

Supporting Information (25 pages)

Theoretical Study on the Mechanism of H₂ Activation Mediated by two transition metal thiolate complexes: Homolytic for Ir, Heterolytic for Rh

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Table S1 E_{elec} (B3LYP/BS2//B3LYP/BS1), thermal correction to Gibbs free energy ($TCGE$), G_{gas}^{253} ($E_{elec} + TCGE$), ΔG_{solv} (kcal/mol) of all stationary points in the reaction of the iridium thiolate complex with H₂. For each species, the relative electronic energy of the triplet state (ΔE_{S-T}) (relative to that of the singlet state) is also listed below.

Species	E_{elec} (a.u.)	TCGE (a.u.)	G_{253}^{gas} (a.u.)	ΔG_{solv}	Species	E_{elec} (a.u.)	ΔE_{S-T} (kcal/mol)
1a¹+H₂	-2285.2467	0.7026	-2284.5441	-14.73	1a³+H₂	-2285.2045	26.5
TS1-a¹	-2285.2254	0.7120	-2284.5134	-16.04	TS1-a³	-2285.1875	23.8
2a¹	-2285.2531	0.7192	-2284.5339	-17.30	2a³	-2285.2081	28.2
TS2-a¹	-2285.2409	0.7159	-2284.5250	-15.34	TS2-a³	-2285.1887	32.8
4a¹	-2285.2623	0.7207	-2284.5416	-15.62	4a³	-2285.2048	36.1

Table S2 E_{elec} (B3LYP/BS2//B3LYP/BS1), thermal correction to Gibbs free energy ($TCGE$), G_{gas}^{233} ($E_{elec} + TCGE$), ΔG_{solv} (kcal/mol) of all stationary points in the reaction of the rhodium thiolate complex with H_2 . For each species, the relative electronic energy of the triplet state (ΔE_{S-T}) (relative to that of the singlet state) is also listed below.

Species	E_{elec} (a.u.)	TCGE (a.u.)	G_{233}^{gas} (a.u.)	ΔG_{solv}	Species	E_{elec} (a.u.)	ΔE_{S-T} (kcal/mol)
1b¹+H₂	-2290.0367	0.7097	-2289.3270	-18.79	1b³+H₂	-2290.0090	17.4
TS1-b¹	-2290.0228	0.7200	-2289.3028	-20.14	TS1-b³	-2289.9915	19.6
3b¹	-2290.0324	0.7228	-2289.3096	-21.30	2b³	-2289.9936	24.3
TS2-b¹	-2290.0233	0.7198	-2289.3035	-20.15	TS2-b³	-2289.9762	29.6
4b¹	-2290.0483	0.7252	-2289.3231	-19.37	4b³	-2290.0043	27.6

Table S3 E_{elec} (BMK/TPSSh/BS2// B3LYP /BS1), G_{gas} ($E_{elec} + TCGE$), ΔG_{solv} (kcal/mol)

and the relative free energies in solution G_{solu} (kcal/mol) of all stationary points in the reaction of the rhodium/rhodium thiolate complex with H_2 . Energies are reported in a.u.

species	E_{elec} (a.u.)		G_{gas} (a.u.)		ΔG_{solv}		G_{solu}	
	BMK	TPSSh	BMK	TPSSh	BMK	TPSSh	BMK	TPSSh
1a+H₂	-2283.3923	-2285.3195	-2282.6897	-2284.6169	-14.97	-14.64	0.0	0.0
TS1-a	-2283.3803	-2285.3028	-2282.6683	-2284.5908	-16.15	-15.91	11.2	15.1
2a	-2283.4020	-2285.3298	-2282.6828	-2284.6106	-17.38	-17.23	1.9	1.4
TS2-a	-2283.3906	-2285.3169	-2282.6747	-2284.6010	-15.25	-15.30	9.1	9.3
4a	-2283.4127	-2285.3360	-2282.6920	-2284.6153	-15.58	-15.58	-2.0	0.1
1b+H₂	-2288.1637	-2290.0999	-2287.4540	-2289.3902	-19.22	-18.68	0.0	0.0
TS1-b	-2288.1587	-2290.0894	-2287.4387	-2289.3694	-20.32	-19.99	8.5	11.8
3b	-2288.1673	-2290.1004	-2287.4445	-2289.3776	-21.33	-21.23	3.9	5.3
TS2-b	-2288.1529	-2290.0905	-2287.4331	-2289.3707	-20.13	-20.09	12.2	10.8
4b	-2288.1766	-2290.1110	-2287.4514	-2289.3858	-19.26	-19.32	1.6	2.1

The coordinates of the optimized structures in gas phase.

For the iridium thiolate complex:

1a

C	0.98423400	-3.16998100	-1.23999300
C	-0.44861700	-3.23126100	-1.23266300
C	-0.94804200	-2.05493800	-1.92591800
C	0.17214900	-1.26681500	-2.35636700
C	1.37104200	-1.93261000	-1.88350000
C	1.93864100	-4.24697600	-0.81471100
H	2.31883900	-4.76735700	-1.70350200
H	2.80412600	-3.84862800	-0.27654200
H	1.45633600	-4.99842900	-0.18586100
C	-1.30910900	-4.36865200	-0.76917000
H	-1.60090600	-4.99048500	-1.62587100
H	-0.78926700	-5.01353900	-0.05715700
H	-2.22677700	-4.00695200	-0.29634300
C	-2.39204100	-1.79664100	-2.21878100
H	-2.70654700	-2.41104700	-3.07397400
H	-3.02699200	-2.05440700	-1.36708600
H	-2.57278800	-0.75087200	-2.46363700
C	0.13966600	-0.07794700	-3.26544800
H	0.16206100	-0.41038900	-4.31214500
H	-0.76328500	0.51806000	-3.12447800
H	1.00209000	0.56795900	-3.10151500
C	2.77538600	-1.47957300	-2.13788400
H	3.48668500	-2.00726800	-1.49790200
H	3.04852500	-1.68296800	-3.18249000
H	2.89020700	-0.40884200	-1.95246500
Ir	0.16315300	-1.37983600	-0.12457100
P	0.54391300	-2.07919100	2.12730600
C	0.33311500	-3.88306200	2.46853600
H	0.55221700	-4.08420100	3.52279300
H	-0.69592100	-4.18845800	2.26114000
H	1.01332200	-4.47694900	1.85499200
C	-0.50096200	-1.31814600	3.44870400
H	-0.24413800	-1.75441100	4.41981800
H	-0.34081200	-0.23910700	3.48382700
H	-1.55769500	-1.50138800	3.23449600
C	2.27696400	-1.72884000	2.66167600

