	4.01542500	-0.30635500	0.00002600
C	-3.54556900	-0.40116300	1.17281400
C	-4.01542800	0.30634000	0.00004700
C	-3.54564000	-0.40083100	-1.17295700
C	-2.83281700	-1.59669300	0.71504100
C	-2.83287100	-1.59649200	-0.71556800
C	-2.19104100	-2.63501900	-1.58214500
H	-1.24177800	-2.96358800	-1.15170000
H	-2.85683200	-3.50042000	-1.68706700
H	-1.97667500	-2.23907000	-2.57552200
C	-2.19093200	-2.63546200	1.58128700
H	-2.85669800	-3.50090900	1.68598900
H	-1.24167600	-2.96388400	1.15071200
H	-1.97652800	-2.23979800	2.57476900
C	-3.81878600	-0.04140700	2.60028500
H	-4.71018200	-0.56489100	2.96748500
H	-2.97386800	-0.31606200	3.23539800
H	-3.98023900	1.03272300	2.70787600
C	-4.82173400	1.56616300	0.00017800
H	-5.89155600	1.32500000	-0.00068300
H	-4.59712700	2.17253900	0.87861200
H	-4.59589100	2.17345600	-0.87730900
C	-3.81903000	-0.04066700	-2.60029100
H	-4.71049300	-0.56401800	-2.96752100
H	-3.98047600	1.03349800	-2.70754700
H	-2.97421000	-0.31516700	-3.23560200
C	2.19102000	2.63509300	1.58203100
H	2.85681800	3.50049000	1.68694200
H	1.24177500	2.96365800	1.15154200
H	1.97661400	2.23918800	2.57541700
C	3.81894200	0.04078200	2.60034700
H	4.71038400	0.56415700	2.96759200
H	2.97409000	0.31530800	3.23560400
H	3.98038700	-1.03337700	2.70766700
C	2.19100000	2.63538900	-1.58140400
H	1.24173800	2.96384300	-1.15086600
H	2.85677900	3.50082300	-1.68612900
H	1.97661800	2.23968100	-2.57487200
C	3.81887400	0.04126400	-2.60022900
H	2.97399200	0.31590700	-3.23539700
H	4.71029900	0.56470900	-2.96741600
H	3.98031000	-1.03287500	-2.70775700
C	4.82171800	-1.56618600	-0.00006800

H	4.59624600	-2.17322800	0.87768600
H	4.59672900	-2.17280900	-0.87823500
H	5.89154400	-1.32503300	0.00027700

**LiOAc**

C	-1.56142000	0.01201600	-0.00000300
H	-1.95059700	1.03027000	0.00159300
H	-1.92186900	-0.53071400	0.87882300
H	-1.92170000	-0.52767300	-0.88079600
C	-0.04644700	0.00774600	0.00007000
O	0.56491100	-1.11425500	0.00002300
O	0.59300900	1.11202300	0.00002000
Li	2.05933800	-0.02419800	-0.00012100

**AgNTf<sub>2</sub>**

N	-0.00009500	0.07740000	-0.00029800
S	-1.18393400	-0.67758800	-0.89021000
S	1.18352600	-0.67766200	0.88996600
O	-1.66916400	0.35018400	-1.81858500
O	-0.83027000	-2.02002500	-1.32806800
O	1.66857700	0.35016200	1.81844400
O	0.82973400	-2.02005000	1.32784200
C	2.52855300	-0.83749500	-0.40185700
C	-2.52850800	-0.83733400	0.40196800
F	2.83728200	0.39259700	-0.85156200
F	3.60896500	-1.38676400	0.14769600
F	2.10552500	-1.57962400	-1.41949800
F	-3.60963200	-1.38537400	-0.14722700
F	-2.10550600	-1.58023900	1.41902800
F	-2.83600300	0.39293700	0.85253700
Ag	0.00021800	2.21760000	-0.00001100

**OAc<sup>-</sup>**

C	-1.35245900	-0.05349100	-0.00000800
H	-1.72216800	-1.08287100	-0.00023200
H	-1.73350400	0.47464900	-0.88150800
H	-1.73361600	0.47429600	0.88166000
C	0.21197400	0.00139500	0.00006300
O	0.69727900	1.16004500	-0.00001600
O	0.80674500	-1.10423200	-0.00001500

**NTf<sub>2</sub><sup>-</sup>**

N	-0.00003400	-0.00027400	0.83084100
S	1.13972100	-0.86824900	0.08969700

S	-1.13958500	0.86805500	0.08970600
O	1.64382200	-1.86233100	1.03431500
O	0.88339800	-1.26765500	-1.29287900
O	-1.64339100	1.86226000	1.03433400
O	-0.88309100	1.26750000	-1.29281200
C	-2.56417800	-0.37728400	-0.03969100
C	2.56400800	0.37742500	-0.03970500
F	-2.96131500	-0.79070200	1.17354900
F	-3.62002700	0.19947500	-0.64611500
F	-2.20974400	-1.45253700	-0.75373700
F	3.62004700	-0.19926100	-0.64575000
F	2.20946200	1.45243300	-0.75409500
F	2.96081800	0.79125700	1.17352500

### LiNTf<sub>2</sub>

N	-0.02478100	0.27297200	-0.63265300
S	1.30469200	1.04079800	-0.04437200
S	-1.08438500	-0.58787600	0.26379000
O	1.85968800	1.82648900	-1.13884000
O	-1.14545600	-1.88193300	-0.49998400
O	1.18307300	1.55737300	1.31028600
O	-0.93816900	-0.62341600	1.71084300
C	-2.70439300	0.27094400	-0.12506600
C	2.44079400	-0.46025500	0.06682800
F	-2.65302200	1.51829000	0.32943600
F	-2.89740000	0.27587300	-1.44562300
F	-3.69137100	-0.39434500	0.47039300
F	2.11153700	-1.24443700	1.08578500
F	3.71567500	-0.12765200	0.12351700
F	2.26225800	-1.22804100	-1.09150300
Li	0.30932500	-1.41566200	-1.67972600

### LiCl

Li	0.00000000	0.00000000	-1.74664400
Cl	0.00000000	0.00000000	0.30823100

### AgOAc

C	-3.02904100	0.00177600	0.00003700
H	-3.42507100	1.01697500	0.00110600
H	-3.38319100	-0.54116400	0.88069800
H	-3.38331900	-0.53919500	-0.88177800
C	-1.50938500	0.00836000	-0.00006100
O	-0.91291300	-1.11419600	-0.00000200
O	-0.90280800	1.12395900	0.00000100

Ag	1.10527500	-0.00160700	0.00000300
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**AgCl**

Cl	0.00000000	0.00000000	-1.70803400
Ag	0.00000000	0.00000000	0.61779900

**Cp\*Ir(OAc)<sub>2</sub>**

Ir	0.03543100	-0.18378000	-0.07128300
C	1.24226700	1.19417600	1.08433900
C	1.14914200	1.68754800	-0.26791100
C	1.68519500	0.68375800	-1.15396100
C	2.18450000	-0.42003200	-0.33249000
C	1.90830900	-0.10800000	1.03564800
C	0.83621800	1.93576200	2.31945000
H	1.60096000	2.67456600	2.59046800
H	0.71198800	1.25138500	3.16164700
H	-0.11756100	2.43647400	2.15099500
C	0.59074500	3.01585200	-0.67337400
H	1.37189400	3.78201700	-0.59525700
H	-0.24880600	3.28594300	-0.03326300
H	0.23775300	2.99587900	-1.70666900
C	1.82073200	0.78370300	-2.64238000
H	2.80212500	1.19240200	-2.91383300
H	1.05166400	1.43334000	-3.06452100
H	1.72048700	-0.19865400	-3.10985500
C	2.85518600	-1.64794000	-0.86752000
H	3.90146000	-1.43514000	-1.11790100
H	2.35241800	-2.00095900	-1.77121900
H	2.83705900	-2.46095200	-0.13930400
C	2.22427400	-0.94831900	2.23447600
H	3.11310800	-0.56199200	2.74717200
H	2.41316200	-1.98659500	1.95548500
H	1.39095900	-0.93942300	2.94097200
O	-1.14832800	-1.61248300	1.11125600
O	-0.73188100	-2.03334200	-0.98837700
C	-1.34283400	-2.34411800	0.08553600
C	-2.29431300	-3.50409000	0.12953200
H	-3.28748400	-3.14468700	-0.15989700
H	-1.98738700	-4.27446900	-0.58016200
H	-2.35442000	-3.91035300	1.14065200
C	-3.91649400	1.58658800	-0.49690400
H	-3.95207100	1.55955200	-1.58916900
H	-4.32722100	2.52565600	-0.12369500
H	-4.52674100	0.75524500	-0.12879800



C	-2.48634700	1.40859900	-0.00316700
O	-2.02018300	2.12080900	0.88602900
O	-1.87098300	0.42888400	-0.61799500

**Cp\*Ir(OAc)(NTf<sub>2</sub>)**

Ir	-1.17137600	-0.10189900	0.10597300
C	-1.67865800	1.20104800	-1.57533400
C	-1.86682500	1.91324100	-0.32054700
C	-2.87079400	1.20020100	0.43887000
C	-3.28741800	0.03820700	-0.31367900
C	-2.53341800	0.04528000	-1.56514200
C	-0.78920000	1.62384300	-2.70162500
H	-1.35169700	2.26489200	-3.39125500
H	-0.40907600	0.76091700	-3.24751400
H	0.06899800	2.18500700	-2.33525200
C	-1.23150900	3.21115500	0.07282400
H	-1.89576300	4.04739200	-0.17712900
H	-0.28602600	3.35889500	-0.44775700
H	-1.01960500	3.23391200	1.14251400
C	-3.34381900	1.58940100	1.80405800
H	-4.13404200	2.34536400	1.72474000
H	-2.52220800	2.00714600	2.38960400
H	-3.74061000	0.73028400	2.34741700
C	-4.34597000	-0.95012900	0.07037700
H	-5.31763300	-0.66083400	-0.34751000
H	-4.44868400	-1.01418400	1.15570400
H	-4.09975300	-1.94764000	-0.30026100
C	-2.61637200	-0.98335200	-2.64942500
H	-3.32437200	-0.66313700	-3.42316100
H	-2.95116400	-1.94366600	-2.25262400
H	-1.63647600	-1.13454800	-3.10582000
O	-0.81573100	-2.24592800	0.35044300
O	-0.85454400	-0.95311000	2.09710600
C	-0.69499700	-2.12202800	1.61708200
C	-0.36330800	-3.29763000	2.48335700
H	0.65406600	-3.62209600	2.25171900
H	-0.43211100	-3.02663600	3.53701100
H	-1.04000700	-4.12523400	2.25492100
N	0.97528800	0.06460900	0.00400600
S	1.82930500	-0.73722300	-1.17998700
S	1.80535400	0.97157800	1.14814100
O	0.89536600	-1.06481700	-2.25850800
O	3.09113400	-0.05125200	-1.45248900
O	0.78691500	1.59315500	1.99299000

O	2.94408600	0.25619200	1.71441100
C	2.55268900	2.42807200	0.17433100
C	2.31860700	-2.41107000	-0.41703100
F	1.92520300	2.59449700	-1.00369900
F	2.36764400	3.53249400	0.90482100
F	3.84606400	2.24784100	-0.03293800
F	1.53333600	-3.37390100	-0.89137500
F	3.58195300	-2.66710100	-0.75029100
F	2.21565800	-2.37193200	0.91636000

**[Cp\*Ir(NTf<sub>2</sub>)]<sup>+</sup>**

Ir	0.96469200	0.11960800	-0.19018500
C	2.17917200	-0.54047700	1.47085400
C	2.84520600	0.58102000	0.79835100
C	3.14437800	0.18869400	-0.55138400
C	2.63596100	-1.15029300	-0.73904300
C	2.05669800	-1.61215200	0.52228800
C	1.74662100	-0.57605000	2.90006600
H	2.55745400	-0.99061600	3.51145300
H	0.86000700	-1.19822900	3.02696600
H	1.52049500	0.42393400	3.27442900
C	3.17762200	1.89041800	1.43455600
H	4.14353800	1.80828000	1.94801100
H	2.42846200	2.17538800	2.17592400
H	3.25462300	2.68909900	0.69520500
C	3.83295700	1.02143300	-1.58754600
H	4.91117000	0.82724500	-1.56061400
H	3.67660000	2.08713700	-1.41257900
H	3.47251000	0.78827400	-2.59112800
C	2.71580400	-1.95542800	-1.99239100
H	3.62489600	-2.56955100	-1.96585200
H	2.76251000	-1.32061000	-2.87846700
H	1.86091200	-2.62754700	-2.08869300
C	1.50936600	-2.97605200	0.79372600
H	2.31209500	-3.61346100	1.18296000
H	1.11829300	-3.43830800	-0.11313700
H	0.70611000	-2.93771300	1.52970100
N	-1.06526300	0.00466000	-0.02499400
S	-2.13963700	-0.97924000	0.85998300
S	-1.47866500	1.34141100	-0.92120100
O	-1.33337700	-1.61457000	1.89339300
O	-3.35922200	-0.23505700	1.12495000
O	-0.05440700	1.61795600	-1.41200000
O	-2.57204400	1.25353700	-1.86078700

C	-1.80638200	2.74124400	0.31966800
C	-2.48409800	-2.28123200	-0.45261200
F	-0.92210400	2.61580900	1.31292200
F	-1.61732900	3.88089700	-0.32275800
F	-3.03624400	2.63986800	0.77306900
F	-1.31451000	-2.83317900	-0.80429500
F	-3.28655000	-3.19894600	0.05693800
F	-3.03534600	-1.69357400	-1.50466500

**Ir-1**

Ir	-0.30026200	-0.00442000	-0.01307700
C	1.50347300	0.49954200	-1.10010900
C	1.51475700	-0.93373200	-0.78111400
C	1.49210700	-1.06618100	0.64088300
C	1.45513000	0.28214200	1.20927200
C	1.49896300	1.24286900	0.13027300
C	1.53956100	1.07307300	-2.47744200
H	2.58370900	1.15567900	-2.80463900
H	1.09502400	2.06895300	-2.51031500
H	1.01544000	0.43481300	-3.19147200
C	1.56961200	-2.04094100	-1.78336000
H	2.61264700	-2.22629900	-2.06682500
H	1.01586800	-1.78746400	-2.68967100
H	1.15729100	-2.96685600	-1.37974100
C	1.51887300	-2.33867500	1.42563000
H	2.55133800	-2.57396300	1.70972600
H	1.12711400	-3.17475500	0.84448800
H	0.92860700	-2.25579000	2.34047600
C	1.43439400	0.60356300	2.66580300
H	2.46706300	0.65885700	3.03348300
H	0.91567400	-0.16634400	3.23990700
H	0.95619300	1.56533900	2.85847000
C	1.52984900	2.73229700	0.27359500
H	2.56742800	3.07478700	0.35939000
H	0.99071900	3.05797300	1.16505900
H	1.08009000	3.22550800	-0.58971000
O	-2.11339900	1.08989100	-0.02399100
O	-2.11252500	-1.08781600	-0.01931100
C	-2.80116900	0.00270400	-0.02407500
C	-4.28599500	-0.00523800	-0.01081800
H	-4.65423800	-0.73780000	-0.73357800
H	-4.62269000	-0.32671600	0.98142700
H	-4.67706900	0.98928800	-0.22430900

**1a**

C	-5.59634100	-0.31227200	0.58576800
H	-5.55211600	0.25013400	1.51587400
H	-6.47828400	-0.92659300	0.42975200
C	-4.61689500	-0.24424600	-0.31566300
H	-4.69977500	-0.82855800	-1.23374700
C	-3.35883400	0.56635400	-0.17335000
H	-3.39659800	1.15425200	0.75268100
H	-3.29455400	1.28941300	-1.00038600
C	-2.08713900	-0.30113600	-0.18343800
H	-2.06576000	-0.90406800	-1.10219100
H	-2.13541300	-1.01580500	0.64866100
C	-0.79798800	0.52085800	-0.08445100
H	-0.82296900	1.12691600	0.83241300
H	-0.75766000	1.23582700	-0.91873000
C	0.47146000	-0.33737100	-0.08998200
H	0.49614100	-0.94352100	-1.00682900
H	0.42999600	-1.05232000	0.74402000
C	1.76195600	0.48304100	0.00966800
H	1.73686000	1.08933300	0.92646600
H	1.80306200	1.19812300	-0.82444500
C	3.03171800	-0.37462000	0.00440900
H	3.05732500	-0.98121600	-0.91234300
H	2.99109100	-1.08990100	0.83852300
C	4.32316200	0.44494300	0.10413000
H	4.29653100	1.05036400	1.02044200
H	4.36277000	1.15899900	-0.72980100
C	5.58536000	-0.42221500	0.09807900
H	5.65214200	-1.01402000	-0.82207900
H	6.49296200	0.18593900	0.17009900
H	5.58549700	-1.12330700	0.94060400

**Ir-2**

Ir	1.56239300	0.17029900	-0.13693100
C	1.24386800	-2.00541700	0.23210700
C	1.15716500	-1.33577300	1.50979000
C	2.39432200	-0.64868800	1.74531700
C	3.28550300	-0.93830900	0.61947200
C	2.57792300	-1.77905400	-0.30479100
C	0.22462400	-2.95373500	-0.31804100
H	0.37980000	-3.94583500	0.12233300
H	0.30813600	-3.06020600	-1.40082000
H	-0.79113500	-2.63417400	-0.08357000
C	-0.04408500	-1.33242500	2.39852900

H	-0.02979700	-2.22346000	3.03743500
H	-0.96741500	-1.35195700	1.81582200
H	-0.06518800	-0.45263600	3.04316400
C	2.77008500	0.14917400	2.95581400
H	3.34117200	-0.47229800	3.65475700
H	1.88762200	0.52097300	3.47952000
H	3.38908300	1.00618100	2.68187200
C	4.69838000	-0.46088800	0.50762800
H	5.34484100	-1.07478900	1.14570300
H	4.78776400	0.57743900	0.83504000
H	5.06792100	-0.52944700	-0.51641400
C	3.13381500	-2.39897000	-1.54918900
H	3.50983400	-3.40336900	-1.32439100
H	3.96125600	-1.81440100	-1.95477900
H	2.37311500	-2.49919600	-2.32645600
O	0.15244400	1.74128800	0.35224600
O	2.26273300	2.19881900	0.18429500
C	1.07852000	2.62159800	0.42176200
C	0.78957400	4.05521700	0.71944100
H	1.67197200	4.54085400	1.13841300
H	0.52407400	4.56330200	-0.21441200
H	-0.05908600	4.13370000	1.40134200
C	1.65294900	0.76254500	-2.28381900
H	1.60694400	1.84799200	-2.32727900
H	2.55460700	0.31817900	-2.69577700
C	0.47384700	0.02118000	-2.18444900
H	0.51860400	-1.03585600	-2.44002300
C	-0.91236700	0.60837500	-2.17654200
H	-0.87445400	1.65996000	-1.87971200
H	-1.25312700	0.58550500	-3.22319000
C	-1.91965400	-0.15217600	-1.30499000
H	-1.56027900	-0.14808700	-0.26870000
H	-1.96038300	-1.20162900	-1.62802300
C	-3.32738900	0.44868700	-1.34956500
H	-3.27857800	1.50289300	-1.04419700
H	-3.69598900	0.44397700	-2.38446200
C	-4.31868900	-0.29661800	-0.44894800
H	-3.94312400	-0.28872200	0.58527300
H	-4.36149500	-1.35310000	-0.75091000
C	-5.73198500	0.29584700	-0.47716700
H	-5.68762800	1.35300900	-0.17957400
H	-6.10770400	0.28628600	-1.50983600
C	-6.71923700	-0.44682500	0.43000200
H	-6.34234000	-0.43738900	1.46315600

H	-6.76226600	-1.50447600	0.13247200
C	-8.13376900	0.14431300	0.40243800
H	-8.08886900	1.20123700	0.69833400
H	-8.50888000	0.13328400	-0.62980600
C	-9.11134200	-0.60431600	1.31336600
H	-8.77584200	-0.58062500	2.35656900
H	-10.11217900	-0.16326200	1.27532300
H	-9.19903000	-1.65614700	1.01819100

Ir-TS<sub>iso</sub>

Ir	1.54581700	-0.03502000	-0.30277700
C	2.54421200	-1.86879100	0.32051600
C	1.37321200	-1.72859400	1.13405800
C	1.52070100	-0.51690000	1.94228800
C	2.74167800	0.11877200	1.58727600
C	3.38147700	-0.68761100	0.54560200
C	2.89202400	-3.02749700	-0.55927500
H	3.46652700	-3.76263400	0.01593200
H	3.50487600	-2.71697600	-1.40746700
H	2.00036400	-3.52730700	-0.94244500
C	0.25118000	-2.71279800	1.25711500
H	0.42928500	-3.37802600	2.10971100
H	0.16146700	-3.33281800	0.36346600
H	-0.70435400	-2.20994900	1.41919000
C	0.53080000	-0.00463100	2.93470300
H	0.41000300	1.07516500	2.83386300
H	0.88529800	-0.22758800	3.94843500
H	-0.44635200	-0.47231900	2.80818400
C	3.28085800	1.39099800	2.15970700
H	2.47207300	2.03588900	2.50600300
H	3.86076300	1.93963900	1.41497700
H	3.93898400	1.17086500	3.00788000
C	4.73422900	-0.43697200	-0.03679900
H	5.50343300	-0.82615100	0.64156500
H	4.91023300	0.63145400	-0.17457600
H	4.85218100	-0.93069800	-1.00263300
O	0.32537000	2.32109900	0.66237400
O	1.87057900	1.93124900	-0.90312300
C	1.14635700	2.74455400	-0.16198200
C	1.40512700	4.21140200	-0.39966300
H	0.66042800	4.81078600	0.12354000
H	2.40470400	4.46767200	-0.03383800
H	1.38624600	4.42962900	-1.47038700
C	1.43250600	-0.36943200	-2.51871600

H	1.48524100	0.63461500	-2.92981300
H	2.17716000	-1.07592500	-2.87374500
C	0.26532900	-0.83885600	-1.91335500
H	0.11741000	-1.91222700	-1.80398400
C	-0.91195800	0.04991600	-1.57714100
H	-0.68289800	0.66757400	-0.67245600
H	-1.04327200	0.80098900	-2.36596300
C	-2.20712900	-0.71873200	-1.29043400
H	-2.01481000	-1.46568300	-0.50779300
H	-2.49445700	-1.27998100	-2.18902600
C	-3.35327300	0.19947300	-0.85553400
H	-3.04718300	0.76152400	0.03846500
H	-3.53426200	0.94797600	-1.63888000
C	-4.65275200	-0.55946500	-0.56476300
H	-4.46905700	-1.30875200	0.21897900
H	-4.95316500	-1.12221800	-1.45952400
C	-5.80160000	0.35835600	-0.13143300
H	-5.49835900	0.92330900	0.76153900
H	-5.98315000	1.10574700	-0.91642700
C	-7.10275600	-0.39680200	0.16169600
H	-6.92136200	-1.14440000	0.94740200
H	-7.40404900	-0.96261100	-0.73138200
C	-8.25342800	0.52095600	0.59176300
H	-7.95034600	1.08621400	1.48365700
H	-8.43270700	1.26670700	-0.19447700
C	-9.54899800	-0.24279300	0.88167900
H	-9.40516200	-0.97301800	1.68624600
H	-10.35333500	0.43410600	1.18584500
H	-9.89070700	-0.79017300	-0.00409600

**Ir-2'**

Ir	1.45554800	-0.06324700	-0.30626600
C	2.43672100	-1.83864000	0.51662800
C	1.08628100	-1.83224600	1.00670800
C	0.91041900	-0.64127900	1.83434400
C	2.12973700	0.09482200	1.82563400
C	3.08338600	-0.61042100	0.97031400
C	3.09218000	-2.92574800	-0.27549800
H	3.57684000	-3.63277800	0.40756900
H	3.86007200	-2.52756100	-0.94134500
H	2.36961200	-3.48307500	-0.87468600
C	0.07225300	-2.91941500	0.82318100
H	0.14959200	-3.64345500	1.64229600
H	0.22656800	-3.45886500	-0.11338500

H	-0.94475000	-2.52284300	0.82522000
C	-0.34127800	-0.22695400	2.53955200
H	-0.53428600	0.83460500	2.36872500
H	-0.23327400	-0.39622900	3.61702100
H	-1.20613000	-0.79474200	2.19314300
C	2.39386100	1.37277200	2.55466700
H	1.48176800	1.96155700	2.65683200
H	3.13682300	1.97649900	2.03070700
H	2.78336900	1.14919500	3.55466700
C	4.51781800	-0.23341600	0.77260000
H	5.11532400	-0.57577600	1.62568900
H	4.62898300	0.84928300	0.68953100
H	4.92713200	-0.68550600	-0.13233300
O	-0.00891300	2.44141100	0.53113000
O	1.81922300	1.95396200	-0.69481800
C	0.97865400	2.79652500	-0.11338400
C	1.36132400	4.24737000	-0.30701000
H	0.52779000	4.88989700	-0.02374900
H	2.22397900	4.47657700	0.32758400
H	1.65806400	4.43489600	-1.34128500
C	1.97768700	-0.20680200	-2.49733600
H	2.10211100	0.83829700	-2.76338400
H	2.79501300	-0.87430600	-2.75330100
C	0.71414900	-0.74857200	-2.23636600
H	0.54792800	-1.82230400	-2.30106600
C	-0.45281000	0.11494200	-1.86861500
H	-0.29557600	0.57425400	-0.79442500
H	-0.47439200	1.04450800	-2.44829400
C	-1.80636700	-0.59067100	-1.76817300
H	-1.66501100	-1.55742300	-1.26800900
H	-2.15123600	-0.81428800	-2.78551300
C	-2.85687900	0.23327700	-1.01641400
H	-2.47675300	0.47277500	-0.01275300
H	-2.99532300	1.19774700	-1.52247200
C	-4.20420900	-0.48644500	-0.89691900
H	-4.05488400	-1.45754600	-0.40201000
H	-4.58688100	-0.71359400	-1.90135400
C	-5.25085900	0.32220600	-0.12216900
H	-4.86215800	0.55327700	0.88013600
H	-5.40118000	1.29039600	-0.61946700
C	-6.59725900	-0.39856200	0.00773200
H	-6.44508700	-1.36890000	0.50227100
H	-6.98546600	-0.62708300	-0.99490600
C	-7.64471800	0.40735300	0.78522800



H	-7.25415500	0.63624600	1.78626000
H	-7.79578800	1.37550100	0.28906900
C	-8.98563600	-0.32220400	0.90985100
H	-8.86756500	-1.27936400	1.43055700
H	-9.71465900	0.27317500	1.46802000
H	-9.41284600	-0.53334300	-0.07693100

### Ir-TS3

Ir	1.40179700	-0.01000400	-0.29965600
C	2.66902500	-1.66931000	0.55401300
C	1.27364500	-2.06651700	0.61149200
C	0.58407000	-1.15515800	1.49781500
C	1.51794900	-0.14881400	1.91130200
C	2.82379200	-0.47119400	1.32895600
C	3.75125800	-2.40935700	-0.16875500
H	4.14751700	-3.20145000	0.47707600
H	4.57806300	-1.75088200	-0.43934000
H	3.37701500	-2.88316300	-1.07902200
C	0.69129700	-3.31006700	0.01135400
H	0.79505400	-4.14747900	0.71084900
H	1.20020900	-3.58821200	-0.91394200
H	-0.37197100	-3.18910400	-0.20535200
C	-0.84904400	-1.25527700	1.91724100
H	-1.25616400	-0.27799000	2.18093100
H	-0.92726300	-1.90408100	2.79756800
H	-1.47188200	-1.68503300	1.13016700
C	1.24716700	0.98602900	2.85012700
H	0.22922400	1.36162300	2.73413900
H	1.93580600	1.81254900	2.66614300
H	1.38301700	0.65741800	3.88657500
C	4.08678900	0.28983300	1.58993500
H	4.44444700	0.08984100	2.60605600
H	3.91595300	1.36437500	1.49106600
H	4.87528000	0.00934600	0.89003100
O	-0.35948300	2.41810000	0.10872200
O	1.82169900	2.05773800	-0.29806200
C	0.80506800	2.83381400	-0.01385200
C	1.15115000	4.29051000	0.18076500
H	0.33023100	4.91342900	-0.17736300
H	1.26957600	4.47581100	1.25395100
H	2.08374500	4.54778400	-0.32187100
C	2.24849700	0.10399000	-2.34456300
H	2.37066000	1.16942300	-2.51603700
H	3.11438600	-0.51581500	-2.55792600

C	0.96484300	-0.49257600	-2.36337900
H	0.84436900	-1.55824100	-2.54884000
C	-0.19214400	0.27866500	-1.95456800
H	-0.08565900	0.82428500	-0.46714000
H	-0.19327100	1.32652300	-2.25739300
C	-1.55224900	-0.38788100	-1.91177800
H	-1.43224300	-1.42573400	-1.57565200
H	-1.91356500	-0.43973900	-2.94874900
C	-2.59086100	0.33114700	-1.04315700
H	-2.20306100	0.43572200	-0.02284900
H	-2.72894300	1.35497200	-1.41126400
C	-3.93558100	-0.40116100	-1.00663500
H	-3.78040500	-1.43140300	-0.65185700
H	-4.33444000	-0.48973100	-2.02641500
C	-4.96812600	0.29210600	-0.11082700
H	-4.56232100	0.38141100	0.90752400
H	-5.12290600	1.32020700	-0.46591600
C	-6.31447700	-0.43832900	-0.05956500
H	-6.15760200	-1.46835800	0.29227600
H	-6.72001700	-0.52438600	-1.07750100
C	-7.34591500	0.25283000	0.84024100
H	-6.93810300	0.33914600	1.85680500
H	-7.50109700	1.28099800	0.48660000
C	-8.68753200	-0.48465500	0.88437100
H	-8.56489800	-1.50534600	1.26433200
H	-9.40485100	0.02829900	1.53229600
H	-9.13168000	-0.55516300	-0.11488400

