

Supporting Information

Mechanism, Selectivity, and Reactivity of Iridium- and Rhodium-Catalyzed Intermolecular Ketone α -Alkylation with Unactivated Olefins via an Enamide Directing Strategy

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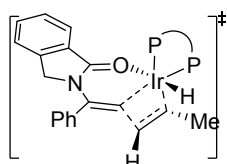
Web: <http://genpinghuang.weebly.com>

[§]These authors contributed equally to this work

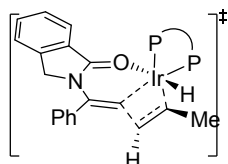
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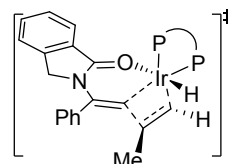
1. Possibilities of migratory insertion into the Ir-C bond.



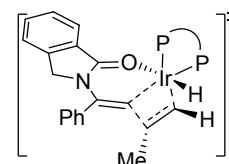
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TS4a



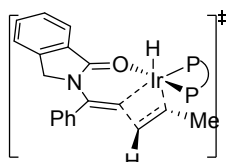
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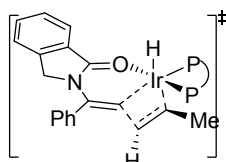
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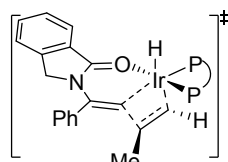
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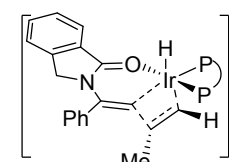
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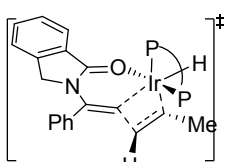
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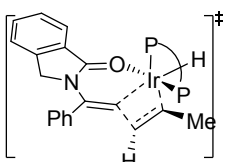
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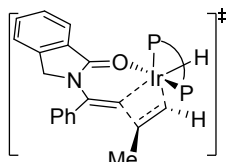
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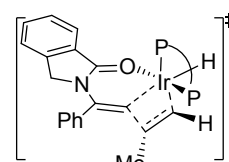
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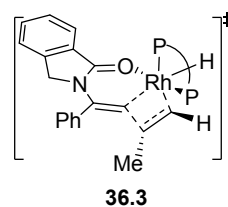
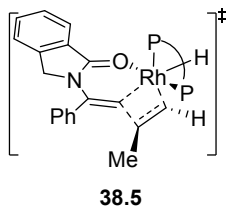
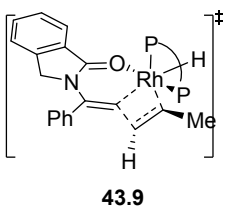
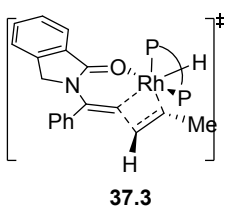
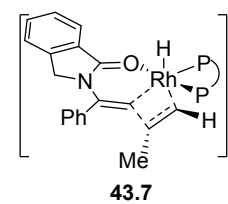
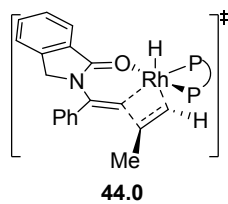
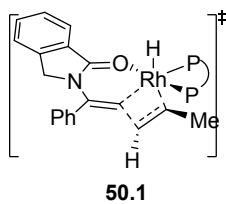
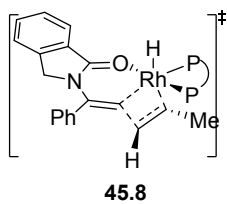
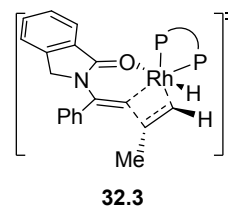
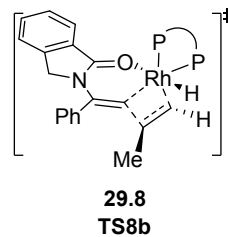
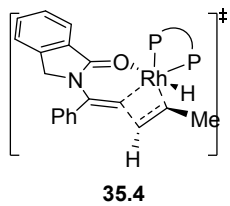
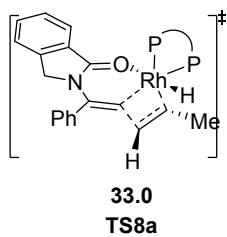


31.8

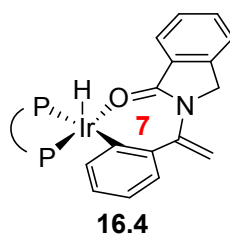
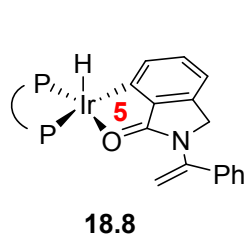


29.5

2. Possibilities of migratory insertion into the Rh-C bond.



3. Intermediates resulted from aromatic C(sp²)-H oxidative addition.



4. Table of calculated energies and energy corrections

Stationary point	Single-point energy- B3LYP 6-311+G(d,p), SDD with DFT-D3(BJ) correction (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	Optimization energy 6-31G(d) , lanl2dz (a.u.)	Solvation energy (a.u.)
2a	-747.7729019	0.207191	-747.5024492	-0.0067879
3a	-117.9535685	0.055102	-117.9060442	-0.0008238
4a	-865.768547	0.287282	-865.4466842	-0.0064069
5a	-865.7665599	0.286709	-865.4464261	-0.0067396
cod	-312.1506082	0.149697	-312.0257964	-0.0013424
[Ir(cod)DIOP] ⁺	-2450.80481	0.666004	-2450.383488	-0.0402285
INT1	-2886.420154	0.721271	-2885.846423	-0.0398697
TS1	-2886.393372	0.716774	-2885.826307	-0.0405951
INT2	-2886.411865	0.717885	-2885.849097	-0.0432361
TS1a	-2886.373295	0.713699	-2885.804908	-0.0404
TS1b	-2886.372525	0.717787	-2885.794364	-0.0416074
INT3a	-3004.389274	0.799099	-3003.745737	-0.038898
INT3b	-3004.389405	0.802229	-3003.742738	-0.0389564
TS2a	-3004.380273	0.797344	-3003.738568	-0.0392394
TS2b	-3004.378233	0.79916	-3003.733975	-0.0393457
INT4a	-3004.395054	0.799266	-3003.772287	-0.04204
INT4b	-3004.393134	0.800279	-3003.764129	-0.0409801
TS3a	-3004.358676	0.799281	-3003.730868	-0.0397065
TS3b	-3004.353403	0.801737	-3003.721009	-0.0396234
INT5a	-3004.421748	0.802551	-3003.79085	-0.0395928
INT5b	-3004.424516	0.802377	-3003.790671	-0.0395316
INT6a	-3004.400305	0.800334	-3003.757215	-0.0392185
INT6b	-3004.394688	0.799456	-3003.752783	-0.0395165
TS4a	-3004.364432	0.799324	-3003.721932	-0.0395966
TS4b	-3004.369116	0.798233	-3003.730671	-0.0403136
INT7a	-3004.387762	0.799853	-3003.759432	-0.0430667
INT7b	-3004.408213	0.802985	-3003.768622	-0.0403976
TS5a	-3004.364858	0.799967	-3003.731073	-0.0399512
TS5b	-3004.370811	0.799332	-3003.734109	-0.0404732
[Rh(cod)DIOP] ⁺	-2456.986477	0.665076	-2455.183908	-0.040075
INT8	-2892.581725	0.716631	-2890.631393	-0.0416097
TS6a	-3010.547241	0.797057	-3008.516062	-0.039057
TS6b	-3010.546226	0.797754	-3008.512299	-0.0391447

INT9a	-3010.566854	0.799	-3008.558149	-0.040656
INT9b	-3010.565491	0.798343	-3008.552004	-0.0401603
TS7a	-3010.544005	0.797987	-3008.533427	-0.0394479
TS7b	-3010.538825	0.800078	-3008.52401	-0.0395198
TS8a	-3010.538002	0.798757	-3008.509413	-0.0392292
TS8b	-3010.541309	0.797757	-3008.516054	-0.0399608
INT10a	-3010.561858	0.79741	-3008.551046	-0.0417991
INT10b	-3010.578391	0.801146	-3008.557352	-0.040304
TS9a	-3010.549459	0.799095	-3008.535482	-0.0396117
TS9b	-3010.552932	0.797998	-3008.536966	-0.0402521

5. Cartesian coordinates

cod

C	0.52272600	1.16375200	6.70902400
H	0.84519300	0.58388900	5.84348300
C	1.06265600	0.66898200	8.03433000
H	0.29652600	0.69129100	8.81347500
H	1.33438400	-0.38818400	7.92171100
C	2.32417100	1.41860900	8.51529700
H	2.70617900	0.91910800	9.42056100
H	3.11529300	1.28366000	7.76256300
C	2.20961700	2.89771500	8.79289500
H	3.17940200	3.38680500	8.90111300
C	1.13358400	3.68326400	8.92698100
H	1.32897800	4.74065400	9.10881900
C	-0.33372400	3.32216200	8.82977500
H	-0.91311200	4.09555000	9.34966900
H	-0.55306800	2.39027200	9.35706500
C	-0.86671000	3.24473400	7.38248700
H	-0.73979400	4.23153600	6.91253700
H	-1.95689000	3.08627000	7.41807800
C	-0.26074000	2.21943400	6.45519000
H	-0.52093900	2.38560400	5.40826500

[Ir(cod)DIOP]⁺

P	-0.41886600	1.70837900	-0.21048400
P	1.48303800	-1.21626200	0.42354400
C	-1.67238200	2.78506200	-1.04562100
C	-3.03741900	2.60941100	-0.76281800
C	-1.29622700	3.76170400	-1.98321000
C	-4.00040500	3.39171700	-1.40165700
H	-3.35207000	1.87764900	-0.02426300
C	-2.26262900	4.54539000	-2.61741700
H	-0.24989200	3.92716200	-2.22221500
C	-3.61579700	4.36101000	-2.33016300
H	-5.05084500	3.24865100	-1.16527600
H	-1.95402500	5.30251300	-3.33245900
H	-4.36580200	4.97290000	-2.82251400
C	-1.08340000	1.63379300	1.50333500
C	-1.06255700	2.76234400	2.34263300
C	-1.70127800	0.46008100	1.95569700
C	-1.62594300	2.70212200	3.61613200
H	-0.61947100	3.69418500	2.00349700
C	-2.27111400	0.40407700	3.23034600
H	-1.73486900	-0.41196300	1.31191800

C	-2.22874200	1.52208900	4.06310200
H	-1.59959800	3.57796700	4.25789000
H	-2.74137100	-0.51470100	3.56811600
H	-2.66761500	1.47965600	5.05571600
C	0.50629600	-2.27223800	1.57049100
C	0.97196400	-2.55183900	2.86577200
C	-0.69467700	-2.85519600	1.13693400
C	0.24056300	-3.38499000	3.71256100
H	1.90752200	-2.12959700	3.21965700
C	-1.42077400	-3.69539500	1.98383200
H	-1.06154400	-2.63777200	0.13748900
C	-0.95552700	-3.95831100	3.27374200
H	0.60867300	-3.59029800	4.71355200
H	-2.34798200	-4.14239400	1.63642000
H	-1.51976100	-4.61065700	3.93393700
C	2.89036400	-2.32310800	-0.04722500
C	2.68451700	-3.70586500	-0.18831100
C	4.17419200	-1.80175100	-0.29050700
C	3.73120300	-4.54461700	-0.57494600
H	1.71356700	-4.13936800	0.03071200
C	5.21779600	-2.64601500	-0.67364800
H	4.38510400	-0.74561700	-0.15844400
C	4.99888300	-4.01676300	-0.82287000
H	3.55534400	-5.61221900	-0.67041900
H	6.20564400	-2.22900300	-0.84699300
H	5.81408600	-4.67031400	-1.11909200
C	1.04979100	2.85956200	-0.12754400
H	1.51443300	2.85225900	-1.11901200
H	0.67963300	3.87505500	0.04765300
C	2.30728200	0.03114000	1.52601300
H	1.57268700	0.35998400	2.26870200
H	3.12317700	-0.45680500	2.06597500
C	2.12944600	2.55564500	0.90818300
H	1.71592700	2.62588600	1.92545200
C	2.89083200	1.23206100	0.76093300
H	2.99637000	1.00795100	-0.31368000
O	3.15856300	3.51827700	0.72282600
O	4.15945000	1.54414700	1.32104000
C	4.39790500	2.96021100	1.18802500
C	5.46317000	3.22519100	0.13118600
H	5.58710800	4.30185700	-0.01985200
H	6.42219400	2.80288900	0.44562100
H	5.17096100	2.77234400	-0.82116400
C	4.75741700	3.51121400	2.56350000