H	2.43375600	-2.01905300	3.70657100
H	2.97338100	-2.28609000	2.02839000
H	2.48579300	-0.66210600	2.53946300
S	-0.10454800	0.63911400	0.82081400
C	-0.32947200	2.19976500	-0.09003000
C	0.80961500	3.00803300	-0.32829800
C	-1.63804900	2.70518500	-0.28503500
C	0.61158600	4.30181900	-0.83143700
C	-1.77566100	4.00808900	-0.78655800
C	-0.66641200	4.80015300	-1.06813400
H	1.48228900	4.92537900	-1.01153600
H	-2.77720900	4.40315100	-0.92919100
H	-0.79781100	5.81095200	-1.44316000
H	3.12416000	3.55888100	-2.81492300
C	2.77863600	2.55607200	-2.53182400
H	1.70398500	2.51966600	-2.72018200
H	3.28559000	1.84082700	-3.18868400
C	3.11737500	2.28867100	-1.07080600
C	4.40914100	1.84856500	-0.76043800
C	2.20321500	2.56460600	-0.02299200
C	4.84136600	1.70882000	0.56292500
H	5.10297200	1.64378500	-1.57100400
C	2.65339500	2.49936100	1.31792900
C	3.95716300	2.06152100	1.58563700
C	6.25526600	1.24594000	0.86809600
C	1.78450200	2.95385100	2.48234500
H	4.29946000	2.03255400	2.61577700
H	6.43799000	0.24512300	0.45859300
H	6.99016700	1.92741500	0.42385300
H	6.43240500	1.21232600	1.94693500
H	1.15564800	2.13622800	2.85609700
H	2.41658300	3.29967900	3.30625400
H	1.12446900	3.77510400	2.18952200
H	-6.27342100	-1.18071000	1.51436400
C	-6.51805900	-0.19096300	1.10825000
H	-7.16080100	-0.33185100	0.23425900
H	-7.08930800	0.35062900	1.87001600
C	-5.25554200	0.56801600	0.73900900
C	-4.43995500	1.12026700	1.73347300
C	-4.89309800	0.76277300	-0.59565400
C	-3.26949400	1.81829100	1.42259100
H	-4.73956200	1.03518700	2.77357400
C	-3.72830000	1.45739700	-0.94865200
H	-5.54282800	0.39095100	-1.38205900

C	-2.87739100	1.94899900	0.06659700
C	-2.49571200	2.50515400	2.53824800
C	-3.46219800	1.74115200	-2.42025900
H	-2.42357000	3.58268800	2.34975100
H	-3.00572300	2.36014200	3.49505400
H	-1.47725200	2.11384100	2.62869800
H	-3.75539300	2.76814400	-2.67133600
H	-2.40290300	1.64157200	-2.67296500
H	-4.04689000	1.06815000	-3.05567500

TS1-a

C	-0.59347200	-3.11724400	-1.28366500
C	-1.94630400	-2.67022900	-1.42203200
C	-1.90986400	-1.36527800	-2.06887200
C	-0.55168600	-0.99921300	-2.30656900
C	0.29313500	-2.05153200	-1.74812500
C	-0.13614800	-4.49188900	-0.89930000
H	0.10817000	-5.04955200	-1.81310300
H	0.76751100	-4.47452900	-0.28455600
H	-0.90939300	-5.05580800	-0.37384600
C	-3.18633800	-3.46510200	-1.13014700
H	-3.52713500	-3.98952200	-2.03245600
H	-3.00977900	-4.21833800	-0.35854200
H	-4.00683300	-2.82774100	-0.79040900
C	-3.11094200	-0.56388700	-2.46899400
H	-3.21084700	-0.56660500	-3.56197700
H	-4.03062200	-0.97844300	-2.05079300
H	-3.02555900	0.47156400	-2.13570200
C	-0.07005700	0.18487700	-3.08926400
H	0.59157100	-0.14629800	-3.89806200
H	-0.90690100	0.72068900	-3.54066100
H	0.48663100	0.88918600	-2.46614400
C	1.78123500	-2.14485500	-1.89957100
H	2.20701600	-2.87898300	-1.21120700
H	2.03309600	-2.46084100	-2.92145400
H	2.26894700	-1.18842000	-1.70187200
Ir	-0.77692200	-1.26214700	-0.08497800
P	-0.39340500	-2.21853900	2.06215300
C	-1.27350500	-3.80534200	2.43250400
H	-1.04937000	-4.11717300	3.45792900
H	-2.35370600	-3.66152900	2.33700300
H	-0.95889300	-4.59909000	1.75257100
C	-0.90070500	-1.16062300	3.49170800

H	-0.71298400	-1.68951800	4.43180700
H	-0.33673300	-0.22611100	3.47420800
H	-1.96653100	-0.92585200	3.41886100
C	1.38540300	-2.59803900	2.38629900
H	1.52641800	-2.93142600	3.41960800
H	1.72596900	-3.38735900	1.70946300
H	1.98152100	-1.70018300	2.20064500
S	0.54448800	0.48904900	0.84979400
C	0.83058900	2.05200500	-0.01509600
C	2.18011800	2.38579600	-0.31873100
C	-0.19346100	3.02764500	-0.15425300
C	2.46935200	3.67465900	-0.78764200
C	0.15515300	4.30341200	-0.62208900
C	1.46914300	4.62940700	-0.94376600
H	3.50264400	3.92633200	-1.00790200
H	-0.62479200	5.05402300	-0.70987700
H	1.71422100	5.62782500	-1.29439800
H	4.10596600	2.07219100	-2.95708100
C	3.59901000	1.15258400	-2.63788300
H	2.52687300	1.31334600	-2.76522600
H	3.91933500	0.34919700	-3.30922900
C	3.96529100	0.82489400	-1.19645000
C	5.02721800	-0.06160100	-0.96077500
C	3.32510100	1.44841500	-0.10296300
C	5.49639200	-0.31872000	0.32760300
H	5.50923800	-0.54028400	-1.80779300
C	3.83689400	1.24678200	1.20499200
C	4.89860900	0.35988100	1.39748100
C	6.65974000	-1.26450500	0.56914200
C	3.29389300	2.02584800	2.39312700
H	5.28604100	0.21422900	2.40139700
H	6.93373600	-1.79276400	-0.34887800
H	7.54016600	-0.71089100	0.91746600
H	6.40955300	-2.00871600	1.33406800
H	2.24414500	1.78344600	2.58838100
H	3.87270500	1.79503100	3.29246400
H	3.36003800	3.10463100	2.21113000
H	-5.94218100	1.42305900	1.97518300
C	-5.82106800	2.21882900	1.23174100
H	-6.41677900	1.96262800	0.35049000
H	-6.23203800	3.14121300	1.66038300
C	-4.35958200	2.41018100	0.86615700
C	-3.38026200	2.50290200	1.86345400
C	-3.96080900	2.56824000	-0.46206300