#### AcOH

C	1.39581500	-0.11015600	-0.00000800
H	1.67847600	-0.69392900	-0.88082600
H	1.67860000	-0.69231100	0.88185100
H	1.91518500	0.84699100	-0.00089800
C	-0.09299300	0.12631600	-0.00002600
O	-0.64425200	1.20365600	0.00000800
O	-0.77694300	-1.04711100	0.00000100
H	-1.71963400	-0.81007300	0.00000600

#### Ir-4

Ir	-1.48652200	0.37995000	-0.29185500
C	-2.82853800	-1.18547800	0.62437700
C	-1.73370000	-0.75570300	1.49548500
C	-0.46394000	-1.22965900	0.92315800
C	-0.76170000	-1.76694300	-0.34846200

C	-2.22958900	-1.73364700	-0.53501800
C	-4.28923500	-1.05905800	0.92826100
H	-4.62618200	-1.92828300	1.50533300
H	-4.88681900	-1.00801900	0.01646600
H	-4.49887200	-0.16593500	1.52050400
C	-1.88501500	-0.17141700	2.86192900
H	-1.97567200	-0.98073800	3.59749300
H	-2.77922900	0.45029100	2.93663600
H	-1.01536500	0.43047400	3.13443900
C	0.85858800	-1.16258500	1.61959200
H	0.87566500	-1.88332000	2.44553100
H	1.04100600	-0.17157500	2.04302500
H	1.68475600	-1.39886300	0.94884100
C	0.19643300	-2.37386500	-1.32615200
H	0.15950900	-3.46762400	-1.25740600
H	1.22251600	-2.05617300	-1.13534300
H	-0.05648300	-2.10140600	-2.35387000
C	-2.93167400	-2.27893500	-1.73817000
H	-2.97622600	-3.37318700	-1.67760800
H	-2.40024100	-2.02490400	-2.65894500
H	-3.95285100	-1.90248200	-1.81550100
C	-2.60892800	2.20357300	-0.54131500
H	-2.69551600	2.28021300	-1.63013100
H	-3.53899800	2.37794600	-0.00915900
C	-1.36608300	2.55942400	0.06745300
H	-1.33457900	2.89629000	1.10291800
C	-0.17636300	2.10364700	-0.55926900
C	1.20210800	2.23625200	0.03740400
H	1.14136700	2.06023700	1.11970100
H	1.55203300	3.27036100	-0.08554800
C	2.21066300	1.27287900	-0.60159000
H	1.76528400	0.27101600	-0.63626800
H	2.37784500	1.56555800	-1.64697700
C	3.55028200	1.20991000	0.13718900
H	3.37042700	0.95522800	1.19192300
H	4.01609500	2.20424400	0.14086600
C	4.51938000	0.18947400	-0.46996000
H	4.04380300	-0.80384700	-0.47371800
H	4.69993600	0.44108800	-1.52423300
C	5.85798000	0.10491900	0.27134300
H	5.67467900	-0.14172800	1.32714400
H	6.33534800	1.09469700	0.26998800
C	6.82214500	-0.92445400	-0.33022800
H	6.34181500	-1.91284600	-0.32989400

H	7.00412700	-0.67497500	-1.38424800
C	8.15591500	-1.00016900	0.41882700
H	8.00449900	-1.27851400	1.46796800
H	8.82485200	-1.74099100	-0.02957200
H	8.67127800	-0.03335700	0.40442000
H	-0.19995600	2.06601100	-1.66104900

**2a**

C	-1.20092300	-0.18030500	-0.00001900
O	-2.30068100	-0.63661500	0.00013000
O	-0.84556900	1.13236100	-0.00006200
O	-0.01619600	-0.90807200	-0.00013900
C	0.98207900	0.01591000	-0.00008800
N	0.57801900	1.23586000	0.00005000
C	2.39041400	-0.44509100	0.00005200
H	2.58452600	-1.05702900	0.88590500
H	2.58444800	-1.05792200	-0.88515500
H	3.05503300	0.41945800	-0.00019800

**Ir-5**

Ir	1.21866100	-0.37706600	-0.28876800
C	1.12282400	-2.46804100	0.42301100
C	0.01716800	-1.78901200	1.08148000
C	0.56259100	-0.72519200	1.85025100
C	2.02841300	-0.79712200	1.75689600
C	2.36581500	-1.90211200	0.91947000
C	0.99819600	-3.71265800	-0.40456300
H	0.98721400	-4.59721100	0.24253200
H	1.83480300	-3.81998500	-1.09865700
H	0.07194500	-3.71374100	-0.98365800
C	-1.41601600	-2.21291200	1.01438100
H	-1.70914800	-2.50223600	0.00372200
H	-2.09258500	-1.42691600	1.35054000
H	-1.56453800	-3.08517600	1.66219000
C	-0.20010700	0.23251300	2.71616900
H	-0.29312500	-0.16533700	3.73325500
H	-1.20391900	0.41089000	2.32622700
H	0.30614000	1.19789200	2.78591600
C	2.97588900	0.05766000	2.54417900
H	3.05883400	-0.31451900	3.57159500
H	2.62629900	1.09186600	2.60274300
H	3.97664400	0.05779000	2.10779400
C	3.73876500	-2.41962800	0.61713900
H	3.98938800	-3.23707100	1.30313000

H	4.49791600	-1.64318200	0.73001200
H	3.80342700	-2.81176800	-0.40030800
C	2.37013900	-0.25381300	-2.14417600
H	2.55699600	0.78730300	-2.39989600
H	3.23681900	-0.90211800	-2.24364600
C	1.07370000	-0.80258200	-2.41079000
H	0.95547100	-1.86360700	-2.62229900
C	-0.06575800	-0.00855500	-2.11923900
C	-1.47741000	-0.52673800	-2.19723100
H	-1.49160200	-1.60201400	-1.97882900
H	-1.83315500	-0.42201600	-3.23263800
C	-2.43189700	0.22208700	-1.25686200
H	-2.00213200	0.22212200	-0.24795800
H	-2.48102700	1.27679700	-1.55828400
C	-3.84301300	-0.37042900	-1.21936000
H	-3.78279800	-1.44101300	-0.97479400
H	-4.29309300	-0.31435600	-2.21954800
C	-4.75568000	0.32621100	-0.20416000
H	-4.29559900	0.26837300	0.79444100
H	-4.81847000	1.39645400	-0.44506600
C	-6.16689600	-0.26824800	-0.14494300
H	-6.10058500	-1.34062300	0.08949000
H	-6.62917700	-0.20399300	-1.13987700
C	-7.07439000	0.41982600	0.88169000
H	-6.60882800	0.35658700	1.87508600
H	-7.14038100	1.49019100	0.64448000
C	-8.48099500	-0.18404800	0.93332800
H	-8.44501200	-1.24665600	1.19938300
H	-9.10780900	0.32384100	1.67271200
H	-8.98015700	-0.10370400	-0.03879700
H	0.02772500	1.06600300	-2.27213100
C	3.70764300	2.38190700	-0.12655400
H	4.12685800	2.95565600	-0.95886700
H	3.91168200	1.32056900	-0.26180700
H	4.17270300	2.74122900	0.79621700
C	2.24676300	2.60322700	-0.05985900
O	1.77016800	3.84746100	0.12593600
N	1.30749000	1.71582700	-0.15592400
O	0.07889200	2.43278500	-0.02226000
C	0.37524100	3.75823500	0.15511300
O	-0.38443000	4.65144200	0.30632300

**Ir-TS6**

Ir	1.31302300	-0.32987400	-0.28852500
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C	1. 71989200	-2. 34415200	0. 64422000
C	0. 34971600	-2. 01649300	0. 97901000
C	0. 35267700	-0. 80782600	1. 74912700
C	1. 73394400	-0. 38040700	1. 89503500
C	2. 58415700	-1. 35439800	1. 25168100
C	2. 18335000	-3. 58923700	-0. 05133300
H	2. 39327800	-4. 37273100	0. 68538600
H	3. 10095400	-3. 41458800	-0. 61764300
H	1. 42702900	-3. 97654500	-0. 73679000
C	-0. 85157500	-2. 84973500	0. 65556500
H	-0. 70165500	-3. 44179800	-0. 24892400
H	-1. 74542800	-2. 23973400	0. 52084800
H	-1. 04029800	-3. 54901000	1. 47849600
C	-0. 82299400	-0. 09912000	2. 34838300
H	-0. 86548800	0. 94002000	2. 01118400
H	-0. 73967600	-0. 10219100	3. 44111000
H	-1. 76398300	-0. 57977200	2. 07942400
C	2. 17287000	0. 80307700	2. 70074900
H	2. 20723500	0. 53642100	3. 76291600
H	1. 47499000	1. 63574700	2. 58777500
H	3. 16790100	1. 14288900	2. 40851800
C	4. 08069200	-1. 38853500	1. 28544000
H	4. 41843700	-1. 97011600	2. 15135600
H	4. 50300700	-0. 38563100	1. 37129900
H	4. 49222800	-1. 85717000	0. 38936500
C	2. 41265400	-0. 48910500	-2. 18979900
H	2. 60710200	0. 52198000	-2. 53477200
H	3. 27261600	-1. 15249100	-2. 19446900
C	1. 11248300	-1. 05474400	-2. 36618200
H	0. 99509900	-2. 13588900	-2. 41880800
C	-0. 03423000	-0. 24605800	-2. 21961100
C	-1. 43043600	-0. 78920500	-2. 20650300
H	-1. 41824700	-1. 86074900	-1. 97557500
H	-1. 82090400	-0. 69722000	-3. 23167400
C	-2. 36889900	-0. 03858700	-1. 24803100
H	-1. 92823600	-0. 04447400	-0. 24535100
H	-2. 41034000	1. 01845300	-1. 53218500
C	-3. 77866300	-0. 63312000	-1. 20333000
H	-3. 72188300	-1. 70382500	-0. 95432700
H	-4. 23196000	-0. 58128700	-2. 20237200
C	-4. 68473700	0. 07581100	-0. 19011600
H	-4. 22856900	0. 01377500	0. 80973000
H	-4. 73121200	1. 14603800	-0. 43296500
C	-6. 10430300	-0. 49877400	-0. 13610300

H	-6.05583200	-1.57144000	0.10158600
H	-6.56062800	-0.42988200	-1.13348300
C	-7.00584900	0.20709800	0.88378400
H	-6.54822900	0.13666800	1.88033200
H	-7.05024400	1.27805300	0.64475300
C	-8.42367800	-0.37055800	0.92605200
H	-8.40969100	-1.43348500	1.19291400
H	-9.04563000	0.14971000	1.66083100
H	-8.91462800	-0.28114000	-0.04944600
H	0.05838900	0.82092300	-2.41052100
C	3.45017200	2.77617500	-0.24772200
H	3.73955600	3.49079300	-1.02230100
H	3.89143200	1.80040500	-0.45036800
H	3.79834200	3.15831600	0.71562400
C	1.93170100	2.71927000	-0.20184300
O	1.31546500	3.81387100	0.02232800
N	1.38582100	1.55982500	-0.43076200
O	-0.58093800	2.41393100	-0.18084700
C	-0.39572300	3.61494400	0.05390000
O	-0.92423500	4.64651500	0.29052100

**CO<sub>2</sub>**

C	0.00000000	0.00000000	-0.00001700
O	0.00000000	0.00000000	1.16931700
O	0.00000000	0.00000000	-1.16930500

**Ir-7**

Ir	1.33251300	-0.08743100	-0.34648900
C	2.67283400	-0.48713500	1.40655000
C	1.90157800	-1.68893000	1.21283200
C	0.51307400	-1.36350500	1.40823700
C	0.41365800	0.03343400	1.75657800
C	1.74838300	0.58548100	1.74176600
C	4.16668500	-0.38371300	1.41331700
H	4.54581100	-0.57131700	2.42490700
H	4.49869500	0.61082700	1.10989000
H	4.62419900	-1.11579300	0.74505600
C	2.46434500	-3.05254000	0.94535900
H	2.74495700	-3.53262400	1.88961300
H	3.36139400	-3.00429800	0.32361600
H	1.73974100	-3.70321200	0.45149800
C	-0.63123000	-2.32859500	1.37237400
H	-0.80831400	-2.72377900	2.37946100
H	-0.42656700	-3.17774300	0.71760300

H	-1.55144000	-1.84882700	1.03580000
C	-0.82160100	0.78333500	2.14525900
H	-0.79074200	0.99908000	3.21999600
H	-1.72527700	0.20630600	1.94561400
H	-0.88277200	1.73000000	1.60311800
C	2.12149100	1.95878000	2.20542200
H	2.28853000	1.93980800	3.28867400
H	1.32638400	2.67602100	1.99631800
H	3.04141300	2.30838100	1.73227800
C	2.44812400	-0.92428800	-2.06608800
H	2.62907100	-0.08449600	-2.72897300
H	3.31861800	-1.52360400	-1.81773800
C	1.16185900	-1.53744400	-2.02665000
H	1.06562700	-2.56009400	-1.66510100
C	-0.00383700	-0.76881800	-2.21748200
C	-1.38970600	-1.28390600	-1.99276100
H	-1.36477900	-2.20384600	-1.39808000
H	-1.79753700	-1.55872300	-2.97758500
C	-2.31680900	-0.24128700	-1.34283700
H	-1.84987300	0.12051100	-0.41988300
H	-2.39081400	0.63553900	-1.99814900
C	-3.71384800	-0.78866400	-1.03795000
H	-3.62594700	-1.69009300	-0.41260100
H	-4.19409300	-1.11516600	-1.97004400
C	-4.60755500	0.23469200	-0.32791900
H	-4.11757200	0.56083000	0.60185100
H	-4.69569300	1.13403100	-0.95252400
C	-6.00587700	-0.30201300	-0.00348200
H	-5.91522300	-1.20492700	0.61776200
H	-6.49617500	-0.62216400	-0.93346500
C	-6.89611000	0.71993700	0.71369500
H	-6.40300200	1.04003900	1.64198900
H	-6.98507900	1.62006000	0.09082600
C	-8.29108600	0.17427600	1.03306700
H	-8.23159600	-0.70806700	1.68046200
H	-8.90538900	0.92193200	1.54396300
H	-8.81743500	-0.12152800	0.11869100
H	0.08419200	0.15453000	-2.78448200
C	2.16336800	3.75063900	-0.98029000
H	3.08861100	3.22710200	-1.23581600
H	2.31548000	4.39174700	-0.10858400
H	1.88080800	4.38508000	-1.82635000
C	1.02512500	2.79689800	-0.68331300
N	1.14567900	1.55410300	-1.25137000



0	0.00767100	3.11776800	-0.06805600
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**Ir-TS8**

Ir	1.50952500	-0.05045800	-0.34558900
C	3.25060200	0.39315500	0.91745800
C	3.17478600	-1.05050300	0.86047600
C	1.91548700	-1.43952100	1.41198900
C	1.22008600	-0.24679900	1.87483500
C	2.04499200	0.89044600	1.58124800
C	4.42541700	1.22821000	0.51603400
H	5.11658500	1.32358100	1.36231400
H	4.11698700	2.23278400	0.22054500
H	4.97133100	0.77935400	-0.31579100
C	4.24163500	-1.96262900	0.33571800
H	4.93522300	-2.23171700	1.14039300
H	4.82183400	-1.48462700	-0.45627700
H	3.82256700	-2.88958000	-0.06202500
C	1.40399000	-2.84017700	1.55621500
H	1.61973600	-3.21370800	2.56365200
H	1.87604400	-3.51874900	0.84307700
H	0.32183100	-2.88828200	1.41257100
C	-0.11553100	-0.19508400	2.54748200
H	0.01675100	-0.04315400	3.62532600
H	-0.67246900	-1.12310500	2.40681100
H	-0.71179900	0.62956100	2.14894800
C	1.78128500	2.30109600	2.00934200
H	2.16370200	2.45776800	3.02438200
H	0.71153700	2.51870200	2.00854400
H	2.27748500	3.01797300	1.35194600
C	1.96754400	-0.90732400	-2.37031900
H	1.95817700	-0.08745600	-3.08044200
H	2.86004800	-1.52458100	-2.36344000
C	0.75521400	-1.44466100	-1.88746000
H	0.72994700	-2.43062000	-1.42528400
C	-0.50688900	-0.74634100	-1.98454500
C	-1.71955300	-1.27127200	-1.29730500
H	-1.44543800	-1.74245500	-0.34592100
H	-2.06422900	-2.09039100	-1.95644900
C	-2.86876900	-0.27280900	-1.11081600
H	-2.52449700	0.54199500	-0.46861700
H	-3.11984300	0.17082900	-2.08374200
C	-4.11330900	-0.92993600	-0.50507200
H	-3.84849100	-1.38632300	0.46008500
H	-4.45186800	-1.75339500	-1.14984100

C	-5.26306000	0.06191000	-0.29547200
H	-4.91703900	0.88659100	0.34309600
H	-5.53001700	0.51521900	-1.26033700
C	-6.50829700	-0.57901600	0.32725300
H	-6.24026100	-1.03296700	1.29226500
H	-6.85146400	-1.40510800	-0.31178100
C	-7.65974700	0.41174300	0.53637600
H	-7.31418300	1.23717500	1.17352800
H	-7.92637600	0.86342000	-0.42867000
C	-8.89856100	-0.23741700	1.16067800
H	-8.66645700	-0.66893200	2.14106100
H	-9.70458400	0.48973000	1.29904200
H	-9.28271000	-1.04467200	0.52685000
H	-0.67037800	-0.10014000	-2.83777800
C	0.34479200	3.58148300	-1.08492900
H	0.23792800	4.29852200	-0.26874800
H	-0.25249300	3.92802800	-1.93502300
H	1.38554300	3.51724800	-1.41172100
C	-0.19962000	2.23798200	-0.62837900
N	0.37900500	1.17027000	-1.30278800
O	-1.08376400	2.13120900	0.21530800

**Ir-9**

Ir	1.53090300	-0.17855100	-0.19001700
C	3.70740500	0.23633800	0.00321300
C	3.46079300	-1.05433100	0.58601300
C	2.51867700	-0.87510200	1.65393900
C	2.24767900	0.56045700	1.79153800
C	2.98835900	1.24479800	0.78601400
C	4.63991200	0.53553900	-1.12746200
H	5.62562400	0.81035300	-0.73378900
H	4.27711000	1.36978700	-1.73175800
H	4.77025100	-0.32953300	-1.78006700
C	4.07715300	-2.35604400	0.16992600
H	4.94773400	-2.57561200	0.79785100
H	4.41761200	-2.32951000	-0.86697200
H	3.37377200	-3.18520200	0.27704300
C	1.99879800	-1.93962200	2.56599100
H	2.62701200	-1.99391400	3.46367800
H	2.01185500	-2.92044000	2.08745500
H	0.97725400	-1.72528500	2.88650700
C	1.39827100	1.19559700	2.84577800
H	2.02824900	1.48419500	3.69610200
H	0.63660200	0.50502200	3.21282100

H	0.89698300	2.08062400	2.45463100
C	3.03222000	2.72391700	0.58859700
H	3.62140500	3.18633300	1.38926900
H	2.02205000	3.14086900	0.62411500
H	3.49088200	2.99073000	-0.36481700
C	1.52808600	-1.31487400	-2.15623600
H	1.64686700	-0.52372300	-2.89386700
H	2.27445000	-2.10280800	-2.18213100
C	0.31752500	-1.52051000	-1.50678400
H	0.10991500	-2.47654300	-1.03173400
C	-0.81964400	-0.48480500	-1.57726500
C	-2.09310200	-1.07202800	-0.94478800
H	-1.82855000	-1.44300900	0.05485800
H	-2.36935800	-1.94927300	-1.54523100
C	-3.29840700	-0.13670700	-0.83617800
H	-3.04876200	0.71754200	-0.19447700
H	-3.54500600	0.27241000	-1.82462700
C	-4.53214800	-0.84264600	-0.25934400
H	-4.28261400	-1.26282000	0.72516700
H	-4.79395400	-1.69683600	-0.89897200
C	-5.74505700	0.08479900	-0.12481500
H	-5.48049800	0.93843000	0.51558200
H	-5.99013800	0.50692500	-1.10971700
C	-6.98121700	-0.61672300	0.44884700
H	-6.73542300	-1.03968900	1.43343400
H	-7.24421000	-1.47078000	-0.19133100
C	-8.19650600	0.30845000	0.58377400
H	-7.93162500	1.16145100	1.22333800
H	-8.43989300	0.73014900	-0.40087900
C	-9.42580900	-0.40284600	1.15712400
H	-9.21875000	-0.80613300	2.15491800
H	-10.27821600	0.27802100	1.24310400
H	-9.73045400	-1.23999900	0.51890900
H	-1.02050500	-0.16138100	-2.60804700
C	-1.52831300	2.52219600	-1.62445400
H	-2.41080800	2.92381700	-1.12139300
H	-1.84484200	1.84982700	-2.42003900
H	-0.99127400	3.36902900	-2.06213300
C	-0.60932900	1.89922000	-0.59274100
N	-0.17218000	0.57430700	-0.77786100
O	-0.16963600	2.55935500	0.33692900

**Ir-10**

Ir	-1.54795600	0.04101400	-0.27777500
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C	-3.72270500	-0.46967300	-0.18648800
C	-3.57508900	0.94479700	-0.46982800
C	-2.91372500	1.52953400	0.66664400
C	-2.59285900	0.48977600	1.62171000
C	-3.11386700	-0.75631000	1.09055200
C	-4.52117400	-1.44247100	-0.99499600
H	-5.53692100	-1.48244000	-0.58392800
H	-4.10766600	-2.45127400	-0.94882300
H	-4.60151200	-1.14216200	-2.04053000
C	-4.14919300	1.68577200	-1.63933900
H	-5.17654000	2.00353800	-1.42585800
H	-4.17379400	1.06196000	-2.53557600
H	-3.56159300	2.57710700	-1.86817100
C	-2.60324300	2.98340600	0.81364700
H	-3.51649800	3.51435800	1.10625100
H	-2.24682200	3.40766600	-0.12680100
H	-1.85001800	3.16043700	1.58200500
C	-1.98595200	0.66966900	2.97870800
H	-2.77797000	0.76829800	3.73034900
H	-1.36659700	1.56767400	3.02310200
H	-1.35846300	-0.18636600	3.22512800
C	-3.16255800	-2.06233000	1.81332200
H	-4.00906100	-2.05191600	2.51090900
H	-2.24567800	-2.23001700	2.37826300
H	-3.30775300	-2.89730600	1.12486300
C	-1.57830700	-1.30046500	-2.15801100
H	-1.69117900	-2.30883300	-1.76938600
H	-2.35642000	-0.95417300	-2.82976900
C	-0.35822900	-0.65677500	-2.11581600
H	-0.17100400	0.20556700	-2.75116400
C	0.78660700	-1.24612000	-1.29273100
C	2.11750500	-0.53807400	-1.58742000
H	1.97070200	0.54419700	-1.49928300
H	2.35997500	-0.71914900	-2.64281200
C	3.29381300	-0.96901600	-0.70829400
H	3.00618000	-0.91648600	0.34931600
H	3.54295100	-2.01842400	-0.91534200
C	4.53774300	-0.09937400	-0.92335600
H	4.28370300	0.94646000	-0.69559900
H	4.82229600	-0.12091500	-1.98436400
C	5.73090600	-0.52924500	-0.06338200
H	5.43788400	-0.51477200	0.99605300
H	5.98657000	-1.57284100	-0.29451000
C	6.96875400	0.35264100	-0.26121200

H	6.71259100	1.39670100	-0.02946700
H	7.25915800	0.33983100	-1.32139600
C	8.16447500	-0.07741700	0.59692000
H	7.87180300	-0.06532500	1.65567000
H	8.41893300	-1.12011300	0.36354600
C	9.39536400	0.81079700	0.39241400
H	9.17674700	1.85362900	0.64931400
H	10.23347600	0.48299800	1.01506800
H	9.72745500	0.79030000	-0.65174800
H	0.89258400	-2.31089500	-1.52804100
C	1.04684600	-3.35762800	0.75764700
H	2.06000900	-3.21313100	0.37706100
H	0.48591300	-3.91743600	0.00015400
H	1.08413200	-3.94374200	1.67511800
C	0.35631700	-2.04221000	1.07057500
N	0.27854300	-1.05128400	0.09304300
O	-0.11872300	-1.83540200	2.18378100
C	1.43111000	3.37290300	0.29171900
H	0.81799800	4.09694900	-0.24289000
H	2.41458600	3.30128500	-0.18496400
H	1.59481800	3.68587600	1.32605200
C	0.79322600	2.01744400	0.27117900
O	1.30985000	1.12870800	1.05914700
H	0.91023400	0.19447700	0.79738700
O	-0.17199500	1.77938800	-0.50078000

### Ir-TS11

Ir	-1.56009300	0.05380600	-0.27701200
C	-3.69621700	-0.60508400	-0.18322100
C	-3.63251500	0.81790500	-0.47596200
C	-3.01784600	1.45147100	0.66075200
C	-2.63234700	0.43773900	1.61914900
C	-3.08058100	-0.84146200	1.09610000
C	-4.42869500	-1.62925300	-0.99119000
H	-5.44966800	-1.71638400	-0.60100000
H	-3.96440300	-2.61449600	-0.92180600
H	-4.50185000	-1.34893700	-2.04279000
C	-4.25299900	1.51400200	-1.64895500
H	-5.30163900	1.75573900	-1.43917900
H	-4.22943700	0.88922600	-2.54454500
H	-3.73127200	2.44587300	-1.87562500
C	-2.79596900	2.92227400	0.79696300
H	-3.74434000	3.40257300	1.06399200
H	-2.44335200	3.35495900	-0.14113800

H	-2.06893900	3.15061900	1.57659300
C	-2.02725000	0.65639000	2.97124300
H	-2.81487800	0.68024000	3.73338500
H	-1.48529300	1.60279100	3.01691400
H	-1.32675500	-0.14587000	3.20348100
C	-3.04555200	-2.14280300	1.82808200
H	-3.90243200	-2.18851400	2.51139600
H	-2.13090300	-2.24212500	2.41233700
H	-3.11865700	-2.99122900	1.14459400
C	-1.51431400	-1.22378800	-2.20045000
H	-1.60731100	-2.25050100	-1.85717300
H	-2.28983900	-0.87061600	-2.87188800
C	-0.31356600	-0.54977000	-2.10766700
H	-0.13917100	0.34441000	-2.70092500
C	0.83506600	-1.13938100	-1.29144100
C	2.16839900	-0.43559200	-1.57652300
H	2.03330000	0.64610400	-1.46538800
H	2.40818800	-0.60076000	-2.63497600
C	3.33738900	-0.89756600	-0.70281400
H	3.05309600	-0.84287100	0.35570800
H	3.56175500	-1.95153900	-0.91647000
C	4.60011200	-0.05517300	-0.91686000
H	4.36996100	0.99455700	-0.68383100
H	4.88193800	-0.07929800	-1.97859200
C	5.78480500	-0.51658200	-0.06141600
H	5.49437600	-0.50002800	0.99866900
H	6.01639500	-1.56470800	-0.29781100
C	7.04187400	0.33803600	-0.25783500
H	6.80971300	1.38630700	-0.02039400
H	7.32968500	0.32386300	-1.31872600
C	8.22936800	-0.12318000	0.59551700
H	7.93906700	-0.11021800	1.65490500
H	8.46025000	-1.17002500	0.35608300
C	9.47923700	0.73867600	0.39333400
H	9.28420900	1.78458400	0.65654600
H	10.31116600	0.38890700	1.01234600
H	9.80867100	0.71679200	-0.65165200
H	0.93683900	-2.20253200	-1.53109100
C	1.02140300	-3.32249900	0.70022600
H	2.03711500	-3.21603900	0.31195100
H	0.42386200	-3.82445600	-0.06942300
H	1.03936900	-3.94083000	1.59688600
C	0.41406200	-1.98316400	1.06739900
N	0.34039700	-0.95996800	0.10619000

O	-0.00249300	-1.76694900	2.19793900
C	1.27823100	3.45617300	0.33351700
H	0.61311300	4.16671200	-0.15560900
H	2.24483700	3.44554800	-0.18101300
H	1.46661800	3.74721600	1.36993900
C	0.70455100	2.06927900	0.30030700
O	1.27029400	1.17818400	1.02541400
H	0.87258800	0.16623800	0.70459800
O	-0.28548100	1.83070500	-0.45863000