H	5.65743000	3.01973900	2.94553200
H	4.94360800	4.58761200	2.50304700
H	3.93984000	3.33304300	3.26844000
Ir	0.16082700	-0.32701800	-1.37004700
C	0.33752500	-2.27801700	-2.49456700
H	0.61984600	-3.03677900	-1.76943700
C	-0.91430000	-2.60602500	-3.29921300
H	-0.68721200	-2.57804600	-4.36906900
H	-1.20879800	-3.63853100	-3.08410600
C	-2.09716400	-1.67083900	-2.96660900
H	-2.82297700	-1.66063900	-3.79387200
H	-2.63576100	-2.06517100	-2.09721600
C	-1.67825400	-0.25442500	-2.63806300
H	-2.41420300	0.30363600	-2.06153400
C	-0.70881300	0.49844200	-3.31369300
H	-0.75919400	1.57477200	-3.18301000
C	0.06352000	0.03878500	-4.54095000
H	0.23922800	0.90284700	-5.19029500
H	-0.54169900	-0.65957700	-5.12596000
C	1.41763100	-0.59292300	-4.16582900
H	2.15907300	0.20110600	-4.01885900
H	1.79679500	-1.21652000	-4.98993900
C	1.36649600	-1.40883300	-2.89436800
H	2.34260500	-1.57861200	-2.44485500

2a

C	-2.25403700	2.99981100	-0.28671300
C	-1.38350000	2.41730700	-1.20565800
C	-0.04482100	2.17911100	-0.90331800
C	0.41276900	2.54629500	0.36260000
C	-0.45895100	3.13377500	1.29176500
C	-1.80212000	3.36728300	0.97775900
C	-3.62210500	3.11847300	-0.90866900
H	0.60742500	1.72042300	-1.64047200
H	1.45074300	2.37674300	0.63507200
H	-0.08411600	3.41237900	2.27304200
H	-2.46748200	3.82314100	1.70672000
H	-4.37549600	2.52410600	-0.37289200
N	-3.41886700	2.58508900	-2.26391700
C	-2.11441500	2.11041000	-2.46239200
O	-1.68106200	1.56117100	-3.46139200
H	-3.98223800	4.15320800	-0.93622900
C	-4.60521400	1.35499300	-3.96907500
H	-3.89910500	0.53648600	-3.92493000

C	-4.49093900	2.43619000	-3.18083700
H	-5.38207000	1.31829500	-4.72474100
C	-5.45040200	3.57309600	-3.25816300
C	-4.99436800	4.90228000	-3.28786300
C	-6.83148900	3.33581400	-3.33544500
C	-5.89426700	5.96080400	-3.40332400
H	-3.92619500	5.09839500	-3.24523700
C	-7.73157900	4.39524800	-3.45349800
H	-7.19460800	2.31302600	-3.28902800
C	-7.26669600	5.71128400	-3.48632500
H	-5.52324800	6.98184500	-3.43629900
H	-8.79780000	4.19221800	-3.50961500
H	-7.96771200	6.53702800	-3.57291000

INT1

P	-0.75882400	1.41332700	0.03378100
P	1.28463300	-1.41470200	0.20488400
C	-2.22905300	2.29265000	-0.65370000
C	-3.51420300	1.84911200	-0.30544500
C	-2.09802100	3.38194000	-1.52708600
C	-4.64499900	2.48849900	-0.81344200
H	-3.63757200	1.01537300	0.37944200
C	-3.23218000	4.02674000	-2.02536700
H	-1.11834500	3.73888600	-1.82618600
C	-4.50717400	3.58155200	-1.67154700
H	-5.63323800	2.13931100	-0.52808100
H	-3.11549700	4.88295900	-2.68419500
H	-5.38807500	4.08727000	-2.05651000
C	-1.20879000	1.23327500	1.80747800
C	-1.13688000	2.32278900	2.69340900
C	-1.71962400	0.01230100	2.26931300
C	-1.54836800	2.18099700	4.01785000
H	-0.77154200	3.28758600	2.35466200
C	-2.13760900	-0.12492700	3.59518600
H	-1.78491000	-0.83412500	1.59476500
C	-2.04763000	0.95659500	4.47147900
H	-1.48369500	3.02823700	4.69442900
H	-2.52483600	-1.07959300	3.93877300
H	-2.36778100	0.85019600	5.50394900
C	0.52680100	-2.51606800	1.47171000
C	1.13761000	-2.71935400	2.72044200
C	-0.65880700	-3.20352600	1.17472600
C	0.56328400	-3.58034400	3.65584000
H	2.06586000	-2.21525400	2.97049300

C	-1.22751500	-4.07153600	2.10971300
H	-1.13677200	-3.05690700	0.21205000
C	-0.62066900	-4.25773300	3.35307000
H	1.04338200	-3.72452600	4.61952500
H	-2.14297000	-4.60172500	1.86261200
H	-1.06359000	-4.93095500	4.08162300
C	2.71996700	-2.42854500	-0.39178800
C	2.70739900	-3.82855100	-0.29769500
C	3.85491400	-1.79824100	-0.93407800
C	3.80096800	-4.57979700	-0.73636700
H	1.85026200	-4.33799300	0.12855500
C	4.94464800	-2.55188000	-1.37067400
H	3.90964700	-0.71686500	-1.00306400
C	4.92017900	-3.94527300	-1.27515900
H	3.77805300	-5.66232100	-0.64619000
H	5.81652000	-2.04740700	-1.77721800
H	5.77158100	-4.53014500	-1.61111000
C	0.57044100	2.71407400	-0.02163700
H	0.86119100	2.81622000	-1.07217800
H	0.15039500	3.67461500	0.29522500
C	2.16406400	-0.12543800	1.23443200
H	1.50646900	0.13960600	2.06915800
H	3.06341900	-0.57724300	1.66162000
C	1.82570600	2.41918600	0.79697600
H	1.58868500	2.42228700	1.87188400
C	2.59035600	1.13238700	0.45426300
H	2.52780800	0.96651500	-0.63363800
O	2.77733500	3.43034900	0.49726100
O	3.92218600	1.46909500	0.82671000
C	4.09575200	2.89206600	0.69852100
C	4.93315700	3.22194400	-0.53224800
H	4.99219500	4.30589100	-0.67087100
H	5.94721900	2.82728100	-0.41788900
H	4.47966600	2.78241000	-1.42603600
C	4.69783200	3.41526800	1.99797700
H	5.66761100	2.94349000	2.18430200
H	4.83940300	4.49862800	1.94024600
H	4.03514000	3.18960300	2.83871000
Ir	-0.08456300	-0.43528500	-1.36942000
C	-2.52588100	-0.89172000	-5.78254900
C	-2.41737700	0.25736100	-4.98552400
C	-3.00702600	1.46904900	-5.34572900
C	-3.71556700	1.50813800	-6.54599100
C	-3.82673500	0.36269800	-7.34900400

C	-3.23742000	-0.85062900	-6.97614800
C	-1.79004700	-2.03343700	-5.12025300
H	-2.91855900	2.34060700	-4.70513000
H	-4.18887900	2.43178500	-6.86463500
H	-4.38415900	0.41822900	-8.27949600
H	-3.33593900	-1.72842600	-7.60838100
H	-2.43184200	-2.89487700	-4.90589200
N	-1.32016200	-1.41020100	-3.87185600
C	-1.62356500	-0.09849000	-3.80950600
O	-1.23918600	0.63348800	-2.86059600
H	-0.93529300	-2.38843100	-5.71069600
C	0.95644100	-1.42218900	-3.01165700
C	-0.34053500	-1.98917600	-2.96560200
H	1.18065400	-0.68341400	-3.77840100
H	1.80955900	-1.98790600	-2.65918300
C	-0.69218500	-3.37623000	-2.55726300
C	0.25485100	-4.41158700	-2.57196200
C	-2.02160100	-3.68247200	-2.20753600
C	-0.11221500	-5.71259000	-2.22306500
H	1.27629100	-4.20583400	-2.87337100
C	-2.38656000	-4.98248000	-1.86496200
H	-2.76391500	-2.88853700	-2.19894300
C	-1.43028700	-6.00305100	-1.86789800
H	0.63206200	-6.50350900	-2.24670600
H	-3.41717400	-5.20154900	-1.59981500
H	-1.71478400	-7.01849400	-1.60794900

TS1

P	0.42351100	1.89381100	-0.73516200
P	1.91700500	-1.24515100	-0.25110900
C	0.83955100	2.81228200	-2.28019000
C	0.07626100	2.56015100	-3.43476400
C	1.88350600	3.74902100	-2.35060800
C	0.35135800	3.23072900	-4.62587800
H	-0.73809300	1.84463200	-3.39529000
C	2.15655200	4.41641500	-3.54729000
H	2.49129500	3.97280400	-1.48092800
C	1.39338900	4.15906400	-4.68626500
H	-0.24880400	3.02704700	-5.50828100
H	2.96653000	5.13930800	-3.58399300
H	1.60779400	4.67957700	-5.61522100
C	-1.06303800	2.73933900	-0.05334400
C	-1.27554600	4.11081100	-0.26292600
C	-1.96769400	2.01719800	0.73985600

C	-2.37316000	4.74827700	0.31684400
H	-0.59056700	4.68172000	-0.88324800
C	-3.06126800	2.65987400	1.32321100
H	-1.81702300	0.95152800	0.88861900
C	-3.26569100	4.02502300	1.11199800
H	-2.52993900	5.80981500	0.14761600
H	-3.75382600	2.09314300	1.93925300
H	-4.11742500	4.52462300	1.56494700
C	2.02965500	-3.08900100	-0.22633700
C	1.23943400	-3.81674600	0.67970200
C	2.84727500	-3.78721800	-1.12673400
C	1.28287200	-5.21093100	0.69672500
H	0.58771200	-3.30123000	1.38008500
C	2.88402300	-5.18407300	-1.11136400
H	3.46232200	-3.24606800	-1.83850500
C	2.10670500	-5.89794100	-0.19893000
H	0.67741600	-5.75933600	1.41292000
H	3.52581200	-5.71074500	-1.81181400
H	2.14290800	-6.98342800	-0.18299300
C	3.48607300	-0.70772000	-1.04014400
C	4.73359000	-0.97526100	-0.44784400
C	3.44539300	-0.03808600	-2.27188900
C	5.91143800	-0.56961100	-1.07360400
H	4.79115100	-1.50826800	0.49729000
C	4.62768400	0.36627600	-2.89750400
H	2.48606800	0.16255100	-2.74074500
C	5.85988700	0.10316600	-2.29850900
H	6.86941400	-0.77983800	-0.60687300
H	4.58165300	0.88494400	-3.85062500
H	6.77961700	0.41722800	-2.78366700
C	1.75722200	2.41648300	0.44684100
H	2.73291600	2.26244000	-0.02625700
H	1.63558800	3.48978600	0.62438200
C	2.12940100	-0.87954900	1.57068500
H	1.16019900	-1.05895200	2.04775600
H	2.82750600	-1.62004100	1.97553300
C	1.70244000	1.70661100	1.80129100
H	0.67137200	1.41602600	2.05867800
C	2.63817000	0.50218700	1.96904700
H	3.58769900	0.72006200	1.45649500
O	2.21615100	2.60292300	2.78091300
O	2.83899200	0.47975200	3.37811000
C	2.75862800	1.83101000	3.86583200
C	4.14859600	2.37178100	4.18298600