C	-2.03082600	2.71522000	1.55894300
H	-3.67959500	2.45206800	2.90611400
C	-2.61759300	2.77600400	-0.81034800
H	-4.71171700	2.56043200	-1.24669700
C	-1.62673100	2.79455300	0.20071200
C	-1.05266900	2.98207700	2.69264900
C	-2.28673700	3.07527900	-2.26681800
H	-0.63338100	3.99090600	2.59873600
H	-1.56509000	2.91645500	3.65721800
H	-0.22148000	2.27185300	2.68801600
H	-2.23108300	4.15950400	-2.42445200
H	-1.32492200	2.65538100	-2.56552800
H	-3.06975200	2.69181100	-2.92937500
H	-2.57330100	-0.59468900	0.85610100
H	-2.32293400	0.12366100	0.75571000

2a

C	-0.58920000	-3.33057600	-0.58790400
C	-1.89970800	-2.93252900	-1.05592400
C	-1.72115200	-1.90699500	-2.07408700
C	-0.31939600	-1.62241000	-2.15561600
C	0.37861700	-2.52011700	-1.24371700
C	-0.30839800	-4.48892100	0.32445100
H	-0.25804300	-5.41727800	-0.25933600
H	0.64585400	-4.37903800	0.84449400
H	-1.09403600	-4.62735400	1.07207300
C	-3.18340400	-3.66721000	-0.79029700
H	-3.28771200	-4.49858000	-1.49966700
H	-3.21625200	-4.09298000	0.21483000
H	-4.05466000	-3.01937100	-0.91135900
C	-2.79860900	-1.38835400	-2.98240600
H	-2.89273100	-2.04537500	-3.85666800
H	-3.76998100	-1.35980400	-2.48317600
H	-2.57778600	-0.38182100	-3.34025000
C	0.36179800	-0.75155500	-3.16782700
H	0.94681100	-1.37232800	-3.85806900
H	-0.35754900	-0.18646400	-3.76173500
H	1.04676400	-0.04647600	-2.69375000
C	1.86508700	-2.60079400	-1.11187200
H	2.17070800	-3.37491100	-0.40463300
H	2.31232300	-2.83943400	-2.08472000
H	2.29062400	-1.64802900	-0.77645100
Ir	-1.14020400	-1.03798300	-0.08781500

P	-1.47247600	-1.20107200	2.24200700
C	-2.92639800	-2.24929500	2.69544400
H	-3.03329100	-2.28849400	3.78427400
H	-3.83724900	-1.82611400	2.26279000
H	-2.79874200	-3.26695100	2.31935200
C	-1.78870300	0.37236600	3.13306400
H	-2.06473500	0.15641000	4.17022900
H	-0.88329800	0.97970400	3.10939800
H	-2.58686300	0.92901200	2.63749200
C	-0.06936600	-1.98018600	3.15530700
H	-0.27356500	-1.96600900	4.23088000
H	0.06063200	-3.01601200	2.83167600
H	0.85119600	-1.42603200	2.95544400
S	0.80547100	0.25245700	0.63888000
C	1.20447000	1.76874600	-0.28315300
C	2.59516300	1.95209500	-0.52639800
C	0.28962700	2.79702600	-0.62185300
C	3.02644900	3.12252100	-1.16375100
C	0.77506000	3.93914000	-1.27908000
C	2.12627100	4.10549100	-1.56231700
H	4.09146400	3.25438100	-1.33124100
H	0.06648000	4.72206200	-1.53476300
H	2.47675700	5.00536800	-2.05906500
H	4.62321900	1.11093500	-2.90435000
C	4.07640800	0.25742900	-2.48441200
H	3.02031100	0.40443800	-2.71848000
H	4.42859800	-0.64646300	-2.99152600
C	4.31948800	0.15766200	-0.98576500
C	5.28867800	-0.74116900	-0.52001900
C	3.63947600	0.98570200	-0.06471900
C	5.63101700	-0.81696900	0.83162700
H	5.79919300	-1.37991900	-1.23422500
C	4.01440800	0.95345200	1.30228000
C	4.99284800	0.05006600	1.72552900
C	6.70853200	-1.77126600	1.31502100
C	3.41869700	1.92875900	2.30740300
H	5.27507700	0.03436800	2.77372000
H	6.88652900	-2.56628700	0.58453800
H	7.65388500	-1.23550800	1.46769500
H	6.42783600	-2.23247000	2.26799400
H	2.33737600	1.79141300	2.41386100
H	3.87955600	1.78685000	3.28938000
H	3.59452200	2.96393900	1.99294500
H	-5.52646800	2.99221000	1.87546900

C	-5.36440500	3.17122000	0.80797500
H	-5.98507300	2.47095900	0.23958000
H	-5.71241200	4.18713300	0.58197800
C	-3.89736600	3.02434100	0.44310300
C	-2.89362500	3.27921200	1.38517600
C	-3.51304000	2.70536700	-0.86303700
C	-1.53566300	3.18718100	1.05808100
H	-3.17301600	3.58716400	2.38867500
C	-2.16496500	2.61948300	-1.23095000
H	-4.27679400	2.55044300	-1.61949200
C	-1.15897800	2.81568500	-0.25431900
C	-0.48603900	3.57314000	2.08767600
C	-1.80294000	2.38181500	-2.68658500
H	0.03182000	4.48821200	1.77579800
H	-0.95207100	3.76139100	3.05960600
H	0.27363000	2.79360000	2.20385400
H	-1.45468000	3.31150600	-3.15273900
H	-0.99782000	1.64980900	-2.78237100
H	-2.67615400	2.03455800	-3.24794100
H	-2.66829200	-0.68312000	0.10368600
H	-1.53103000	0.48090200	-0.29288800

TS2-a

C	-0.67455900	-3.31440700	-0.63694300
C	-1.97114800	-2.83646600	-1.11939900
C	-1.71491200	-1.83297600	-2.14232400
C	-0.30766600	-1.61158500	-2.18551400
C	0.33617700	-2.54493500	-1.26038000
C	-0.46888300	-4.49240300	0.26967900
H	-0.45359700	-5.41774400	-0.32112600
H	0.47968300	-4.43260800	0.80903600
H	-1.27418300	-4.59510500	1.00209400
C	-3.29011100	-3.52744500	-0.91880300
H	-3.45236200	-4.26144500	-1.71917900
H	-3.33027600	-4.06771100	0.02942200
H	-4.12478400	-2.82200700	-0.94141700
C	-2.75265600	-1.23751200	-3.04828900
H	-2.87877400	-1.87303400	-3.93487900
H	-3.72338800	-1.16370500	-2.55221700
H	-2.47239900	-0.23870600	-3.38626300
C	0.43718800	-0.74650600	-3.15941100
H	1.11285400	-1.36452100	-3.76349200
H	-0.24326700	-0.23554600	-3.84310200