**P-C3**

C	3.93030900	2.42938400	0.38697700
H	3.83139300	2.35418100	1.46775500
H	4.65903200	3.14197500	0.01318200
C	3.18753400	1.68528600	-0.43159300
H	3.30597700	1.77263300	-1.51191400
C	2.14898200	0.68393300	0.02151500
C	0.73085600	1.12634200	-0.38452900
H	0.67479800	1.17400300	-1.48238300
H	0.58434500	2.15309400	-0.02963200
C	-0.38149000	0.22210400	0.15738200
H	-0.21270200	-0.80935300	-0.17485400
H	-0.32233400	0.19962900	1.25469600
C	-1.78108100	0.67742100	-0.26870800
H	-1.83737700	0.70008500	-1.36644600
H	-1.94694900	1.71196200	0.06410200
C	-2.89941100	-0.21686400	0.27707300
H	-2.73073300	-1.25128200	-0.05422600
H	-2.84393600	-0.23796500	1.37480800
C	-4.30071200	0.23113300	-0.15114200
H	-4.35664000	0.25130100	-1.24906700
H	-4.46891200	1.26639000	0.17903100
C	-5.42016600	-0.66190600	0.39547700
H	-5.25074800	-1.69573700	0.06509100
H	-5.36343400	-0.68098800	1.49239400
C	-6.81600900	-0.20585700	-0.03889400
H	-6.90915200	-0.20859900	-1.13096500
H	-7.59677200	-0.85906700	0.36399400
H	-7.02258300	0.81368500	0.30640500
H	2.17952300	0.61443300	1.11527400
C	4.07316500	-1.25685300	1.19140200
H	3.35697800	-1.21360800	2.01921700
H	4.59280000	-0.29464500	1.14914400
H	4.78960200	-2.05618600	1.37683000

C	3.37057700	-1.55266300	-0.12303000
N	2.41526900	-0.64901200	-0.52655100
O	3.61153500	-2.55135200	-0.78845300
H	2.03333400	-0.86080400	-1.44053100

**Ir-TS8'**

Ir	-1.20990300	-0.07364300	-0.22713300
C	-2.20832500	1.91198600	-0.08465300
C	-0.83914600	2.16408000	-0.45635500
C	0.00065600	1.65336300	0.58837300
C	-0.85051500	1.08701900	1.62219600
C	-2.22355500	1.26190600	1.21733000
C	-3.41851200	2.33524400	-0.85721200
H	-3.71913300	3.34323400	-0.54768600
H	-4.26372500	1.66765600	-0.67750900
H	-3.22163300	2.36449200	-1.93098100
C	-0.37489800	2.89333000	-1.68140100
H	-0.33620300	3.97135100	-1.48807600
H	-1.04917900	2.73516100	-2.52649100
H	0.62598300	2.57562400	-1.98070000
C	1.48372800	1.82567500	0.67308400
H	1.70182400	2.83313800	1.04752300
H	1.96472400	1.72342400	-0.30054100
H	1.94020400	1.11050100	1.35714600
C	-0.40370500	0.47374400	2.91143000
H	-0.49120500	1.21064300	3.71883600
H	0.63634800	0.14815600	2.85939800
H	-1.01940700	-0.39402500	3.15767200
C	-3.42777600	0.95660900	2.05200300
H	-3.61836700	1.78648700	2.74212900
H	-3.27938100	0.05087600	2.64336700
H	-4.32012000	0.82479800	1.43633000
C	-2.17034900	-1.42379200	-2.04984000
H	-2.26094900	-2.49921800	-1.99972400
H	-3.07027500	-0.88857900	-2.33847200
C	-0.88464400	-0.81432500	-2.30072100
H	-0.84299400	0.06259800	-2.94514500
C	0.27515300	-1.30459400	-1.68844100
C	1.65451200	-0.77549500	-1.95034200
H	1.61896900	0.30441500	-2.14077500
H	2.01481800	-1.23315900	-2.88463100
C	2.63968400	-1.10519400	-0.82011300
H	2.21093000	-0.77848800	0.13445600
H	2.74172900	-2.19557800	-0.74483500



C	4.01983600	-0.47232800	-1.01723800
H	3.91158000	0.61563300	-1.14033700
H	4.45843200	-0.83774000	-1.95567700
C	4.98000200	-0.75439800	0.14353300
H	4.53361700	-0.38755800	1.07990600
H	5.09128300	-1.84041300	0.26691000
C	6.36135800	-0.11742700	-0.04340600
H	6.24741700	0.96878000	-0.17230000
H	6.80835100	-0.48799900	-0.97653300
C	7.31940400	-0.39177300	1.12195100
H	6.86991100	-0.02198500	2.05385800
H	7.43179500	-1.47694300	1.24823100
C	8.69633400	0.24918000	0.92446600
H	8.61501600	1.33775800	0.82651400
H	9.35989700	0.03907000	1.76879900
H	9.18076400	-0.12910000	0.01732400
H	0.21827600	-2.28026200	-1.21296400
C	-4.17258900	-2.49043000	0.56927600
H	-4.15713800	-3.31060100	-0.15486200
H	-4.61555400	-1.61774100	0.07716400
H	-4.78018400	-2.77367300	1.42975400
C	-2.77328100	-2.16926700	1.04170100
N	-1.82318200	-1.87076500	0.07662200
O	-2.41398400	-2.21418800	2.21401300

**Ir-9'**

Ir	-1.22466400	0.06921000	0.13095600
C	-1.13790500	-1.78362400	1.29846100
C	0.15459200	-1.67155600	0.67783600
C	-0.04674800	-1.64512500	-0.73875000
C	-1.47296000	-1.82870800	-1.01157400
C	-2.14513000	-1.93117300	0.24325200
C	-1.40242200	-1.89424900	2.76592500
H	-1.38773600	-2.94933100	3.06586600
H	-2.38145400	-1.48710300	3.02630800
H	-0.64445500	-1.36903600	3.35019900
C	1.46457400	-1.67877700	1.40364500
H	1.75762600	-2.71410900	1.61288700
H	1.39912300	-1.15903000	2.36191200
H	2.26131400	-1.21869600	0.82073000
C	0.99890000	-1.61525400	-1.80888800
H	1.00172100	-2.57631500	-2.33615700
H	1.99746700	-1.45288700	-1.40418400
H	0.79186900	-0.83693000	-2.54811300

C	-2.07913000	-1.98232500	-2.36780100
H	-2.12674100	-3.04721300	-2.62755500
H	-1.47817600	-1.47842800	-3.12767000
H	-3.08559700	-1.56565800	-2.39101500
C	-3.59763700	-2.21280800	0.45212500
H	-3.76429300	-3.29618200	0.41222800
H	-4.20030100	-1.73412000	-0.31988200
H	-3.93690200	-1.85845900	1.42751600
C	-2.14844100	2.63330600	0.48514700
H	-1.97663700	3.49836100	-0.16872900
H	-2.87064200	2.92458300	1.25542200
C	-0.86386500	2.10792700	1.12382300
H	-0.82016200	1.99655400	2.20548100
C	0.28521800	1.98816800	0.36804100
C	1.66429700	1.78907600	0.93279800
H	1.63235300	1.08790600	1.77351500
H	1.96608400	2.75583100	1.36347400
C	2.70626400	1.36606800	-0.10761900
H	2.35218600	0.46971700	-0.62739500
H	2.78270100	2.14602300	-0.87686300
C	4.08995000	1.10499300	0.49506200
H	4.00571200	0.35806000	1.29797600
H	4.45582800	2.02189700	0.97635000
C	5.11329900	0.62344700	-0.53945400
H	4.74072400	-0.29459800	-1.01871200
H	5.19829700	1.36978000	-1.34134600
C	6.49911600	0.35558500	0.05765700
H	6.41128100	-0.38796600	0.86297700
H	6.87260700	1.27373500	0.53227800
C	7.52124500	-0.13372200	-0.97528000
H	7.14484000	-1.05049300	-1.44977800
H	7.60749200	0.61108100	-1.77785700
C	8.90193200	-0.39811600	-0.36737900
H	8.84863700	-1.16208600	0.41657900
H	9.61175900	-0.74579600	-1.12405100
H	9.31441100	0.51099300	0.08428200
H	0.24565100	2.32924300	-0.66917700
C	-4.65548700	2.58425300	-0.96826600
H	-4.10083200	3.42921800	-1.38954200
H	-4.98310300	2.87356900	0.03636600
H	-5.53040000	2.38017900	-1.58414900
C	-3.80009700	1.33623200	-0.91554200
N	-2.57230800	1.43885400	-0.24680100
O	-4.13804400	0.28310400	-1.43443900

**Ir-10'**

Ir	0.92327200	-0.18828300	-0.06844800
C	1.28318400	-2.36389200	-0.09912000
C	-0.10629500	-2.15885700	0.31621600
C	-0.08824500	-1.41074600	1.52434200
C	1.31065800	-1.15400200	1.88853400
C	2.14146500	-1.81533400	0.92519900
C	1.73285700	-3.22662900	-1.23846000
H	1.86089000	-4.25974600	-0.89516000
H	2.68924400	-2.88857400	-1.64323100
H	1.00221400	-3.23793800	-2.04954800
C	-1.30738400	-2.75072400	-0.35268600
H	-1.50936300	-3.74069800	0.07288000
H	-1.14888600	-2.88233100	-1.42443400
H	-2.19681800	-2.13547000	-0.21259900
C	-1.26258700	-0.95810800	2.33225000
H	-1.25154800	-1.45491700	3.30854800
H	-2.20813200	-1.19080200	1.84087800
H	-1.21685800	0.12113700	2.50114900
C	1.77719500	-0.44632400	3.12238800
H	1.98332900	-1.16896000	3.92047200
H	1.01393900	0.24617000	3.48236100
H	2.68357400	0.12369400	2.91215800
C	3.62884500	-1.94007300	0.98108200
H	3.88540300	-2.85054200	1.53628400
H	4.08151500	-1.08603400	1.48339000
H	4.06312100	-2.02915000	-0.01725900
C	2.37121900	0.65103400	-2.29263000
H	2.44483400	1.51352400	-2.96840700
H	3.13739100	-0.07442700	-2.58582500
C	0.99626400	-0.00991400	-2.31817100
H	0.89211900	-0.97475000	-2.80791900
C	-0.14388400	0.69218000	-1.93508700
C	-1.55576000	0.23463300	-2.18954900
H	-1.57684000	-0.84953800	-2.34002200
H	-1.87750400	0.68222000	-3.14144300
C	-2.54269000	0.64198500	-1.08749700
H	-2.18030400	0.26009500	-0.12612800
H	-2.54472500	1.73626500	-0.99028600
C	-3.96932000	0.14619200	-1.34000400
H	-3.95790500	-0.94483300	-1.48087200
H	-4.34318800	0.56628100	-2.28334000
C	-4.93386500	0.49886000	-0.20226700

H	-4.55466200	0.07353200	0.73949200
H	-4.94315800	1.58857500	-0.05933700
C	-6.36455900	0.00447200	-0.44148800
H	-6.35352200	-1.08516100	-0.58852200
H	-6.74329500	0.43284700	-1.37998600
C	-7.32732700	0.35257600	0.69995100
H	-6.94657200	-0.07627700	1.63728700
H	-7.33595000	1.44138300	0.84478900
C	-8.75397500	-0.14461300	0.44838100
H	-8.77748600	-1.23395500	0.33088500
H	-9.42031800	0.11597500	1.27631500
H	-9.16912800	0.29536200	-0.46523000
H	-0.03830100	1.76119100	-1.75450800
C	4.93397000	1.35143100	-1.10015400
H	4.74843200	2.03355400	-1.93504900
H	5.23688600	0.38651300	-1.52441300
H	5.74782200	1.73252700	-0.48416100
C	3.70820100	1.16994000	-0.22632600
N	2.48007500	1.01586900	-0.86586000
O	3.76795000	1.20502200	0.99771900
C	-0.23827800	3.83899400	1.61294000
H	-1.11264400	3.43616500	2.12228900
H	-0.51217600	4.68922500	0.98375700
H	0.48587900	4.19777500	2.35214400
C	0.41988900	2.78367500	0.77893800
O	0.09871200	1.57770300	0.91569300
O	1.31408000	3.19522600	-0.06609500
H	1.80683600	2.37266200	-0.47511600

### Ir-TS11'

Ir	0.91928700	-0.17435900	-0.06199900
C	1.27420800	-2.36402500	-0.15161900
C	-0.11064600	-2.14569700	0.26555500
C	-0.08507600	-1.42594800	1.49538500
C	1.31334200	-1.19008100	1.86135900
C	2.13598300	-1.83967500	0.87774400
C	1.71128500	-3.20388200	-1.31295900
H	1.80541400	-4.25093300	-1.00244400
H	2.68133900	-2.88228400	-1.69821700
H	0.98944500	-3.16788900	-2.13132700
C	-1.31857800	-2.71574600	-0.40926600
H	-1.52731100	-3.70966800	0.00382100
H	-1.16384100	-2.83417600	-1.48299500
H	-2.20207700	-2.09517700	-0.25737500

C	-1.25489000	-0.97932000	2.31277300
H	-1.23374200	-1.47795700	3.28780400
H	-2.20317400	-1.21471500	1.82817700
H	-1.20997400	0.10020300	2.48144500
C	1.78738800	-0.51444700	3.11013700
H	1.97290100	-1.25413400	3.89753400
H	1.03640200	0.18885000	3.47464800
H	2.70676600	0.04114900	2.91881800
C	3.62263400	-1.97717000	0.93063400
H	3.87114700	-2.90444200	1.46102800
H	4.08354500	-1.14426900	1.46055100
H	4.05900200	-2.04363400	-0.06870000
C	2.34998700	0.76018700	-2.27072600
H	2.40843600	1.64657900	-2.91451300
H	3.12409400	0.05624700	-2.58518200
C	0.98535500	0.07999700	-2.30663900
H	0.89564700	-0.87119300	-2.82538200
C	-0.16148700	0.76122900	-1.90966000
C	-1.56871100	0.29772100	-2.17332600
H	-1.58290800	-0.78231100	-2.35170800
H	-1.89279200	0.76731400	-3.11391200
C	-2.55784600	0.67404100	-1.06206900
H	-2.19320900	0.27338000	-0.10945200
H	-2.56489000	1.76541800	-0.93941700
C	-3.98165700	0.17698300	-1.32745500
H	-3.96539400	-0.91022000	-1.49545600
H	-4.35727600	0.61843200	-2.26031300
C	-4.94828100	0.49700000	-0.18185200
H	-4.56815200	0.04929600	0.74907600
H	-4.96147000	1.58258400	-0.01117600
C	-6.37696700	0.00370400	-0.43485400
H	-6.36200400	-1.08174500	-0.61005500
H	-6.75666600	0.45489100	-1.36222200
C	-7.34169900	0.31878500	0.71448400
H	-6.96027200	-0.13317800	1.64061100
H	-7.35383800	1.40337200	0.88773200
C	-8.76658500	-0.17611000	0.44881400
H	-8.78661800	-1.26205800	0.30260000
H	-9.43432500	0.06048200	1.28281400
H	-9.18251300	0.28651000	-0.45319500
H	-0.06515500	1.82369600	-1.69255000
C	4.98123100	1.20876400	-1.07389800
H	4.85613600	1.90612200	-1.90735900
H	5.18936600	0.21949000	-1.49888500

H	5.82977300	1.50991700	-0.46051500
C	3.75113900	1.14895400	-0.19611000
N	2.48579000	1.09169700	-0.83059800
O	3.80506700	1.19087500	1.02056800
C	-0.19945400	3.79423100	1.65664200
H	-1.10881100	3.40596600	2.11479100
H	-0.41096900	4.69028600	1.06955600
H	0.51028100	4.07383600	2.44267200
C	0.44933400	2.75795300	0.78265900
O	0.10017800	1.54279700	0.93856300
O	1.31860700	3.14245300	-0.06594900
H	1.91118400	2.18605400	-0.50318300

**P-C1**

C	-3.60336600	-0.79978600	0.32048100
H	-3.55644000	-1.04838500	1.39161600
H	-4.32631200	-1.48545500	-0.13298400
C	-2.25237000	-0.99674500	-0.31156500
H	-2.20631100	-0.83259600	-1.38826200
C	-1.14904600	-1.32974500	0.36161900
C	0.21576500	-1.51240800	-0.23832100
H	0.16304400	-1.40606800	-1.32912300
H	0.56650400	-2.53627900	-0.04099200
C	1.24977400	-0.52253900	0.32900600
H	0.91398400	0.50229700	0.12285000
H	1.28260700	-0.61869800	1.42333700
C	2.65574000	-0.73043400	-0.24308100
H	2.61965700	-0.63891500	-1.33793400
H	2.98396500	-1.75898200	-0.03564500
C	3.68893900	0.25445100	0.31423700
H	3.35962600	1.28240900	0.10634500
H	3.72367300	0.16339900	1.40928800
C	5.09606300	0.04785700	-0.25618700
H	5.06166600	0.13872000	-1.35140100
H	5.42561600	-0.98039400	-0.04855300
C	6.13080500	1.03229100	0.30030000
H	5.80067100	2.05906100	0.09175200
H	6.16399000	0.94080900	1.39453800
C	7.53312400	0.81654900	-0.27592600
H	7.53357700	0.93409300	-1.36564500
H	8.25265200	1.53106300	0.13683400
H	7.89941000	-0.19230500	-0.05368500
H	-1.21658100	-1.46993600	1.44269400
C	-6.44450300	-0.04443600	-0.22621100

H	-6.50356900	-0.70085400	0.64835200
H	-6.25771000	-0.67359500	-1.10317300
H	-7.39474000	0.47286400	-0.35318800
C	-5.36176500	1.01262000	-0.06080700
N	-4.07563400	0.56536200	0.11106500
O	-5.61318000	2.21056500	-0.09490900
H	-3.40905600	1.30964200	0.27352600

**<sup>1</sup>[Cp\*CoCl<sub>2</sub>]<sub>2</sub>**

Co	-1.63591900	-0.22029000	-0.00001800
Co	1.63596900	0.22039600	0.00002000
Cl	0.00001600	-0.00002100	1.63071600
Cl	-0.00000600	0.00041400	-1.63071400
Cl	-1.55656500	-2.47587500	-0.00032900
Cl	1.55702500	2.47599500	0.00031700
C	2.56281300	-1.56558200	-0.70705900
C	2.56282100	-1.56576700	0.70662100
C	3.24724000	-0.36896100	1.15707600
C	3.24723000	-0.36866100	-1.15720900
C	3.74678800	0.30944900	0.00001900
C	-3.24730100	0.36876100	-1.15707300
C	-3.74672300	-0.30972800	-0.00000600
C	-3.24728500	0.36848400	1.15721300
C	-2.56310500	1.56569900	-0.70663200
C	-2.56309000	1.56552600	0.70704900
C	-1.93523600	2.62082500	1.56141900
H	-0.92834700	2.85563700	1.20589200
H	-2.54209400	3.53400900	1.52441400
H	-1.85697300	2.30080000	2.60072600
C	-1.93525800	2.62120600	-1.56074900
H	-2.54211200	3.53438300	-1.52351100
H	-0.92836300	2.85592500	-1.20517600
H	-1.85700800	2.30143800	-2.60013700
C	-3.45179600	-0.04207900	-2.58189000
H	-4.35881000	0.41297900	-2.99820800
H	-2.60220700	0.26391900	-3.19592200
H	-3.54271100	-1.12721500	-2.66148300
C	-4.60924100	-1.52928700	-0.00014100
H	-5.66317000	-1.22245400	0.00002700
H	-4.42473000	-2.14641100	-0.87960000
H	-4.42454100	-2.14673600	0.87905100
C	-3.45177300	-0.04267200	2.58193900
H	-4.35868000	0.41245200	2.99841700
H	-3.54288700	-1.12781000	2.66127800

H	-2.60209500	0.26302500	3.19599900
C	1.93476800	-2.62075500	-1.56144200
H	2.54149100	-3.53403100	-1.52449500
H	0.92785600	-2.85542700	-1.20588600
H	1.85651200	-2.30068000	-2.60073500
C	3.45179700	0.04247600	-2.58193000
H	4.35864500	-0.41277400	-2.99839900
H	2.60208400	-0.26309500	-3.19600400
H	3.54306600	1.12760200	-2.66125800
C	1.93477600	-2.62116200	1.56073100
H	0.92784700	-2.85570800	1.20514000
H	2.54147200	-3.53444400	1.52351100
H	1.85656000	-2.30137400	2.60011500
C	3.45180900	0.04182400	2.58189800
H	2.60214700	-0.26399300	3.19592000
H	4.35871800	-0.41343700	2.99822200
H	3.54296300	1.12693900	2.66150100
C	4.60952600	1.52885300	0.00017400
H	4.42500900	2.14630100	-0.87905700
H	4.42505400	2.14604400	0.87959500
H	5.66340000	1.22183100	0.00010400

**<sup>3</sup>[Cp\*CoCl<sub>2</sub>]<sub>2</sub>**

Co	1.61170600	0.42932400	0.00154100
Co	-1.69662300	-0.23565200	-0.00019400
Cl	-0.08528000	-0.01936600	1.65612400
Cl	-0.08510800	-0.01805000	-1.65529300
Cl	1.69581300	2.66488600	-0.00169200
Cl	-1.60067600	-2.49118400	-0.00185700
C	-2.62053400	1.55093200	-0.70683200
C	-2.61998500	1.55116900	0.70635200
C	-3.30913700	0.35724400	1.15772200
C	-3.30958100	0.35664100	-1.15724100
C	-3.80783600	-0.32140700	0.00059600
C	3.37129400	-0.49606300	-1.18250600
C	3.82752500	0.21360900	0.00316500
C	3.36830300	-0.49904200	1.18411000
C	2.63968600	-1.60210400	-0.74393500
C	2.63705900	-1.60393100	0.73916700
C	1.95226300	-2.65891000	1.53844600
H	0.90127400	-2.74086200	1.23934400
H	2.42778600	-3.63195900	1.35995700
H	1.98733900	-2.44565800	2.60732900
C	1.95648100	-2.65467300	-1.54801300



H	2.43203600	-3.62824400	-1.37257300
H	0.90505000	-2.73788400	-1.25093200
H	1.99300100	-2.43745400	-2.61607200
C	3.64136800	-0.06188100	-2.59215300
H	4.68821200	-0.23338700	-2.87059000
H	3.00857200	-0.60407500	-3.29708600
H	3.43328200	1.00541800	-2.71540700
C	4.76293200	1.37409100	0.00498900
H	5.79817100	1.00512900	0.00031500
H	4.61763800	2.00185800	-0.87537600
H	4.62325000	1.99517200	0.89095800
C	3.63367600	-0.07147000	2.59679400
H	4.67515800	-0.26026000	2.88404700
H	3.44136500	0.99865400	2.72046500
H	2.98609000	-0.60457000	3.29524800
C	-1.98744500	2.60431800	-1.56067600
H	-2.60018000	3.51407100	-1.53989800
H	-0.98740900	2.85163100	-1.19410100
H	-1.89081200	2.27601100	-2.59557900
C	-3.51809500	-0.05071200	-2.58230100
H	-4.41834400	0.41724100	-2.99907600
H	-2.66266800	0.24289500	-3.19409900
H	-3.62430800	-1.13435700	-2.66282500
C	-1.98619200	2.60480400	1.55939400
H	-0.98628300	2.85169600	1.19217300
H	-2.59865200	3.51473500	1.53857400
H	-1.88908600	2.27691400	2.59438800
C	-3.51714300	-0.04915700	2.58312900
H	-2.66108100	0.24394800	3.19428200
H	-4.41666200	0.41996700	3.00016000
H	-3.62448900	-1.13263600	2.66436800
C	-4.66603600	-1.54428800	0.00113000
H	-4.47878900	-2.16083300	-0.87820900
H	-4.47748800	-2.16098300	0.88009400
H	-5.72154200	-1.24319100	0.00194000

**<sup>5</sup>[Cp\*CoCl<sub>2</sub>]<sub>2</sub>**

Co	-1.55075500	0.47040600	-0.00062300
Co	1.70785700	-0.24309100	0.00000600
Cl	0.08073400	-0.06573600	-1.65814100
Cl	0.08054800	-0.06508500	1.65775100
Cl	-1.77389900	2.71047800	-0.00036900
Cl	1.66105900	-2.49342600	0.00036800
C	2.58895700	1.56492900	0.70632100

C	2.58901200	1.56471300	-0.70677800
C	3.30295000	0.38448400	-1.15737900
C	3.30281800	0.38481500	1.15733300
C	3.81732300	-0.28228200	0.00009400
C	-3.36567400	-0.50026700	1.16911100
C	-3.87563500	0.17481900	0.00045200
C	-3.36637200	-0.50117700	-1.16840800
C	-2.64052100	-1.63246600	0.72771100
C	-2.64087000	-1.63285200	-0.72692000
C	-1.96105200	-2.67724500	-1.54859200
H	-0.91737700	-2.79544700	-1.23785200
H	-2.46146300	-3.64540000	-1.41513100
H	-1.97282200	-2.42959600	-2.61097400
C	-1.96051400	-2.67649100	1.54961500
H	-2.46103200	-3.64466900	1.41668000
H	-0.91695400	-2.79491300	1.23854600
H	-1.97192300	-2.42839000	2.61189000
C	-3.62098200	-0.09334200	2.58992300
H	-4.58019700	-0.48217900	2.95416100
H	-2.83358800	-0.46534600	3.24938100
H	-3.64388700	0.99559300	2.68652100
C	-4.81586000	1.33420500	0.00020900
H	-5.85428900	0.97534800	-0.00020700
H	-4.67346800	1.96224000	0.88152100
H	-4.67283600	1.96238600	-0.88090500
C	-3.62275400	-0.09479200	-2.58916300
H	-4.58306900	-0.48233700	-2.95188900
H	-3.64411700	0.99412100	-2.68646400
H	-2.83682500	-0.46850400	-3.24939000
C	1.93667200	2.60474400	1.56249500
H	2.54410800	3.51818100	1.56052200
H	0.94061300	2.85318200	1.18618700
H	1.82819700	2.26499100	2.59249900
C	3.51913000	-0.02028700	2.58180500
H	4.42048100	0.45035100	2.99298500
H	2.66690500	0.27159700	3.19869700
H	3.62850900	-1.10363600	2.66207300
C	1.93678800	2.60426600	-1.56331800
H	0.94072800	2.85286700	-1.18711700
H	2.54425000	3.51768600	-1.56163100
H	1.82833400	2.26417900	-2.59321400
C	3.51942200	-0.02102000	-2.58171200
H	2.66727700	0.27070400	-3.19879200
H	4.42082700	0.44949100	-2.99291800

H	3.62880000	-1.10439300	-2.66166700
C	4.70444200	-1.48402300	0.00031300
H	4.53190700	-2.10461600	0.87973600
H	4.53195500	-2.10489900	-0.87892000
H	5.75202600	-1.15639400	0.00028900

**<sup>1</sup>Cp\*Co(OAc)<sub>2</sub>**

Co	0.10482500	0.16856300	-0.12491800
C	1.03498800	-1.40947600	-1.04754500
C	0.26771400	-1.91337000	0.06079400
C	0.72888800	-1.27529400	1.24467300
C	1.84206300	-0.41590300	0.88411600
C	2.04963500	-0.53330200	-0.51572500
C	0.84334900	-1.76710800	-2.48951900
H	1.30284300	-2.73439400	-2.72713900
H	1.28792700	-1.01127600	-3.14118700
H	-0.22112800	-1.82696400	-2.72975600
C	-0.85661700	-2.89409200	-0.03478000
H	-0.46068800	-3.91679100	-0.00706000
H	-1.40101100	-2.76725100	-0.97316200
H	-1.56242000	-2.75742700	0.78373600
C	0.14532500	-1.43655600	2.61411700
H	0.32295900	-2.44890500	2.99548300
H	-0.93142500	-1.25497400	2.56824400
H	0.58692100	-0.72606500	3.31568100
C	2.56993700	0.47248400	1.84724400
H	3.10048800	-0.11974200	2.60080500
H	1.86073600	1.12601400	2.36380200
H	3.29928000	1.10563000	1.33809600
C	3.02829800	0.22595500	-1.35795600
H	3.70459000	0.82779800	-0.74858100
H	2.49846100	0.90034000	-2.03739500
H	3.62984100	-0.46500100	-1.95773900
O	0.37151300	1.88788300	-1.08141400
O	-0.31245100	1.76923400	0.97797500
C	-0.06208400	2.48896300	-0.04261200
C	-0.31488500	3.96806500	-0.04104100
H	-1.34847000	4.14111500	-0.35918900
H	-0.19260000	4.37179300	0.96554900
H	0.35164600	4.46849600	-0.74567900
C	-4.00749900	0.05929100	-0.68374400
H	-4.80788700	-0.31416700	-0.04376600
H	-4.03545100	-0.43713700	-1.65789500
H	-4.15104500	1.12996500	-0.86169000

C	-2.65615900	-0.16140900	-0.01351600
O	-1.65353600	0.10296300	-0.81330800
O	-2.57322100	-0.54654800	1.15232200

**<sup>3</sup>Cp\*Co(OAc)<sub>2</sub>**

Co	-0.00481400	0.34444200	-0.02815100
C	-0.70366400	-1.81816000	-0.81418000
C	-1.12577400	-1.50917800	0.57682000
C	0.02573500	-1.38220000	1.38527200
C	1.15035700	-1.50034900	0.50945300
C	0.67639800	-1.82091800	-0.84772600
C	-1.66958000	-1.98921000	-1.94130200
H	-2.42086900	-2.75196500	-1.70642700
H	-1.16332400	-2.27874300	-2.86411600
H	-2.19092500	-1.04238100	-2.12251600
C	-2.55254900	-1.45383600	1.01185700
H	-2.92894300	-2.46456900	1.21782100
H	-3.17773700	-1.02333400	0.22512900
H	-2.67044400	-0.84611300	1.90956700
C	0.09201100	-1.07505400	2.85195100
H	0.43419500	-1.94217900	3.42932600
H	-0.88591800	-0.77666100	3.23412100
H	0.78097300	-0.24527800	3.03482200
C	2.58671500	-1.43324100	0.90556300
H	2.95530100	-2.43499300	1.16428600
H	2.72510500	-0.77897200	1.76749900
H	3.19875300	-1.05660400	0.08209300
C	1.58819100	-1.98929900	-2.02184500
H	2.34282600	-2.76081400	-1.83040700
H	2.10753100	-1.04604300	-2.22362200
H	1.03588200	-2.26952300	-2.92101000
O	1.53970400	1.15471800	-1.21433300
O	1.50074200	1.48223300	0.95547100
C	2.04310600	1.68803500	-0.17336700
C	3.25580800	2.58089600	-0.28885400
H	2.91713400	3.61080300	-0.44384100
H	3.84118800	2.54976300	0.63190500
H	3.86455500	2.28954900	-1.14677700
C	-3.27391200	2.56743300	-0.31200300
H	-3.83425700	2.61513900	0.62304900
H	-3.90481500	2.20179500	-1.12490600
H	-2.94365200	3.57886600	-0.57140700
C	-2.05583400	1.68808700	-0.15508500
O	-1.52554400	1.15347800	-1.18773300