H	4.08854300	3.42568600	4.47192800
H	4.59618000	1.80682500	5.00615000
H	4.79575800	2.28931300	3.30467500
C	1.81552200	1.84728600	5.06387900
H	2.19163600	1.18617600	5.85078600
H	1.73207500	2.86117400	5.46652100
H	0.82060200	1.50257800	4.76652800
Ir	-0.00190300	-0.45105400	-1.20105300
C	-4.93524800	-1.00637600	-3.06805000
C	-4.15738100	0.05918300	-2.60621800
C	-4.70326800	1.31544300	-2.33583200
C	-6.06992100	1.48102500	-2.55484700
C	-6.85542700	0.41601900	-3.02343500
C	-6.29871700	-0.84087000	-3.28422700
C	-4.05667100	-2.21331100	-3.24590000
H	-4.08243600	2.12415000	-1.96414400
H	-6.53541100	2.44217700	-2.35933900
H	-7.91836600	0.57012100	-3.18450300
H	-6.92015900	-1.65666600	-3.64217300
H	-4.33380100	-3.04830200	-2.59181800
N	-2.71423900	-1.71074300	-2.86089100
C	-2.78061300	-0.41031100	-2.45591500
O	-1.82718800	0.28562100	-2.01866600
H	-4.04606200	-2.58629200	-4.27275300
C	-0.46006200	-2.24428600	-2.08816300
C	-1.56918900	-2.54157600	-2.82252700
H	-0.75210800	-1.80542500	-0.65096000
H	0.30982500	-3.00767900	-2.12119400
C	-1.60942100	-3.75977200	-3.67820000
C	-1.83694100	-3.66549900	-5.06315000
C	-1.36916000	-5.02345600	-3.11593900
C	-1.83146900	-4.80816700	-5.86116300
H	-1.98912100	-2.68979800	-5.51862600
C	-1.36553500	-6.16583300	-3.91730000
H	-1.19013700	-5.10597200	-2.04765100
C	-1.60000400	-6.06238100	-5.28945800
H	-1.99780900	-4.71902100	-6.93090300
H	-1.18479100	-7.13773600	-3.46713300
H	-1.59882200	-6.95241800	-5.91187000
INT2			
P	0.38598700	1.92546400	-0.69654300
P	1.95356800	-1.25296200	-0.35503500
C	0.84530300	2.87081000	-2.21428100

C	0.12460700	2.61713500	-3.39609800
C	1.87970600	3.82034000	-2.24670500
C	0.43222000	3.29511700	-4.57548100
H	-0.68712600	1.89679400	-3.38630600
C	2.18590200	4.49573300	-3.43082000
H	2.45300200	4.04972600	-1.35514500
C	1.46577300	4.23441700	-4.59693000
H	-0.13684400	3.09006300	-5.47798700
H	2.98737800	5.22903300	-3.43679000
H	1.70593600	4.76147300	-5.51583400
C	-1.10439400	2.79559800	-0.04661900
C	-1.26623900	4.17965000	-0.22179900
C	-2.07020500	2.08413800	0.68094000
C	-2.36784800	4.83678000	0.32638400
H	-0.53637000	4.74604300	-0.79304800
C	-3.16929500	2.74507100	1.23360500
H	-1.96890300	1.01110900	0.80759600
C	-3.32006300	4.12139200	1.05693900
H	-2.48181200	5.90752900	0.18280100
H	-3.90764000	2.18278800	1.79840900
H	-4.17582900	4.63540800	1.48540400
C	2.11790200	-3.08983700	-0.38817500
C	1.38005200	-3.86579700	0.52166200
C	2.92835100	-3.73546700	-1.33307000
C	1.47266900	-5.25721900	0.50140100
H	0.72877900	-3.39082600	1.24986400
C	3.01286700	-5.12976700	-1.35520100
H	3.50096600	-3.15577500	-2.04982400
C	2.29068500	-5.89213600	-0.43683700
H	0.90824300	-5.84437900	1.22030200
H	3.64829100	-5.61650200	-2.08943500
H	2.36388300	-6.97575100	-0.45084300
C	3.49665900	-0.64866500	-1.14440600
C	4.75624500	-0.92129500	-0.58033600
C	3.43026300	0.07478900	-2.34384900
C	5.91882600	-0.46729700	-1.20118200
H	4.83495000	-1.49554600	0.33863300
C	4.59701500	0.52589100	-2.96625200
H	2.46501100	0.29065800	-2.79374400
C	5.84076100	0.25769500	-2.39440100
H	6.88585100	-0.68103300	-0.75529400
H	4.52928400	1.08661100	-3.89378700
H	6.74876600	0.60896900	-2.87598700
C	1.69410300	2.42985500	0.52598200

H	2.67738500	2.33762700	0.05246800
H	1.53818200	3.48573700	0.76853800
C	2.16633800	-0.93050900	1.47208200
H	1.21027500	-1.15940300	1.95424100
H	2.89141900	-1.66159900	1.84480100
C	1.66536000	1.63621500	1.83411700
H	0.64352100	1.30298500	2.07921900
C	2.63856600	0.45024300	1.92214500
H	3.57028200	0.72063000	1.40173900
O	2.16187400	2.48583700	2.86271100
O	2.87080800	0.35723700	3.32337100
C	2.73147500	1.66949000	3.89767200
C	4.09684300	2.24451200	4.25722400
H	3.99225000	3.27230200	4.61837400
H	4.56658700	1.64293100	5.04109200
H	4.74753100	2.25031100	3.37765800
C	1.78526900	1.56759600	5.08952600
H	2.18653000	0.87219600	5.83328500
H	1.65840500	2.54840100	5.55753900
H	0.80599500	1.20220000	4.76574500
Ir	-0.00156700	-0.43384200	-1.24877600
C	-4.91370500	-0.97386600	-3.18342300
C	-4.13084600	0.08907000	-2.72332600
C	-4.66105100	1.36186400	-2.50496800
C	-6.01649900	1.54658100	-2.77399100
C	-6.80649900	0.48447800	-3.24119000
C	-6.26552600	-0.78894200	-3.45028700
C	-4.05097700	-2.19930700	-3.30123100
H	-4.03802200	2.16921100	-2.13403900
H	-6.46932900	2.52115000	-2.61930900
H	-7.86029000	0.65382700	-3.44210200
H	-6.89011900	-1.60243200	-3.80805100
H	-4.36443900	-3.01559500	-2.64056900
N	-2.71420800	-1.71218100	-2.87954500
C	-2.77035900	-0.40611100	-2.51885400
O	-1.81310500	0.28858300	-2.07392600
H	-4.00950200	-2.59538100	-4.31867300
C	-0.46078400	-2.21720600	-2.07124900
C	-1.57971700	-2.55682700	-2.77095400
H	-0.59234400	-0.70423700	0.16617500
H	0.27455700	-3.01820700	-2.08292600
C	-1.68082700	-3.86266200	-3.48897000
C	-1.84726500	-3.91446700	-4.88429300
C	-1.55401200	-5.06602500	-2.77846600

C	-1.89415900	-5.13955000	-5.54828900
H	-1.91084000	-2.99007300	-5.45393200
C	-1.60332700	-6.29163200	-3.44464000
H	-1.41625700	-5.03436000	-1.70145500
C	-1.77720600	-6.33202100	-4.82898400
H	-2.01192800	-5.16344600	-6.62797500
H	-1.50923200	-7.21505900	-2.88024600
H	-1.81632800	-7.28603800	-5.34671900

3a

C	-2.74074100	0.89785000	-0.07009600
C	-1.41918200	0.84752800	-0.24285500
H	-3.29169700	1.83240300	-0.13460600
H	-3.32311200	0.00338700	0.14347300
H	-0.88034000	1.77259200	-0.45412700
C	-0.58285800	-0.39830100	-0.17083100
H	0.18550500	-0.31795300	0.61004400
H	-1.19456300	-1.28134700	0.04322800
H	-0.05066300	-0.57393500	-1.11596200

INT3a

P	0.92543100	0.41701300	-3.23038000
P	2.05717900	-1.31262900	-0.35605900
C	0.52809600	-0.43424700	-4.81968300
C	-0.74743700	-0.25984300	-5.38412700
C	1.44958400	-1.25747600	-5.48510100
C	-1.09305900	-0.89789500	-6.57471900
H	-1.46373100	0.40490900	-4.91231800
C	1.10125600	-1.89599900	-6.67869600
H	2.45045800	-1.40133000	-5.09340500
C	-0.17058800	-1.72192100	-7.22477400
H	-2.07803900	-0.73681100	-7.00421500
H	1.83302000	-2.51799200	-7.18654300
H	-0.43674300	-2.21131300	-8.15720500
C	0.31052200	2.13430000	-3.54097200
C	0.58483600	2.72879300	-4.78668200
C	-0.35718000	2.88779900	-2.56589800
C	0.20710900	4.04522400	-5.04473000
H	1.08967400	2.16417000	-5.56516700
C	-0.73585100	4.20695100	-2.82876000
H	-0.58180900	2.44368400	-1.60480900
C	-0.45469600	4.78876200	-4.06461300
H	0.43127500	4.48885100	-6.01046200
H	-1.24880300	4.77953500	-2.06082600

H	-0.74798600	5.81533700	-4.26501800
C	1.89438700	-2.21940800	1.24442100
C	2.08991100	-1.58954400	2.48328300
C	1.53643200	-3.57885000	1.22299300
C	1.93545700	-2.30485300	3.67387600
H	2.37418300	-0.54303100	2.53513600
C	1.38172400	-4.28914200	2.41284100
H	1.39251000	-4.08914500	0.27493100
C	1.58092500	-3.65342200	3.64134100
H	2.09828200	-1.80508000	4.62434400
H	1.11195800	-5.34075500	2.37974300
H	1.46472400	-4.20875100	4.56739800
C	3.09029100	-2.49545300	-1.32980100
C	4.29373400	-2.96022400	-0.76629200
C	2.72598600	-2.94102800	-2.60628600
C	5.11466700	-3.83692100	-1.47270900
H	4.58927100	-2.64715500	0.23102500
C	3.54751800	-3.82759600	-3.30967000
H	1.79376300	-2.61281700	-3.04876300
C	4.74288600	-4.27341500	-2.74785500
H	6.04168500	-4.18360400	-1.02544600
H	3.24389600	-4.17215500	-4.29423500
H	5.38071800	-4.96191000	-3.29451800
C	2.76382900	0.67770300	-3.33056600
H	3.27213400	-0.28561200	-3.43167800
H	2.95231900	1.24732400	-4.24555000
C	3.25223900	0.05145600	0.07636500
H	2.67866600	0.84931700	0.55726500
H	3.96472500	-0.33937300	0.81016800
C	3.34787200	1.46372600	-2.15094800
H	2.58874900	2.10657500	-1.68068900
C	4.06504800	0.63202600	-1.07841500
H	4.62917300	-0.17158000	-1.57617700
O	4.42251100	2.25836400	-2.64516500
O	4.96366700	1.58347900	-0.52161300
C	5.33283700	2.50989100	-1.56102300
C	6.74669900	2.22575100	-2.05518600
H	6.99015000	2.87569400	-2.90140800
H	7.47073300	2.40508600	-1.25482100
H	6.83038800	1.18491500	-2.38171000
C	5.15285100	3.92406900	-1.01999200
H	5.78466500	4.07567400	-0.13930600
H	5.42953200	4.65907300	-1.78176400
H	4.11024800	4.08941700	-0.73226800