H	1.04749200	0.00533100	-2.65446900
C	1.81763400	-2.68206900	-1.08991700
H	2.07097600	-3.32286200	-0.24204100
H	2.25750300	-3.13461600	-1.98891900
H	2.30317100	-1.71560100	-0.93119800
Ir	-1.11679300	-1.08804900	-0.09692600
P	-1.69361600	-1.30042000	2.16213100
C	-3.20361500	-2.31517900	2.48697100
H	-3.44277400	-2.29215100	3.55535900
H	-4.04770200	-1.91021900	1.92231600
H	-3.04636000	-3.35438600	2.18815400
C	-2.06821200	0.28270500	3.02746000
H	-2.37068600	0.07994700	4.06008400
H	-1.17835000	0.91529600	3.02780000
H	-2.86471900	0.81649600	2.50402200
C	-0.40181500	-2.08191300	3.22989000
H	-0.74392400	-2.13216400	4.26911200
H	-0.18222300	-3.09377600	2.87903500
H	0.51660100	-1.48972600	3.18364900
S	0.72939900	0.43673200	0.76622400
C	1.28909500	1.84928600	-0.23605200
C	2.68430300	1.92239700	-0.48349900
C	0.43220000	2.92030700	-0.58776600
C	3.18266000	3.05487300	-1.14372200
C	0.98314900	4.01985500	-1.26052700
C	2.34395400	4.08936000	-1.54674200
H	4.25175200	3.11675300	-1.32335000
H	0.32609900	4.84158800	-1.53046800
H	2.75162900	4.95739700	-2.05644500
H	4.80242200	0.87624100	-2.85579800
C	4.09782200	0.14959000	-2.43120000
H	3.09095900	0.48753200	-2.68190900
H	4.28046500	-0.81236000	-2.92100800
C	4.30502400	0.03245800	-0.92768200
C	5.21754000	-0.91966800	-0.45180700
C	3.65901600	0.89278500	-0.01195400
C	5.53485800	-1.02043800	0.90345900
H	5.70294200	-1.58195300	-1.16199000
C	4.01458000	0.83669600	1.36105100
C	4.93315600	-0.12235800	1.79315400
C	6.54518600	-2.03829000	1.40167500
C	3.46879900	1.84462000	2.36394100
H	5.20131800	-0.15650000	2.84452900
H	6.77631100	-2.77486600	0.62656400

H	7.48084300	-1.54194200	1.68737200
H	6.16626100	-2.56945100	2.28189900
H	2.38630700	1.74510200	2.50092300
H	3.94598700	1.70093200	3.33764000
H	3.66981300	2.86949400	2.03212500
H	-5.41666900	3.19652600	1.82062600
C	-5.23491500	3.36420000	0.75447700
H	-5.85196600	2.66451500	0.18150500
H	-5.56963900	4.38117500	0.51344900
C	-3.76347500	3.20117900	0.41601200
C	-2.77414700	3.45130500	1.37360000
C	-3.36109500	2.86447800	-0.88104200
C	-1.41187200	3.34896100	1.06870300
H	-3.06691700	3.76003000	2.37258100
C	-2.00927400	2.76457500	-1.22742100
H	-4.11453500	2.70281700	-1.64609800
C	-1.01934400	2.97169300	-0.23825900
C	-0.37760600	3.71472400	2.12070100
C	-1.62732900	2.48282100	-2.67060600
H	0.19857500	4.59209100	1.80358500
H	-0.86594600	3.95331500	3.07013200
H	0.33251600	2.89791900	2.28866300
H	-1.22189300	3.38302100	-3.14789900
H	-0.86223900	1.70511100	-2.73731600
H	-2.50606200	2.16834000	-3.24227300
H	-2.40475800	-0.15964100	-0.05146200
H	-0.81343200	0.58741000	0.14532300

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C	-1.09679500	-3.42895300	0.75744500
C	0.26765400	-3.56207200	0.29551200
C	1.06447400	-2.59225700	0.99151600
C	0.19675900	-1.92062200	1.95171600
C	-1.12015800	-2.43508200	1.82617300
C	-2.21308800	-4.38697600	0.45749200
H	-2.22629900	-5.18569800	1.21119200
H	-3.19286200	-3.90158100	0.48503100
H	-2.09166200	-4.86190000	-0.51905700
C	0.76911600	-4.59810700	-0.66839700
H	1.04424400	-5.51075000	-0.12341500
H	0.00860500	-4.86642200	-1.40577200
H	1.65302900	-4.25197800	-1.20900200
C	2.55767600	-2.46358700	0.92302700

H	3.03041700	-3.03434100	1.73444200
H	2.94753400	-2.85235900	-0.02148100
H	2.88956800	-1.42826900	1.00710300
C	0.67820200	-0.93493600	2.97463700
H	1.43810500	-1.40353800	3.61227200
H	1.13517700	-0.05739600	2.51044000
H	-0.13233200	-0.59451800	3.62160600
C	-2.28936500	-2.16766100	2.72882400
H	-3.24037100	-2.24830200	2.19610100
H	-2.31310500	-2.90055300	3.54707200
H	-2.24471700	-1.17233400	3.17528700
Ir	-0.50321200	-1.54279200	-0.24866000
P	-2.46421100	-1.07612200	-1.42972600
C	-2.95086900	-2.47392400	-2.54420200
H	-3.84799200	-2.21257500	-3.11579700
H	-2.13274200	-2.68525000	-3.23852300
H	-3.15660200	-3.37696900	-1.96549600
C	-2.42169300	0.33920600	-2.61342400
H	-3.33807700	0.34226900	-3.21321600
H	-2.35265900	1.28293700	-2.06981200
H	-1.55941800	0.24191700	-3.27880700
C	-4.00888600	-0.75860800	-0.46592200
H	-4.86029900	-0.63084200	-1.14379000
H	-4.21982000	-1.59566400	0.20522500
H	-3.88099900	0.15248900	0.12381600
S	0.45053900	0.64710700	-0.82741400
C	0.93792700	1.98585800	0.32687500
C	-0.06243500	2.86009700	0.80097200
C	2.31348800	2.23706600	0.57454200
C	0.32848000	3.93325700	1.61683700
C	2.64255000	3.33554500	1.38242000
C	1.66526900	4.16631200	1.92080900
H	-0.44122800	4.60812800	1.97923000
H	3.69276200	3.54050100	1.56504400
H	1.94681300	5.01120800	2.54214600
H	-1.58054600	2.58146400	3.31274100
C	-2.06883300	1.81190100	2.70399100
H	-1.36269700	0.98477500	2.58722200
H	-2.94483900	1.45085800	3.25135100
C	-2.48022100	2.36645300	1.35133800
C	-3.83782500	2.48977400	1.03803700
C	-1.50774900	2.80455700	0.42169300
C	-4.26420500	3.05129500	-0.17279400
H	-4.57769900	2.16824500	1.76557100