0	-1.53673200	1.49136000	0.98111500
<b><sup>5</sup>Cp*Co(OAc)<sub>2</sub></b>			
Co	-0.00353000	-0.55592000	-0.06953600
C	0.68773300	1.87199600	-0.72487100
C	1.15044700	1.47739500	0.60513400
C	0.01414500	1.21424200	1.42276800
C	-1.13779200	1.48869600	0.63129700
C	-0.70144300	1.87893100	-0.70878400
C	1.60695200	2.13735000	-1.87507700
H	2.34741200	2.90582900	-1.62303000
H	1.06082900	2.47251200	-2.75933100
H	2.14878800	1.22223500	-2.13954400
C	2.58328100	1.39424900	1.01513000
H	2.93472300	2.36198700	1.39813300
H	3.21729700	1.12987800	0.16397800
H	2.72721400	0.64618000	1.79712800
C	0.02948900	0.80867000	2.86788800
H	0.04434600	1.67908400	3.53578900
H	0.90696000	0.19535200	3.08728300
H	-0.85087100	0.20817500	3.10986000
C	-2.56209500	1.42035100	1.07147900
H	-2.90457800	2.40135100	1.42826400
H	-2.69325200	0.69847800	1.87944800
H	-3.21331000	1.12989600	0.24192900
C	-1.64448800	2.15179800	-1.83758900
H	-2.37908300	2.91883900	-1.56509400
H	-2.19200900	1.23813300	-2.09550600
H	-1.11734000	2.49195200	-2.73141500
O	-1.65459500	-1.03431700	-1.25089000
O	-1.61466700	-1.56935000	0.87868300
C	-2.20207800	-1.60425100	-0.24710500
C	-3.51560500	-2.32503800	-0.41260400
H	-3.31664800	-3.32964100	-0.80078600
H	-4.02572700	-2.41682600	0.54719000
H	-4.14250900	-1.80371200	-1.13892300
C	3.53459000	-2.28105800	-0.39401600
H	4.30271200	-1.57919600	-0.05062400
H	3.73446500	-2.53706100	-1.43525600
H	3.58334800	-3.16756000	0.24117500
C	2.18675400	-1.61994900	-0.25829100
O	1.64559700	-1.04476500	-1.26094300
O	1.59156800	-1.59361100	0.86498100

**<sup>1</sup>Cp\*Co(OAc)(NTf<sub>2</sub>)**

Co	-1.29319700	-0.05276900	-0.08592200
C	-1.64183500	-1.26031900	1.61241600
C	-1.69876700	-2.07093500	0.41058900
C	-2.72688500	-1.54707400	-0.41973600
C	-3.27431800	-0.38179600	0.22378800
C	-2.62296000	-0.24017000	1.50681300
C	-0.73064200	-1.50362300	2.77286500
H	-1.10951300	-2.34548000	3.36547800
H	-0.65711800	-0.62512400	3.41196200
H	0.27552100	-1.75374200	2.43595500
C	-0.89146300	-3.30493900	0.15206400
H	-1.46717400	-4.19067600	0.44754700
H	0.03282900	-3.30045400	0.72786900
H	-0.62343300	-3.39326800	-0.90054400
C	-3.08167300	-2.00987100	-1.79735200
H	-4.13349600	-2.31309000	-1.83849400
H	-2.46206500	-2.85192700	-2.10653900
H	-2.92808800	-1.19852700	-2.51514200
C	-4.34398600	0.50734000	-0.33143600
H	-5.32697000	0.24614900	0.07685900
H	-4.39470800	0.41786200	-1.41888700
H	-4.14099600	1.55295900	-0.08757800
C	-2.83179400	0.86690500	2.49220600
H	-3.30001500	0.48177600	3.40510000
H	-3.47189600	1.64846200	2.08101700
H	-1.87162800	1.31675500	2.75636400
O	-1.39183000	1.91616000	-0.19396500
O	-1.32912000	0.64098700	-1.94061700
C	-1.37784000	1.82355600	-1.46961200
C	-1.39276200	3.03725700	-2.34461300
H	-0.41012900	3.51229100	-2.28567900
H	-1.60116000	2.75878400	-3.37799500
H	-2.13525700	3.74935700	-1.97655800
N	0.69061200	-0.03273700	0.03062600
S	1.45662700	0.97435900	1.10895400
S	1.60149700	-0.81245300	-1.13593000
O	0.51997300	1.24957000	2.19865800
O	2.81270500	0.49909300	1.37902000
O	0.65966700	-1.60297800	-1.92749200
O	2.58677200	0.05895600	-1.76948700
C	2.62188900	-2.10010800	-0.16917700
C	1.67796000	2.64046200	0.20781800
F	2.12201000	-2.29718900	1.06285100

F	2.54972300	-3.25448800	-0.83994700
F	3.88545600	-1.71941000	-0.07696900
F	0.84732700	3.54322800	0.72444800
F	2.93325400	3.04726000	0.37505100
F	1.42917200	2.51581100	-1.10236100

**<sup>3</sup>Cp\*Co(OAc)(NTf<sub>2</sub>)**

Co	-1.24100600	0.07121500	0.02410100
C	-1.68447100	-1.49253600	1.54902700
C	-1.71146500	-2.19066700	0.23533000
C	-2.73122600	-1.63525400	-0.54435000
C	-3.31774100	-0.56503400	0.22717200
C	-2.69637700	-0.52810400	1.54927400
C	-0.72929100	-1.83514200	2.64649600
H	-0.98569300	-2.80559000	3.08903900
H	-0.73652200	-1.07890800	3.43134100
H	0.29116700	-1.90648400	2.26161200
C	-0.82597500	-3.33705300	-0.12442800
H	-1.29373500	-4.27857500	0.19310800
H	0.14140100	-3.26552900	0.37152200
H	-0.64596000	-3.37913300	-1.19878200
C	-3.09700500	-1.97155500	-1.95797300
H	-4.16065900	-2.22028700	-2.04169000
H	-2.51944700	-2.82203700	-2.32344100
H	-2.88568700	-1.12018000	-2.61250500
C	-4.44523300	0.30562600	-0.21304400
H	-5.39295500	-0.07627800	0.18847600
H	-4.52203600	0.32813000	-1.30214800
H	-4.30738000	1.32658900	0.14905400
C	-3.05595100	0.45227500	2.62376600
H	-4.05350800	0.24540500	3.02848000
H	-3.05412900	1.47063900	2.22368000
H	-2.33629800	0.42138900	3.44248000
O	-1.82171600	1.95992100	-0.29782700
O	-1.32266500	0.75010400	-2.05429900
C	-1.65451000	1.86556500	-1.57023800
C	-1.80997700	3.09364000	-2.42513200
H	-0.89402500	3.68565100	-2.32889600
H	-1.94508500	2.81754400	-3.47135700
H	-2.64306200	3.70404500	-2.07007200
N	0.78320300	-0.08395100	0.01940400
S	1.31506900	0.93175600	1.20007800
S	1.76763400	-0.68507700	-1.17474700
O	0.08234100	1.18705300	1.97052500

O	2.54199000	0.49336200	1.85783200
O	0.92612200	-1.52993600	-2.01656300
O	2.65328100	0.33835300	-1.72422800
C	2.90429200	-1.88575200	-0.25156500
C	1.73623700	2.57461700	0.35203300
F	2.26981200	-2.41839400	0.80836500
F	3.22684800	-2.86858100	-1.09456600
F	4.00360800	-1.27033900	0.15939300
F	1.40499500	3.55989500	1.18715900
F	3.03593600	2.62326600	0.09212400
F	1.04573900	2.70492900	-0.78397000

**<sup>5</sup>Cp\*Co(OAc)(NTf<sub>2</sub>)**

Co	-1.19392600	0.25291000	0.04626600
C	-1.57400100	-1.58397000	1.58071100
C	-1.60239300	-2.29442300	0.33135500
C	-2.65793000	-1.77960200	-0.43360000
C	-3.30740300	-0.71221600	0.33679900
C	-2.62757100	-0.58010600	1.56534900
C	-0.61313200	-1.82727700	2.69683900
H	-0.88445600	-2.73975900	3.24413100
H	-0.59956700	-0.99593400	3.40222600
H	0.40270800	-1.96561400	2.31658100
C	-0.68859700	-3.41132700	-0.07978300
H	-1.25159800	-4.34401700	-0.20264500
H	0.08950400	-3.58780600	0.66275700
H	-0.19748900	-3.18721200	-1.03039800
C	-3.04680800	-2.17352600	-1.81833800
H	-4.11365500	-2.42104200	-1.87375900
H	-2.47163500	-3.03406500	-2.16497700
H	-2.86133100	-1.33978000	-2.50517500
C	-4.49376100	0.05829600	-0.14402500
H	-5.41469700	-0.52224400	-0.00361000
H	-4.40131400	0.27321600	-1.21258300
H	-4.60138900	1.00430600	0.38906200
C	-2.97204300	0.34003900	2.69974100
H	-3.54947300	-0.18208200	3.47236500
H	-3.56444500	1.18729600	2.34776100
H	-2.06892300	0.74424200	3.16244400
O	-1.94590200	2.11574300	-0.31152900
O	-1.69317200	0.70727700	-1.97558600
C	-1.98699000	1.87330100	-1.57007600
C	-2.34258300	2.97138300	-2.53349300
H	-1.47936500	3.63912000	-2.62471400



H	-2.58195400	2.56139400	-3.51497400
H	-3.17568500	3.55882300	-2.14096100
N	0.83605100	-0.01930200	-0.07651800
S	1.34204600	0.94372600	1.15218800
S	1.84054000	-0.62287600	-1.25678000
O	0.05029000	1.18128600	1.85024200
O	2.51672400	0.48169900	1.88116100
O	0.99398400	-1.40384300	-2.15201500
O	2.76753900	0.39517400	-1.74400900
C	2.90605800	-1.88029600	-0.32767400
C	1.78979300	2.61317500	0.38554400
F	2.21794600	-2.41610300	0.69189400
F	3.23687500	-2.84748800	-1.18349500
F	4.00206600	-1.29725600	0.13946700
F	1.53311100	3.55676500	1.29043100
F	3.07544300	2.63199300	0.06469100
F	1.04294800	2.81928200	-0.70141500

**<sup>1</sup>[Cp\*Co(NTf<sub>2</sub>)]<sup>+</sup>**

Co	1.13788900	-0.10560100	-0.23042400
C	2.14215900	-0.75466600	1.43519100
C	2.90848200	0.23593400	0.69352200
C	3.14893800	-0.26919400	-0.62230900
C	2.49392100	-1.54359400	-0.71816100
C	1.88800200	-1.85268800	0.56496600
C	1.67393000	-0.60567100	2.84452900
H	2.39997200	-1.08220700	3.51515400
H	0.70313700	-1.07861300	2.99508100
H	1.59812300	0.44457800	3.13238500
C	3.30395500	1.57808200	1.21587300
H	4.08846000	1.46384000	1.97328200
H	2.45814300	2.07974700	1.69492500
H	3.68426700	2.22313500	0.42338600
C	3.84508600	0.47120200	-1.72140600
H	4.92107000	0.51032200	-1.52026300
H	3.47750800	1.49797600	-1.79649500
H	3.70018400	-0.00945000	-2.68916600
C	2.38092500	-2.39507100	-1.93744600
H	3.17040700	-3.15753500	-1.92146800
H	2.49416800	-1.81463900	-2.85425600
H	1.42240000	-2.91807100	-1.96976300
C	1.14887300	-3.10880600	0.89477400
H	1.87286600	-3.90417100	1.10860100
H	0.52576200	-3.44007300	0.06246100

H	0.50541800	-2.97923200	1.76349300
N	-0.74128400	0.04528700	-0.06965300
S	-2.02000700	-0.62944300	0.81982800
S	-0.83352400	1.42924600	-0.96023500
O	-1.40495000	-1.42302400	1.87462700
O	-3.02437700	0.39370300	1.06271200
O	0.63756400	1.39593000	-1.39083700
O	-1.87401600	1.58388300	-1.95037100
C	-0.89932600	2.88274200	0.26247300
C	-2.67143700	-1.83026000	-0.47179200
F	-0.18574200	2.54091200	1.34283800
F	-0.34215600	3.92017100	-0.34033800
F	-2.14797600	3.12654100	0.58720400
F	-1.66436700	-2.63842600	-0.83331300
F	-3.65394200	-2.53583700	0.05909600
F	-3.08961600	-1.14116500	-1.52350600

**<sup>3</sup>[Cp\*Co(NTf<sub>2</sub>)]<sup>+</sup>**

Co	1.08931300	0.11380800	-0.30196600
C	2.39015300	-0.47766100	1.43272400
C	2.99809300	0.58540900	0.75942300
C	3.20622100	0.16681300	-0.63727300
C	2.75981100	-1.19165500	-0.79039200
C	2.21868000	-1.59056600	0.46445900
C	1.95649600	-0.55498400	2.85876100
H	2.57206700	-1.28947800	3.39252500
H	0.91659000	-0.88624800	2.93394600
H	2.05742300	0.40442400	3.36725700
C	3.36943200	1.93352200	1.29294500
H	4.45997900	2.03007400	1.34901500
H	2.96456500	2.09809500	2.29219800
H	3.00726200	2.73438000	0.64100700
C	3.84795000	1.01660100	-1.67973100
H	4.93596500	1.01354100	-1.52939800
H	3.51557900	2.05576900	-1.61012900
H	3.64931400	0.65021500	-2.68780500
C	2.86006300	-2.02613400	-2.03373900
H	3.83316000	-2.52814000	-2.07710900
H	2.76071000	-1.41876900	-2.93625200
H	2.08702200	-2.79665500	-2.06176200
C	1.66513700	-2.92407200	0.82686700
H	2.42639700	-3.48109700	1.39004500
H	1.40162800	-3.51138100	-0.05300500
H	0.78587500	-2.82973300	1.46755700

N	-0.82269400	0.01456700	-0.03142300
S	-1.94406000	-0.91226000	0.83390300
S	-1.16030800	1.35671700	-0.92862100
O	-1.17995600	-1.55861600	1.89527700
O	-3.14891000	-0.13442000	1.06894400
O	0.29018200	1.61177900	-1.36207100
O	-2.20913400	1.30355900	-1.92231100
C	-1.51000600	2.76954000	0.28858700
C	-2.30250800	-2.22861400	-0.45782500
F	-0.70124400	2.60473200	1.33895400
F	-1.22686700	3.90016300	-0.33657600
F	-2.77076200	2.72440700	0.65777100
F	-1.13987700	-2.82052100	-0.77305700
F	-3.14073800	-3.11465300	0.04939900
F	-2.81282700	-1.64731800	-1.53394900

**<sup>5</sup>[Cp\*Co(NTf<sub>2</sub>)]<sup>+</sup>**

Co	0.92340200	-0.42064900	-0.26958600
C	2.47774900	-0.41131500	1.39536300
C	2.95050900	0.58956500	0.51918100
C	3.24050100	-0.03762200	-0.77371000
C	2.89811400	-1.42447000	-0.68780500
C	2.49596500	-1.68276700	0.67229500
C	2.04238400	-0.26828500	2.82127800
H	2.78562800	-0.71532000	3.49219500
H	1.09263000	-0.78425700	2.99532400
H	1.91896200	0.77796700	3.10377100
C	3.09814100	2.05053000	0.77964100
H	4.14441900	2.35382100	0.65608800
H	2.78233900	2.32148100	1.78739300
H	2.50780200	2.62870900	0.06026400
C	3.74886200	0.70553400	-1.95738400
H	4.71825100	1.16407700	-1.72613400
H	3.06502800	1.52284900	-2.21626900
H	3.87293700	0.06278800	-2.82915600
C	3.08931100	-2.45521000	-1.76357600
H	4.10080800	-2.87448500	-1.71549500
H	2.95430400	-2.02489100	-2.75817600
H	2.38357100	-3.28232300	-1.65867300
C	2.11325300	-2.99301700	1.27379600
H	2.81122700	-3.24499700	2.08242600
H	2.12981300	-3.80232600	0.54338100
H	1.11427600	-2.94325200	1.72334500
N	-0.95672200	-0.05440100	-0.36024700

S	-2.02841900	-0.75735100	0.72996600
S	-0.91724100	1.46721600	-1.01121000
O	-1.15330300	-1.66265000	1.48723200
O	-2.88803400	0.23115400	1.35988100
O	0.55207000	1.45463400	-1.37443700
O	-1.93118900	1.81420600	-1.98291200
C	-0.99303800	2.68711600	0.44058600
C	-3.05176000	-1.80262000	-0.44935600
F	-0.36518200	2.12061000	1.48181400
F	-0.33698900	3.77596300	0.06430200
F	-2.24211500	2.96022400	0.73951600
F	-2.22799900	-2.64704700	-1.07171800
F	-3.95714200	-2.46689600	0.24780200
F	-3.62419100	-0.98982400	-1.32613800

**<sup>1</sup>Co-1**

Co	-0.28929900	-0.00006100	-0.30485100
C	1.64105200	0.73293900	-0.55615700
C	1.64102600	-0.73319800	-0.55584200
C	1.10327600	-1.17842000	0.67306500
C	0.70250200	0.00031500	1.42156000
C	1.10330400	1.17870200	0.67256300
C	2.09917500	1.57129000	-1.70566600
H	3.19462300	1.56254300	-1.75548700
H	1.77080300	2.60687400	-1.61288700
H	1.73056800	1.17872700	-2.65792300
C	2.09906900	-1.57202600	-1.70504200
H	3.19452900	-1.56362200	-1.75473100
H	1.73070000	-1.17963100	-2.65745800
H	1.77038800	-2.60749000	-1.61200800
C	0.84419700	-2.58468500	1.10985900
H	1.45178200	-2.81816600	1.99087200
H	1.08539700	-3.30489200	0.32795900
H	-0.20675000	-2.71911600	1.38197800
C	0.04533900	0.00064600	2.76029200
H	0.81485900	0.00152400	3.54329400
H	-0.57222100	-0.88824900	2.90346900
H	-0.57322200	0.88900700	2.90251100
C	0.84412900	2.58514400	1.10874300
H	1.45160800	2.81902900	1.98972100
H	-0.20685500	2.71962200	1.38069600
H	1.08537300	3.30504200	0.32657300
O	-1.86670400	1.08170000	-0.42172900
O	-1.86663300	-1.08191000	-0.42178300

C	-2.55878200	-0.00012800	-0.50696500
C	-4.03681500	-0.00015600	-0.66341100
H	-4.36010000	-0.90208900	-1.18541200
H	-4.48848900	0.00022700	0.33592600
H	-4.36003900	0.90145500	-1.18601600

**<sup>1</sup>Co-2**

Co	1.90813000	0.14738000	-0.18950000
C	1.68427000	-1.79694800	0.66068200
C	1.38796600	-0.80344300	1.63412900
C	2.53248100	0.05541000	1.75470700
C	3.58257900	-0.47179800	0.90616000
C	3.05464800	-1.58895600	0.21114300
C	0.81875900	-2.96796900	0.30995200
H	0.93272800	-3.74263500	1.07748600
H	1.10052500	-3.41788900	-0.64382600
H	-0.23638700	-2.69613000	0.26346100
C	0.08718000	-0.59390700	2.34050500
H	0.23068600	-0.68334000	3.42253700
H	-0.66531200	-1.32063500	2.03335100
H	-0.29891300	0.40903100	2.13404100
C	2.65004500	1.24429700	2.65371600
H	3.07939000	0.95015000	3.61834200
H	1.67166300	1.69035700	2.84549700
H	3.29838700	2.00459500	2.21369700
C	4.93132300	0.15238800	0.75061700
H	5.49305700	0.06216700	1.68682500
H	4.83254800	1.21706000	0.51978700
H	5.51352200	-0.31987300	-0.04143100
C	3.77506300	-2.46754900	-0.76293100
H	4.11484900	-3.37864200	-0.25721300
H	4.65228000	-1.97478100	-1.18537800
H	3.12699600	-2.77867900	-1.58657500
O	0.51553500	1.52529400	-0.05397400
O	2.58482400	1.98782900	-0.45282200
C	1.39683900	2.42656400	-0.27718200
C	1.05217500	3.87589800	-0.36880200
H	1.93275600	4.48866000	-0.17163600
H	0.69813500	4.08960000	-1.38360300
H	0.24585100	4.11473200	0.32722700
C	2.07670900	0.02603200	-2.39399400
H	2.07274800	1.06791200	-2.69803100
H	3.02223100	-0.49602100	-2.49863000
C	0.90634300	-0.64863400	-2.19030700

H	0.95417100	-1.72599500	-2.04983400
C	-0.47196000	-0.07900900	-2.35394300
H	-0.42868200	1.01381200	-2.33932000
H	-0.80997800	-0.37111300	-3.35999100
C	-1.48518500	-0.58847000	-1.31882900
H	-1.10251800	-0.37037300	-0.31580200
H	-1.56992700	-1.68076000	-1.40332700
C	-2.87085500	0.04348500	-1.47608300
H	-2.77698600	1.13574500	-1.40338600
H	-3.25900600	-0.16679200	-2.48202600
C	-3.87094000	-0.45216200	-0.42563100
H	-3.47389900	-0.24184000	0.57868600
H	-3.96067100	-1.54568300	-0.49581500
C	-5.26024400	0.18042800	-0.56313900
H	-5.16887300	1.27382500	-0.49645000
H	-5.65604500	-0.03073900	-1.56631900
C	-6.25813200	-0.31172900	0.49095600
H	-5.86149100	-0.10061100	1.49478800
H	-6.34822000	-1.40547200	0.42425300
C	-7.64863000	0.31976600	0.35339600
H	-7.55672400	1.41246700	0.41887800
H	-8.04310300	0.10742700	-0.64942200
C	-8.63762700	-0.17821700	1.41156300
H	-8.28215000	0.05041200	2.42286900
H	-9.62087900	0.28686900	1.29106900
H	-8.77199400	-1.26391300	1.34599300

**<sup>1</sup>Co-2'**

Co	1.77289000	-0.10211900	-0.31821600
C	2.81979700	-1.73642500	0.47216800
C	1.48455800	-1.74779200	0.97533100
C	1.27010800	-0.51376600	1.70086100
C	2.46375700	0.25837900	1.62412300
C	3.41542200	-0.46618500	0.81175700
C	3.47802200	-2.84523700	-0.28379200
H	3.88405700	-3.57163500	0.43025200
H	4.30722100	-2.48753900	-0.89575600
H	2.77418400	-3.37975300	-0.92589400
C	0.51312400	-2.88262600	0.87298400
H	0.65437600	-3.56767700	1.71707900
H	0.65385400	-3.46205500	-0.04214300
H	-0.52078100	-2.53492100	0.90353900
C	0.01455300	-0.09427400	2.39483900
H	-0.21900800	0.94454600	2.15267300

H	0.14539700	-0.17990000	3.47980900
H	-0.83494500	-0.71622200	2.10849000
C	2.70295200	1.58418800	2.26588900
H	3.14885200	1.42985500	3.25571100
H	1.77305600	2.13969300	2.38653200
H	3.39576700	2.18588900	1.67554600
C	4.78439500	0.01980900	0.46055100
H	5.44264300	-0.03300400	1.33521400
H	4.73973200	1.05996700	0.12894600
H	5.23417300	-0.57313100	-0.33722800
O	0.29027900	2.33665100	0.25894400
O	2.16860500	1.69961700	-0.80217400
C	1.31314900	2.60783700	-0.37419400
C	1.71353200	4.02776100	-0.71232600
H	0.85792100	4.69192100	-0.59011300
H	2.50949500	4.34382400	-0.02933000
H	2.10921400	4.08936500	-1.72836500
C	2.30961000	-0.49224300	-2.45273700
H	2.47385800	0.54299400	-2.72765200
H	3.11781900	-1.19113500	-2.63895300
C	1.07837900	-0.96513800	-2.07450700
H	0.92598500	-2.03828400	-1.97706200
C	-0.06542400	-0.08273900	-1.69496700
H	0.09465100	0.37523400	-0.63925300
H	-0.07737800	0.83711200	-2.28692100
C	-1.43727500	-0.75884100	-1.61015400
H	-1.33803600	-1.71231300	-1.07689600
H	-1.75677400	-1.00866400	-2.62959600
C	-2.48985600	0.11680100	-0.92245200
H	-2.13912800	0.38002300	0.08534700
H	-2.58172800	1.06795100	-1.46281700
C	-3.86046400	-0.56150700	-0.83004200
H	-3.75867800	-1.51712200	-0.29486300
H	-4.21068100	-0.81513400	-1.84005100
C	-4.91223700	0.30460100	-0.12759100
H	-4.55666000	0.56132600	0.88070300
H	-5.01358800	1.25765900	-0.66500600
C	-6.28390300	-0.37173000	-0.02665600
H	-6.18125400	-1.32617900	0.50969000
H	-6.63823600	-0.62740300	-1.03529200
C	-7.33680900	0.49357000	0.67609800
H	-6.98019500	0.74935400	1.68325700
H	-7.43797100	1.44589500	0.13830800
C	-8.70340000	-0.19129500	0.77204900

H	-8.63583900	-1.13061500	1.33268300
H	-9.43581700	0.44617100	1.27675300
H	-9.09661800	-0.42791200	-0.22306200

**<sup>1</sup>Co-TS3**

Co	1.79443400	-0.07370900	-0.36780000
C	3.06156300	-1.50986000	0.50240200
C	1.68446600	-1.83541900	0.77998400
C	1.11291000	-0.75396400	1.53807500
C	2.10878500	0.25160300	1.67876000
C	3.31791700	-0.20546100	1.01872200
C	4.03808400	-2.40498300	-0.19222500
H	4.47479700	-3.09909000	0.53553800
H	4.85451100	-1.84205400	-0.64717300
H	3.55872900	-3.00696500	-0.96773300
C	1.02993800	-3.15350500	0.50129900
H	1.20327700	-3.83288000	1.34416600
H	1.43693300	-3.63541600	-0.39027500
H	-0.04992200	-3.05770800	0.37729300
C	-0.27932500	-0.68740600	2.08161000
H	-0.65588100	0.33712700	2.07612700
H	-0.29031500	-1.04643400	3.11748700
H	-0.97008500	-1.30784500	1.50862900
C	1.97096700	1.54097200	2.42188900
H	2.25155300	1.39043200	3.47080700
H	0.94549500	1.91206400	2.39490900
H	2.63144700	2.30563100	2.00912200
C	4.58884700	0.57822000	0.93559300
H	5.05489500	0.65213200	1.92437900
H	4.38494300	1.59055000	0.57747900
H	5.30661100	0.11554400	0.25680400
O	0.00069600	2.09123200	-0.14433100
O	2.13827100	1.81826300	-0.70624700
C	1.13492500	2.57322400	-0.42760200
C	1.33982600	4.06245900	-0.43852300
H	0.56525200	4.53066100	-1.05076500
H	1.21902100	4.44000400	0.58184000
H	2.33091600	4.32009100	-0.81067500
C	2.43270900	-0.40616700	-2.38582300
H	2.56130700	0.62527200	-2.69528400
H	3.27128800	-1.07254500	-2.55382300
C	1.18379600	-0.93467000	-2.09549800
H	1.06232500	-2.01297300	-2.02106600
C	0.05695500	-0.08773400	-1.70892200



H	0.16882100	0.78307100	-0.63438900
H	-0.01012400	0.80476400	-2.34065200
C	-1.29034900	-0.77453100	-1.49447900
H	-1.15171700	-1.64577200	-0.84381600
H	-1.61815500	-1.17337900	-2.46432700
C	-2.38862400	0.12946700	-0.92355000
H	-2.07023300	0.53855600	0.04194100
H	-2.52468900	0.99585500	-1.58387800
C	-3.72147600	-0.60651300	-0.75178000
H	-3.57315600	-1.47964200	-0.09876400
H	-4.04738300	-1.00647900	-1.72188700
C	-4.82652400	0.28025200	-0.16725300
H	-4.49509700	0.68186000	0.80125500
H	-4.97597500	1.15059600	-0.82124400
C	-6.15929700	-0.45404600	0.01594100
H	-6.00805900	-1.32638000	0.66815100
H	-6.49017900	-0.85388400	-0.95302900
C	-7.26493800	0.43147900	0.60292200
H	-6.93171400	0.83136000	1.57044300
H	-7.41482000	1.30157600	-0.05045500
C	-8.59180500	-0.31216400	0.78253200
H	-8.47635200	-1.16838100	1.45688300
H	-9.36303700	0.34101000	1.20218900
H	-8.96279500	-0.69367300	-0.17541300