Ir	0.04621700	-0.53704100	-1.21966200
C	-4.71066800	-0.73345500	-3.73800100
C	-3.96289300	0.23161300	-3.05885700
C	-4.39741300	1.55217700	-2.93465000
C	-5.62352700	1.88353400	-3.51033300
C	-6.38176800	0.91618700	-4.18792200
C	-5.93385300	-0.40366800	-4.31141600
C	-3.96155400	-2.03409800	-3.70021900
H	-3.79378500	2.28985500	-2.41597200
H	-5.99815800	2.89989000	-3.43569300
H	-7.33443200	1.19837800	-4.62652300
H	-6.52977800	-1.14178500	-4.84076000
H	-4.51855500	-2.83689200	-3.20753200
N	-2.74391200	-1.70675900	-2.92460300
C	-2.73403300	-0.40204300	-2.56648800
O	-1.84336200	0.23015100	-1.92706800
H	-3.67657800	-2.39562000	-4.69454500
C	-0.55926300	-2.38417600	-2.06517400
C	-1.71464600	-2.68249600	-2.68595600
H	0.52726300	0.96167100	-0.68131000
H	0.06652500	-3.26710000	-1.94767600
C	-2.04403500	-4.06728300	-3.15855300
C	-1.48811600	-4.56310000	-4.34777200
C	-2.88251400	-4.90603000	-2.40547500
C	-1.76234900	-5.86530100	-4.77219600
H	-0.83848700	-3.92223400	-4.93773500
C	-3.15887000	-6.20594000	-2.83104500
H	-3.30702700	-4.54038500	-1.47318400
C	-2.59962200	-6.68829800	-4.01700100
H	-1.32237500	-6.23627400	-5.69398800
H	-3.80404300	-6.84428200	-2.23367600
H	-2.81287600	-7.70086800	-4.34759300
C	-1.19884200	-1.37116000	0.48565200
C	-0.78650500	-0.11808700	0.94243700
H	-0.72197700	-2.27447700	0.84451100
H	-2.20365400	-1.49397800	0.09321900
H	0.08356900	-0.08921900	1.59073000
C	-1.69497300	1.08041800	1.04499900
H	-1.13258400	2.01816100	1.02690600
H	-2.43807800	1.09800900	0.24619000
H	-2.22581000	1.02933000	2.00628000
INT3b			
P	0.87786600	0.30600500	-3.13392800

P	2.20540500	-1.38330200	-0.31419900
C	0.40489700	-0.54282500	-4.70611000
C	-0.86081800	-0.30064300	-5.26749200
C	1.27135600	-1.42921300	-5.36552300
C	-1.25090200	-0.93400600	-6.44765100
H	-1.53494500	0.41263100	-4.80453800
C	0.87913100	-2.06137700	-6.54850900
H	2.26417500	-1.62752400	-4.97750400
C	-0.38354300	-1.82022400	-7.09065500
H	-2.22665400	-0.71848200	-6.87440000
H	1.57033500	-2.73160200	-7.05188900
H	-0.68366000	-2.30603700	-8.01454900
C	0.25524200	2.02718900	-3.41221000
C	0.49726100	2.63144600	-4.66018200
C	-0.38416400	2.77503400	-2.41360700
C	0.11595500	3.95061200	-4.89783200
H	0.97978200	2.07258900	-5.45666300
C	-0.76710800	4.09684800	-2.65643500
H	-0.58410900	2.32503600	-1.44999600
C	-0.51781500	4.68784400	-3.89467900
H	0.31611400	4.40140800	-5.86550300
H	-1.25783100	4.66417000	-1.87033800
H	-0.81361900	5.71669500	-4.07905100
C	2.15780300	-2.27621000	1.30232800
C	2.38684400	-1.61891500	2.52115400
C	1.85514600	-3.64917200	1.31794700
C	2.31833100	-2.31970500	3.72786600
H	2.63128100	-0.56137000	2.54475600
C	1.78626100	-4.34514300	2.52432700
H	1.68630800	-4.18065600	0.38582700
C	2.01753900	-3.68179400	3.73231100
H	2.50570200	-1.79809500	4.66192000
H	1.55845500	-5.40715300	2.51961300
H	1.96799100	-4.22580400	4.67096600
C	3.18533800	-2.56484100	-1.34092300
C	4.44800900	-2.97839600	-0.87559600
C	2.71536800	-3.07080800	-2.55894200
C	5.22380500	-3.86209900	-1.62287500
H	4.82672800	-2.62004000	0.07742600
C	3.49263900	-3.96436600	-3.30296400
H	1.73578000	-2.78342200	-2.92086500
C	4.74753700	-4.35759000	-2.84043600
H	6.19765200	-4.16816700	-1.25203200
H	3.10846900	-4.35600400	-4.24072700

H	5.35095300	-5.05120600	-3.41875500
C	2.70894600	0.56044900	-3.33507600
H	3.20761100	-0.40725900	-3.43990300
H	2.85070800	1.10604300	-4.27259600
C	3.40804200	-0.00293900	0.03751800
H	2.85255100	0.79458500	0.53984400
H	4.16304900	-0.37619900	0.73699200
C	3.35412100	1.37476600	-2.20802300
H	2.61621400	2.01545800	-1.70262900
C	4.14735600	0.57341500	-1.16763200
H	4.69598700	-0.22861800	-1.68489100
O	4.38512800	2.17565100	-2.77908000
O	5.05939600	1.54875500	-0.67860700
C	5.34434200	2.47025900	-1.74977300
C	6.73706800	2.21932300	-2.31586000
H	6.91455400	2.86265300	-3.18325800
H	7.49773200	2.43258800	-1.55896700
H	6.83378800	1.17621300	-2.63120200
C	5.15204900	3.88671200	-1.21858000
H	5.82268900	4.06797100	-0.37292200
H	5.36934300	4.61812200	-2.00274500
H	4.12110900	4.02790200	-0.88027800
Ir	0.13350600	-0.62989100	-1.05740000
C	-4.55595200	-0.73666500	-3.65969200
C	-3.85520900	0.18816800	-2.88128400
C	-4.30016500	1.50024600	-2.71197000
C	-5.48759300	1.86477600	-3.34576900
C	-6.19752600	0.93835500	-4.12515800
C	-5.73935900	-0.37305500	-4.29309100
C	-3.81106700	-2.03999400	-3.64226500
H	-3.73429100	2.20655800	-2.11351700
H	-5.86925900	2.87546500	-3.23752100
H	-7.12047100	1.24586500	-4.60808400
H	-6.29814500	-1.07969400	-4.90025800
H	-4.40136100	-2.86337400	-3.22954000
N	-2.64665000	-1.75836500	-2.77375400
C	-2.65500500	-0.47168100	-2.35354500
O	-1.79920200	0.12560000	-1.63715300
H	-3.46006700	-2.35004200	-4.63317800
C	-0.51757600	-2.48883600	-1.82432100
C	-1.65980900	-2.76280500	-2.48274800
H	0.64926800	0.89076800	-0.62442800
H	0.07010800	-3.39052300	-1.65781600
C	-2.01201500	-4.14496300	-2.94686800

C	-1.35580200	-4.70556800	-4.05325500
C	-2.96785000	-4.92064000	-2.26887400
C	-1.64370700	-6.00780500	-4.46830700
H	-0.62009000	-4.11197500	-4.58899200
C	-3.25784200	-6.22042200	-2.68477900
H	-3.47579300	-4.50804500	-1.40001800
C	-2.59603800	-6.76739400	-3.78698800
H	-1.12519800	-6.42780600	-5.32600300
H	-3.99380400	-6.80889700	-2.14387400
H	-2.82007000	-7.78011000	-4.10982900
C	-0.50443500	-0.14956900	1.07695300
C	-0.98974700	-1.44060200	0.86574900
H	0.39216800	0.02113600	1.65980500
H	-1.18523500	0.69534600	1.01902500
H	-0.37798200	-2.27398600	1.19308200
C	-2.45731700	-1.74590100	0.73033600
H	-2.83126500	-2.05562500	1.71612700
H	-3.03424000	-0.87260800	0.41758900
H	-2.64090700	-2.57203000	0.03887200

TS2a

P	0.90510100	0.47068300	-3.23271600
P	2.01836700	-1.35967500	-0.38666400
C	0.46491100	-0.32561400	-4.84086600
C	-0.81994100	-0.11802500	-5.37206300
C	1.35100000	-1.16015700	-5.53978800
C	-1.20939800	-0.73428900	-6.56083000
H	-1.51052100	0.55405000	-4.87254400
C	0.95919100	-1.77723400	-6.73135200
H	2.35927600	-1.32824100	-5.17697600
C	-0.32208400	-1.57064400	-7.24305900
H	-2.20134300	-0.54677400	-6.96290300
H	1.66460800	-2.40827300	-7.26485500
H	-0.62210200	-2.04432600	-8.17332500
C	0.31769800	2.20679800	-3.48798700
C	0.58885900	2.84996700	-4.70961000
C	-0.34444400	2.92250300	-2.48249500
C	0.21341800	4.17650100	-4.91276800
H	1.08783400	2.31383300	-5.51170700
C	-0.72060900	4.25264000	-2.68770000
H	-0.56890500	2.43857700	-1.54028000
C	-0.44235500	4.88217000	-3.90053200
H	0.43383800	4.65847500	-5.86088400
H	-1.23035700	4.79509200	-1.89611100

H	-0.73405300	5.91649700	-4.05897100
C	1.84555400	-2.23557600	1.22931000
C	2.08367600	-1.59931600	2.45713300
C	1.41171600	-3.57295000	1.23062800
C	1.89948900	-2.28778100	3.65973500
H	2.42545700	-0.56953400	2.49308200
C	1.22899600	-4.25643400	2.43162200
H	1.22403200	-4.08594000	0.29167300
C	1.47257300	-3.61513800	3.64970700
H	2.09605700	-1.78356500	4.60148800
H	0.90066000	-5.29167400	2.41617900
H	1.33307300	-4.14993600	4.58459700
C	3.04639100	-2.55621100	-1.34688200
C	4.19502900	-3.09191000	-0.73484300
C	2.75047800	-2.92379100	-2.66584000
C	5.02899700	-3.96359900	-1.43247000
H	4.43703200	-2.83781200	0.29302100
C	3.58486200	-3.80434800	-3.36075300
H	1.85929400	-2.54296800	-3.14870900
C	4.72550100	-4.32249500	-2.74878100
H	5.91256500	-4.36647000	-0.94608000
H	3.33400000	-4.08875200	-4.37880600
H	5.37278300	-5.00695100	-3.28934900
C	2.74663600	0.70706600	-3.37092400
H	3.23744200	-0.26084900	-3.50909200
H	2.93276000	1.30222900	-4.26990700
C	3.22865000	-0.00148400	0.02821300
H	2.67395900	0.81005500	0.50951000
H	3.93668700	-0.39976100	0.76234500
C	3.36230000	1.44225700	-2.17590200
H	2.62511700	2.09762100	-1.68583300
C	4.05446000	0.56255500	-1.12572200
H	4.58336900	-0.25404200	-1.64036300
O	4.45812800	2.21523100	-2.65631200
O	4.99305900	1.46802000	-0.55644900
C	5.38876000	2.40340100	-1.57719100
C	6.78521300	2.07503000	-2.09350500
H	7.04655000	2.73575600	-2.92593100
H	7.52386200	2.20455400	-1.29686900
H	6.82351100	1.04032100	-2.44685700
C	5.27164300	3.81056900	-1.00162100
H	5.91822500	3.91661200	-0.12498900
H	5.56958600	4.55138100	-1.74961500
H	4.23950400	4.01092400	-0.69871800