C	-1.92454200	3.39707400	-0.79422300
C	-3.29460200	3.49695300	-1.07424100
C	-5.74480100	3.20534600	-0.47075000
C	-0.91937300	3.98557700	-1.77205800
H	-3.60694200	3.96101500	-2.00430700
H	-6.27430700	2.25407000	-0.34264100
H	-6.19897500	3.93438200	0.21106200
H	-5.90549600	3.55385500	-1.49489200
H	-0.20914200	3.23021900	-2.12470700
H	-1.43506300	4.40311800	-2.64139400
H	-0.34305500	4.78850400	-1.29787200
H	6.39106900	-1.37935400	-2.61827800
C	6.74603000	-0.74726300	-1.79615500
H	7.23770600	-1.38698300	-1.05789000
H	7.49527400	-0.05789500	-2.20321000
C	5.59737000	0.02290500	-1.17148900
C	4.79348400	0.85890600	-1.95624300
C	5.33892300	-0.04504100	0.19832400
C	3.73518200	1.58839000	-1.40882200
H	5.01444200	0.96875100	-3.01320100
C	4.28506000	0.66518600	0.79029700
H	5.97966000	-0.65280900	0.82933500
C	3.43636200	1.45278400	-0.02317600
C	2.99263000	2.58606100	-2.28755600
C	4.14609500	0.61744300	2.30586300
H	3.06704100	3.59467600	-1.86502600
H	3.43218900	2.60124900	-3.28868200
H	1.92843000	2.34886800	-2.39198700
H	4.69635700	1.45060100	2.76169300
H	3.10743500	0.69646800	2.63140700
H	4.56978200	-0.31141400	2.70022700
H	0.00583800	-1.74605600	-1.74601400
H	1.73659300	0.28115000	-1.05436400

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C	-0.91083300	3.34724000	-1.25770800
C	0.51649600	3.38571600	-1.21178600
C	1.01713100	2.21330500	-1.90947400
C	-0.10064100	1.45459900	-2.38223100
C	-1.29813700	2.13162800	-1.93938100
C	-1.85930000	4.42840200	-0.83230200
H	-2.23521200	4.95645300	-1.71879600
H	-2.72947400	4.03270600	-0.29934200

H	-1.37335800	5.17169400	-0.19655300
C	1.37909100	4.49492000	-0.69061000
H	1.69676400	5.14424500	-1.51800400
H	0.85014600	5.12046000	0.03197700
H	2.28487400	4.10972100	-0.21258600
C	2.46126200	1.92834600	-2.16709700
H	2.80928400	2.53737600	-3.01415500
H	3.08432200	2.17454900	-1.30266100
H	2.62824400	0.87929000	-2.40998800
C	-0.04865800	0.27517500	-3.30311800
H	0.20238500	0.60646400	-4.31986800
H	0.70500500	-0.45274500	-2.99561800
H	-1.01138000	-0.23460200	-3.34728900
C	-2.70161900	1.70083900	-2.22862600
H	-3.42530100	2.27843400	-1.64835300
H	-2.92896500	1.85120300	-3.29332100
H	-2.85086500	0.64297300	-1.99514500
P	-0.59692100	2.18911100	2.15381100
C	-0.47013000	3.99599300	2.54067400
H	-0.70567000	4.17071700	3.59614900
H	0.54735000	4.34809600	2.34711700
H	-1.16840900	4.57103900	1.92885200
C	0.47797200	1.44528700	3.46322300
H	0.17844400	1.81379100	4.45024100
H	0.39636600	0.35683600	3.44137800
H	1.52153500	1.71469500	3.27548900
C	-2.31910800	1.75054100	2.66809100
H	-2.48889200	1.98724400	3.72427000
H	-3.03641800	2.30890700	2.05809300
H	-2.48679200	0.68341800	2.49535800
S	0.06570600	-0.52566900	0.78322900
C	0.28230400	-2.09193300	-0.10185000
C	-0.86566800	-2.88281900	-0.35874900
C	1.58478100	-2.61797800	-0.28681800
C	-0.68397300	-4.17897000	-0.85919900
C	1.70736700	-3.92345300	-0.78511600
C	0.58913900	-4.69804400	-1.08027500
H	-1.56282000	-4.78665200	-1.05429500
H	2.70417900	-4.33397300	-0.91728800
H	0.70903700	-5.70987200	-1.45638000
H	-3.05528900	-3.28635600	-2.90208400
C	-2.76050000	-2.27869000	-2.58149100
H	-1.68506900	-2.18822600	-2.74521500
H	-3.28653400	-1.56607500	-3.22622700

C	-3.13462200	-2.07027000	-1.12042200
C	-4.42625100	-1.61384700	-0.81759400
C	-2.25394000	-2.41223700	-0.07017900
C	-4.88214100	-1.52245000	0.49837200
H	-5.09671500	-1.35535000	-1.63196300
C	-2.72878100	-2.38942200	1.26700600
C	-4.02399300	-1.93361100	1.52708000
C	-6.29554300	-1.06248600	0.81013000
C	-1.88705100	-2.93526500	2.41096100
H	-4.38486600	-1.93198800	2.55134200
H	-6.75979900	-0.59727700	-0.06454700
H	-6.91811400	-1.91465600	1.10961400
H	-6.30323300	-0.33848900	1.63250100
H	-0.96146200	-2.36621500	2.54506100
H	-2.45245400	-2.89872800	3.34699700
H	-1.61134900	-3.97867500	2.21913100
H	6.34600100	0.87619900	1.98201800
C	6.50214000	0.19979400	1.13469800
H	6.88942200	0.78222400	0.29321600
H	7.27155100	-0.52692100	1.42420200
C	5.21485000	-0.51327700	0.75964900
C	4.38592600	-1.05403200	1.74932400
C	4.85942600	-0.70527000	-0.57741700
C	3.21222700	-1.74338000	1.43150700
H	4.67501100	-0.96243400	2.79190600
C	3.69204700	-1.39162600	-0.93712800
H	5.51515400	-0.33530000	-1.35991400
C	2.83035600	-1.87609700	0.07260700
C	2.42066100	-2.41499800	2.54353700
C	3.42661200	-1.66677300	-2.41043100
H	2.35485300	-3.49541200	2.36949600
H	2.91279500	-2.25421000	3.50726800
H	1.39943600	-2.02598400	2.60966800
H	3.68700300	-2.70250900	-2.66103900
H	2.37277900	-1.53227800	-2.66899600
H	4.03582700	-1.01199200	-3.04187000
Rh	-0.15133700	1.52429100	-0.14168500