#### **<sup>1</sup>Co-4**

Co	1.86698800	-0.34762800	-0.45340700
C	3.30279600	0.75813900	0.58061600
C	2.24926500	0.23386600	1.42699800
C	0.99041100	0.85852700	1.05000600
C	1.24079000	1.63223900	-0.10212500
C	2.67334500	1.56435800	-0.39675800
C	4.76750200	0.47911300	0.72178200
H	5.22528800	1.22295700	1.38402700
H	5.28409600	0.52575000	-0.23888200
H	4.95103100	-0.50479400	1.15827900
C	2.42889700	-0.69336600	2.58548600
H	2.59927800	-0.11682600	3.50320100
H	3.28733400	-1.35389500	2.44721400
H	1.53994100	-1.30828500	2.74559700
C	-0.29296500	0.69499500	1.80103800
H	-0.21372600	1.19644800	2.77241900
H	-0.51749600	-0.35636400	1.99751400
H	-1.14012300	1.12676900	1.26839800

C	0.25905600	2.43172600	-0.90326200
H	0.43875000	3.50297100	-0.75665300
H	-0.77153600	2.21938300	-0.61671000
H	0.35943100	2.23292100	-1.97477500
C	3.32621500	2.25839000	-1.55158400
H	3.44063800	3.32650700	-1.33102900
H	2.72026400	2.18258700	-2.45944300
H	4.31662500	1.85251900	-1.76402600
C	2.96998100	-1.92435400	-1.00756000
H	3.03312600	-1.73074400	-2.08269500
H	3.91506100	-2.16055300	-0.53087200
C	1.75208700	-2.39559400	-0.45843300
H	1.74982300	-2.91566900	0.49836700
C	0.55439600	-1.84044300	-0.93922100
C	-0.81499200	-2.09934600	-0.37535000
H	-0.75397100	-2.14323900	0.71991700
H	-1.14996700	-3.09595000	-0.69577600
C	-1.84325600	-1.04978500	-0.81719400
H	-1.42115200	-0.05023400	-0.65792200
H	-2.00466200	-1.13986100	-1.89989500
C	-3.18321300	-1.16131800	-0.08508100
H	-3.01063700	-1.09151400	0.99872700
H	-3.61413300	-2.15611800	-0.26021200
C	-4.18743900	-0.08372900	-0.50874400
H	-3.74776300	0.91037300	-0.33473900
H	-4.35955500	-0.15272800	-1.59185100
C	-5.52811400	-0.17938200	0.22760200
H	-5.35408600	-0.11360800	1.31128600
H	-5.96819000	-1.17071800	0.05078400
C	-6.53002400	0.90282300	-0.19214400
H	-6.08733400	1.89297400	-0.01592700
H	-6.70191200	0.83447200	-1.27480800
C	-7.86611900	0.79696900	0.54906300
H	-7.72593200	0.89358700	1.63167700
H	-8.56226400	1.57930200	0.23180100
H	-8.34453600	-0.17098800	0.36263700
H	0.56788500	-1.48444600	-1.98446100

**<sup>1</sup>Co-5**

Co	1.49499800	-0.47882700	-0.31047500
C	1.84372800	-2.39796500	0.43375700
C	0.52565800	-2.00297400	0.86996900
C	0.65317300	-0.80889600	1.62229600
C	2.06975700	-0.49950400	1.71222100

C	2. 80352400	-1. 48842700	1. 00284200
C	2. 19032400	-3. 64609700	-0. 32015700
H	2. 51764200	-4. 42555000	0. 37730900
H	3. 00747900	-3. 47926900	-1. 02718000
H	1. 33658200	-4. 04229000	-0. 87325600
C	-0. 73465100	-2. 77106900	0. 62283600
H	-0. 69485300	-3. 33206100	-0. 31269200
H	-1. 61295900	-2. 12550000	0. 59690400
H	-0. 87871100	-3. 49883300	1. 43032000
C	-0. 43126900	-0. 05762800	2. 33567300
H	-0. 36008400	-0. 22634400	3. 41637100
H	-1. 42319100	-0. 37811300	2. 01440400
H	-0. 35916600	1. 01842500	2. 16175300
C	2. 63771600	0. 62940800	2. 51517200
H	2. 74176700	0. 32013700	3. 56150800
H	1. 98231500	1. 50386400	2. 50395600
H	3. 62828100	0. 92659500	2. 16451700
C	4. 29430600	-1. 61754000	0. 91701300
H	4. 66349800	-2. 27398000	1. 71364200
H	4. 79501900	-0. 65325700	1. 03291200
H	4. 60828800	-2. 05095800	-0. 03497900
C	2. 60026900	-0. 57209000	-2. 02683700
H	2. 82588500	0. 43884900	-2. 35492000
H	3. 44551800	-1. 25281800	-2. 04932600
C	1. 29760400	-1. 09621700	-2. 25791800
H	1. 15945000	-2. 17223800	-2. 33325800
C	0. 16876300	-0. 29138800	-2. 09413800
C	-1. 24802100	-0. 78152900	-2. 14534700
H	-1. 28996000	-1. 85098400	-1. 91514800
H	-1. 60547900	-0. 67876300	-3. 18111200
C	-2. 18295700	0. 00889000	-1. 21694800
H	-1. 75560600	0. 01561700	-0. 20759900
H	-2. 20357600	1. 05971800	-1. 53414700
C	-3. 60902700	-0. 54657800	-1. 17428400
H	-3. 57962500	-1. 60778500	-0. 88596000
H	-4. 04276300	-0. 52092800	-2. 18299000
C	-4. 51698800	0. 21719800	-0. 20386500
H	-4. 07491100	0. 18996700	0. 80370000
H	-4. 54609400	1. 27722300	-0. 49188800
C	-5. 94540700	-0. 33478500	-0. 14461100
H	-5. 91436800	-1. 39643500	0. 14010400
H	-6. 38788600	-0. 30357400	-1. 15013600
C	-6. 85042400	0. 42597300	0. 83176000
H	-6. 40520100	0. 39489300	1. 83586000

H	-6.87985300	1.48575500	0.54474700
C	-8.27526300	-0.13350300	0.88291700
H	-8.27625200	-1.18322800	1.19788800
H	-8.89986400	0.42619000	1.58585100
H	-8.75380600	-0.08343700	-0.10154800
H	0.28169600	0.77963600	-2.24670100
C	3.87061500	2.26317700	-0.45772800
H	4.19570500	2.73725800	-1.38933600
H	4.13131000	1.20586500	-0.46920400
H	4.37555000	2.76976300	0.36973400
C	2.40737300	2.41565900	-0.30299700
O	1.88312600	3.64636500	-0.15291600
N	1.51364700	1.48107900	-0.27946200
O	0.26773400	2.14251400	-0.08670100
C	0.50271100	3.49128100	-0.00978200
O	-0.29352900	4.35049600	0.14935200

**<sup>1</sup>Co-TS6**

Co	1.58590500	-0.44704800	-0.27926700
C	2.03120300	-2.35866100	0.49768600
C	0.66948500	-2.04231500	0.83872500
C	0.67236400	-0.84131600	1.60962700
C	2.04292300	-0.41483200	1.75062600
C	2.88622900	-1.35890800	1.07567400
C	2.49682600	-3.58919200	-0.21736100
H	2.75320800	-4.36278900	0.51567900
H	3.39172200	-3.40317300	-0.81545500
H	1.72636000	-4.00540800	-0.86914500
C	-0.52798100	-2.87599200	0.50531100
H	-0.39806600	-3.41915400	-0.43289900
H	-1.43535600	-2.27581100	0.43111500
H	-0.68321300	-3.62248100	1.29323100
C	-0.49731100	-0.13627700	2.22262900
H	-0.36525500	-0.07696600	3.30861500
H	-1.43431800	-0.65827400	2.02633500
H	-0.58378600	0.88174700	1.83434800
C	2.47758800	0.77744600	2.53969400
H	2.52559100	0.51367200	3.60258700
H	1.76874900	1.60105300	2.43232700
H	3.46690900	1.12678700	2.24017300
C	4.38211000	-1.34532900	1.03744400
H	4.78192800	-1.91822800	1.88254800
H	4.77802800	-0.33062900	1.11141600
H	4.76807800	-1.79784100	0.12171100

C	2.59549200	-0.66823600	-2.07375900
H	2.86571100	0.32219000	-2.41999400
H	3.40498100	-1.39011500	-2.05080100
C	1.26523900	-1.14056000	-2.23740400
H	1.08554800	-2.21313800	-2.24057600
C	0.15664400	-0.29588600	-2.19557300
C	-1.25421100	-0.77250900	-2.21250800
H	-1.29866500	-1.85386000	-2.04367000
H	-1.62970800	-0.60304900	-3.23480900
C	-2.17315400	-0.02333400	-1.22792900
H	-1.73104000	-0.06887900	-0.22810300
H	-2.18949600	1.04107800	-1.48422300
C	-3.59418000	-0.59117300	-1.19864800
H	-3.55706200	-1.66625900	-0.96651900
H	-4.04260200	-0.51397500	-2.19829200
C	-4.48973800	0.11762200	-0.17588100
H	-4.03296100	0.03882500	0.82215000
H	-4.52496600	1.19083600	-0.40722900
C	-5.91537000	-0.44270600	-0.12656800
H	-5.87731100	-1.51813100	0.09998300
H	-6.37242700	-0.35865600	-1.12245100
C	-6.80800100	0.26136000	0.90240300
H	-6.34815100	0.17771900	1.89684000
H	-6.84429200	1.33481200	0.67337100
C	-8.23034000	-0.30523400	0.94344600
H	-8.22409000	-1.37045500	1.20122600
H	-8.84596100	0.21363600	1.68448900
H	-8.72328600	-0.20347100	-0.02983000
H	0.30409700	0.77505400	-2.30045500
C	3.81906100	2.42769300	-0.45566800
H	4.08130800	3.04598900	-1.31800200
H	4.21445400	1.41995600	-0.57950000
H	4.23766200	2.89339900	0.44010300
C	2.30139300	2.44161800	-0.31490700
O	1.74740300	3.57318400	-0.13710600
N	1.71510600	1.28614000	-0.42177700
O	-0.22695300	2.23444800	-0.16169500
C	-0.00766300	3.43981900	-0.02234800
O	-0.47409400	4.51021000	0.15230900

**<sup>1</sup>Co-7**

Co	-1.66326800	-0.11824300	0.35243200
C	-3.03675700	-0.36779600	-1.19559500
C	-2.33585300	-1.60872800	-1.04082500

C	-0.94102900	-1.36196500	-1.25507200
C	-0.76995200	0.02684800	-1.57305400
C	-2.06770400	0.64176600	-1.54120900
C	-4.51609800	-0.16095700	-1.10962000
H	-4.96608400	-0.27190000	-2.10353300
H	-4.75814500	0.83988300	-0.74623000
H	-4.99113600	-0.88892500	-0.44923500
C	-2.96699700	-2.94320500	-0.78779500
H	-3.25170900	-3.39958600	-1.74280600
H	-3.87505800	-2.86276800	-0.18646600
H	-2.28529200	-3.63756300	-0.29198700
C	0.14674200	-2.38964400	-1.23265200
H	0.26950400	-2.81633500	-2.23524600
H	-0.08305600	-3.21541900	-0.55586200
H	1.10474600	-1.95856200	-0.93784700
C	0.49615600	0.72353500	-1.96263500
H	0.42233800	1.05499100	-3.00482600
H	1.36270000	0.06615100	-1.88309700
H	0.66199900	1.60321500	-1.33490500
C	-2.36411000	2.04872700	-1.94978100
H	-2.58331800	2.06694300	-3.02413900
H	-1.50986400	2.70411700	-1.77289100
H	-3.23432300	2.45210700	-1.42879100
C	-2.74860300	-0.90322400	1.98134000
H	-2.92975000	-0.05378700	2.62796400
H	-3.62081600	-1.47659100	1.68864500
C	-1.47579700	-1.51849000	1.94050600
H	-1.38379000	-2.51751600	1.52165600
C	-0.29999700	-0.82906800	2.25357300
C	1.07480000	-1.34667200	2.03874000
H	1.05836100	-2.28026100	1.46720100
H	1.48940800	-1.58753500	3.03048400
C	1.98961400	-0.29942500	1.36636600
H	1.50164400	0.05518800	0.45332300
H	2.06994700	0.58062700	2.01550200
C	3.38109800	-0.84725000	1.03993300
H	3.28380600	-1.74594600	0.41246000
H	3.87465400	-1.17643800	1.96409100
C	4.26274700	0.18057500	0.32079800
H	3.75855000	0.51053000	-0.59957000
H	4.35990500	1.07684200	0.94828100
C	5.65606300	-0.35500800	-0.02676700
H	5.55611700	-1.25449900	-0.65145200
H	6.16006200	-0.67993100	0.89419800

C	6.53543200	0.67098600	-0.75162000
H	6.02858100	0.99578700	-1.67078700
H	6.63353200	1.56776800	-0.12532700
C	7.92552600	0.12704800	-1.09438900
H	7.85645800	-0.75176200	-1.74559600
H	8.53215100	0.87752500	-1.61027200
H	8.46532500	-0.17356600	-0.18947100
H	-0.38745200	0.10601700	2.79677100
C	-2.21570200	3.65680900	1.08191500
H	-3.20146700	3.19735400	1.19720600
H	-2.22575000	4.37254300	0.25617400
H	-1.97354200	4.19915800	2.00109700
C	-1.12868100	2.63428200	0.81933100
N	-1.41123200	1.36227600	1.19035500
O	-0.00097100	2.92548800	0.40477700

**<sup>1</sup>Co-TS8**

Co	-1.81520900	-0.06808900	0.37796000
C	-3.38440000	0.17295900	-0.93736900
C	-3.18398700	-1.23740600	-0.74912300
C	-1.85069900	-1.54873400	-1.15136400
C	-1.22157000	-0.33744100	-1.61712500
C	-2.17980200	0.71934500	-1.51754200
C	-4.63880400	0.93647800	-0.65311200
H	-5.28669800	0.93542300	-1.53799500
H	-4.42292800	1.97654800	-0.40066200
H	-5.20113200	0.49555800	0.17228700
C	-4.19992900	-2.21813900	-0.25017400
H	-3.74888200	-2.98934100	0.38006400
H	-4.67063100	-2.72737000	-1.09884300
H	-4.99160400	-1.72867400	0.31975900
C	-1.23492600	-2.91348500	-1.16525200
H	-1.36611500	-3.36254700	-2.15679600
H	-1.70415500	-3.58395400	-0.44203500
H	-0.16202300	-2.88487300	-0.96473400
C	0.17712200	-0.18893900	-2.12750700
H	0.16744200	-0.09244900	-3.21960000
H	0.79395900	-1.05350400	-1.87693500
H	0.64641300	0.70426400	-1.70703700
C	-1.99657300	2.11155900	-2.03072300
H	-2.29083000	2.13993700	-3.08655900
H	-0.95580100	2.43290900	-1.96496900
H	-2.62001000	2.82993500	-1.49620400
C	-2.55027600	-0.74665300	2.32449000

H	-2.59983700	0.17251500	2.89456700
H	-3.45587000	-1.33837200	2.26265400
C	-1.33174700	-1.31445100	1.96845600
H	-1.29880100	-2.32587500	1.56953300
C	-0.09223300	-0.58037300	1.99997700
C	1.15866100	-1.15829300	1.42316000
H	0.93552500	-1.70401200	0.50076700
H	1.46726400	-1.92633700	2.15590000
C	2.31627500	-0.17562700	1.21458300
H	1.98108900	0.63709500	0.56508900
H	2.57305300	0.28383600	2.17840200
C	3.55200600	-0.85782100	0.61903500
H	3.28110100	-1.32306100	-0.34089000
H	3.87916500	-1.67857000	1.27304200
C	4.71562400	0.11459500	0.39600900
H	4.37920000	0.93867900	-0.24844900
H	4.99217200	0.57291500	1.35560900
C	5.94905000	-0.54996400	-0.22525000
H	5.67110300	-1.00852000	-1.18542100
H	6.28250900	-1.37534300	0.41981100
C	7.11397000	0.42208800	-0.44727000
H	6.77769500	1.24742500	-1.08950000
H	7.39118500	0.87749600	0.51297100
C	8.34049300	-0.24997900	-1.07155100
H	8.09807000	-0.68561200	-2.04763200
H	9.15639200	0.46425100	-1.21886700
H	8.71555800	-1.05779300	-0.43302400
H	0.03410900	0.16025200	2.77910600
C	-1.22158400	3.63499100	0.89511500
H	-1.07960600	4.30343200	0.04356200
H	-0.80843400	4.11628000	1.78726500
H	-2.28513500	3.45158400	1.06792900
C	-0.43693800	2.35374000	0.63753700
N	-1.03370700	1.25970800	1.20307100
O	0.64671300	2.34945100	0.05517700

**<sup>1</sup>Co-9**

Co	1.89900800	-0.11983400	-0.26799600
C	3.93551300	0.00659300	0.21723600
C	3.46117700	-1.30999000	0.49649400
C	2.36101100	-1.19392500	1.40540200
C	2.21137400	0.20436200	1.76227200
C	3.18314400	0.94348500	1.03027600
C	5.04226200	0.37918800	-0.71863700



H	5. 97095800	0. 53947400	-0. 15856100
H	4. 81774100	1. 30634500	-1. 25201200
H	5. 23122900	-0. 40199500	-1. 45708600
C	3. 97720100	-2. 59957700	-0. 06565100
H	4. 53695800	-3. 13992100	0. 70560900
H	4. 65123900	-2. 44060300	-0. 90882300
H	3. 16395100	-3. 25387100	-0. 39303400
C	1. 53817000	-2. 31710200	1. 94956600
H	1. 95084600	-2. 65003700	2. 91020700
H	1. 53125800	-3. 17790400	1. 27768400
H	0. 50669700	-2. 00439400	2. 12652700
C	1. 25513300	0. 72979600	2. 78333500
H	1. 63967400	0. 49797300	3. 78435000
H	0. 27421800	0. 25854700	2. 68725400
H	1. 11968200	1. 80417400	2. 68639400
C	3. 37828900	2. 42194600	1. 08544900
H	3. 75303500	2. 70781000	2. 07505300
H	2. 42361000	2. 93537900	0. 93500800
H	4. 09671000	2. 76655100	0. 34031300
C	2. 14388100	-0. 88068400	-2. 33601400
H	2. 30802900	0. 08138000	-2. 81729000
H	2. 93948200	-1. 61072200	-2. 42856800
C	0. 92487100	-1. 22755100	-1. 83028900
H	0. 73219600	-2. 25088000	-1. 51508900
C	-0. 21388100	-0. 20486300	-1. 72875100
C	-1. 48415300	-0. 89895600	-1. 19989700
H	-1. 21379000	-1. 42815800	-0. 27523400
H	-1. 76001900	-1. 66736100	-1. 93447600
C	-2. 68828100	0. 00458400	-0. 93190000
H	-2. 43306300	0. 73895600	-0. 15758500
H	-2. 93645800	0. 57407300	-1. 83679800
C	-3. 92145300	-0. 78467400	-0. 47456200
H	-3. 66822500	-1. 36536400	0. 42390800
H	-4. 19122400	-1. 51831000	-1. 24666700
C	-5. 12877400	0. 11190700	-0. 17750200
H	-4. 85399500	0. 84756400	0. 59202800
H	-5. 38006900	0. 69129900	-1. 07712500
C	-6. 36368100	-0. 66931300	0. 28500900
H	-6. 11146000	-1. 24942000	1. 18428900
H	-6. 63757800	-1. 40532100	-0. 48416100
C	-7. 57202500	0. 22665400	0. 58239100
H	-7. 29553100	0. 96253600	1. 34975900
H	-7. 82253900	0. 80462200	-0. 31746200
C	-8. 79986900	-0. 56329200	1. 04519700

H	-8.58541700	-1.12490000	1.96155500
H	-9.64710500	0.09823400	1.25032600
H	-9.11602700	-1.28363500	0.28226700
H	-0.41652100	0.26462900	-2.70098200
C	-0.94352700	2.74363300	-1.45804200
H	-1.90053700	2.97615300	-0.98495100
H	-1.13110500	2.20942600	-2.38849100
H	-0.45119700	3.69439000	-1.67900800
C	-0.06485300	2.00994200	-0.45938500
N	0.39812800	0.72462600	-0.76898000
O	0.30688300	2.57293100	0.56095300

**<sup>3</sup>Co-1**

Co	-0.45537600	-0.00199500	-0.21741400
C	1.20331400	-0.69811700	1.14115200
C	1.19941400	0.69913000	1.14321000
C	1.36455800	1.15090500	-0.25112500
C	1.52551000	0.00462400	-1.09237500
C	1.37097100	-1.14491900	-0.25448400
C	1.04582000	-1.63198300	2.29817400
H	1.97870600	-2.18310800	2.46580300
H	0.26318300	-2.37279200	2.10691500
H	0.79661100	-1.10171200	3.21797000
C	1.03668700	1.62879300	2.30288500
H	1.96638000	2.18484100	2.47197500
H	0.79066900	1.09449200	3.22120700
H	0.24974200	2.36557300	2.11374700
C	1.43599900	2.58372600	-0.65952000
H	2.42297400	2.98799500	-0.39841600
H	0.69048700	3.18682400	-0.13420700
H	1.29669100	2.71187200	-1.73385800
C	1.81861700	0.00759100	-2.56479900
H	2.90126400	0.01109100	-2.73448600
H	1.40413600	0.88988200	-3.05726600
H	1.40945900	-0.87579300	-3.05975000
C	1.45056700	-2.57616100	-0.66701500
H	2.44025200	-2.97521900	-0.40816700
H	1.31087600	-2.70211500	-1.74157000
H	0.70931800	-3.18528800	-0.14264000
O	-2.07079300	-1.09416400	-0.16601400
O	-2.07298300	1.08252100	-0.16410200
C	-2.76036900	-0.00728400	-0.14663700
C	-4.24818300	-0.00330800	-0.12565600
H	-4.60661600	0.78186200	0.54368000

H	-4.60729200	0.23107800	-1.13437300
H	-4.62891100	-0.98044800	0.17168800

**<sup>3</sup>Co-2**

Co	-1.98828100	0.22557600	0.30120700
C	-1.49577200	-1.90153800	-0.55155600
C	-1.10728900	-0.96625700	-1.51814500
C	-2.27326200	-0.16985600	-1.83066300
C	-3.42282100	-0.68335900	-1.08066400
C	-2.94549700	-1.71108000	-0.26068200
C	-0.67657000	-3.01819800	0.00556800
H	-0.83910600	-3.91951400	-0.60011800
H	-0.96334300	-3.27238900	1.02859400
H	0.38994700	-2.79259900	-0.01244500
C	0.25031200	-0.74989600	-2.11362900
H	0.22336500	-0.88379600	-3.20018100
H	0.98484600	-1.44713500	-1.70823300
H	0.60012700	0.26670100	-1.90669800
C	-2.33251400	0.92476600	-2.83654300
H	-2.69271600	0.52391200	-3.79357700
H	-1.34759300	1.36373700	-3.00689300
H	-3.02534000	1.70807100	-2.52171500
C	-4.81282800	-0.13719100	-1.20023200
H	-5.22153500	-0.34507700	-2.19520800
H	-4.81445000	0.94759600	-1.05716200
H	-5.48543000	-0.57951500	-0.46345100
C	-3.72583500	-2.58032300	0.67467200
H	-3.85607700	-3.57992500	0.24291100
H	-4.71764700	-2.17144100	0.87453400
H	-3.21058700	-2.71215500	1.63136000
O	-0.49668600	1.71424500	0.10774600
O	-2.64152600	2.11640900	0.09865800
C	-1.43851500	2.56373700	0.03443000
C	-1.17665200	4.03494200	-0.09178900
H	-1.96564200	4.51327300	-0.67444200
H	-1.18322000	4.47848500	0.91009600
H	-0.19793000	4.20980700	-0.54006100
C	-2.11834700	0.30272500	2.55581800
H	-2.10057800	1.37797500	2.71292700
H	-3.08677400	-0.18979800	2.63662600
C	-0.96680300	-0.42062300	2.51085100
H	-1.04457100	-1.50674900	2.46067500
C	0.41716100	0.13962200	2.60533900
H	0.38281500	1.22782400	2.50129700

H	0.78414000	-0.08269000	3.61896600
C	1.38602600	-0.46398700	1.57529200
H	0.96071600	-0.32145800	0.57637600
H	1.46740200	-1.54654800	1.74376700
C	2.77869100	0.16976300	1.61786500
H	2.68260600	1.25326100	1.46689800
H	3.21704600	0.03208300	2.61555000
C	3.72005200	-0.41060700	0.55625700
H	3.27056200	-0.27180300	-0.43840700
H	3.81020800	-1.49669100	0.70275400
C	5.11651900	0.22085200	0.57117400
H	5.02407600	1.30693400	0.43002000
H	5.56651600	0.08038400	1.56374700
C	6.05280100	-0.35332100	-0.49787300
H	5.60066000	-0.21403400	-1.49080600
H	6.14474700	-1.43975700	-0.35597900
C	7.44980600	0.27864500	-0.48540700
H	7.35592200	1.36403500	-0.62595000
H	7.89982200	0.13829300	0.50658000
C	8.37671900	-0.30136100	-1.55789700
H	7.96500400	-0.14581500	-2.56174400
H	9.36575600	0.16600400	-1.52755400
H	8.51326200	-1.37999200	-1.42000500

**<sup>3</sup>Co-TS3**

Co	2.23923000	-0.08677700	-0.53295200
C	4.13634000	-0.76634400	0.24761000
C	3.02908500	-1.29659500	1.07438300
C	2.38149300	-0.20374600	1.71671200
C	3.03107100	0.98386500	1.26916000
C	4.13188500	0.63178800	0.38348500
C	5.12873500	-1.61550000	-0.48533100
H	5.89135400	-1.98747700	0.20942300
H	5.63899700	-1.05384400	-1.26998700
H	4.65707200	-2.48721600	-0.94571300
C	2.78406000	-2.75155600	1.31258100
H	3.52336900	-3.13100000	2.02911500
H	2.89371400	-3.34292600	0.40012900
H	1.79502100	-2.93886300	1.73451800
C	1.20545300	-0.26236400	2.64883000
H	0.44565200	0.47383100	2.37254000
H	1.51421600	-0.06036700	3.68021200
H	0.73167700	-1.24600700	2.63417100
C	2.67424300	2.38385900	1.64251800

H	3.41202500	2.77981500	2.35112900
H	1.69099400	2.44241200	2.11239000
H	2.68808100	3.03659300	0.76484800
C	5.05287400	1.62843500	-0.25210900
H	5.69856000	1.16345300	-0.99887100
H	5.69575400	2.09392900	0.50354700
H	4.49001600	2.42924600	-0.74197800
O	-0.48023800	1.23054400	-0.14503600
O	1.46197400	1.53213700	-1.22582300
C	0.33781600	1.96287800	-0.79144800
C	-0.03091400	3.39507400	-1.04961900
H	-0.96056000	3.42615600	-1.62548700
H	-0.23270500	3.88733600	-0.09312200
H	0.76219200	3.91788200	-1.58291900
C	1.61598300	-1.58715800	-1.76424000
H	1.58440800	-1.11850900	-2.75064700
H	2.33834800	-2.39677700	-1.68035900
C	0.37111300	-1.78814600	-1.09691900
H	0.38664400	-2.46826800	-0.24303700
C	-0.82189900	-1.09169300	-1.32383400
H	-0.52236000	0.01849600	-0.60841200
H	-0.89750300	-0.60518500	-2.30254700
C	-2.14381800	-1.55874100	-0.72182800
H	-1.97429500	-1.90547500	0.30667800
H	-2.49735300	-2.43235100	-1.28696300
C	-3.23530300	-0.47974600	-0.73452100
H	-2.89727500	0.39229200	-0.16147800
H	-3.38135800	-0.13132800	-1.76679600
C	-4.57046100	-0.98092600	-0.17413700
H	-4.42152100	-1.33726400	0.85517700
H	-4.90536600	-1.85316900	-0.75273600
C	-5.66746300	0.08966900	-0.18660900
H	-5.32945300	0.96230900	0.39055900
H	-5.81578100	0.44494100	-1.21624400
C	-7.00412200	-0.40525700	0.37696300
H	-6.85545200	-0.76175800	1.40635600
H	-7.34128000	-1.27791800	-0.20027100
C	-8.10232100	0.66473600	0.36517600
H	-7.76326600	1.53634700	0.94171200
H	-8.24941700	1.01931000	-0.66407100
C	-9.43328100	0.15980900	0.93049100
H	-9.32054500	-0.17111300	1.96921300
H	-10.19932100	0.94120300	0.91078700
H	-9.80979300	-0.69126000	0.35180600