Ir	0.00576600	-0.58267200	-1.24508300
C	-4.71089100	-0.88508300	-3.78340400
C	-4.00428000	0.09998800	-3.08851000
C	-4.48547700	1.40387900	-2.96019900
C	-5.71614900	1.69722600	-3.54685300
C	-6.43329200	0.70948300	-4.23937700
C	-5.93860800	-0.59317500	-4.36743200
C	-3.91741900	-2.15955100	-3.74841200
H	-3.91420700	2.15894600	-2.42973900
H	-6.12621700	2.69958200	-3.46921300
H	-7.39038400	0.96197600	-4.68633800
H	-6.50283800	-1.34731800	-4.90877100
H	-4.45220700	-2.98587600	-3.27061400
N	-2.72209900	-1.79646000	-2.95498100
C	-2.76002700	-0.49573100	-2.58967100
O	-1.89096400	0.15578000	-1.93987700
H	-3.60625400	-2.49965100	-4.74254800
C	-0.50442600	-2.39528700	-2.11086100
C	-1.66114500	-2.73224800	-2.71361500
H	0.27253500	0.88143000	-0.37887200
H	0.15143200	-3.25576600	-1.99916800
C	-1.94389100	-4.13316200	-3.16640400
C	-1.34967000	-4.63515400	-4.33416200
C	-2.77658600	-4.97987400	-2.41542900
C	-1.57971900	-5.95195600	-4.73954100
H	-0.70678500	-3.98647600	-4.92312900
C	-3.00932300	-6.29397400	-2.82270100
H	-3.22963500	-4.60902100	-1.49878700
C	-2.41121600	-6.78298400	-3.98692900
H	-1.11052200	-6.32764100	-5.64482700
H	-3.65025400	-6.93842300	-2.22731500
H	-2.59045200	-7.80680900	-4.30271000
C	-1.11342100	-1.06413300	0.55954400
C	-0.66068200	0.26032800	0.87745400
H	-0.69302500	-1.90142600	1.10404100
H	-2.16175400	-1.17898500	0.29184800
H	0.18858400	0.32342400	1.55438200
C	-1.62177700	1.42491500	0.96179300
H	-1.10459400	2.38928900	0.97306100
H	-2.33411100	1.40803000	0.13422300
H	-2.18552500	1.33364800	1.89964000
TS2b			
P	0.86490100	0.37094200	-3.14823200

P	2.16211100	-1.43636300	-0.35509600
C	0.36445800	-0.42076500	-4.74298200
C	-0.90523700	-0.14827100	-5.28087000
C	1.20198000	-1.31551400	-5.42844800
C	-1.32728700	-0.75951200	-6.46203700
H	-1.55957600	0.56897400	-4.79581700
C	0.77809200	-1.92595700	-6.61188200
H	2.19796200	-1.53629400	-5.06052000
C	-0.48843500	-1.65447200	-7.13015500
H	-2.30619800	-0.52041400	-6.86865800
H	1.44776900	-2.60316300	-7.13479800
H	-0.81307300	-2.12374000	-8.05433900
C	0.26301400	2.10816700	-3.36973700
C	0.52204500	2.77306100	-4.58253900
C	-0.39701800	2.80487300	-2.34888400
C	0.13836000	4.10061800	-4.76202800
H	1.01866900	2.25350100	-5.39679000
C	-0.78154700	4.13620600	-2.53031900
H	-0.61771800	2.30506100	-1.41440200
C	-0.51399800	4.78679300	-3.73435300
H	0.35069300	4.59888400	-5.70353200
H	-1.28881900	4.66279500	-1.72657900
H	-0.81127300	5.82222400	-3.87398100
C	2.11819100	-2.32265500	1.26459200
C	2.37885200	-1.67027500	2.47963900
C	1.75854300	-3.68141800	1.28714100
C	2.28864400	-2.36350200	3.68960200
H	2.66295900	-0.62260300	2.49922500
C	1.66884000	-4.36973000	2.49604900
H	1.55738300	-4.20765000	0.35852100
C	1.93386600	-3.71225500	3.70063900
H	2.50087400	-1.84630400	4.62085000
H	1.39669600	-5.42124900	2.49672900
H	1.86683500	-4.25044000	4.64156100
C	3.14741700	-2.60830700	-1.38601400
C	4.37776200	-3.07172600	-0.88284800
C	2.72892800	-3.04055200	-2.65060900
C	5.17237900	-3.93305100	-1.63669700
H	4.71586200	-2.76929000	0.10415600
C	3.52453500	-3.91180200	-3.40109400
H	1.77406400	-2.71592300	-3.04497200
C	4.74722900	-4.35564300	-2.89954700
H	6.12061700	-4.27862800	-1.23546000
H	3.17993500	-4.24675000	-4.37548400

H	5.36471100	-5.03208600	-3.48332500
C	2.69778200	0.61615800	-3.37359900
H	3.18527500	-0.35213100	-3.51967900
H	2.84019300	1.19652000	-4.28977700
C	3.36728100	-0.05528000	-0.00491300
H	2.82338600	0.74921000	0.50023800
H	4.11605600	-0.43620000	0.69713700
C	3.36279500	1.37444400	-2.22011300
H	2.64116200	2.02217100	-1.69772000
C	4.12504700	0.51886400	-1.19974500
H	4.64526100	-0.29009600	-1.73469200
O	4.41823200	2.16240300	-2.76255600
O	5.07000600	1.44888400	-0.68377100
C	5.39144400	2.38682800	-1.72888800
C	6.77139900	2.09374300	-2.30647700
H	6.97378100	2.75289400	-3.15635100
H	7.54208000	2.25362800	-1.54653800
H	6.82375100	1.05677600	-2.65122000
C	5.26046000	3.79484600	-1.15816700
H	5.94067000	3.92479700	-0.31069100
H	5.50593000	4.53783300	-1.92288300
H	4.23724900	3.96993000	-0.81226900
Ir	0.08731600	-0.68679400	-1.09010400
C	-4.55230900	-0.88772600	-3.74186500
C	-3.88413600	0.06037400	-2.96245100
C	-4.36165800	1.36317200	-2.81125300
C	-5.54897700	1.69399000	-3.46366400
C	-6.22680800	0.74404100	-4.24318100
C	-5.73579800	-0.55770000	-4.39317700
C	-3.77605800	-2.17263000	-3.70577800
H	-3.82069300	2.08857100	-2.21235000
H	-5.95547500	2.69641000	-3.36993400
H	-7.15034700	1.02536500	-4.74070000
H	-6.26982100	-1.28263300	-5.00102200
H	-4.35279600	-3.01005300	-3.30316600
N	-2.63577000	-1.85795700	-2.81655000
C	-2.67671100	-0.56712400	-2.41468100
O	-1.83680700	0.05068900	-1.69810500
H	-3.39661000	-2.47258500	-4.68944300
C	-0.46534200	-2.51157200	-1.89476700
C	-1.61995500	-2.82544000	-2.51618400
H	0.38177400	0.81894700	-0.31882300
H	0.14754300	-3.39364900	-1.72150300
C	-1.94981200	-4.23171100	-2.91495200

C	-1.26879200	-4.84458000	-3.97727700
C	-2.91220100	-4.97738100	-2.21256300
C	-1.53854900	-6.16997700	-4.32609100
H	-0.53002600	-4.27256700	-4.53209100
C	-3.18499000	-6.29951200	-2.56372500
H	-3.43593900	-4.52262100	-1.37463000
C	-2.49808300	-6.89945100	-3.62246200
H	-1.00131100	-6.63100600	-5.15048300
H	-3.92622000	-6.86449100	-2.00525100
H	-2.70863500	-7.92983800	-3.89439100
C	-0.40797800	0.20913800	0.97564400
C	-0.88155200	-1.14392300	0.84621900
H	0.43964600	0.41579000	1.62339900
H	-1.14133700	1.01314800	0.93771800
H	-0.29298600	-1.89598900	1.36064500
C	-2.36605600	-1.44600600	0.84926400
H	-2.70658000	-1.59052500	1.88365600
H	-2.95545200	-0.63388400	0.41687900
H	-2.58486300	-2.36874600	0.30266900

INT4a

P	1.09709800	0.63954800	-3.41725000
P	1.94899300	-1.88567700	-1.00241000
C	1.20989900	0.04241900	-5.16438500
C	0.33951700	-0.96654500	-5.61051900
C	2.14027800	0.57459300	-6.07357700
C	0.40754100	-1.44102300	-6.92234700
H	-0.40882400	-1.37131800	-4.93685600
C	2.20810600	0.09865100	-7.38363200
H	2.81568500	1.36849600	-5.77250900
C	1.34523300	-0.91284600	-7.81072500
H	-0.27451100	-2.22148600	-7.24816100
H	2.93532400	0.52182500	-8.07068400
H	1.40029800	-1.28196200	-8.83082200
C	0.14385100	2.21865800	-3.56106500
C	-0.56698100	2.54169500	-4.72744300
C	0.11056700	3.11875700	-2.48213600
C	-1.28413300	3.73779000	-4.81372500
H	-0.55142500	1.86872100	-5.57786600
C	-0.60245900	4.31464500	-2.57271000
H	0.64426600	2.89858400	-1.56288100
C	-1.30364300	4.62740500	-3.73883200
H	-1.81718900	3.97741900	-5.72988600
H	-0.60691000	5.00219200	-1.73167500

H	-1.85594000	5.55995000	-3.81000600
C	1.69420600	-3.11923900	0.34933000
C	1.42094100	-2.69723200	1.66101200
C	1.71728100	-4.49529200	0.07189500
C	1.18827200	-3.63066500	2.67224900
H	1.39704100	-1.64065300	1.90926600
C	1.48039300	-5.42632600	1.08471300
H	1.92895900	-4.84510400	-0.93382400
C	1.21754800	-4.99687600	2.38657000
H	0.99050800	-3.28799600	3.68393300
H	1.50636600	-6.48747300	0.85434700
H	1.04011100	-5.72253600	3.17503700
C	3.11094900	-2.74511600	-2.14146700
C	4.36309500	-3.19497900	-1.68443800
C	2.75183000	-2.97896400	-3.47572600
C	5.23582000	-3.85090900	-2.55073300
H	4.65735100	-3.04485600	-0.64950100
C	3.62613500	-3.64052500	-4.34207100
H	1.78892400	-2.64118000	-3.84639800
C	4.86915700	-4.07385000	-3.88170300
H	6.20095700	-4.19092200	-2.18658600
H	3.33270400	-3.81159900	-5.37366900
H	5.55104300	-4.58657900	-4.55398000
C	2.84537600	1.23862700	-3.12765500
H	3.52110400	0.51763300	-3.60079200
H	2.96116000	2.18991900	-3.65529300
C	3.01542700	-0.63709800	-0.11529700
H	2.36687800	-0.02331300	0.51818800
H	3.66601400	-1.20438900	0.55792600
C	3.28179800	1.46689000	-1.67836500
H	2.46227400	1.87214800	-1.06463300
C	3.91542500	0.27071000	-0.94916400
H	4.49836300	-0.32408900	-1.66870200
O	4.36074600	2.39424700	-1.71888400
O	4.78676700	0.91596300	-0.02505500
C	5.24172000	2.14484100	-0.60982100
C	6.65933300	1.99339000	-1.15279800
H	6.96536100	2.90587700	-1.67372800
H	7.36040200	1.80391600	-0.33445500
H	6.70660500	1.15915200	-1.85918300
C	5.10998300	3.24595200	0.43607400
H	5.72703600	3.01533500	1.30999700
H	5.43501600	4.20403700	0.01978200
H	4.06860100	3.33559800	0.75935000

Ir	0.02513300	-1.11404900	-2.01126900
C	-5.19694900	-1.13276000	-3.07628800
C	-4.09888200	-0.36009800	-3.46507000
C	-4.24314500	0.80987100	-4.21226800
C	-5.53629000	1.18507600	-4.57436100
C	-6.64200800	0.40935300	-4.19293900
C	-6.48606800	-0.75822100	-3.43777500
C	-4.70695300	-2.30720200	-2.27656200
H	-3.37753300	1.40373600	-4.48786500
H	-5.69346300	2.08874500	-5.15540700
H	-7.63927400	0.72368500	-4.48653400
H	-7.35123600	-1.34607300	-3.14471900
H	-5.07867600	-2.31514300	-1.24577000
N	-3.23547700	-2.12025300	-2.26943900
C	-2.88930500	-0.98885100	-2.93379300
O	-1.71987200	-0.53421700	-3.07828900
H	-4.96674600	-3.26832600	-2.72752900
C	-1.05059000	-2.66103200	-1.30081500
C	-2.35085100	-2.97335200	-1.55800400
H	-2.51877500	-0.01584500	-0.32958500
H	-0.56821900	-3.43617600	-0.71011600
C	-2.94071500	-4.27072100	-1.10542200
C	-3.37939300	-5.23084700	-2.03413300
C	-3.01821200	-4.57131000	0.26279800
C	-3.88902500	-6.45527800	-1.60344500
H	-3.29697800	-5.02569100	-3.09919200
C	-3.52908200	-5.79741300	0.69291500
H	-2.67644000	-3.83772000	0.98759800
C	-3.96878400	-6.74012300	-0.23764000
H	-4.21502900	-7.19069300	-2.33363600
H	-3.58646900	-6.01328300	1.75608600
H	-4.36741100	-7.69333100	0.09746800
C	-0.35907200	0.09714800	-0.32125200
C	-1.73651800	0.75265100	-0.31431600
H	0.42032000	0.86492200	-0.28444900
H	-0.25071100	-0.54256500	0.56010700
H	-1.86994900	1.36935900	-1.20881100
C	-1.91927000	1.62554400	0.94053400
H	-2.91299800	2.08717500	0.94922400
H	-1.81619100	1.03505300	1.85866600
H	-1.17736700	2.43227300	0.97737700
INT4b			
P	1.03083100	0.64128900	-3.17183400