TS1-b

C	-0.44526500	-3.32863600	-1.10381800
C	-1.76939000	-2.97368000	-1.49190100
C	-1.68384100	-1.73673200	-2.25038600
C	-0.32147500	-1.32397000	-2.32022200

C	0.46031300	-2.27237000	-1.54854200
C	0.00206400	-4.63055500	-0.51263100
H	0.39227100	-5.26937300	-1.31670000
H	0.81066900	-4.50401800	0.21229300
H	-0.81638700	-5.17506700	-0.03767800
C	-3.01327500	-3.79618000	-1.32072700
H	-3.21894500	-4.37482000	-2.23129500
H	-2.92069200	-4.50705800	-0.49580900
H	-3.89076100	-3.17195700	-1.12901200
C	-2.84949200	-1.07245700	-2.91265900
H	-3.01148100	-1.52119100	-3.90271600
H	-3.77109000	-1.20566300	-2.34028200
H	-2.68565100	-0.00345500	-3.05078500
C	0.23648300	-0.19310700	-3.12981100
H	1.03315200	-0.55911000	-3.78749300
H	-0.53152700	0.25973000	-3.76005800
H	0.66247100	0.58830000	-2.49537500
C	1.95406600	-2.30902000	-1.45855500
H	2.29062200	-2.88048100	-0.58987800
H	2.36509000	-2.79630500	-2.35479800
H	2.38613100	-1.31025900	-1.37898300
P	-0.85541300	-2.12986300	2.16209100
C	-1.80346000	-3.68308600	2.51335600
H	-1.81351600	-3.87685400	3.59133200
H	-2.83420200	-3.57421600	2.16377600
H	-1.34879200	-4.53968600	2.01184300
C	-1.60310300	-0.93781800	3.36130700
H	-1.56434600	-1.35156000	4.37464600
H	-1.05218900	0.00362400	3.32225000
H	-2.64432600	-0.74013400	3.09141700
C	0.82526500	-2.46332100	2.85214200
H	0.75715800	-2.75356200	3.90581100
H	1.30669200	-3.26928400	2.29107800
H	1.43745800	-1.56245200	2.75655100
S	0.42385900	0.40029000	0.82900000
C	0.75611600	1.91487800	-0.08751600
C	2.11309500	2.24421700	-0.36689300
C	-0.26928000	2.87308600	-0.31495800
C	2.40396400	3.50645400	-0.90261300
C	0.07974000	4.12114900	-0.84979100
C	1.40101000	4.43901600	-1.15192800
H	3.44169400	3.75620000	-1.10312600
H	-0.70407700	4.85738400	-1.00255400
H	1.64990500	5.41617500	-1.55579600

H	4.29272700	1.84595300	-2.90330900
C	3.71285700	0.97616400	-2.56767900
H	2.66184500	1.19268500	-2.76132400
H	4.01841700	0.12166500	-3.18116000
C	3.98763700	0.70589200	-1.09391500
C	5.06194400	-0.13721100	-0.76853200
C	3.26132400	1.33745400	-0.05932900
C	5.46348100	-0.33893800	0.55130500
H	5.60853900	-0.62316300	-1.57119900
C	3.70568200	1.19464800	1.28119700
C	4.78369400	0.35338000	1.56206400
C	6.64349000	-1.23318800	0.88854800
C	3.08144100	2.00325800	2.40792800
H	5.11918200	0.25556200	2.59006100
H	6.96814100	-1.80236800	0.01242000
H	7.49338100	-0.63358300	1.23697700
H	6.38574300	-1.94101100	1.68459900
H	2.04040600	1.71185600	2.58288900
H	3.64154100	1.85199000	3.33549700
H	3.09474600	3.07324700	2.17074000
H	-6.04551100	1.41420300	1.83332000
C	-5.90652200	2.20621400	1.08815400
H	-6.51201100	1.96289100	0.21010000
H	-6.29144500	3.13901100	1.51746100
C	-4.44173700	2.35644300	0.71636900
C	-3.47501500	2.57207400	1.70734700
C	-4.02655300	2.33841800	-0.61637300
C	-2.12280000	2.73954500	1.39541900
H	-3.78717900	2.64893700	2.74471500
C	-2.67895100	2.50254100	-0.97002300
H	-4.76709100	2.22582300	-1.40251600
C	-1.70403000	2.65610000	0.04244800
C	-1.14315200	3.09820800	2.50034900
C	-2.31527200	2.60990300	-2.44406400
H	-0.64705200	4.05032400	2.27903200
H	-1.66772400	3.20087300	3.45502000
H	-0.36482000	2.33571800	2.60764700
H	-2.14084800	3.65743700	-2.71819200
H	-1.40157200	2.05962400	-2.68177200
H	-3.13478800	2.24151200	-3.06970500
H	-2.84477600	-0.61320200	0.46394800
H	-2.64681700	0.09668200	0.28577100
Rh	-0.86478300	-1.37282000	-0.11901000

3b

C	-1.11261600	-3.25842500	-0.80815600
C	-2.37795400	-2.70901400	-1.22976400
C	-2.09390700	-1.64535200	-2.16322000
C	-0.67258600	-1.51286200	-2.28941600
C	-0.05910500	-2.50690600	-1.43712700
C	-0.91953700	-4.53179400	-0.04012100
H	-0.83705700	-5.36648800	-0.74958400
H	-0.00176000	-4.52435100	0.55247800
H	-1.76118600	-4.75617900	0.61904800
C	-3.73704600	-3.28951800	-0.96390900
H	-4.00419300	-4.00747400	-1.75138100
H	-3.77710000	-3.82291100	-0.01115700
H	-4.51253100	-2.51837600	-0.94979500
C	-3.13169500	-0.88459500	-2.93162400
H	-3.43757900	-1.46591200	-3.81205200
H	-4.02788200	-0.70272200	-2.33205600
H	-2.75596400	0.07778600	-3.28244800
C	0.07381400	-0.64954500	-3.25910900
H	0.53431800	-1.27430400	-4.03593400
H	-0.58314300	0.06501800	-3.75754500
H	0.87445600	-0.09477100	-2.76520600
C	1.40885300	-2.79076500	-1.36419900
H	1.64500000	-3.50982400	-0.57592700
H	1.74992400	-3.21749200	-2.31734300
H	1.98755700	-1.88316800	-1.16900600
P	-1.42542400	-1.54873400	2.21803200
C	-2.84796100	-2.63815800	2.69129000
H	-2.87541400	-2.76361900	3.77919200
H	-3.78819000	-2.18459000	2.36427300
H	-2.75325500	-3.62398900	2.23146700
C	-1.67567800	-0.08156100	3.30448000
H	-1.86316400	-0.41370600	4.33115000
H	-0.77884300	0.53870300	3.27624900
H	-2.52026700	0.51304400	2.94863800
C	0.04714900	-2.38416100	2.95846700
H	-0.08784700	-2.49483100	4.03978600
H	0.18697200	-3.37376000	2.51730800
H	0.93802100	-1.78029700	2.76464200
S	0.78615000	0.11507900	0.58924900
C	1.20682500	1.70474900	-0.16922700