**<sup>3</sup>Co-4**

Co	-1.86985300	0.43425100	-0.50696000
C	-3.27018600	-0.92823800	0.31359700
C	-2.45631000	-0.47303500	1.42045200
C	-1.11005900	-0.84957700	1.15865000
C	-1.07962600	-1.56503200	-0.10148500
C	-2.41114800	-1.62783100	-0.61324000
C	-4.76521100	-0.84717000	0.23138000
H	-5.21257100	-1.73084700	0.70212400
H	-5.11362500	-0.81582400	-0.80334300
H	-5.15408900	0.03193700	0.74962300
C	-2.96047000	0.26265300	2.62559700
H	-3.30726900	-0.44288800	3.38978900
H	-3.80419600	0.91256000	2.37923200
H	-2.18059500	0.87746500	3.08151200
C	0.06745000	-0.60422000	2.05255600
H	0.19462400	-1.44048600	2.75041300
H	-0.06065800	0.30090800	2.65120300
H	0.99587500	-0.50614500	1.48688100
C	0.10826600	-2.25860900	-0.70125400
H	0.03979200	-3.33567100	-0.50652100
H	1.04929100	-1.90841700	-0.27523800
H	0.15573900	-2.12892800	-1.78586000
C	-2.85285900	-2.36750100	-1.84307800
H	-3.12584800	-3.39839600	-1.58749200
H	-2.05923000	-2.41594900	-2.59258400
H	-3.72820700	-1.90406200	-2.30462400
C	-2.96587200	2.14423700	-0.80942200
H	-3.05894000	2.08310600	-1.89700000
H	-3.89182700	2.30978700	-0.27021200
C	-1.72642600	2.50793000	-0.23150900
H	-1.70547000	2.84839300	0.80343000
C	-0.52687200	2.09418000	-0.82633500
C	0.82891700	2.23101400	-0.19328000
H	0.73679300	2.12819500	0.89507900
H	1.19944500	3.25059800	-0.37549800
C	1.84159200	1.21688600	-0.74269300
H	1.39604000	0.21568500	-0.69823200
H	2.01876300	1.42138500	-1.80705500
C	3.17362800	1.21744700	0.01313200
H	2.98445700	1.04312400	1.08246500
H	3.63213900	2.21296700	-0.05442400
C	4.15500400	0.16105900	-0.50700600

H	3.68570800	-0.83257000	-0.44354600
H	4.34712200	0.33719200	-1.57443700
C	5.48488300	0.14104600	0.25451800
H	5.29017300	-0.03091100	1.32292000
H	5.95569700	1.13174700	0.18755800
C	6.46279300	-0.92181100	-0.26053400
H	5.98841900	-1.91082300	-0.19555900
H	6.65667700	-0.74656300	-1.32732000
C	7.78725800	-0.93470800	0.50845900
H	7.62408800	-1.13939800	1.57264900
H	8.46620900	-1.70074300	0.12182200
H	8.29693100	0.03221200	0.43194000
H	-0.53393700	1.93426500	-1.91279700

**<sup>3</sup>Co-5**

Co	-1.57239500	-0.47231500	0.36388500
C	-1.96404200	-2.48473500	-0.60389900
C	-0.62267700	-2.16088000	-0.89755600
C	-0.61162000	-0.89581200	-1.60909700
C	-1.95792500	-0.46705700	-1.78466900
C	-2.80608900	-1.40987600	-1.10953200
C	-2.46673600	-3.71797000	0.08347700
H	-2.81314900	-4.45609000	-0.64950700
H	-3.31233600	-3.50215100	0.74322500
H	-1.68687900	-4.19796700	0.67983500
C	0.58729500	-2.98904700	-0.58336100
H	0.42486800	-3.63096700	0.28612400
H	1.46381500	-2.36908400	-0.38299600
H	0.83601500	-3.64309600	-1.42749200
C	0.58896500	-0.22128100	-2.20684800
H	0.58053800	-0.33593100	-3.29723100
H	1.52366900	-0.64724900	-1.83945500
H	0.60318100	0.85092400	-1.99107300
C	-2.39750300	0.72993700	-2.57588400
H	-2.50101000	0.47741400	-3.63746400
H	-1.67040600	1.54475800	-2.50995300
H	-3.36749400	1.10701300	-2.24056200
C	-4.30640100	-1.42086400	-1.12159500
H	-4.67571000	-1.98120800	-1.98899300
H	-4.72017400	-0.41126500	-1.18867800
H	-4.71575200	-1.89671300	-0.22736100
C	-2.63947700	-0.75009800	2.10768800
H	-2.89440900	0.26432600	2.41210000
H	-3.46743700	-1.45053100	2.08831600

C	-1.32318700	-1.23854300	2.35128100
H	-1.16496300	-2.31573700	2.33293200
C	-0.20838500	-0.41383000	2.32596400
C	1.20978500	-0.89225700	2.33482600
H	1.24580200	-1.96228900	2.10043200
H	1.61045900	-0.78098100	3.35361900
C	2.09793800	-0.09944100	1.35969200
H	1.62637900	-0.11115500	0.37009700
H	2.12214800	0.95471500	1.66429300
C	3.52496000	-0.64467600	1.25778900
H	3.49055300	-1.70901700	0.98267000
H	4.00522600	-0.60305400	2.24454900
C	4.37766600	0.11624500	0.23610200
H	3.88787300	0.07327000	-0.74850700
H	4.41063900	1.17976800	0.51048400
C	5.80654600	-0.42413000	0.11407800
H	5.77141700	-1.48950400	-0.15557800
H	6.29733900	-0.37595200	1.09619600
C	6.65514100	0.33208300	-0.91509700
H	6.16153500	0.28365100	-1.89563100
H	6.68826900	1.39576700	-0.64332700
C	8.08107400	-0.21517200	-1.02906000
H	8.07673700	-1.26892700	-1.33013900
H	8.66483200	0.34075100	-1.76907900
H	8.60690800	-0.14756200	-0.07011800
H	-0.35394000	0.65607200	2.46873500
C	-3.70722400	2.65310500	0.36150300
H	-4.05685200	3.25771000	1.20405200
H	-4.02650000	1.61793200	0.49252600
H	-4.14536700	3.06343000	-0.55288700
C	-2.23147400	2.71470600	0.27504200
O	-1.61524000	3.88908200	0.04690700
N	-1.41009100	1.72517500	0.39252800
O	-0.11633600	2.27333200	0.22081800
C	-0.24337000	3.62483500	0.00484100
O	0.62406700	4.40555700	-0.18158200

**<sup>3</sup>Co-TS6**

Co	-1.61708600	-0.36788900	0.30187900
C	-1.98646500	-2.52014700	-0.01569200
C	-0.60172300	-2.25152300	-0.39954800
C	-0.61395400	-1.29421100	-1.43086600
C	-2.00599600	-0.96192800	-1.71058700
C	-2.84805100	-1.74118300	-0.83628500



C	-2.41694100	-3.55435500	0.97437400
H	-2.51901200	-4.52262500	0.46876400
H	-3.38623300	-3.31921900	1.41929100
H	-1.68800900	-3.69070100	1.77615200
C	0.59105200	-2.94904500	0.17443900
H	0.48265400	-3.12628000	1.24700400
H	1.51016700	-2.38476600	0.01468900
H	0.70917000	-3.92961000	-0.30236900
C	0.53940500	-0.68920400	-2.16752000
H	0.43625200	-0.87092700	-3.24283300
H	1.49445400	-1.10541400	-1.84595300
H	0.56612300	0.39449400	-2.01288600
C	-2.42853000	-0.11281100	-2.86196300
H	-2.22511100	-0.65589500	-3.79341200
H	-1.85526300	0.81683700	-2.89587800
H	-3.49205500	0.12287200	-2.84061200
C	-4.34555600	-1.79556400	-0.86204700
H	-4.68390200	-2.58088000	-1.54805800
H	-4.78038900	-0.85390800	-1.20339900
H	-4.75865900	-2.01996500	0.12389500
C	-2.56304500	-0.28175200	2.13274900
H	-2.86731800	0.76244800	2.14819000
H	-3.35146400	-1.00903100	2.29459700
C	-1.22056300	-0.63251400	2.43064400
H	-1.00141900	-1.66958500	2.67407900
C	-0.14911000	0.24113900	2.26519400
C	1.27278400	-0.16578400	2.39055800
H	1.35779200	-1.24476300	2.56374300
H	1.67633200	0.33493500	3.28470700
C	2.12454500	0.26556900	1.17347100
H	1.62720000	-0.08477500	0.26271100
H	2.12763700	1.35638100	1.10425800
C	3.55120300	-0.28544200	1.23208700
H	3.52356400	-1.38060500	1.33603900
H	4.05361800	0.09149100	2.13275100
C	4.37159500	0.08683800	-0.00870800
H	3.86268200	-0.29279600	-0.90816200
H	4.39384300	1.17977900	-0.11369900
C	5.80499600	-0.45461700	0.02688700
H	5.77989300	-1.54820200	0.13982300
H	6.31508300	-0.06896600	0.92045500
C	6.62075300	-0.09127800	-1.21966200
H	6.10775200	-0.47616300	-2.11206400
H	6.64383400	1.00116100	-1.32922500

C	8.05185400	-0.63499600	-1.17381200
H	8.05708300	-1.72813800	-1.09512100
H	8.61172900	-0.36256000	-2.07362000
H	8.59625300	-0.23858700	-0.30954600
H	-0.33667100	1.29686100	2.08410300
C	-3.57206000	2.33959500	-0.89459800
H	-4.18593900	2.96766500	-0.24334900
H	-3.92212100	1.30916000	-0.84436300
H	-3.66893000	2.72350700	-1.91314500
C	-2.13107900	2.46788500	-0.44269400
O	-1.70525600	3.68502200	-0.37130700
N	-1.40811300	1.42810800	-0.14391300
O	0.22605300	2.75215300	0.58360400
C	-0.20049700	3.87183800	0.23533400
O	0.13417800	5.01331700	0.21502300

**<sup>3</sup>Co-7**

Co	-1.72266400	0.09637100	0.34933000
C	-3.14433900	-0.62841100	-1.06463700
C	-2.40846700	-1.75023700	-0.55211200
C	-1.01683800	-1.59711400	-0.90793800
C	-0.87807500	-0.37097600	-1.60090800
C	-2.20384000	0.24316400	-1.69432300
C	-4.62968800	-0.43738600	-1.02432400
H	-5.07880500	-0.78327800	-1.96274800
H	-4.89311400	0.61543300	-0.90103800
H	-5.09114900	-1.00218200	-0.21189400
C	-3.01553400	-2.95675400	0.09224300
H	-3.41550600	-3.61832600	-0.68528800
H	-3.84791700	-2.69886900	0.75126600
H	-2.28567700	-3.53435800	0.66263800
C	0.06670600	-2.59666100	-0.64386400
H	0.12832800	-3.30989500	-1.47434100
H	-0.12232700	-3.17447300	0.26358900
H	1.04284000	-2.11896000	-0.54615000
C	0.35406400	0.16899200	-2.25065200
H	0.25899500	0.06928200	-3.33894300
H	1.24820100	-0.37595900	-1.94408600
H	0.48204800	1.23016300	-2.02616800
C	-2.53334800	1.48090900	-2.46266700
H	-2.76038200	1.20358100	-3.50002200
H	-1.70123400	2.18360800	-2.45704900
H	-3.41382600	1.98003900	-2.05292900
C	-2.92344300	-0.09721200	2.04815900

H	-3.04477700	0.93711100	2.35333600
H	-3.83801700	-0.66734700	1.93411400
C	-1.70347100	-0.77972200	2.26876400
H	-1.68184500	-1.86489100	2.20906500
C	-0.48606500	-0.09579600	2.32419700
C	0.86231400	-0.73105200	2.28662400
H	0.78421200	-1.78257100	1.99241500
H	1.26892100	-0.71741400	3.30955400
C	1.83303600	0.02334200	1.35576200
H	1.36261700	0.12915400	0.37152500
H	1.97467600	1.04470500	1.73247400
C	3.19169700	-0.66768500	1.21211200
H	3.04077700	-1.70274100	0.87219800
H	3.67373500	-0.74036300	2.19600400
C	4.12084300	0.05834100	0.23235200
H	3.62600200	0.13591600	-0.74732200
H	4.27458700	1.09095300	0.57493800
C	5.47915400	-0.63067600	0.06132700
H	5.32280400	-1.66493400	-0.27767500
H	5.97471100	-0.70362000	1.03946300
C	6.40474000	0.09216900	-0.92463300
H	5.90548600	0.16638100	-1.90056400
H	6.55981900	1.12434000	-0.58287400
C	7.75846700	-0.60478300	-1.09006200
H	7.63313600	-1.62836100	-1.46102400
H	8.39903900	-0.06979400	-1.79763200
H	8.29178500	-0.66211900	-0.13462600
H	-0.50983900	0.95999900	2.58136500
C	-0.08369400	3.73394100	1.34726600
H	-0.94134900	3.99503000	1.97359100
H	0.38673100	4.63851600	0.95827500
H	0.64113700	3.19748400	1.97040100
C	-0.50097900	2.85866700	0.18256700
N	-1.32557800	1.81453300	0.49627000
O	-0.14041000	3.06557900	-0.97764300

**<sup>3</sup>Co-TS8**

Co	1.82035400	-0.14465600	-0.53188800
C	3.80714000	-0.45071600	0.32931600
C	3.15987300	-1.70745200	0.20231000
C	1.96096600	-1.70682600	1.04794800
C	1.85343900	-0.44535500	1.65176400
C	2.99306600	0.35222700	1.19737900
C	5.10065400	-0.02480700	-0.29800600

H	5.93004600	-0.14124900	0.40911800
H	5.06864100	1.02527500	-0.59981800
H	5.33385100	-0.62003200	-1.18321900
C	3.68303300	-2.89980500	-0.53611900
H	4.30858400	-3.50035900	0.13559800
H	4.29910100	-2.61233100	-1.39048800
H	2.87934300	-3.54959600	-0.89022700
C	1.06280900	-2.88753200	1.26122900
H	1.45986500	-3.52385300	2.06072500
H	0.98562300	-3.51247600	0.36743000
H	0.05543300	-2.58305300	1.55383100
C	0.81395400	0.04844500	2.60962000
H	1.25816800	0.22126700	3.59647800
H	0.00476700	-0.67335500	2.73250600
H	0.38784200	0.99402100	2.26138100
C	3.34151200	1.70260300	1.72797100
H	3.93698600	1.57500700	2.64127500
H	2.45179100	2.27615400	1.99258300
H	3.94319100	2.27760000	1.02183500
C	1.40712700	-1.14599900	-2.42195800
H	1.66904500	-0.33400800	-3.09426400
H	1.90238200	-2.09621200	-2.58070800
C	0.29113200	-1.06593000	-1.59686900
H	-0.05047400	-1.94586800	-1.05649000
C	-0.37436400	0.17939200	-1.30858700
C	-1.45630500	0.25147500	-0.28665600
H	-1.44592100	1.23948400	0.17813400
H	-1.28388300	-0.48911800	0.50206000
C	-2.83287400	0.00002800	-0.95644400
H	-2.99239600	0.74406200	-1.74713400
H	-2.83534400	-0.98321200	-1.44514600
C	-3.97732900	0.07484000	0.06286900
H	-3.96077900	1.05831100	0.55111600
H	-3.80680500	-0.66670200	0.85577300
C	-5.35225100	-0.16238900	-0.57256800
H	-5.51845800	0.57985800	-1.36554500
H	-5.36159900	-1.14452900	-1.06584300
C	-6.50111000	-0.09066600	0.44042200
H	-6.48932700	0.89096000	0.93479100
H	-6.33409900	-0.83312600	1.23386200
C	-7.87893500	-0.32431700	-0.19098700
H	-8.04308600	0.41845600	-0.98326200
H	-7.88764500	-1.30489300	-0.68598700
C	-9.02014700	-0.25131000	0.82791000

H	-9.05307100	0.73037400	1.31378600
H	-9.99119600	-0.42069700	0.35273100
H	-8.89691700	-1.00544900	1.61350000
H	-0.39261100	0.92084000	-2.09992900
C	1.91964400	3.88491500	-0.71830600
H	1.89522000	4.62491400	0.08360000
H	1.45312200	4.31443600	-1.61181100
H	2.94989200	3.62884300	-0.97812200
C	1.12567600	2.66386400	-0.29059100
N	1.45734500	1.52123100	-0.99656100
O	0.25743500	2.71365700	0.57911100

**<sup>3</sup>Co-9**

Co	1.74113000	-0.05307900	-0.32868800
C	3.89137200	-0.36233300	0.15441000
C	3.22123100	-1.62241100	-0.19271700
C	2.21566200	-1.88861300	0.78048800
C	2.18941700	-0.77271200	1.67670100
C	3.26309700	0.15903100	1.29570400
C	5.08388900	0.20090000	-0.55793700
H	6.00368500	-0.25210000	-0.16938400
H	5.16348500	1.28084900	-0.41875600
H	5.05433500	-0.00266000	-1.63098600
C	3.62810300	-2.52409900	-1.31574200
H	4.44012400	-3.18372700	-0.98537400
H	4.00062600	-1.96286300	-2.17584400
H	2.80494000	-3.16059300	-1.64760200
C	1.32374600	-3.09393900	0.85039000
H	1.73226900	-3.83027600	1.55209200
H	1.22812600	-3.58502100	-0.12051400
H	0.32113900	-2.83192100	1.19751000
C	1.33600200	-0.61987200	2.88830700
H	1.93299300	-0.86685200	3.77664700
H	0.47555900	-1.29072700	2.86760300
H	0.98841200	0.40983700	2.98148100
C	3.60968200	1.39328900	2.06145400
H	3.99045300	1.11946400	3.05283200
H	2.72105700	2.01367700	2.20600500
H	4.37977500	1.97933100	1.55717200
C	2.16077700	0.76389200	-2.47404400
H	2.40789200	1.76430100	-2.12602900
H	2.93412400	0.22480500	-3.01085900
C	0.90005600	0.26210300	-2.37931300
H	0.67642800	-0.69236500	-2.85592500

C	-0.23630600	0.97383600	-1.62475100
C	-1.48185900	0.06593800	-1.60483500
H	-1.18452600	-0.89606900	-1.15965200
H	-1.76437900	-0.14421200	-2.64537300
C	-2.68803300	0.61858500	-0.84617600
H	-2.39612200	0.85109700	0.18599000
H	-3.00915800	1.56257800	-1.30718400
C	-3.87030500	-0.35826700	-0.82607900
H	-3.55049100	-1.30421400	-0.36584400
H	-4.15915300	-0.60259400	-1.85766100
C	-5.08726700	0.18870300	-0.07154900
H	-4.79468400	0.43604900	0.95888400
H	-5.40473600	1.13424200	-0.53324800
C	-6.27026600	-0.78551300	-0.04474800
H	-5.95273000	-1.73136900	0.41734700
H	-6.56028900	-1.03369900	-1.07564100
C	-7.48978000	-0.23874500	0.70695600
H	-7.19780900	0.00948600	1.73647000
H	-7.80491800	0.70602800	0.24376200
C	-8.66601600	-1.21949600	0.72732300
H	-8.38666500	-2.16092300	1.21399700
H	-9.52241800	-0.80587300	1.26860700
H	-8.99778700	-1.45864900	-0.28937500
H	-0.47133000	1.92738300	-2.11579300
C	-0.71911800	3.39834800	0.04642400
H	-1.72682900	3.09732400	-0.24537100
H	-0.24087200	3.85193200	-0.82899100
H	-0.78053500	4.13986500	0.84209800
C	0.10306800	2.22815900	0.56159200
N	0.35478000	1.16687000	-0.29045000
O	0.58164500	2.24409900	1.69293500

**<sup>5</sup>Co-1**

Co	0.57227400	0.03248800	-0.04671100
C	-1.41531600	0.50484700	1.12296500
C	-1.45264400	-0.93706600	0.80000800
C	-1.44774000	-1.06785300	-0.59520500
C	-1.42163500	0.28378100	-1.17102900
C	-1.35626400	1.23899100	-0.09646900
C	-1.47854100	1.06178100	2.50388900
H	-2.52268000	1.07245000	2.84682000
H	-1.10831700	2.08743500	2.55061700
H	-0.91955600	0.44950200	3.21721900
C	-1.51614000	-2.02047400	1.82784700

H	-2.49955900	-2.02057700	2.31433700
H	-0.77100100	-1.87457200	2.61648200
H	-1.35858900	-3.00668600	1.38974500
C	-1.51752400	-2.32697000	-1.40366600
H	-2.51510900	-2.43974500	-1.84477100
H	-1.31886900	-3.20971700	-0.79447400
H	-0.79858200	-2.31905800	-2.22848500
C	-1.51824000	0.59453300	-2.62569000
H	-2.57684500	0.62608300	-2.92052300
H	-1.04047100	-0.17195100	-3.24125800
H	-1.08668700	1.56797300	-2.86789300
C	-1.37430500	2.73384300	-0.24396900
H	-2.40466500	3.09959000	-0.31838900
H	-0.84245000	3.05583100	-1.14219100
H	-0.90670500	3.22676300	0.61085500
O	2.27656400	1.06943900	0.00266600
O	2.20638000	-1.10910400	-0.00084400
C	2.92204700	-0.04148600	0.02005500
C	4.41272000	-0.08985200	0.03205600
H	4.75648100	-0.99775600	0.52939600
H	4.76418500	-0.11338500	-1.00600600
H	4.81596800	0.80350600	0.51039700

**<sup>5</sup>Co-2**

Co	-1.53492900	0.28966700	0.24658900
C	-1.62686800	-1.95580100	-0.62617500
C	-1.25382700	-0.95482000	-1.59810400
C	-2.41727600	-0.18059200	-1.86560000
C	-3.49316300	-0.64587000	-0.98280500
C	-3.00160900	-1.72464300	-0.23075200
C	-0.77295700	-3.09680400	-0.18629800
H	-0.87328100	-3.92518100	-0.90091600
H	-1.06992200	-3.48286000	0.79163700
H	0.28516200	-2.82836300	-0.15410500
C	0.05915700	-0.87782000	-2.32487600
H	0.03500700	-1.48657700	-3.23600200
H	0.88295700	-1.24139100	-1.70608000
H	0.29358400	0.14949800	-2.61281100
C	-2.56663900	0.92562800	-2.85306900
H	-3.20784800	0.60315500	-3.68335200
H	-1.60661500	1.23365300	-3.27037400
H	-3.04830600	1.79185700	-2.38937000
C	-4.84435800	-0.01521300	-0.93695800
H	-5.33355800	-0.08456100	-1.91568600

H	-4.75571000	1.04860500	-0.69109400
H	-5.49572900	-0.48886800	-0.20111600
C	-3.74853200	-2.55003600	0.77161800
H	-4.02347200	-3.52207400	0.34558200
H	-4.66951100	-2.06021300	1.09340400
H	-3.14596600	-2.75454200	1.66257900
O	-0.43053700	1.93184300	0.13481900
O	-2.61652600	2.13349600	0.16335300
C	-1.47830900	2.69224800	0.11422200
C	-1.31563700	4.17839500	0.04010900
H	-2.28534500	4.67404300	0.01086500
H	-0.74374800	4.51941200	0.90848700
H	-0.73045200	4.43202000	-0.84876900
C	-2.15045800	0.11554600	2.53336700
H	-2.14757900	1.18579400	2.72776900
H	-3.12137400	-0.36714800	2.48587600
C	-0.99883000	-0.59906200	2.49582900
H	-1.06804800	-1.68047600	2.37654900
C	0.38885600	-0.04342100	2.65570600
H	0.35596300	1.05101000	2.64211700
H	0.76469500	-0.34795500	3.64218100
C	1.35230100	-0.55812000	1.57051100
H	0.94080700	-0.32920300	0.57392800
H	1.41982900	-1.65225600	1.63416500
C	2.75076500	0.05792200	1.65347400
H	2.66389200	1.15117500	1.60302700
H	3.19110900	-0.17590100	2.63218700
C	3.67758600	-0.43445200	0.53636700
H	3.22461100	-0.19660900	-0.43800400
H	3.75323300	-1.53047600	0.58120500
C	5.08277700	0.17426100	0.60068500
H	5.00469700	1.26976500	0.56095400
H	5.53586200	-0.06401600	1.57296200
C	6.00461100	-0.31176500	-0.52323300
H	5.54963500	-0.07377500	-1.49584700
H	6.08067200	-1.40791500	-0.48346400
C	7.41112300	0.29565800	-0.46067300
H	7.33314200	1.39064800	-0.49910400
H	7.86376300	0.05679800	0.51108400
C	8.32360500	-0.19576700	-1.58834900
H	7.90962700	0.05904900	-2.57071600
H	9.31987300	0.25180600	-1.52058600
H	8.44403000	-1.28447700	-1.55240100



**<sup>5</sup>Co-TS3**

Co	2. 22785600	0. 14694600	-0. 70448600
C	3. 37695200	-1. 57700500	0. 75431300
C	2. 37620100	-0. 89796000	1. 54936700
C	2. 65999800	0. 51671000	1. 53703800
C	3. 82788900	0. 71120100	0. 76450900
C	4. 26605600	-0. 60691100	0. 26081000
C	3. 42858900	-3. 05571000	0. 52955900
H	3. 72508300	-3. 57683700	1. 44730400
H	4. 14726600	-3. 32352200	-0. 24689100
H	2. 45289000	-3. 45772600	0. 23688800
C	1. 24802000	-1. 53690700	2. 28606000
H	0. 31939600	-0. 96872800	2. 16840500
H	1. 46670800	-1. 56217900	3. 36212900
H	1. 07503300	-2. 56548800	1. 96371400
C	1. 89236100	1. 55588000	2. 29906800
H	2. 07913900	2. 55740200	1. 90579000
H	2. 18772800	1. 55581500	3. 35464600
H	0. 81602200	1. 37156800	2. 25479700
C	4. 56707500	1. 99389800	0. 54890800
H	3. 91763000	2. 86045200	0. 68436400
H	5. 00393200	2. 04855900	-0. 45205000
H	5. 39330300	2. 07746100	1. 26661600
C	5. 49522000	-0. 82456400	-0. 56328500
H	6. 39074300	-0. 77570700	0. 06936300
H	5. 60894200	-0. 05567800	-1. 33341500
H	5. 48973400	-1. 79917400	-1. 05451600
O	-0. 56004000	1. 44581400	-0. 13271000
O	1. 42524000	1. 88403100	-1. 08754200
C	0. 31021000	2. 25930100	-0. 58776200
C	-0. 00642100	3. 72616800	-0. 55070300
H	0. 90765200	4. 32008000	-0. 56181400
H	-0. 59120600	3. 97058800	-1. 44514700
H	-0. 62108900	3. 95871100	0. 32042600
C	1. 65252400	-1. 36580200	-2. 02771800
H	1. 58868700	-0. 84417300	-2. 98596700
H	2. 39870400	-2. 15533500	-1. 98970600
C	0. 45207200	-1. 56157800	-1. 30456000
H	0. 49163700	-2. 28762400	-0. 48947300
C	-0. 74825100	-0. 83326700	-1. 42680300
H	-0. 51381100	0. 31492800	-0. 66208400
H	-0. 87599600	-0. 31510700	-2. 38393900
C	-2. 03406500	-1. 36867400	-0. 79850300
H	-1. 82829900	-1. 69457400	0. 23115300

H	-2.34554900	-2.27024600	-1.34530500
C	-3.19271800	-0.36282700	-0.80246000
H	-2.90607400	0.53509100	-0.24192700
H	-3.37754400	-0.03499800	-1.83508000
C	-4.48311500	-0.94514600	-0.21564800
H	-4.29409700	-1.28244200	0.81367100
H	-4.77003100	-1.84236000	-0.78173300
C	-5.64823600	0.05093900	-0.21656800
H	-5.35835100	0.94910400	0.34749900
H	-5.83757200	0.38657500	-1.24600400
C	-6.93919700	-0.52570100	0.37508600
H	-6.74907300	-0.86297000	1.40420900
H	-7.22854500	-1.42354900	-0.18936800
C	-8.10557500	0.46960200	0.37589300
H	-7.81428500	1.36658500	0.93948700
H	-8.29436100	0.80487900	-0.65299200
C	-9.38984000	-0.11686700	0.96976600
H	-9.23656900	-0.43087800	2.00857400
H	-10.20596400	0.61225300	0.95884400
H	-9.72001200	-0.99574000	0.40447900

**<sup>5</sup>Co-4**

Co	-2.56638800	0.69007800	-0.32297400
C	-2.82585100	-0.74031500	1.38517600
C	-1.51923800	-0.97085900	0.84315400
C	-1.66751000	-1.33518300	-0.53310700
C	-3.07764600	-1.34275400	-0.84583500
C	-3.79375900	-0.97677800	0.34573300
C	-3.13578500	-0.37652200	2.80703800
H	-3.25530700	-1.28276200	3.41352100
H	-4.06540700	0.19196700	2.88988200
H	-2.33481900	0.21235500	3.26154200
C	-0.23161400	-0.89084700	1.60747600
H	0.61734600	-0.68652000	0.95295500
H	-0.03026100	-1.84049400	2.11756500
H	-0.26197500	-0.11350900	2.37585400
C	-0.56478300	-1.72645700	-1.47183800
H	-0.81705800	-1.50335800	-2.51153600
H	-0.37478500	-2.80482300	-1.40852300
H	0.37156600	-1.21667800	-1.23474800
C	-3.69036300	-1.78486200	-2.14378600
H	-3.04449200	-1.56238600	-2.99676600
H	-4.65797500	-1.30876800	-2.31954100
H	-3.85640100	-2.86881000	-2.13448500