P	2.19494100	-1.85805900	-0.89110200
C	0.96880000	0.04134600	-4.92111400
C	0.03456000	-0.94063800	-5.29002800
C	1.82132100	0.56304300	-5.90845400
C	-0.03725100	-1.39717000	-6.60837100
H	-0.65021000	-1.33935000	-4.54831500
C	1.75173200	0.10223200	-7.22353900
H	2.54297500	1.33555100	-5.66386200
C	0.82463100	-0.88059700	-7.57686500
H	-0.76808800	-2.15527500	-6.87635800
H	2.42108700	0.51539700	-7.97270700
H	0.77125000	-1.23651300	-8.60175100
C	0.11698900	2.24816900	-3.28003000
C	-1.01812200	2.35170000	-4.10112800
C	0.52037600	3.37540500	-2.54479600
C	-1.73080600	3.54862600	-4.18089800
H	-1.32984400	1.50441100	-4.70284400
C	-0.19826600	4.57029800	-2.62446100
H	1.40779100	3.34890200	-1.92162400
C	-1.32723900	4.66038000	-3.43864900
H	-2.59433700	3.61728300	-4.83717500
H	0.13504000	5.43321100	-2.05499200
H	-1.88061500	5.59258600	-3.50478800
C	2.22613000	-3.27031100	0.30943100
C	2.46163300	-3.08973000	1.68134400
C	2.00198600	-4.57262800	-0.16927500
C	2.47300000	-4.18290400	2.55100400
H	2.65162100	-2.10247000	2.08931800
C	2.01006300	-5.66191300	0.70116800
H	1.83307200	-4.74190900	-1.22867700
C	2.24573500	-5.47007600	2.06435700
H	2.66613700	-4.02363200	3.60798400
H	1.83822200	-6.66110400	0.31157700
H	2.25780400	-6.31950300	2.74108400
C	3.19267800	-2.56461200	-2.27334600
C	4.54233900	-2.91147600	-2.08108700
C	2.59672700	-2.82993200	-3.51307400
C	5.27808800	-3.48542000	-3.11630100
H	5.02150700	-2.74683300	-1.12003100
C	3.33341400	-3.40999600	-4.54942900
H	1.55289800	-2.58202100	-3.67773700
C	4.67549500	-3.73332400	-4.35373000
H	6.32078800	-3.74397100	-2.95602800
H	2.85512200	-3.60196100	-5.50538600

H	5.25148600	-4.18192900	-5.15796900
C	2.80351700	1.20238200	-3.02259100
H	3.43159900	0.44646000	-3.50591100
H	2.91529600	2.12918100	-3.59229600
C	3.34946200	-0.65184700	-0.05826700
H	2.77481400	-0.10499300	0.69486200
H	4.09880400	-1.23817800	0.48225700
C	3.30754400	1.47593400	-1.59989100
H	2.48864200	1.78123900	-0.93041200
C	4.10515600	0.35153700	-0.92647100
H	4.70266500	-0.17276100	-1.68689600
O	4.27339800	2.51839900	-1.68557800
O	4.95659000	1.07551600	-0.04410500
C	5.23686200	2.35635800	-0.62868700
C	6.63012400	2.37523800	-1.24929600
H	6.79972600	3.32215200	-1.77105400
H	7.39251300	2.26046900	-0.47297600
H	6.73436300	1.55907000	-1.97050900
C	5.03918400	3.42108300	0.44421000
H	5.72237600	3.24675800	1.28116400
H	5.23604500	4.41526900	0.03208600
H	4.01257200	3.39080300	0.82166400
Ir	0.12145900	-1.09776900	-1.59985700
C	-5.17416700	-1.43761900	-2.23074800
C	-4.15749300	-0.61942100	-2.73218100
C	-4.43384400	0.49861700	-3.52043200
C	-5.77041200	0.77184800	-3.80795300
C	-6.79321500	-0.05232300	-3.31443600
C	-6.50709200	-1.16598300	-2.51749700
C	-4.55603900	-2.53360800	-1.41077200
H	-3.63344100	1.13581100	-3.87987700
H	-6.02636600	1.63322000	-4.41743900
H	-7.82692500	0.18167300	-3.55138300
H	-7.30818800	-1.79217200	-2.13526900
H	-4.85927200	-2.51087700	-0.35809200
N	-3.10384100	-2.25473800	-1.51440400
C	-2.87433600	-1.14567100	-2.26021000
O	-1.74591300	-0.63590300	-2.51674700
H	-4.77907700	-3.53214500	-1.79573100
C	-0.82347400	-2.63321600	-0.70337400
C	-2.12363500	-3.01596700	-0.82460300
H	-1.45734800	1.59238200	-1.11663500
H	-0.26083200	-3.33935300	-0.09821300
C	-2.61488500	-4.29551800	-0.22404200

C	-3.04786800	-5.35797200	-1.03643900
C	-2.60420700	-4.47227700	1.16758800
C	-3.46505000	-6.56196700	-0.46964600
H	-3.03460500	-5.24680800	-2.11846500
C	-3.02153900	-5.67810700	1.73448000
H	-2.26731800	-3.65892300	1.80434100
C	-3.45577600	-6.72376500	0.91842100
H	-3.78853100	-7.37679700	-1.11133300
H	-3.01018800	-5.79777000	2.81418400
H	-3.78171400	-7.66129400	1.35959600
C	-1.39454500	1.09682600	-0.14738800
C	-0.11817300	0.27621500	0.03309300
H	-1.41633800	1.87649600	0.62903600
H	-2.29136400	0.48318600	-0.00797000
H	0.74572900	0.94334200	-0.05415600
C	-0.11029300	-0.38249500	1.40921600
H	-0.12901900	0.39991700	2.18359600
H	-0.99170700	-1.01414700	1.55180800
H	0.76912600	-1.00212000	1.59294300

TS3a

P	1.04722500	0.55307800	-3.35946300
P	1.96179400	-1.36672700	-0.58823000
C	0.56193600	-0.18065100	-4.97831700
C	-0.64800100	0.19333300	-5.58709800
C	1.35755800	-1.15789500	-5.59854200
C	-1.04594900	-0.39139500	-6.78971300
H	-1.27486700	0.95029800	-5.12874200
C	0.95622900	-1.73862400	-6.80286900
H	2.29349700	-1.47747000	-5.15252800
C	-0.24543300	-1.35810200	-7.40173700
H	-1.97969000	-0.08352200	-7.25208600
H	1.58926600	-2.48471200	-7.27497300
H	-0.55289000	-1.80706500	-8.34185200
C	0.48792900	2.30633400	-3.44407700
C	0.73682400	3.08168600	-4.58967200
C	-0.13310200	2.90349300	-2.33733600
C	0.36871600	4.42613500	-4.62443300
H	1.20936600	2.63715200	-5.46132100
C	-0.49927800	4.25097900	-2.37458800
H	-0.33036500	2.30936900	-1.44962000
C	-0.24941900	5.01290000	-3.51686700
H	0.56606200	5.01542000	-5.51530500
H	-0.97742700	4.70331500	-1.51026600

H	-0.53301800	6.06116200	-3.54527800
C	1.74334300	-2.19096400	1.05263100
C	1.66324400	-1.42599900	2.22850600
C	1.59844400	-3.58494900	1.14204600
C	1.45129900	-2.04095300	3.46293500
H	1.77006800	-0.34561900	2.19205700
C	1.38067200	-4.19730900	2.37838400
H	1.67737700	-4.20011900	0.25088700
C	1.30735300	-3.42795400	3.54069100
H	1.40234400	-1.43561500	4.36356800
H	1.28066300	-5.27775300	2.43181900
H	1.14569800	-3.90603100	4.50246800
C	2.92508300	-2.62098000	-1.53650900
C	4.19974400	-3.03177200	-1.10575900
C	2.36929300	-3.21287000	-2.67980300
C	4.90702600	-3.99991500	-1.81661400
H	4.64141200	-2.60560500	-0.20899300
C	3.07861700	-4.18867500	-3.38694600
H	1.37833800	-2.91092300	-3.00554600
C	4.34786700	-4.57923000	-2.96000400
H	5.89215500	-4.30575300	-1.47633900
H	2.63417900	-4.64430900	-4.26741900
H	4.89970700	-5.33620300	-3.50995600
C	2.89031200	0.74003100	-3.52308900
H	3.35070700	-0.23341900	-3.71771500
H	3.07083400	1.36824800	-4.40110700
C	3.21079200	-0.04588400	-0.14174400
H	2.65688500	0.79336900	0.29186500
H	3.84872500	-0.45346600	0.64918900
C	3.54162600	1.40482400	-2.30974500
H	2.84970600	2.11641800	-1.83121600
C	4.12641800	0.46363700	-1.25115800
H	4.61177000	-0.38269000	-1.76001800
O	4.70925400	2.08817100	-2.75235400
O	5.11072100	1.29117400	-0.63974400
C	5.60869100	2.20430100	-1.63614000
C	6.99798800	1.78421500	-2.10223700
H	7.33611300	2.43139600	-2.91748000
H	7.71224500	1.85708000	-1.27663800
H	6.97923200	0.75185000	-2.46388400
C	5.56638900	3.61242000	-1.05226000
H	6.18292000	3.66674700	-0.14962100
H	5.94490500	4.33584200	-1.78060200
H	4.53966500	3.88247600	-0.78751300

Ir	0.02180700	-0.65832000	-1.57864300
C	-5.03412300	-0.95796600	-3.23916300
C	-4.05319200	0.03682100	-3.20544800
C	-4.31659800	1.35139100	-3.59374700
C	-5.60713500	1.64646000	-4.03231300
C	-6.59444300	0.64997600	-4.07409300
C	-6.31995500	-0.66422000	-3.67848000
C	-4.43566400	-2.24810500	-2.75105800
H	-3.54222200	2.11090200	-3.54690300
H	-5.85443900	2.65706200	-4.34277000
H	-7.59281800	0.90435200	-4.41765200
H	-7.09547300	-1.42408200	-3.71318700
H	-4.90364200	-2.61756200	-1.83101900
N	-3.02502500	-1.88262100	-2.47276100
C	-2.81344000	-0.55771200	-2.70519500
O	-1.73988600	0.07522200	-2.52448200
H	-4.48607200	-3.04960700	-3.49215700
C	-0.99874400	-2.38649900	-1.19083000
C	-2.11080700	-2.78927000	-1.88241900
H	-3.34683700	-1.54556100	0.17455500
H	-0.43277500	-3.21261300	-0.77243400
C	-2.37096700	-4.23571200	-2.10878100
C	-2.52628200	-4.75168900	-3.40950500
C	-2.42366100	-5.12648100	-1.02343900
C	-2.73506600	-6.11450700	-3.61356000
H	-2.45451200	-4.08256700	-4.26367300
C	-2.62658600	-6.49136900	-1.23047400
H	-2.31770300	-4.74070000	-0.01317900
C	-2.78708000	-6.98935300	-2.52464000
H	-2.84566800	-6.49673300	-4.62454900
H	-2.67052000	-7.16397900	-0.37849400
H	-2.95039000	-8.05098700	-2.68530900
C	-1.22518500	-1.12850900	0.33262600
C	-2.68756700	-0.72891600	0.48838600
H	-0.58782700	-0.29034100	0.65686700
H	-0.96023700	-1.96477500	0.97899400
H	-2.91817500	0.13966900	-0.13722500
C	-2.99242900	-0.37852000	1.95556100
H	-4.04604100	-0.10226900	2.07352500
H	-2.79231300	-1.22827800	2.61841000
H	-2.38494900	0.46622400	2.30040100
TS3b			
P	0.95310900	0.55220200	-3.09032900