C	2.60012400	1.88291000	-0.40417300
C	0.31858300	2.78648300	-0.39940500
C	3.06125100	3.10903600	-0.89774700
C	0.83090700	3.98917000	-0.91049400
C	2.18720800	4.15796200	-1.16758300
H	4.12920000	3.23131100	-1.05525200
H	0.14185500	4.81306700	-1.07502100
H	2.56086700	5.10356900	-1.54904100
H	4.30865200	1.26514100	-2.89460300
C	3.89572600	0.30640900	-2.55909100
H	2.81754700	0.34022800	-2.73562800
H	4.32695400	-0.48408800	-3.18079100
C	4.21587000	0.06448700	-1.09216700
C	5.16238100	-0.91040900	-0.75122600
C	3.61434900	0.83509900	-0.07279100
C	5.55320400	-1.12172700	0.57322400
H	5.61650000	-1.50189300	-1.54023900
C	4.03376500	0.66031200	1.26870500
C	4.98625400	-0.31740800	1.56815500
C	6.60708800	-2.15727100	0.92369900
C	3.50421200	1.55450100	2.38007200
H	5.30471600	-0.44333000	2.59847900
H	6.74888500	-2.86758200	0.10351400
H	7.57129300	-1.67170300	1.11993300
H	6.32598400	-2.71756900	1.82213000
H	2.41888100	1.45622900	2.49095000
H	3.97262400	1.29145100	3.33315900
H	3.72509200	2.60705000	2.16840500
H	-5.58009700	2.40302700	1.87433300
C	-5.37998000	2.85779200	0.89874700
H	-5.98026900	2.34085000	0.14352800
H	-5.71927000	3.90052200	0.94043000
C	-3.90100500	2.80246000	0.55807100
C	-2.93020000	2.92853900	1.56112900
C	-3.47257200	2.71016300	-0.77014500
C	-1.56223300	2.92684700	1.26643900
H	-3.24694700	3.07059000	2.59051100
C	-2.11176700	2.71148700	-1.10416100
H	-4.21100500	2.66562300	-1.56512600
C	-1.13890100	2.76564400	-0.07558600
C	-0.55037600	3.18938200	2.36922000
C	-1.70312800	2.71238900	-2.56786700
H	-0.07063400	4.16302200	2.21184100
H	-1.04119600	3.20699200	3.34699600

H	0.23954900	2.43257300	2.37919000
H	-1.34405500	3.70548800	-2.86231300
H	-0.89018900	2.00790700	-2.76119500
H	-2.55720000	2.46555600	-3.20652000
H	-2.44672900	0.08515400	0.26080900
H	-1.80447500	0.56320500	-0.01975300
Rh	-1.23645200	-1.09014400	-0.10916300

TS2-b

C	-0.48867000	-3.48903600	-0.57637500
C	-1.78310600	-3.14439500	-1.16273500
C	-1.55138300	-2.16302900	-2.18806300
C	-0.15863800	-1.83886600	-2.18022200
C	0.50186200	-2.68473300	-1.19614000
C	-0.23775500	-4.62262200	0.37544400
H	-0.06664000	-5.54949700	-0.18818000
H	0.64741400	-4.44977500	0.99273800
H	-1.08749600	-4.80655600	1.03824000
C	-3.06310000	-3.90478500	-0.97627500
H	-3.13091600	-4.70510300	-1.72599600
H	-3.12425600	-4.37806600	0.00522600
H	-3.94151100	-3.26575400	-1.10195100
C	-2.58525700	-1.64853500	-3.14553700
H	-2.64667300	-2.31313100	-4.01788300
H	-3.57759000	-1.61312300	-2.68867400
H	-2.34430000	-0.64777700	-3.50869200
C	0.55641700	-0.96757800	-3.16630600
H	1.00028600	-1.58858300	-3.95662500
H	-0.11775700	-0.25688300	-3.64802900
H	1.36690400	-0.40902800	-2.69695500
C	1.97867200	-2.71889600	-0.95000600
H	2.22532000	-3.27320300	-0.04141800
H	2.48476300	-3.21679000	-1.78851500
H	2.40490800	-1.71709800	-0.85114800
P	-1.79042100	-1.53907900	2.10753100
C	-3.19737300	-2.70827200	2.38982100
H	-3.53216600	-2.63731800	3.43018500
H	-4.03110200	-2.45505500	1.72952800
H	-2.89239000	-3.73925700	2.19497400
C	-2.40214100	0.01884900	2.88462000
H	-2.74542200	-0.18308000	3.90479300
H	-1.59405800	0.75245500	2.91025900
H	-3.22206300	0.43747400	2.29601800

C	-0.48958900	-2.12546800	3.28451700
H	-0.88908500	-2.18336000	4.30280200
H	-0.12920100	-3.11366700	2.98683900
H	0.35246700	-1.42776300	3.26752600
S	0.52038500	0.46763500	0.81662100
C	1.03146700	1.88522500	-0.18868500
C	2.42342800	2.05727700	-0.41454300
C	0.11162800	2.89623600	-0.56555700
C	2.85457400	3.22817100	-1.05520600
C	0.59595600	4.03559500	-1.22169800
C	1.95528800	4.20485000	-1.47134600
H	3.91993000	3.36421000	-1.21525600
H	-0.11234100	4.80736500	-1.50915300
H	2.31291000	5.10284400	-1.96661600
H	4.77551400	1.12968400	-2.80262800
C	3.99633900	0.46615200	-2.40546300
H	3.03238400	0.90953400	-2.66233200
H	4.09461300	-0.49742300	-2.91688700
C	4.17364200	0.30123000	-0.90155000
C	5.13244500	-0.61630100	-0.44779400
C	3.46035000	1.08157200	0.03681400
C	5.43511700	-0.75257100	0.90761400
H	5.66798700	-1.21899300	-1.17541500
C	3.80120100	0.99336500	1.41124600
C	4.77036600	0.07475700	1.82061200
C	6.50398000	-1.72303600	1.37771500
C	3.18606500	1.93013500	2.44158600
H	5.02709400	0.01667900	2.87375300
H	6.67042900	-2.51340900	0.63934200
H	7.45583200	-1.19872300	1.53027100
H	6.22266100	-2.18911900	2.32777700
H	2.11755000	1.73448700	2.58577400
H	3.68540100	1.80616000	3.40694600
H	3.29580400	2.97517000	2.13075500
H	-5.80736000	3.13382400	1.63913700
C	-5.61549800	2.88662500	0.59105200
H	-6.07785900	1.91605400	0.37523900
H	-6.11409300	3.63879900	-0.03157900
C	-4.12449100	2.85878800	0.30213400
C	-3.19005800	3.20187400	1.28469700
C	-3.65401600	2.53261200	-0.97573400
C	-1.81384200	3.20553800	1.02485800
H	-3.53923000	3.50214300	2.26765000
C	-2.28769400	2.53444400	-1.27601000