C	-5.28678700	-0.95083000	0.50606000
H	-5.65184900	-1.93660600	0.81823300
H	-5.79216900	-0.69797800	-0.42918500
H	-5.60299400	-0.23176400	1.26578500
C	-2.17626700	2.69016800	-0.65015800
H	-2.16765100	2.83700500	-1.73193000
H	-2.98917900	3.18688400	-0.11753200
C	-0.94307300	2.48886400	0.02549400
H	-0.94037100	2.57462400	1.11224500
C	0.27587900	2.24037500	-0.60326400
H	0.28593500	2.18853800	-1.69290800
C	1.58074300	2.10670900	0.10099000
H	1.41902300	1.88576100	1.16352100
H	2.08081300	3.09006400	0.07195400
C	2.53209100	1.07507300	-0.53558900
H	2.04971800	0.08903400	-0.54967300
H	2.70598600	1.34486600	-1.58552500
C	3.87065200	0.97377200	0.20309700
H	3.68671100	0.71456800	1.25526900
H	4.35437300	1.96008300	0.21154200
C	4.81948500	-0.05760900	-0.41798500
H	4.33071300	-1.04262100	-0.42726200
H	5.00035500	0.20282400	-1.47020200
C	6.16016000	-0.16313100	0.31789800
H	5.97827600	-0.42187000	1.37080300
H	6.64780400	0.82179900	0.32701600
C	7.11149900	-1.19427800	-0.30100200
H	6.62181400	-2.17771000	-0.31002500
H	7.29101900	-0.93365500	-1.35281700
C	8.44797200	-1.29112300	0.44081100
H	8.29872100	-1.58120600	1.48702900
H	9.10789900	-2.03251200	-0.01987600
H	8.97226800	-0.32893000	0.43593400

**<sup>5</sup>Co-5**

Co	-1.44256600	-0.36729900	0.28467300
C	-2.11050000	-2.43623200	-0.29042500
C	-0.69795600	-2.27073900	-0.49130900
C	-0.51594000	-1.26997000	-1.50812200
C	-1.81219800	-0.82555800	-1.92848500
C	-2.79534600	-1.53570600	-1.16892700
C	-2.76626800	-3.43031500	0.62266900
H	-2.93607300	-4.38169300	0.10433900
H	-3.74110400	-3.07916300	0.97316200

H	-2.15179500	-3.65246400	1.49980400
C	0.38826500	-3.09274100	0.14348800
H	0.10067700	-3.45013400	1.13611400
H	1.31791900	-2.52785700	0.24960000
H	0.61045100	-3.97793400	-0.46379300
C	0.78324400	-0.83273500	-2.12241500
H	0.89303200	-1.25104800	-3.13005200
H	1.64156400	-1.16581900	-1.53641400
H	0.84665200	0.25657000	-2.21722100
C	-2.04937400	0.17689000	-3.02001200
H	-1.82868200	-0.25885700	-4.00135500
H	-1.40025900	1.05373000	-2.91365500
H	-3.08614300	0.51985800	-3.04723800
C	-4.28865500	-1.43493700	-1.30271000
H	-4.69110700	-2.30453800	-1.83524200
H	-4.59238100	-0.54917600	-1.86658000
H	-4.78641000	-1.40190200	-0.32758500
C	-2.51174700	-0.37087700	2.54438700
H	-2.78567400	0.67550200	2.64863800
H	-3.30994000	-1.10027600	2.48303300
C	-1.17664200	-0.77469900	2.64184700
H	-0.97166600	-1.84419500	2.60679800
C	-0.07782200	0.07582100	2.83282800
C	1.33852700	-0.38260800	2.78970100
H	1.38355800	-1.47772100	2.81535100
H	1.88335600	-0.01359600	3.66863800
C	2.05192200	0.13632200	1.51581900
H	1.45079700	-0.13273400	0.63453600
H	2.08120800	1.23181100	1.53780200
C	3.46849200	-0.42520100	1.35749800
H	3.42192600	-1.52211400	1.29974100
H	4.05148400	-0.19328900	2.25875800
C	4.19307200	0.12466900	0.12347900
H	3.59765700	-0.08796600	-0.77631900
H	4.25101800	1.21958600	0.19576700
C	5.60238300	-0.45053500	-0.05676100
H	5.54246300	-1.54625000	-0.12431600
H	6.19999200	-0.23379200	0.83954500
C	6.32539800	0.09563600	-1.29377700
H	5.72456200	-0.12100200	-2.18804400
H	6.38348900	1.19021600	-1.22352600
C	7.73223700	-0.48489600	-1.46576500
H	7.69947500	-1.57539600	-1.56917500
H	8.22579100	-0.08011400	-2.35455700

H	8.36235500	-0.25363600	-0.59975300
H	-0.26162300	1.14592000	2.92024700
C	-3.56345600	2.46001700	-0.74997000
H	-4.21520700	3.05477300	-0.10243600
H	-3.84474400	1.40790000	-0.69555000
H	-3.68053900	2.82313700	-1.77492400
C	-2.15818800	2.62452600	-0.32291600
O	-1.58324400	3.83669200	-0.33620000
N	-1.36301900	1.69528000	0.10197300
O	-0.13708400	2.33640500	0.40357900
C	-0.27212300	3.67540000	0.12861000
O	0.54287600	4.51997500	0.25805700

**<sup>5</sup>Co-7**

Co	1.89819100	0.34002400	0.18934700
C	3.27965900	-1.35158500	-0.16070100
C	2.86737900	-0.74937900	-1.41406700
C	1.44103200	-0.96298100	-1.58301000
C	0.97374200	-1.62383200	-0.43157900
C	2.12355500	-1.86531500	0.46189100
C	4.68831200	-1.40789600	0.35394800
H	5.23091100	-2.24231100	-0.10537600
H	4.71367000	-1.55127000	1.43583900
H	5.24173400	-0.49339800	0.12324400
C	3.79024100	-0.20423700	-2.45720000
H	4.06519600	-1.00419200	-3.15590500
H	4.71586900	0.18026500	-2.02365400
H	3.32396100	0.58982500	-3.04608100
C	0.62740900	-0.59982000	-2.79080200
H	0.48697000	-1.47538700	-3.43483200
H	1.11566000	0.16736100	-3.39584100
H	-0.36496000	-0.23416400	-2.51351100
C	-0.41024100	-2.11282800	-0.15950000
H	-0.42149400	-3.20966700	-0.18682700
H	-1.12118000	-1.75291700	-0.90491700
H	-0.74277400	-1.80342000	0.83488400
C	2.02883400	-2.61191200	1.75097400
H	1.91675600	-3.68395600	1.54411000
H	1.15674600	-2.28780700	2.32331900
H	2.92334900	-2.48264400	2.36259200
C	2.61441500	2.28081100	-0.44393400
H	2.81434700	2.71708700	0.53425900
H	3.47031100	2.13893000	-1.09477900
C	1.32792700	2.39640500	-1.00389200

H	1.19841200	2.09746500	-2.04249800
C	0.19046200	2.83083900	-0.31877600
C	-1.18857100	2.71493000	-0.85491300
H	-1.16946700	2.56265600	-1.94042200
H	-1.75312600	3.63475000	-0.65711900
C	-1.93120000	1.52491200	-0.18243700
H	-1.32480700	0.62008000	-0.30440600
H	-1.99442600	1.70179000	0.89803500
C	-3.33298000	1.29856600	-0.75472700
H	-3.26366100	1.14005700	-1.84014300
H	-3.93728200	2.20464300	-0.61570800
C	-4.03926000	0.10152500	-0.10609700
H	-3.42745200	-0.80158900	-0.24646500
H	-4.09905300	0.25881900	0.97969800
C	-5.44491200	-0.14625600	-0.66512900
H	-5.38349500	-0.29750000	-1.75232400
H	-6.05774600	0.75392500	-0.51792600
C	-6.14684300	-1.34933500	-0.02368900
H	-5.53125600	-2.24745400	-0.17143400
H	-6.20543000	-1.19582000	1.06226100
C	-7.55080900	-1.58867600	-0.58706400
H	-7.51676200	-1.77582700	-1.66631300
H	-8.02934700	-2.45144000	-0.11379000
H	-8.19517900	-0.71788400	-0.42259200
H	0.31644700	3.18742400	0.70140200
C	-0.24674600	1.66268300	3.57743900
H	0.66528900	2.17447700	3.89829200
H	-0.79149400	1.28683500	4.44509000
H	-0.87440700	2.39112800	3.05178600
C	0.07376800	0.50873000	2.65628300
N	0.95110100	0.73697500	1.64576200
O	-0.43384000	-0.61380800	2.76840600

**<sup>5</sup>Co-TS8**

Co	2.05288600	-0.12791200	-0.46548400
C	3.92091100	0.79296400	0.26977600
C	3.87551300	-0.61366400	0.58891000
C	2.77671700	-0.83202400	1.51264900
C	2.13606100	0.41306800	1.72286000
C	2.85305600	1.42591200	0.96019500
C	4.95425400	1.45869600	-0.59241300
H	4.56770300	2.36839100	-1.05745000
H	5.30500100	0.79656500	-1.38833900
H	5.82870700	1.74046800	0.00600500

C	4.91377600	-1.62516700	0.20930400
H	5.74968100	-1.58420800	0.91845600
H	5.32386800	-1.43709300	-0.78600700
H	4.52223100	-2.64509700	0.23475300
C	2.42505200	-2.14415400	2.14889400
H	3.00669100	-2.29788300	3.06528900
H	2.64196600	-2.98823100	1.48794900
H	1.36803800	-2.18955000	2.42258400
C	0.94516300	0.70186300	2.58330300
H	1.25297500	1.23702400	3.48961400
H	0.43983700	-0.21406300	2.89677600
H	0.22866100	1.33162900	2.04907000
C	2.51417800	2.88146300	0.97014500
H	2.79817400	3.32033200	1.93483700
H	1.43968500	3.03929100	0.84291200
H	3.04447300	3.42893700	0.18867300
C	2.04588200	-1.89494400	-1.79011900
H	2.04466300	-1.36768600	-2.74451800
H	2.92603600	-2.48905200	-1.57150000
C	0.84485300	-2.15316900	-1.13370700
H	0.85753900	-2.79209800	-0.25273700
C	-0.37715100	-1.48312300	-1.43413000
C	-1.60781400	-1.72311700	-0.62646300
H	-1.33823400	-1.84897000	0.42961800
H	-1.99026600	-2.70668000	-0.95455200
C	-2.72581900	-0.68480400	-0.78108800
H	-2.37889200	0.27827300	-0.39166300
H	-2.94470000	-0.54225900	-1.84831000
C	-4.01019700	-1.08942200	-0.04899800
H	-3.78437400	-1.25429300	1.01382800
H	-4.36722700	-2.05210900	-0.44025900
C	-5.12059700	-0.04038900	-0.17624900
H	-4.75706400	0.92127300	0.21273500
H	-5.34340900	0.12468700	-1.23998100
C	-6.40805900	-0.43230100	0.55742100
H	-6.18445000	-0.59769400	1.62097800
H	-6.76946400	-1.39517300	0.16936900
C	-7.52043700	0.61541000	0.43017100
H	-7.15646200	1.57687700	0.81720700
H	-7.74184200	0.77908000	-0.63322900
C	-8.80202600	0.21523400	1.16715600
H	-8.61452300	0.07649500	2.23793400
H	-9.57900600	0.97841800	1.06098900
H	-9.20386600	-0.72663600	0.77691000

H	-0.50147900	-1.09359800	-2.44240800
C	-0.86846000	2.03206300	-2.51704200
H	-1.66535200	1.33449400	-2.79579900
H	-0.07857200	1.96061400	-3.27101100
H	-1.27603700	3.04395900	-2.49372800
C	-0.34359100	1.67712900	-1.14918200
N	0.41400100	0.52912600	-1.02385500
O	-0.56553100	2.33126900	-0.13228700

**<sup>5</sup>Co-9**

Co	1.51985700	0.06018400	0.00300400
C	3.61695800	-0.66382900	-0.60075200
C	2.58937700	-1.13550200	-1.51557900
C	1.73028000	-2.05679000	-0.80472200
C	2.27429300	-2.22287700	0.49505000
C	3.44552200	-1.34935700	0.62011800
C	4.71647400	0.29291000	-0.96162800
H	5.52277500	-0.22791400	-1.49116200
H	5.14796600	0.76025400	-0.07433400
H	4.35739400	1.08988400	-1.61851500
C	2.48069500	-0.75696700	-2.95727200
H	3.17052700	-1.37225600	-3.55084200
H	2.75697500	0.28747600	-3.12639000
H	1.47563100	-0.92184600	-3.35082900
C	0.56724800	-2.80526600	-1.39278900
H	0.90623700	-3.72704800	-1.87941900
H	0.04334500	-2.21180500	-2.14633400
H	-0.15840500	-3.08157000	-0.62483000
C	1.74337300	-3.04818900	1.61368600
H	2.51850200	-3.72287900	1.99521000
H	0.88336800	-3.64828400	1.31426600
H	1.44700000	-2.39592000	2.44450400
C	4.21971100	-1.19441700	1.88282300
H	4.58580300	-2.16658400	2.23200700
H	3.56789000	-0.79196100	2.66770500
H	5.07593600	-0.52945100	1.76386300
C	1.92633400	3.23919600	-1.17551000
H	2.49816700	2.63175700	-0.47693000
H	2.49487300	3.80500700	-1.90634300
C	0.59686400	3.33638600	-1.10416300
H	0.07387200	4.00143900	-1.78955400
C	-0.30572300	2.60086300	-0.13549000
C	-1.53917100	2.02128400	-0.86374800
H	-1.18284700	1.29594300	-1.61011900



H	-2.02537200	2.82957800	-1.42320700
C	-2.55336900	1.35549700	0.06996200
H	-2.05611300	0.56393700	0.64769200
H	-2.91245000	2.09463300	0.80036600
C	-3.75095100	0.75397300	-0.67434600
H	-3.38826100	0.02361500	-1.41219900
H	-4.25551400	1.54184900	-1.24980200
C	-4.76143200	0.07590300	0.25770300
H	-4.25220500	-0.70855100	0.83676900
H	-5.12487800	0.80802100	0.99245500
C	-5.95574400	-0.53505300	-0.48362200
H	-5.59198900	-1.26612900	-1.22013900
H	-6.46433500	0.24948100	-1.06141700
C	-6.96677700	-1.21431400	0.44784100
H	-6.45626100	-1.99684300	1.02602500
H	-7.32951800	-0.48188500	1.18157800
C	-8.15513900	-1.82177100	-0.30360300
H	-7.82239500	-2.57994600	-1.02171800
H	-8.86087000	-2.29963200	0.38278700
H	-8.70167900	-1.05427700	-0.86305000
H	-0.66332400	3.32105000	0.61569000
C	-0.13042400	2.04673300	2.92633600
H	-1.21971500	1.99347200	2.83272300
H	0.15761800	3.10071400	2.86405800
H	0.17300000	1.64040900	3.89070900
C	0.51218500	1.26063400	1.82499300
N	0.42216800	1.52959700	0.52656900
O	1.22680400	0.21747900	2.08123400

**[Cp\*RhCl<sub>2</sub>]<sub>2</sub>**

Cl	0.00002500	0.00018200	-1.72643100
Cl	-0.00002400	-0.00013100	1.72644200
Cl	-1.49722500	2.63122000	0.00017900
Cl	1.49716700	-2.63120400	-0.00022500
C	2.77234700	1.56721500	0.71230300
C	2.77235800	1.56735800	-0.71191600
C	3.47360900	0.37058900	-1.16689500
C	3.47358900	0.37035600	1.16705300
C	3.94693300	-0.33256200	0.00001300
C	-3.47357000	-0.37066000	1.16692400
C	-3.94694000	0.33252600	0.00005900
C	-3.47361000	-0.37033700	-1.16702300
C	-2.77230100	-1.56739500	0.71187900
C	-2.77233500	-1.56720000	-0.71233900

C	-2.13687300	-2.61399500	-1.57231800
H	-1.15940200	-2.89918500	-1.17346600
H	-2.77854000	-3.50321900	-1.61004300
H	-1.98381000	-2.25211400	-2.58935000
C	-2.13679900	-2.61442400	1.57154400
H	-2.77844200	-3.50367500	1.60902900
H	-1.15932800	-2.89947300	1.17259200
H	-1.98372200	-2.25283200	2.58867600
C	-3.72016500	0.00125400	2.59554700
H	-4.58955100	-0.53856800	2.99101600
H	-2.85303200	-0.24627100	3.21189200
H	-3.90504600	1.07229200	2.69498000
C	-4.75631100	1.58966100	0.00018400
H	-5.82513200	1.34248000	-0.00063700
H	-4.53572100	2.19747400	0.87846600
H	-4.53454900	2.19835400	-0.87719800
C	-3.72031600	0.00198500	-2.59552000
H	-4.58973000	-0.53773000	-2.99107400
H	-3.90522700	1.07305000	-2.69462000
H	-2.85323400	-0.24535200	-3.21201100
C	2.13688200	2.61405600	1.57222500
H	2.77856200	3.50327200	1.60992900
H	1.15942500	2.89924500	1.17334000
H	1.98379000	2.25221900	2.58926700
C	3.72023100	-0.00191100	2.59557500
H	4.58963400	0.53781100	2.99114400
H	2.85312400	0.24546300	3.21201700
H	3.90512100	-1.07297400	2.69473100
C	2.13690100	2.61436800	-1.57163700
H	1.15942700	2.89945600	-1.17271900
H	2.77856600	3.50360300	-1.60913800
H	1.98384200	2.25274100	-2.58875900
C	3.72025400	-0.00139000	-2.59549200
H	2.85316100	0.24614200	-3.21188900
H	4.58968000	0.53838300	-2.99094100
H	3.90510300	-1.07243900	-2.69487000
C	4.75627700	-1.58971500	-0.00008300
H	4.53485600	-2.19817000	0.87754900
H	4.53531900	-2.19775700	-0.87811600
H	5.82510300	-1.34255700	0.00025100
Rh	-1.77686200	0.24601100	-0.00000400
Rh	1.77685700	-0.24599900	0.00000500

**Rh-1**

C	1.60483000	0.73384300	-0.79330100
C	1.60473500	-0.73425700	-0.79298500
C	1.34820300	-1.18208500	0.53420500
C	1.14591200	0.00025600	1.36010800
C	1.34833200	1.18222100	0.53369900
C	1.85480300	1.58538700	-1.99438600
H	2.93588600	1.66652400	-2.16368800
H	1.45602200	2.59268000	-1.86699700
H	1.41321700	1.15005000	-2.89388900
C	1.85458200	-1.58640200	-1.99368300
H	2.93563500	-1.66742400	-2.16322200
H	1.41267900	-1.15165500	-2.89331800
H	1.45602600	-2.59369700	-1.86562900
C	1.27608600	-2.59604100	1.01533300
H	2.23065400	-2.87717800	1.47568200
H	1.07649000	-3.28986100	0.19769200
H	0.49167700	-2.72207000	1.76480500
C	0.86935800	0.00066000	2.82454700
H	1.82478900	0.00077100	3.36619100
H	0.31306300	-0.88717800	3.13038700
H	0.31313400	0.88871700	3.12988100
C	1.27642800	2.59637700	1.01428200
H	2.23059200	2.87710300	1.47571600
H	0.49117700	2.72309200	1.76276600
H	1.07823200	3.29004700	0.19618100
O	-2.14239700	1.09351100	-0.15804500
O	-2.14247900	-1.09346500	-0.15765000
C	-2.81946700	0.00003600	-0.19493600
C	-4.30695900	0.00008700	-0.24776300
H	-4.66734600	-0.90129000	-0.74605400
H	-4.68744600	-0.00013300	0.78065000
H	-4.66731000	0.90166400	-0.74570900
Rh	-0.34887200	-0.00002300	-0.15570200

## Rh-2

C	1.54305200	-1.98352200	0.21565800
C	1.34078300	-1.28998300	1.46041300
C	2.53110100	-0.54155800	1.75942400
C	3.50273000	-0.81760400	0.70925100
C	2.89272000	-1.69695300	-0.24185200
C	0.60168700	-2.97796100	-0.38867900
H	0.72339600	-3.94455100	0.11489800
H	0.80090800	-3.13679600	-1.44987300
H	-0.43868700	-2.66953400	-0.27694100

C	0.09108000	-1.31135000	2.27869900
H	0.17355900	-2.08237300	3.05434400
H	-0.78405400	-1.53982000	1.66811900
H	-0.07752000	-0.35234100	2.77236500
C	2.78221800	0.30011700	2.97085000
H	3.30315800	-0.28716200	3.73605700
H	1.84873800	0.66341700	3.40454400
H	3.40521000	1.16308600	2.72617600
C	4.88512100	-0.25183000	0.66542300
H	5.51197500	-0.75713700	1.40971800
H	4.87687200	0.81520800	0.90280200
H	5.34858000	-0.38262600	-0.31315500
C	3.54096000	-2.29320000	-1.45207300
H	3.91777500	-3.29465900	-1.21427300
H	4.38401900	-1.69228200	-1.79705300
H	2.83434800	-2.39728400	-2.27899200
O	0.31544600	1.69905700	0.33061400
O	2.40920000	2.23545500	0.08596200
C	1.21334700	2.61007400	0.33774900
C	0.87188700	4.04468000	0.58462100
H	1.74159300	4.58173000	0.96602700
H	0.56951200	4.50366600	-0.36332000
H	0.03327200	4.11809100	1.27947900
C	1.86914900	0.71139300	-2.36486000
H	1.85338400	1.79710600	-2.39281100
H	2.79494300	0.24045900	-2.68133600
C	0.69605200	-0.00695100	-2.28808100
H	0.74242400	-1.07974900	-2.46968600
C	-0.68770300	0.57803300	-2.27194000
H	-0.64817200	1.63149000	-1.98077200
H	-1.04322700	0.54796400	-3.31355600
C	-1.68285700	-0.18262000	-1.38434000
H	-1.30730700	-0.18280400	-0.35431400
H	-1.73330100	-1.23071300	-1.71175200
C	-3.08854900	0.42444400	-1.40256600
H	-3.02887500	1.47648300	-1.09196700
H	-3.47462200	0.42697500	-2.43106400
C	-4.06759800	-0.32079900	-0.48862400
H	-3.67277900	-0.32186600	0.53843800
H	-4.12299300	-1.37491700	-0.79664500
C	-5.47717300	0.28120200	-0.48650200
H	-5.42000900	1.33589700	-0.18241000
H	-5.87207100	0.28144900	-1.51201700
C	-6.45239500	-0.46123000	0.43376900

H	-6.05577300	-0.46249400	1.45957500
H	-6.50899900	-1.51619600	0.12911100
C	-7.86272000	0.14051900	0.43783700
H	-7.80423800	1.19464100	0.74126700
H	-8.25740100	0.14065800	-0.58713300
C	-8.82843700	-0.60827200	1.36118500
H	-8.47295400	-0.59572500	2.39794900
H	-9.82640000	-0.15941400	1.34587000
H	-8.92979700	-1.65692900	1.05919200
Rh	1.76736900	0.19207100	-0.14470400

**Rh-TS<sub>iso</sub>**

C	2.77076600	-1.85458500	0.29034600
C	1.59377300	-1.74538200	1.09175400
C	1.69635700	-0.51942200	1.87925700
C	2.90856600	0.14158700	1.53277400
C	3.57342500	-0.65497500	0.51215900
C	3.14851600	-3.00197100	-0.59061900
H	3.73617800	-3.72431500	-0.01165700
H	3.76165900	-2.67906300	-1.43387200
H	2.27175500	-3.52384300	-0.97869500
C	0.49011000	-2.75081900	1.20373700
H	0.65095400	-3.38801400	2.08118800
H	0.44416200	-3.39852500	0.32646200
H	-0.48156400	-2.26552700	1.32046700
C	0.68912000	-0.02053500	2.86087300
H	0.49783900	1.04280600	2.70217200
H	1.07494100	-0.15873200	3.87830000
H	-0.25614200	-0.55881000	2.78167900
C	3.40841100	1.42915900	2.10299500
H	2.57886600	2.05893000	2.42683500
H	3.99334800	1.98306900	1.36635700
H	4.05275800	1.22823000	2.96688700
C	4.90870200	-0.35617600	-0.08530900
H	5.70007200	-0.67887200	0.60276100
H	5.02778400	0.71506700	-0.25987600
H	5.05272600	-0.87672200	-1.03333300
O	0.52621200	2.28330600	0.59521800
O	2.09222000	1.89759400	-0.95022300
C	1.34810600	2.70484700	-0.23276200
C	1.57987100	4.17611700	-0.48483800
H	0.81074900	4.76540600	0.01435300
H	2.56452300	4.45895100	-0.09844500
H	1.58149800	4.38143100	-1.55820200

C	1.66811700	-0.40302400	-2.59959300
H	1.76844700	0.62022000	-2.94688900
H	2.42518300	-1.10958700	-2.92632000
C	0.50398100	-0.85813000	-2.01524100
H	0.36323500	-1.93063700	-1.88462400
C	-0.64777400	0.03031200	-1.61610900
H	-0.40769800	0.56665000	-0.65981500
H	-0.75450700	0.85155900	-2.33487300
C	-1.96701300	-0.71960300	-1.39369300
H	-1.79717300	-1.54055800	-0.68274900
H	-2.27323700	-1.18824100	-2.33782700
C	-3.08296200	0.19034500	-0.87157400
H	-2.75645400	0.66159500	0.06668900
H	-3.24427300	1.01085800	-1.58375700
C	-4.40306500	-0.55327900	-0.64042300
H	-4.23701100	-1.37744800	0.06861200
H	-4.72610400	-1.02132800	-1.58064700
C	-5.52095500	0.35319600	-0.11266000
H	-5.19487800	0.82320700	0.82616600
H	-5.68566300	1.17565100	-0.82270300
C	-6.84171800	-0.38844900	0.12148100
H	-6.67629600	-1.21246500	0.83057600
H	-7.16676900	-0.85773300	-0.81797200
C	-7.96119800	0.51674000	0.64929100
H	-7.63438700	0.98536300	1.58762400
H	-8.12468600	1.33897900	-0.06038800
C	-9.27636800	-0.23383000	0.87921800
H	-9.14763800	-1.04143000	1.60892100
H	-10.05787300	0.43364500	1.25522700
H	-9.64124800	-0.68406500	-0.05089700
Rh	1.72086400	-0.04945900	-0.32653500

**Rh-2'**

C	2.67142000	-1.85342800	0.42362700
C	1.36650000	-1.81459300	1.00543300
C	1.26696800	-0.60092800	1.80994200
C	2.49685500	0.11084800	1.70316200
C	3.36789100	-0.63068600	0.80387600
C	3.24598400	-2.95864500	-0.40390800
H	3.76949100	-3.66669100	0.24947900
H	3.96930100	-2.58322400	-1.13017000
H	2.47171300	-3.51166600	-0.93917100
C	0.31435400	-2.87492900	0.90588800
H	0.39382500	-3.56016100	1.75798500

H	0.42119500	-3.46573500	-0.00589900
H	-0.68969900	-2.44588500	0.92002400
C	0.07933700	-0.15558100	2.59904400
H	-0.12676300	0.89932000	2.40324400
H	0.28165500	-0.27969800	3.66952000
H	-0.81142200	-0.73577100	2.35402100
C	2.83428200	1.39406300	2.38928300
H	1.94179700	2.00208900	2.54024800
H	3.55341300	1.97400900	1.80834000
H	3.28316400	1.17884300	3.36635400
C	4.77774900	-0.26727900	0.46705500
H	5.44544800	-0.57719500	1.28027400
H	4.88171600	0.81153600	0.33517200
H	5.11153400	-0.75691300	-0.44920600
O	0.30046100	2.39492600	0.53777900
O	2.03933900	1.91203000	-0.80558100
C	1.23515000	2.75212000	-0.18536600
C	1.57321700	4.20789300	-0.42908800
H	1.76331900	4.38665600	-1.48992200
H	0.76025100	4.84094500	-0.07359300
H	2.49070000	4.45864400	0.11364200
C	2.03170800	-0.28561000	-2.61316800
H	2.17980500	0.76478300	-2.84030800
H	2.82495000	-0.97043600	-2.89759400
C	0.79870400	-0.78494500	-2.24018100
H	0.63500500	-1.86172900	-2.23728900
C	-0.35346900	0.08136300	-1.81990500
H	-0.16148100	0.53756900	-0.77888300
H	-0.40215900	0.99480500	-2.42363300
C	-1.70200200	-0.63475000	-1.69865100
H	-1.55798400	-1.57695300	-1.15291500
H	-2.04137100	-0.91024000	-2.70514400
C	-2.76398000	0.21408300	-0.99240200
H	-2.39240200	0.50453200	0.00108800
H	-2.90745200	1.15174000	-1.54556400
C	-4.10699600	-0.50915000	-0.84646200
H	-3.95473100	-1.45174900	-0.30012900
H	-4.47917900	-0.79137100	-1.84089200
C	-5.16672300	0.33051100	-0.12415200
H	-4.78803200	0.61867300	0.86708400
H	-5.32139600	1.26910500	-0.67416900
C	-6.50810000	-0.39382900	0.03466000
H	-6.35198200	-1.33385300	0.58352700
H	-6.88602300	-0.68101500	-0.95678800

C	-7.56875100	0.44469400	0.75793500
H	-7.18805800	0.73306800	1.74732300
H	-7.72444900	1.38203100	0.20703500
C	-8.90418000	-0.28893100	0.91372200
H	-8.78178900	-1.21396600	1.48868300
H	-9.64284900	0.33029200	1.43188000
H	-9.32171100	-0.55953900	-0.06264800
Rh	1.66041700	-0.07231700	-0.33868100