P	2.24703700	-1.36098500	-0.48212200
C	0.31860100	-0.18157500	-4.65911300
C	-0.94147500	0.18396100	-5.16027800
C	1.06463400	-1.15196600	-5.34835400
C	-1.43685100	-0.40050300	-6.32654600
H	-1.53251800	0.93306800	-4.64598800
C	0.56615800	-1.73294000	-6.51543800
H	2.03671700	-1.46697300	-4.98374100
C	-0.68502400	-1.35922700	-7.00825900
H	-2.40942400	-0.09908700	-6.70563500
H	1.16135400	-2.47397600	-7.04160600
H	-1.06899400	-1.80815600	-7.91983300
C	0.30539300	2.27703800	-3.06297800
C	0.37118000	3.08787900	-4.20900600
C	-0.19695300	2.81938700	-1.87136000
C	-0.06224100	4.41248500	-4.16092600
H	0.74976900	2.68647500	-5.14494200
C	-0.62852500	4.14690400	-1.82544500
H	-0.24753500	2.19504500	-0.98373000
C	-0.56265200	4.94395700	-2.96926500
H	-0.00737000	5.02930700	-5.05333900
H	-1.01351400	4.55686300	-0.89590400
H	-0.89719600	5.97685600	-2.93352200
C	2.32567500	-2.19235400	1.16962000
C	2.34947400	-1.42708600	2.34803700
C	2.34214500	-3.59249500	1.27277100
C	2.39523000	-2.04722100	3.59725900
H	2.34187600	-0.34169400	2.30130100
C	2.38396200	-4.21084000	2.52487200
H	2.34037800	-4.20525700	0.37686600
C	2.41153700	-3.44078300	3.68875500
H	2.42403300	-1.44065400	4.49800100
H	2.40471200	-5.29521500	2.58736100
H	2.45187000	-3.92262500	4.66131000
C	3.12379700	-2.57085700	-1.56345400
C	4.46999400	-2.90920000	-1.33411500
C	2.43072200	-3.20761900	-2.60332900
C	5.10921300	-3.85056600	-2.13922200
H	5.02237800	-2.44779100	-0.52012500
C	3.07247100	-4.15725400	-3.40449700
H	1.38744500	-2.95918600	-2.77554700
C	4.41126700	-4.47613800	-3.17699400
H	6.15010300	-4.09971800	-1.95400900
H	2.52175900	-4.64823800	-4.20200900

H	4.91040500	-5.21277100	-3.80007600
C	2.74835100	0.83700900	-3.48641900
H	3.22421700	-0.10688500	-3.76891900
H	2.77782000	1.49247500	-4.36251900
C	3.50076300	0.00549900	-0.19369000
H	2.98228400	0.82607400	0.31392100
H	4.24522300	-0.38460800	0.50778100
C	3.52529600	1.50231100	-2.35200000
H	2.87808400	2.18303300	-1.77580600
C	4.25797800	0.55356800	-1.39934400
H	4.68811500	-0.27139800	-1.98662600
O	4.60994600	2.22726200	-2.92072100
O	5.29818500	1.38836300	-0.90005300
C	5.65167100	2.32647700	-1.93311500
C	6.96776500	1.92980200	-2.59283000
H	7.18628500	2.59626100	-3.43297100
H	7.78764400	1.99385900	-1.87115500
H	6.90770000	0.90463300	-2.97031000
C	5.67978200	3.72114200	-1.31746100
H	6.41548200	3.76333400	-0.50825500
H	5.94737400	4.46410600	-2.07477500
H	4.69740500	3.97341400	-0.90713600
Ir	0.17537900	-0.73869700	-1.23316600
C	-5.01913900	-1.17564100	-2.41447600
C	-4.05214900	-0.17298200	-2.52976300
C	-4.37027800	1.11656900	-2.95879400
C	-5.70070100	1.37677700	-3.28611500
C	-6.67388100	0.37120900	-3.18054900
C	-6.34503300	-0.91686700	-2.74293500
C	-4.36111300	-2.43173500	-1.91354200
H	-3.60645500	1.88531500	-3.02375000
H	-5.99035800	2.36741400	-3.62319400
H	-7.70384700	0.59821300	-3.43964500
H	-7.11001800	-1.68377300	-2.66109600
H	-4.73541700	-2.75046100	-0.93344000
N	-2.93589500	-2.03947700	-1.79143200
C	-2.76309100	-0.72957500	-2.11749200
O	-1.68492300	-0.08315700	-2.06383800
H	-4.47191200	-3.27536100	-2.59909600
C	-0.79122200	-2.44575100	-0.67558300
C	-1.95343100	-2.90096700	-1.24183600
H	-2.17390700	0.60452700	0.26829500
H	-0.17940700	-3.24313800	-0.26536000
C	-2.18847900	-4.35951300	-1.42225100

C	-2.46580300	-4.88769600	-2.69835800
C	-2.09088900	-5.24868800	-0.33879700
C	-2.64883500	-6.25732200	-2.87910900
H	-2.50901700	-4.22068800	-3.55609600
C	-2.26977100	-6.62029600	-0.52292000
H	-1.88402400	-4.86118300	0.65412600
C	-2.55346200	-7.12947200	-1.79111200
H	-2.85459100	-6.64626300	-3.87250800
H	-2.19703000	-7.29019100	0.32927800
H	-2.69700000	-8.19668000	-1.93250900
C	-2.22353000	-0.27796000	0.90699600
C	-0.93695700	-1.09117100	0.91259200
H	-2.40610000	0.06394700	1.93590000
H	-3.09091700	-0.88085000	0.62042300
H	-0.09178800	-0.44910100	1.17518000
C	-1.01837300	-2.21974500	1.94160200
H	-1.07436100	-1.75857700	2.93772400
H	-1.92186400	-2.82151200	1.80337000
H	-0.15188100	-2.88024200	1.94338500

INT5a

P	1.47699900	0.78192900	-0.25744900
P	-1.60988700	1.02193400	1.29784800
C	2.80719900	0.72008500	-1.54563200
C	3.50264700	-0.46107600	-1.84192200
C	3.14130500	1.89504200	-2.24248200
C	4.52300300	-0.46198100	-2.79656700
H	3.25779500	-1.39003200	-1.33771200
C	4.15148700	1.88826600	-3.20381200
H	2.62481100	2.82408800	-2.02000700
C	4.84995900	0.70959800	-3.47870500
H	5.05975200	-1.38328800	-3.00379700
H	4.40273400	2.80685000	-3.72646600
H	5.64651300	0.70738500	-4.21724600
C	1.90747400	2.36854000	0.58435900
C	3.13797700	2.52371600	1.24796600
C	1.03628300	3.46359200	0.50539500
C	3.47228800	3.74034800	1.84010900
H	3.84506900	1.69990900	1.29425600
C	1.37433900	4.68446300	1.09724200
H	0.09479000	3.35940400	-0.02575200
C	2.58910700	4.82245500	1.76828600
H	4.42377300	3.84626900	2.35329200
H	0.68664700	5.52245700	1.03019400

H	2.85342600	5.77012600	2.22874800
C	-2.34112900	2.70001500	1.47671400
C	-2.17089200	3.48230100	2.62985700
C	-3.10482300	3.21121500	0.41116900
C	-2.75042600	4.75086200	2.71450200
H	-1.59136300	3.11731600	3.47088500
C	-3.68379000	4.47638000	0.50380800
H	-3.25026800	2.61211200	-0.48182100
C	-3.50576500	5.25053000	1.65337800
H	-2.61059900	5.34455400	3.61335500
H	-4.27393500	4.85904200	-0.32422800
H	-3.95560000	6.23688100	1.72188500
C	-2.99578100	-0.14737900	1.63074700
C	-4.08237900	0.22846000	2.43452000
C	-2.93405900	-1.45816200	1.13389200
C	-5.08510500	-0.69412200	2.73750500
H	-4.15301000	1.24052200	2.82144100
C	-3.93507300	-2.37963900	1.44285300
H	-2.10345200	-1.74790100	0.49576700
C	-5.01296700	-1.99838800	2.24458200
H	-5.92283200	-0.39147700	3.35930600
H	-3.87542100	-3.39289300	1.05516700
H	-5.79411300	-2.71445000	2.48337800
C	2.04014500	-0.55881900	0.91941900
H	1.62744000	-1.50307800	0.54932500
H	3.13022800	-0.63298800	0.85223600
C	-0.57087700	0.81041500	2.82345700
H	0.09846700	1.67017000	2.92972900
H	-1.25018200	0.80390600	3.68174000
C	1.69364300	-0.39652500	2.39794200
H	2.10798800	0.54892300	2.77799200
C	0.22893100	-0.49591600	2.84394200
H	-0.28142700	-1.28876600	2.27422200
O	2.28226400	-1.49686800	3.08489300
O	0.37496000	-0.89403700	4.20334800
C	1.57168100	-1.68281600	4.32138800
C	1.22981800	-3.16296600	4.45364700
H	2.14422000	-3.76440100	4.45755900
H	0.68576200	-3.34406700	5.38542200
H	0.60652700	-3.48279300	3.61315300
C	2.38118000	-1.14250900	5.49528100
H	1.79849200	-1.20733500	6.41943300
H	3.30168400	-1.72086000	5.61891200
H	2.64254100	-0.09417300	5.32320900

Ir	-0.71817200	0.62836700	-0.90196400
C	-3.98294300	-1.55106300	-4.07142400
C	-4.29317700	-0.69162100	-3.00711900
C	-5.60816600	-0.36214900	-2.67861800
C	-6.62461800	-0.91893500	-3.45380400
C	-6.32119700	-1.77998100	-4.51949900
C	-4.99887600	-2.10822000	-4.83962500
C	-2.48298200	-1.70872100	-4.16633600
H	-5.82477700	0.30215400	-1.84806900
H	-7.66184300	-0.68698100	-3.23249400
H	-7.13042300	-2.20168900	-5.10848000
H	-4.78215400	-2.77761400	-5.66720200
H	-2.14878800	-2.74583300	-4.05188200
N	-2.01719600	-0.88746600	-3.03764800
C	-3.03003800	-0.28096600	-2.39399800
O	-2.83354700	0.50816400	-1.43061300
H	-2.07503900	-1.32543700	-5.11034900
C	-0.21801400	0.79214900	-3.06698900
C	-0.62694100	-0.53460400	-2.76177600
H	0.85621700	0.92731000	-3.15506000
C	0.26900100	-1.73335600	-2.82826800
C	1.23696200	-1.84350200	-3.83619000
C	0.08533500	-2.81404300	-1.94755300
C	2.01214100	-2.99992500	-3.95492300
H	1.37805500	-1.02530300	-4.53612100
C	0.86406800	-3.96389400	-2.05982000
H	-0.66991300	-2.73968000	-1.17042600
C	1.83147000	-4.06003000	-3.06668300
H	2.75296200	-3.07071000	-4.74622700
H	0.71518700	-4.78797300	-1.36763900
H	2.43212800	-4.96021200	-3.16042000
C	-1.01422600	1.81030600	-3.86034700
C	-0.57605700	3.26279900	-3.61587500
H	-0.86984800	1.57899800	-4.92976700
H	-2.08872400	1.72453000	-3.67141200
H	0.50554400	3.34795500	-3.78902400
C	-1.31867800	4.26032900	-4.51002600
H	-1.14089400	4.05308900	-5.57228700
H	-2.40170800	4.21716500	-4.34072200
H	-0.99254200	5.28718400	-4.31324200
H	-0.74219000	3.51198100	-2.56004400
INT5b			
P	-0.69951300	0.13024600	1.14541500