H	-4.36609700	2.30256000	-1.76284100
C	-1.34989100	2.84030900	-0.26071500
C	-0.84445300	3.65789900	2.10412200
C	-1.83472600	2.26078500	-2.70069500
H	-0.30376300	4.55614700	1.78385000
H	-1.38195700	3.89406600	3.02719400
H	-0.09942400	2.88413900	2.32053800
H	-1.46463800	3.17865900	-3.17257400
H	-1.02062900	1.53036700	-2.72887000
H	-2.66960600	1.88687600	-3.30143100
H	-2.06786900	-0.06312900	-0.18068900
H	-1.11701000	0.40558700	0.13298300
Rh	-1.01773800	-1.30923500	-0.13333600

4b

C	1.15034700	3.45523100	1.11908400
C	0.07625600	3.82305000	0.20105700
C	-1.10926600	3.10366600	0.60189300
C	-0.73091200	2.24659600	1.68276800
C	0.65811600	2.47876600	2.02167100
C	2.47990100	4.14351600	1.20256000
H	2.37204700	5.08078200	1.76534600
H	3.22422000	3.53653500	1.72422700
H	2.87617100	4.40699900	0.21827400
C	0.12003800	4.96690400	-0.77090600
H	-0.12978700	5.90637300	-0.25898700
H	1.11149200	5.09068500	-1.21393400
H	-0.59658000	4.83144800	-1.58461700
C	-2.49950100	3.30803300	0.06843800
H	-3.03060100	4.05897800	0.66918800
H	-2.48263500	3.66513700	-0.96459500
H	-3.09069500	2.38829000	0.09443100
C	-1.64973000	1.34695500	2.44644600
H	-2.00038000	1.85596100	3.35487500
H	-2.52362300	1.06915000	1.85609200
H	-1.14571500	0.42848700	2.76096300
C	1.35897600	1.93745400	3.23297000
H	2.44635600	1.95513800	3.11750500
H	1.11402100	2.53896500	4.11970600
H	1.06496900	0.90822100	3.44844200
P	2.44260600	1.38750900	-1.44321800
C	2.87743800	2.84353900	-2.50051800
H	3.79452500	2.64571800	-3.06639400

H	2.06049400	3.04004300	-3.20075100
H	3.03297800	3.73823100	-1.89203200
C	2.46974700	0.00440600	-2.66335100
H	3.39041400	0.05759000	-3.25496600
H	2.44057700	-0.95492100	-2.14218200
H	1.60763300	0.07722500	-3.33170800
C	3.97315600	1.09599900	-0.44674800
H	4.85133400	1.04179400	-1.10083000
H	4.11863500	1.90783900	0.27007100
H	3.87354800	0.15111500	0.09429800
S	-0.32552700	-0.64517000	-0.77932600
C	-0.82517200	-2.11477300	0.18428700
C	0.18908700	-3.00299200	0.59115600
C	-2.19714000	-2.43550400	0.34409700
C	-0.18655000	-4.20519700	1.20733700
C	-2.51448000	-3.66092700	0.94725100
C	-1.52602400	-4.53610500	1.38802000
H	0.59524200	-4.88947100	1.52377900
H	-3.56219300	-3.92344100	1.05729500
H	-1.79909000	-5.47883400	1.85262400
H	1.51451300	-2.80239000	3.27857100
C	1.84310200	-1.90160500	2.74611100
H	0.96661600	-1.25802400	2.61660300
H	2.57140400	-1.38115700	3.37466800
C	2.45603100	-2.26761000	1.40549700
C	3.83951100	-2.17923600	1.21914700
C	1.64435400	-2.76459500	0.36051900
C	4.44487400	-2.58857600	0.02269000
H	4.46022000	-1.81865100	2.03438700
C	2.23985600	-3.18628900	-0.85005500
C	3.63056700	-3.08450700	-0.99921300
C	5.95360700	-2.52683500	-0.13591700
C	1.40281400	-3.78788700	-1.96773100
H	4.08455400	-3.42369000	-1.92496700
H	6.33609600	-1.52751200	0.10284700
H	6.43895100	-3.23990800	0.54124700
H	6.25176200	-2.77494700	-1.15853000
H	0.58668300	-3.11878100	-2.26177400
H	2.02319500	-3.98308500	-2.84700500
H	0.95504000	-4.73619200	-1.64755000
H	-6.03654000	1.97009900	-2.00466800
C	-6.46749400	1.11069100	-1.47660300
H	-7.05899300	1.48685700	-0.63710500
H	-7.14345800	0.59743500	-2.16950000

C	-5.37642200	0.17081200	-0.99625600
C	-4.61578000	-0.56311100	-1.91481500
C	-5.12780200	-0.01479700	0.36643800
C	-3.60214000	-1.43326500	-1.50197300
H	-4.83526200	-0.47885500	-2.97446100
C	-4.12100100	-0.87718000	0.82452300
H	-5.74690300	0.50087900	1.09381600
C	-3.30890100	-1.55292700	-0.11641000
C	-2.89903900	-2.30370500	-2.53506800
C	-3.99720800	-1.12678800	2.32176300
H	-3.07880300	-3.36372800	-2.32096200
H	-3.28576400	-2.08669500	-3.53465200
H	-1.81477200	-2.14841900	-2.54955200
H	-4.53728100	-2.04240800	2.59391100
H	-2.95907800	-1.25162300	2.63766100
H	-4.44300100	-0.30234200	2.88661600
H	-0.08109800	1.78716600	-1.69060500
H	-1.60318400	-0.26930200	-1.02115200
Rh	0.46826200	1.70031300	-0.22216500