**Rh-TS3**

C	2.90877000	-1.62098300	0.50984300
C	1.51876800	-2.02456100	0.58418900
C	0.82897400	-1.10391500	1.46105200
C	1.75582400	-0.09225900	1.85324100
C	3.05618000	-0.41296800	1.26574200
C	3.99310800	-2.36609900	-0.20335000
H	4.40343900	-3.13843800	0.45800900
H	4.81090700	-1.70589200	-0.49639500
H	3.61727600	-2.86596500	-1.09884000
C	0.94459300	-3.28630000	0.01697800
H	1.06898400	-4.10627400	0.73416500
H	1.44641600	-3.58034900	-0.90735200
H	-0.12322100	-3.18777900	-0.18785300
C	-0.60467500	-1.20073800	1.87555100
H	-1.00882000	-0.22587400	2.15237400
H	-0.69079600	-1.86204400	2.74628800
H	-1.22864300	-1.61682500	1.08207900
C	1.48478200	1.06640400	2.76046200
H	0.45462400	1.41441200	2.66525000
H	2.15036700	1.90137600	2.53360500
H	1.65509100	0.77523600	3.80343300
C	4.30767700	0.37559700	1.48845300
H	4.65758900	0.23947700	2.51820000
H	4.12484000	1.44121500	1.32819100
H	5.10633600	0.06349300	0.81418200
O	-0.13401200	2.30986400	-0.11633000
O	2.07165100	2.05144700	-0.38282300
C	1.03350900	2.78144500	-0.15001100
C	1.26125200	4.25082400	0.09617200
H	2.29401300	4.53055600	-0.10944800
H	0.57442400	4.83294400	-0.52255500
H	1.02245200	4.46983800	1.14190300
C	2.36321300	0.00553400	-2.47769700
H	2.49570100	1.07221900	-2.62907800



H	3.21030600	-0.62742800	-2.72365600
C	1.09026000	-0.56009200	-2.35511300
H	0.95363100	-1.63259300	-2.48100700
C	-0.05623600	0.24013900	-1.91493000
H	0.06253700	0.98880900	-0.74858500
H	-0.10729800	1.20850000	-2.42545100
C	-1.40061300	-0.46922800	-1.79793400
H	-1.24384300	-1.45045100	-1.33124200
H	-1.76366400	-0.67140300	-2.81507200
C	-2.46788300	0.30848200	-1.01969900
H	-2.09666100	0.53668600	-0.01349000
H	-2.63407400	1.28019300	-1.50156100
C	-3.79151400	-0.45562500	-0.91618400
H	-3.61205400	-1.43284800	-0.44240000
H	-4.16897300	-0.67423900	-1.92455100
C	-4.86181300	0.30186200	-0.12272900
H	-4.47977000	0.51986500	0.88527400
H	-5.04027400	1.27711100	-0.59632300
C	-6.18673700	-0.46039800	-0.01098000
H	-6.00692700	-1.43717300	0.46119500
H	-6.56717900	-0.67686200	-1.01923100
C	-7.25804000	0.29660900	0.78296600
H	-6.87588800	0.51279500	1.79011200
H	-7.43571500	1.27155400	0.30941300
C	-8.57796600	-0.47332100	0.88706300
H	-8.43376600	-1.43888800	1.38516700
H	-9.32465100	0.08773200	1.45732500
H	-8.99715500	-0.67293800	-0.10552800
Rh	1.64846100	-0.02028200	-0.35270700

**Rh-4**

C	-3.06863300	-1.04083600	0.60575000
C	-1.97587600	-0.56894000	1.44964500
C	-0.71089700	-1.10046600	0.92735000
C	-1.00514900	-1.72581500	-0.29755600
C	-2.47034400	-1.68217000	-0.50101000
C	-4.53012200	-0.87504200	0.89099600
H	-4.88216800	-1.69214600	1.53171600
H	-5.12367600	-0.88835000	-0.02496100
H	-4.73389600	0.06347500	1.41115800
C	-2.12559600	0.12461900	2.76376400
H	-2.22858100	-0.62322900	3.56077100
H	-3.01364900	0.75918400	2.78824700
H	-1.24959100	0.73460900	2.99562400

C	0.60490800	-1.00342100	1.63362800
H	0.59130800	-1.63786700	2.52766000
H	0.81506600	0.01824300	1.96116500
H	1.43180200	-1.33012500	1.00260700
C	-0.04993200	-2.41010300	-1.22544500
H	-0.11932000	-3.49763200	-1.10147300
H	0.98247700	-2.11254500	-1.03536100
H	-0.27950300	-2.18826200	-2.27122900
C	-3.16745100	-2.30160300	-1.67045700
H	-3.20489300	-3.39102400	-1.54609500
H	-2.63583400	-2.10278500	-2.60526900
H	-4.19142800	-1.93872000	-1.77216700
C	-2.83087300	2.24748100	-0.67551600
H	-2.91796000	2.26715500	-1.76494200
H	-3.76112300	2.41550200	-0.14180800
C	-1.59229100	2.59513700	-0.07444700
H	-1.56358200	2.93274100	0.96076300
C	-0.39996400	2.16186200	-0.69340500
C	0.97236400	2.29068400	-0.08953900
H	0.90276000	2.16206400	0.99889200
H	1.33994200	3.31422100	-0.25024600
C	1.97397000	1.28996000	-0.68269800
H	1.52090700	0.29075400	-0.67517700
H	2.14689200	1.53544600	-1.73920000
C	3.31070400	1.24746300	0.06298200
H	3.12511000	1.04649400	1.12820300
H	3.78817100	2.23529500	0.01968200
C	4.26881900	0.18689900	-0.49046100
H	3.77971400	-0.79900200	-0.44976500
H	4.45773600	0.38606300	-1.55443200
C	5.60249100	0.11911500	0.26138500
H	5.41045000	-0.07480800	1.32658600
H	6.09393800	1.10090700	0.21595300
C	6.55464700	-0.95113600	-0.28553700
H	6.05954400	-1.93127400	-0.24240700
H	6.74641900	-0.75364500	-1.34879800
C	7.88271900	-1.01165400	0.47492400
H	7.72099200	-1.23908000	1.53474300
H	8.54308400	-1.78212100	0.06548600
H	8.41257200	-0.05421800	0.41938200
H	-0.42155000	2.07032600	-1.78935400
Rh	-1.71118000	0.42560300	-0.40982400

**Rh-5**

C	1. 27954500	-2. 51611400	0. 39546400
C	0. 16174300	-1. 84536800	1. 03987500
C	0. 68917600	-0. 77227500	1. 79477600
C	2. 15747600	-0. 83309900	1. 71263700
C	2. 51318000	-1. 94087900	0. 89922000
C	1. 17247600	-3. 76785900	-0. 42198900
H	1. 17370800	-4. 64590000	0. 23480300
H	2. 01150000	-3. 87301400	-1. 11368300
H	0. 24546900	-3. 79028500	-0. 99959300
C	-1. 26578600	-2. 28740700	0. 96044900
H	-1. 55623300	-2. 55283400	-0. 05806300
H	-1. 95358900	-1. 52053800	1. 31792000
H	-1. 40533700	-3. 17977000	1. 58245900
C	-0. 08140900	0. 19742400	2. 63884900
H	-0. 13989600	-0. 16124200	3. 67327400
H	-1. 09914100	0. 33184900	2. 26780500
H	0. 39718700	1. 17918000	2. 65906100
C	3. 08593600	0. 04970200	2. 48999400
H	3. 15366000	-0. 29486300	3. 52846400
H	2. 72788600	1. 08235900	2. 51749200
H	4. 09467900	0. 04487700	2. 07224600
C	3. 89187800	-2. 45771900	0. 62084300
H	4. 13571200	-3. 27052600	1. 31506200
H	4. 64901400	-1. 68001300	0. 74051600
H	3. 97426900	-2. 85729100	-0. 39267000
C	2. 51094600	-0. 40321400	-2. 19183500
H	2. 72715300	0. 63779500	-2. 41804400
H	3. 36128600	-1. 07474500	-2. 27230200
C	1. 20555700	-0. 91096600	-2. 44792900
H	1. 06321500	-1. 97526500	-2. 62452000
C	0. 08246500	-0. 10001300	-2. 18618600
C	-1. 33805200	-0. 58629700	-2. 25002900
H	-1. 37448600	-1. 66395100	-2. 04672300
H	-1. 70360600	-0. 46005600	-3. 28012700
C	-2. 26681300	0. 17329800	-1. 29097000
H	-1. 82913600	0. 15210600	-0. 28576700
H	-2. 29541100	1. 23213300	-1. 57997700
C	-3. 68985200	-0. 38951200	-1. 24645000
H	-3. 64999200	-1. 46357700	-1. 01351300
H	-4. 14795900	-0. 31285100	-2. 24160400
C	-4. 57697600	0. 31613600	-0. 21492600
H	-4. 10832600	0. 23773400	0. 77829700
H	-4. 61888200	1. 38994600	-0. 44419600
C	-6. 00012000	-0. 24825000	-0. 14727000

H	-5.95478600	-1.32412400	0.07571900
H	-6.47087100	-0.16368200	-1.13668400
C	-6.88180700	0.44895400	0.89558400
H	-6.40760500	0.36544400	1.88337700
H	-6.92678000	1.52285600	0.66972600
C	-8.30066600	-0.12468000	0.95586700
H	-8.28521200	-1.19044300	1.21101600
H	-8.90858200	0.38924800	1.70675000
H	-8.80785400	-0.02360600	-0.01014300
H	0.20266400	0.97616500	-2.29820000
C	3.87874700	2.32865000	-0.20774500
H	4.28700200	2.89484500	-1.05063700
H	4.08009700	1.26590400	-0.33887700
H	4.35997600	2.69206300	0.70498000
C	2.41914400	2.55353400	-0.11939700
O	1.94806000	3.80002500	0.07333800
N	1.48049900	1.66707500	-0.20430800
O	0.25837900	2.38248100	-0.05368400
C	0.55437000	3.70939000	0.12070300
O	-0.20573800	4.60067000	0.28262100
Rh	1.36495900	-0.45358800	-0.33597500

**Rh-TS6**

C	1.86892100	-2.36594500	0.64713500
C	0.50202600	-2.02232300	0.97923600
C	0.51763800	-0.79254000	1.70406300
C	1.90296400	-0.37237800	1.83092800
C	2.74118700	-1.36841400	1.21977200
C	2.31939000	-3.63275200	-0.01494700
H	2.53343800	-4.39338600	0.74481400
H	3.23318900	-3.48254600	-0.59453000
H	1.55457000	-4.04046200	-0.67887400
C	-0.70335300	-2.86014600	0.68460400
H	-0.56954600	-3.45989200	-0.21772200
H	-1.60103800	-2.25311900	0.56084900
H	-0.87813000	-3.55429800	1.51524600
C	-0.64656200	-0.05638800	2.29149900
H	-0.68773000	0.97045500	1.91843100
H	-0.55021200	-0.01849100	3.38268500
H	-1.59404400	-0.54063500	2.05300000
C	2.35046900	0.83123400	2.59937600
H	2.36365800	0.59936200	3.67068500
H	1.66923600	1.67223900	2.45119300
H	3.35651100	1.14349300	2.31456700

C	4.23774200	-1.40975400	1.24293600
H	4.58169100	-1.96237400	2.12552800
H	4.66734900	-0.40726100	1.29132600
H	4.64106000	-1.91190600	0.36115700
C	2.54343200	-0.65469000	-2.24205900
H	2.75840400	0.35049700	-2.58801400
H	3.38966000	-1.33456800	-2.21407700
C	1.23483700	-1.18887300	-2.38374900
H	1.09659500	-2.26871100	-2.37942200
C	0.10206400	-0.36427900	-2.28180900
C	-1.30089100	-0.88007200	-2.24316000
H	-1.30850200	-1.94728800	-1.99296700
H	-1.70194800	-0.79834600	-3.26571100
C	-2.21592400	-0.09144100	-1.29031600
H	-1.76353500	-0.08131200	-0.29292800
H	-2.24522100	0.95886800	-1.60033300
C	-3.63373400	-0.66321600	-1.21388400
H	-3.58901300	-1.72737000	-0.93659300
H	-4.09803100	-0.63114900	-2.20867000
C	-4.51679800	0.08609500	-0.20939600
H	-4.04775900	0.04669600	0.78562200
H	-4.55353000	1.14947000	-0.48242500
C	-5.94253000	-0.46850200	-0.11966000
H	-5.90390100	-1.53407000	0.14948300
H	-6.41148300	-0.42357500	-1.11252400
C	-6.82121300	0.27894800	0.89053100
H	-6.35030900	0.23337000	1.88232300
H	-6.85657300	1.34259000	0.61941400
C	-8.24489400	-0.28005800	0.97016600
H	-8.23941000	-1.33429700	1.26973100
H	-8.85027200	0.27010700	1.69695200
H	-8.74854100	-0.21492100	-0.00076500
H	0.21683800	0.70018000	-2.47162900
C	3.67229800	2.63477300	-0.35615400
H	3.96711200	3.34918700	-1.12890500
H	4.08307600	1.64989000	-0.57762000
H	4.04584600	2.99575200	0.60560200
C	2.15019000	2.62831900	-0.28409800
O	1.57272100	3.72694200	-0.01304700
N	1.57388400	1.48971900	-0.55927400
O	-0.36870400	2.35754800	-0.28689500
C	-0.19620900	3.54420000	-0.00157600
O	-0.69639500	4.57627100	0.27493900
Rh	1.46191100	-0.40037900	-0.33459100

**Rh-7**

C	-2.87173900	-0.44378100	-1.34828200
C	-2.12742600	-1.65957600	-1.16416900
C	-0.73334700	-1.36148400	-1.35490500
C	-0.60474900	0.03558400	-1.68273400
C	-1.92574200	0.60991200	-1.66766900
C	-4.36226300	-0.30642200	-1.34863300
H	-4.74859200	-0.46518800	-2.36288200
H	-4.67277400	0.68952200	-1.02667100
H	-4.83641300	-1.04137100	-0.69512600
C	-2.71699900	-3.01492400	-0.91475600
H	-2.99070000	-3.48419000	-1.86673300
H	-3.62336700	-2.95710300	-0.30749200
H	-2.01167700	-3.68256800	-0.41529600
C	0.38964200	-2.35081100	-1.32696300
H	0.55555900	-2.74614900	-2.33628200
H	0.16962400	-3.19949000	-0.67615400
H	1.32227500	-1.89304800	-0.99304300
C	0.64334800	0.76785500	-2.06371100
H	0.60275900	1.02713200	-3.12852000
H	1.53551200	0.16165300	-1.90177000
H	0.73716900	1.69251500	-1.48828100
C	-2.26350000	1.99922400	-2.10625100
H	-2.40029800	2.00830600	-3.19433100
H	-1.46031500	2.69723000	-1.86281900
H	-3.19047900	2.35523100	-1.65222400
C	-2.61123700	-0.98749100	2.12854300
H	-2.78754100	-0.13461500	2.77409600
H	-3.48220700	-1.58015500	1.86762000
C	-1.32622800	-1.57906100	2.05687800
H	-1.22744100	-2.58636300	1.65587100
C	-0.15927800	-0.82957600	2.28086100
C	1.22318500	-1.33342500	2.03685400
H	1.19986300	-2.25384200	1.44296100
H	1.64658800	-1.60298500	3.01723500
C	2.13513500	-0.27981400	1.37855500
H	1.65233700	0.08492800	0.46532500
H	2.21417400	0.59301700	2.03829200
C	3.52968300	-0.81901500	1.04885500
H	3.43621100	-1.71498200	0.41660900
H	4.02489700	-1.15150800	1.97093200
C	4.40789600	0.21514800	0.33495000
H	3.90182600	0.54873000	-0.58337500

H	4.50276800	1.10836300	0.96725500
C	5.80272600	-0.31311300	-0.01739700
H	5.70521900	-1.20971800	-0.64666500
H	6.30912700	-0.64115000	0.90112500
C	6.67745100	0.71978400	-0.73801900
H	6.16794200	1.04805600	-1.65451800
H	6.77358100	1.61343200	-0.10695900
C	8.06881100	0.18260800	-1.08625000
H	8.00164000	-0.69276500	-1.74228700
H	8.67203300	0.93803600	-1.59890000
H	8.61116600	-0.12130600	-0.18397300
H	-0.24886500	0.09784400	2.83960300
C	-2.28193800	3.73176200	1.06137600
H	-3.21333600	3.23567700	1.34755600
H	-2.43406700	4.33525900	0.16271500
H	-1.97833500	4.39957600	1.87359900
C	-1.16017600	2.74890700	0.79446800
N	-1.32873200	1.50765400	1.33331500
O	-0.11194000	3.04977700	0.21555600
Rh	-1.52530600	-0.10714600	0.39591700

**Rh-TS8**

C	3.41281000	0.33095400	0.92834000
C	3.30517100	-1.10352600	0.80919400
C	2.01818100	-1.48271500	1.29851700
C	1.33354100	-0.29052900	1.77498800
C	2.19673800	0.82956700	1.55728900
C	4.61225200	1.15565200	0.58687000
H	5.27299500	1.22371400	1.46025400
H	4.33085500	2.17156600	0.30274600
H	5.18494700	0.71572100	-0.23171100
C	4.37039700	-2.02312600	0.29435900
H	5.01449100	-2.34999800	1.11886800
H	5.00455700	-1.52905900	-0.44463800
H	3.94617300	-2.91859500	-0.16552500
C	1.47504600	-2.87561800	1.38368500
H	1.63232800	-3.27466800	2.39255900
H	1.97088100	-3.54896800	0.68174800
H	0.40021600	-2.90243500	1.18716500
C	-0.02592300	-0.22875300	2.39494300
H	0.06544400	-0.10242200	3.48058200
H	-0.59430300	-1.14267200	2.21316400
H	-0.59049300	0.61683200	1.99342800
C	1.94089700	2.23100800	2.01472300

H	2.25748400	2.33898000	3.05877700
H	0.87887000	2.47782500	1.95455600
H	2.49966400	2.95759300	1.42151700
C	2.20272600	-0.90766800	-2.47703000
H	2.21186000	-0.03927200	-3.12553400
H	3.09711300	-1.52180500	-2.46546800
C	1.00150100	-1.42444500	-1.98601100
H	0.97892100	-2.40939800	-1.52186100
C	-0.24247800	-0.68837000	-2.00973600
C	-1.45376800	-1.22337100	-1.31806600
H	-1.17870600	-1.67827000	-0.35889900
H	-1.78499400	-2.05860200	-1.96292300
C	-2.61673600	-0.23973900	-1.14780200
H	-2.28183500	0.59965200	-0.53291800
H	-2.88382300	0.17112000	-2.13089000
C	-3.84488400	-0.90065900	-0.51336800
H	-3.56556300	-1.32002200	0.46467900
H	-4.17117000	-1.75143100	-1.12843200
C	-5.01310500	0.07432300	-0.32863900
H	-4.68032500	0.92543800	0.28167700
H	-5.29335700	0.49160400	-1.30588800
C	-6.24275700	-0.57057800	0.32027200
H	-5.96189200	-0.98819300	1.29800700
H	-6.57224600	-1.42322900	-0.29048300
C	-7.41272300	0.40355000	0.50312700
H	-7.08112300	1.25531500	1.11242600
H	-7.69167100	0.81923000	-0.47452500
C	-8.63631700	-0.24959700	1.15275200
H	-8.39232300	-0.64538400	2.14525800
H	-9.45598600	0.46566800	1.27152800
H	-9.00679700	-1.08378500	0.54623500
H	-0.41729900	-0.02255600	-2.84548700
C	0.68125200	3.61980100	-1.05631800
H	0.69979000	4.25132600	-0.16530700
H	0.02025700	4.08536900	-1.79469200
H	1.67923800	3.53903100	-1.49307300
C	0.09205200	2.26723800	-0.67651200
N	0.67374300	1.23133300	-1.37378700
O	-0.82598400	2.15518900	0.13471400
Rh	1.72058400	-0.05503300	-0.40981300

**Rh-9**

C	3.91400900	0.20041300	-0.03112200
C	3.66266900	-1.08015000	0.56324300



C	2.72570000	-0.88544300	1.63174300
C	2.44459000	0.54566000	1.74310600
C	3.18739100	1.21498600	0.72888100
C	4.83739800	0.48401000	-1.17194400
H	5.82032100	0.78243000	-0.78723200
H	4.46417600	1.30101700	-1.79372100
H	4.98069800	-0.39394600	-1.80432000
C	4.27538100	-2.38847400	0.16309500
H	5.14124000	-2.60585200	0.79875200
H	4.62264500	-2.37426000	-0.87172100
H	3.56909900	-3.21467600	0.27498700
C	2.19616200	-1.93932300	2.54857000
H	2.81359200	-1.98001000	3.45506800
H	2.21854200	-2.92765200	2.08584700
H	1.17135900	-1.72221200	2.85753100
C	1.60211800	1.19814300	2.79133100
H	2.24029100	1.51137800	3.62721000
H	0.85001300	0.51171600	3.18498100
H	1.09126100	2.07042800	2.38427100
C	3.22569800	2.69020600	0.51072000
H	3.72875200	3.17489100	1.35580300
H	2.20749700	3.08906500	0.45541400
H	3.76416900	2.95373800	-0.40077400
C	1.70872200	-1.39493700	-2.22137600
H	1.86416200	-0.56822100	-2.91133500
H	2.45149300	-2.18643100	-2.23950500
C	0.51477100	-1.56736500	-1.56897900
H	0.30762000	-2.50593500	-1.05855400
C	-0.59829400	-0.50521900	-1.59359300
C	-1.87964700	-1.09779000	-0.97599700
H	-1.61982500	-1.49672300	0.01427200
H	-2.16556300	-1.95667700	-1.59832300
C	-3.07324000	-0.15148900	-0.84098400
H	-2.81128500	0.67957200	-0.17447900
H	-3.31393800	0.28961100	-1.81689000
C	-4.31635000	-0.85731000	-0.28456300
H	-4.07212700	-1.31136700	0.68621900
H	-4.59161200	-1.68736900	-0.94979900
C	-5.51519900	0.08347800	-0.11923700
H	-5.23672600	0.91285700	0.54662800
H	-5.75518300	0.53951500	-1.09017700
C	-6.76122100	-0.61627900	0.43492200
H	-6.52025400	-1.07403900	1.40505200
H	-7.03901100	-1.44539500	-0.23126400

C	-7.96140100	0.32328500	0.60215400
H	-7.68161500	1.15128000	1.26770900
H	-8.20000400	0.77984400	-0.36801600
C	-9.20081200	-0.38609000	1.15581900
H	-8.99821000	-0.82403100	2.13983200
H	-10.04208300	0.30517000	1.26546000
H	-9.52007400	-1.19767700	0.49222700
H	-0.79884400	-0.16533800	-2.61956600
C	-1.29628200	2.48287000	-1.65969000
H	-2.21164400	2.81711000	-1.16567200
H	-1.56150900	1.82930000	-2.48959700
H	-0.79287800	3.37312400	-2.04649500
C	-0.37202400	1.86220100	-0.62755200
N	0.04124600	0.53615200	-0.77856500
O	0.08062800	2.54425700	0.28493600
Rh	1.75046300	-0.21852600	-0.20845900

**Rh-TS8'**

C	-2.39667700	1.88376000	-0.05411100
C	-1.02734100	2.14540000	-0.40210000
C	-0.19660600	1.59689600	0.63206400
C	-1.05513100	0.98856100	1.62892100
C	-2.42063200	1.17479300	1.21074200
C	-3.60029100	2.33074300	-0.82226100
H	-3.91280500	3.32248800	-0.47334900
H	-4.44418700	1.65203800	-0.68108900
H	-3.39275600	2.40995900	-1.89161900
C	-0.54741600	2.92212600	-1.59098000
H	-0.47492200	3.98732700	-1.34279400
H	-1.22971900	2.82959800	-2.43931200
H	0.44297600	2.59208000	-1.91213000
C	1.28611300	1.76222400	0.73088700
H	1.50733400	2.75557700	1.14056700
H	1.77147900	1.69356800	-0.24394800
H	1.73807200	1.02233300	1.39166400
C	-0.62975400	0.32353000	2.89888100
H	-0.79553400	1.00357100	3.74333200
H	0.42844900	0.05884800	2.87957200
H	-1.20774300	-0.58858700	3.06835100
C	-3.62980400	0.82094600	2.01731300
H	-3.82569100	1.61303500	2.74965500
H	-3.48162700	-0.11205500	2.56559800
H	-4.51983300	0.72064100	1.39258500
C	-2.30694900	-1.26743900	-2.12161200

H	-2.43143200	-2.34102500	-2.11684600
H	-3.19442000	-0.69760700	-2.38281400
C	-1.00682500	-0.69846000	-2.38186200
H	-0.95086700	0.23076700	-2.94687300
C	0.14882400	-1.26110500	-1.85242000
C	1.53313700	-0.73699700	-2.07579700
H	1.50957100	0.34646000	-2.24966400
H	1.91105300	-1.18096900	-3.01024500
C	2.49480000	-1.09344400	-0.93108200
H	2.04133200	-0.79805000	0.02244400
H	2.60424900	-2.18459100	-0.88527400
C	3.87255500	-0.44156900	-1.07598800
H	3.75512800	0.64885300	-1.16508700
H	4.33612300	-0.77106000	-2.01568400
C	4.80833900	-0.75311400	0.09715000
H	4.33469000	-0.42581700	1.03484500
H	4.93133700	-1.84132600	0.18438900
C	6.18492700	-0.09204600	-0.03280000
H	6.05916000	0.99661200	-0.12474800
H	6.65922800	-0.42231300	-0.96755300
C	7.11820500	-0.39680000	1.14505900
H	6.64074900	-0.06847600	2.07861200
H	7.24335100	-1.48428900	1.23362100
C	8.48995100	0.27004600	1.00596200
H	8.39507900	1.36034100	0.94710600
H	9.13582100	0.03710800	1.85797800
H	9.00173300	-0.06680100	0.09752400
H	0.06914500	-2.24220000	-1.39082500
C	-4.32836900	-2.43601400	0.44792000
H	-4.35835900	-3.23396300	-0.30039700
H	-4.72838800	-1.52772400	-0.01485700
H	-4.94501400	-2.71656800	1.30314800
C	-2.91043900	-2.20830100	0.92298200
N	-1.95479400	-1.88441200	-0.01468500
O	-2.54297600	-2.35402400	2.08839200
Rh	-1.37509100	-0.07904700	-0.26936500

**Rh-9'**

C	-1.27192500	-1.70577000	1.37304800
C	0.01899600	-1.60457900	0.74634200
C	-0.18183800	-1.65675800	-0.66508600
C	-1.60598100	-1.85062800	-0.92591300
C	-2.27707100	-1.90531800	0.33267900
C	-1.53110100	-1.73919200	2.84422200

H	-1.50219300	-2.77744100	3.19883400
H	-2.51564900	-1.33448600	3.08763600
H	-0.77710300	-1.17775200	3.39953300
C	1.32615200	-1.54666800	1.47524700
H	1.61583400	-2.55771500	1.78476100
H	1.25900500	-0.93786800	2.37974700
H	2.12706700	-1.14595600	0.85538300
C	0.86157200	-1.64915500	-1.73656700
H	0.86883000	-2.62337500	-2.23957100
H	1.86043400	-1.46848000	-1.34004900
H	0.64726700	-0.89402300	-2.49833500
C	-2.21812400	-2.06556200	-2.27069800
H	-2.31937400	-3.14241000	-2.45675800
H	-1.59497300	-1.64645600	-3.06332000
H	-3.20498300	-1.60485800	-2.32087100
C	-3.72219400	-2.20914800	0.55515800
H	-3.86808600	-3.29629200	0.52789200
H	-4.33824800	-1.75227000	-0.21970100
H	-4.06301100	-1.85177100	1.52882200
C	-2.35455300	2.62192900	0.39414000
H	-2.21466100	3.45463000	-0.30842400
H	-3.07533300	2.94234300	1.15548800
C	-1.04225300	2.20579800	1.05312500
H	-1.01815600	2.07991100	2.13450300
C	0.11374900	2.13646200	0.32677800
C	1.49444300	1.96116700	0.89125200
H	1.46452700	1.31621700	1.77673900
H	1.81797300	2.94900000	1.25256800
C	2.51525500	1.45138300	-0.13293600
H	2.13399300	0.53170700	-0.59011000
H	2.59723900	2.17887800	-0.95135200
C	3.90109700	1.19715900	0.46719700
H	3.81066100	0.51248200	1.32311700
H	4.29831400	2.13606500	0.87541500
C	4.89399400	0.61464400	-0.54488700
H	4.49036500	-0.32641600	-0.94922900
H	4.98316800	1.29725700	-1.40120200
C	6.28311000	0.35482300	0.04803000
H	6.19105000	-0.32445500	0.90781800
H	6.68797800	1.29537900	0.44687000
C	7.27373500	-0.23638600	-0.96205600
H	6.86596400	-1.17561700	-1.36078200
H	7.36397200	0.44441500	-1.81916300
C	8.65818600	-0.49121700	-0.35865300

H	8.60010800	-1.19339000	0.48077900
H	9.34526000	-0.91239800	-1.09878600
H	9.10128100	0.43771500	0.01726400
H	0.06514500	2.42063000	-0.72749700
C	-4.90052500	2.45655700	-0.95648400
H	-4.38795900	3.31224700	-1.40823100
H	-5.21495100	2.75515100	0.04968700
H	-5.78155000	2.20807800	-1.54687700
C	-3.99866200	1.23906400	-0.89951300
N	-2.76446900	1.38897200	-0.27077300
O	-4.32238300	0.16604400	-1.39398500
Rh	-1.37345000	0.07441200	0.12973700

**TS-CO<sub>2</sub>**

C	2.57359100	-0.25960600	-0.00004800
H	2.82203600	-0.82178400	0.90199500
H	3.10279700	0.69441500	-0.00023200
H	2.82180400	-0.82176000	-0.90218200
C	1.00773300	-0.15189500	0.00003900
O	0.24202200	-1.12515900	0.00015400
N	0.87850000	1.12930900	-0.00008700
O	-1.06273000	1.16397800	0.00015500
C	-1.64467700	0.11306800	-0.00007000
O	-2.49379500	-0.68449900	-0.00012100