P	0.98780800	-1.92163300	-1.07608900
C	0.13753400	1.67855400	1.67974300
C	0.88753300	1.76198700	2.86357700
C	0.01022500	2.82252400	0.87055100
C	1.50039300	2.96333900	3.22865300
H	1.00162000	0.90068600	3.51254800
C	0.62166500	4.01940600	1.24230400
H	-0.57585500	2.77388600	-0.04110300
C	1.37037900	4.09250000	2.41984700
H	2.07717800	3.01248500	4.14781200
H	0.51372200	4.89647500	0.61029600
H	1.84752600	5.02542500	2.70601700
C	-2.46437400	0.33810900	1.63728100
C	-2.82927700	1.20510000	2.67793500
C	-3.45599500	-0.43348500	1.01186000
C	-4.16146000	1.29308400	3.08584800
H	-2.07882900	1.81621300	3.16995800
C	-4.78560900	-0.34755500	1.42558400
H	-3.18291900	-1.09570600	0.19467000
C	-5.14071200	0.51723600	2.46294700
H	-4.43215500	1.96922500	3.89182900
H	-5.54382200	-0.95275100	0.93631600
H	-6.17617100	0.58675000	2.78378200
C	1.70625000	-2.63838900	-2.62688300
C	1.17905400	-3.79446500	-3.22009900
C	2.82062200	-2.02053000	-3.22158200
C	1.76700000	-4.33346800	-4.36705800
H	0.30834300	-4.28568000	-2.79850800
C	3.39743300	-2.55331800	-4.37422900
H	3.25444900	-1.13301800	-2.77057000
C	2.87551200	-3.71639500	-4.94622000
H	1.35313100	-5.23707400	-4.80520200
H	4.26382600	-2.06863900	-4.81535700
H	3.33386100	-4.13980700	-5.83538100
C	2.53586600	-1.47238600	-0.17321100
C	3.45907600	-2.46379700	0.20626100
C	2.84143700	-0.12854900	0.08222600
C	4.64546700	-2.11583700	0.84952600
H	3.26121300	-3.50994800	-0.01081100
C	4.03407400	0.21940900	0.72407800
H	2.14810100	0.64700400	-0.22850700
C	4.93374900	-0.77277500	1.11247100
H	5.34768600	-2.89152400	1.14125300
H	4.25479000	1.26527300	0.91685300

H	5.86022900	-0.50414500	1.61190100
C	-0.11893800	-1.14619900	2.36525500
H	0.97452800	-1.12968900	2.41401300
H	-0.50517100	-0.85866600	3.34823100
C	0.36174300	-3.46368600	-0.22035200
H	-0.65178900	-3.64326600	-0.59330800
H	0.97992100	-4.30663300	-0.54530700
C	-0.62218400	-2.55942200	2.05700600
H	-1.58914500	-2.53377100	1.53024000
C	0.35162500	-3.47603200	1.30610000
H	1.36598100	-3.29533700	1.69162800
O	-0.76331700	-3.25199500	3.29324900
O	-0.09755200	-4.76701300	1.70751600
C	-0.62015800	-4.66119700	3.04339400
C	0.37118700	-5.22321600	4.05655000
H	0.00635900	-5.05858200	5.07516200
H	0.50460300	-6.29789000	3.90032700
H	1.34078800	-4.72739200	3.95129000
C	-1.97774200	-5.35486300	3.07727100
H	-1.87223100	-6.40784400	2.79800300
H	-2.40708500	-5.29898900	4.08205400
H	-2.66450000	-4.87538900	2.37317200
Ir	-0.54828700	-0.22916100	-1.22665900
C	-4.45826800	1.62999100	-3.81900100
C	-3.93722800	2.12467100	-2.61421000
C	-4.51298500	3.20490000	-1.94534100
C	-5.63877400	3.79306200	-2.52056800
C	-6.16486100	3.30299400	-3.72559000
C	-5.58372100	2.21538400	-4.38739700
C	-3.62078800	0.46155400	-4.28464800
H	-4.09561300	3.56765900	-1.01141300
H	-6.11592000	4.63764700	-2.03311100
H	-7.04295900	3.77758900	-4.15371900
H	-6.00534500	1.84776400	-5.31856500
H	-4.18987300	-0.47118400	-4.36667300
N	-2.61610000	0.35993200	-3.21467400
C	-2.77564900	1.30406700	-2.27071800
O	-2.00227700	1.39535700	-1.27954000
H	-3.13478700	0.64540200	-5.25065600
C	-0.17285200	0.06825300	-3.40543700
C	-1.45180500	-0.52243200	-3.21433400
H	0.60414300	-0.62915200	-3.71003800
C	-1.81649800	-1.90892800	-3.65161500
C	-1.36047300	-2.40992500	-4.87879400

C	-2.70777300	-2.68787800	-2.89279500
C	-1.77437500	-3.66511400	-5.33232200
H	-0.68672200	-1.81213200	-5.48549000
C	-3.11337600	-3.94371100	-3.34011600
H	-3.07346200	-2.29958000	-1.94630900
C	-2.64686600	-4.43607300	-4.56441700
H	-1.41618300	-4.03539500	-6.28870000
H	-3.79698400	-4.53750300	-2.73967600
H	-2.97026200	-5.41093700	-4.91797600
C	1.44916400	2.00534500	-3.30193100
C	0.10893700	1.49517300	-3.85456100
H	2.27825100	1.36591600	-3.62945800
H	1.65113400	3.02106800	-3.65977300
H	1.44331200	2.01946300	-2.20773800
H	-0.67853800	2.16448200	-3.49204500
C	0.10934900	1.54868700	-5.39770800
H	0.30009800	2.57028400	-5.74574200
H	0.89352700	0.90363300	-5.81265100
H	-0.84908500	1.22423600	-5.81924500

INT6a

P	1.89384300	1.53937400	0.02121400
P	-1.11116100	-0.33829900	0.83652200
C	3.39687300	1.92081300	-0.99371800
C	4.48051500	1.02741000	-1.03768000
C	3.45785700	3.09233500	-1.76697700
C	5.59789900	1.30249800	-1.82868500
H	4.46995400	0.11733200	-0.44449000
C	4.57522600	3.36319000	-2.55879100
H	2.63884500	3.80511700	-1.74033100
C	5.64781100	2.47002700	-2.59187700
H	6.43066200	0.60512900	-1.84183800
H	4.60906900	4.27824100	-3.14334700
H	6.51871600	2.68477600	-3.20414600
C	1.35528000	3.22253200	0.55380200
C	2.19106300	4.04215100	1.33399800
C	0.10040600	3.70928200	0.15904100
C	1.76978200	5.31136700	1.72741500
H	3.17704600	3.69617200	1.63128900
C	-0.31611500	4.98578100	0.55224700
H	-0.53715100	3.09676700	-0.46983400
C	0.51260800	5.78469700	1.33969700
H	2.42306000	5.93181100	2.33413600
H	-1.28979400	5.35467200	0.24035200

H	0.18627500	6.77412100	1.64712600
C	-2.84010900	0.26633800	0.63851300
C	-3.13261100	1.62925500	0.81287300
C	-3.88047000	-0.61112300	0.29456300
C	-4.43739300	2.09960000	0.65897200
H	-2.34795500	2.33367100	1.06964300
C	-5.18532300	-0.13727900	0.14480400
H	-3.67632500	-1.66777600	0.16149400
C	-5.46750600	1.21810500	0.32627600
H	-4.64900000	3.15471400	0.80659700
H	-5.98435400	-0.83202900	-0.10006200
H	-6.48430400	1.58398600	0.21646600
C	-1.28745900	-2.08755300	1.39558500
C	-2.19328400	-2.37976800	2.43297000
C	-0.49189700	-3.12341700	0.88588700
C	-2.30551200	-3.67538300	2.93391400
H	-2.82335000	-1.59927000	2.84924500
C	-0.60482800	-4.42075400	1.39137700
H	0.22218700	-2.91759000	0.09785500
C	-1.51174100	-4.70023800	2.41297300
H	-3.01089200	-3.88253000	3.73337900
H	0.01883400	-5.21077500	0.98303800
H	-1.59942000	-5.70959000	2.80450400
C	2.71952800	0.83141700	1.54855100
H	2.96602700	-0.21326500	1.33217300
H	3.66397000	1.36294800	1.70130000
C	-0.60489900	0.48395100	2.42812500
H	-0.57431900	1.56827400	2.28299300
H	-1.39425100	0.27374100	3.15572300
C	1.92460600	0.90212900	2.84682600
H	1.59859400	1.93572500	3.03652200
C	0.72152200	-0.03053900	2.99730100
H	0.97340900	-1.02101500	2.58769100
O	2.76896400	0.45744900	3.90277600
O	0.60531900	-0.11275000	4.41417200
C	1.92789800	-0.01309900	4.97345500
C	2.43544300	-1.38424100	5.40629800
H	3.47311800	-1.31364600	5.74691500
H	1.82248200	-1.77385300	6.22459300
H	2.39269300	-2.08618700	4.56809200
C	1.88451700	1.00248000	6.10951000
H	1.17660400	0.67961300	6.87921500
H	2.87459100	1.10514900	6.56376800
H	1.56533200	1.97838900	5.73188800

Ir	0.24885500	-0.01044500	-1.05144900
C	-4.00444600	1.79021300	-3.90156300
C	-2.99388500	2.38431600	-3.14476800
C	-2.87398200	3.77005900	-3.03230000
C	-3.81277200	4.55668600	-3.69864400
C	-4.83597400	3.96303400	-4.45419400
C	-4.94338200	2.57281000	-4.56551500
C	-3.84546800	0.29871100	-3.83209100
H	-2.07147800	4.21408200	-2.45144500
H	-3.75299400	5.63921400	-3.63770000
H	-5.55505500	4.59575100	-4.96628700
H	-5.73633200	2.12645000	-5.15901000
H	-4.71510700	-0.19462200	-3.38796700
N	-2.65559600	0.11995300	-2.97062300
C	-2.15319300	1.32186200	-2.57613500
O	-1.13124800	1.53673400	-1.87693500
H	-3.67002100	-0.16128600	-4.81090300
C	-0.97512300	-1.37146900	-1.98315200
C	-2.09040300	-1.17307700	-2.71627600
H	-0.70771800	-2.42417100	-1.90786900
C	-2.80770900	-2.32586600	-3.35600300
C	-2.19293300	-3.04060200	-4.39590500
C	-4.07094800	-2.75010000	-2.90998200
C	-2.82141700	-4.14433200	-4.97584800
H	-1.21453300	-2.72777300	-4.75023700
C	-4.70103500	-3.85121800	-3.49009200
H	-4.55477600	-2.22252700	-2.09262400
C	-4.07844600	-4.55094500	-4.52645700
H	-2.32885100	-4.68382000	-5.77999000
H	-5.67451200	-4.16879100	-3.12668400
H	-4.56870200	-5.40898600	-4.97720800
C	1.82737000	-0.69502400	-2.67459000
C	1.37060400	0.48003800	-3.22568100
H	2.75221400	-0.71177100	-2.11125000
H	1.47262000	-1.65428000	-3.03944900
H	1.90753800	1.39149000	-2.98341000
C	0.46084600	0.57405300	-4.41585800
H	1.08838200	0.66577800	-5.31371900
H	-0.16629900	-0.31198300	-4.53263800
H	-0.16736500	1.46774000	-4.37824100
H	1.13412100	-1.16597900	-0.42137300
INT6b			
P	1.74308000	1.07753700	-0.04258300

P	-0.87300900	-1.20842900	0.52761700
C	3.36780000	0.23106900	-0.28113800
C	4.37593100	0.27815800	0.69761700
C	3.62866900	-0.45898000	-1.47591000
C	5.60422400	-0.35060600	0.48650000
H	4.21643400	0.80819900	1.63048700
C	4.85894500	-1.08284500	-1.68908000
H	2.85733700	-0.52841700	-2.23506100
C	5.84982700	-1.03174900	-0.70705600
H	6.36869600	-0.30550000	1.25687400
H	5.04012200	-1.61201400	-2.62042500
H	6.80666500	-1.51919200	-0.87035100
C	2.12011500	2.85968500	-0.39374900
C	3.42833800	3.32418100	-0.59684900
C	1.06167400	3.78463800	-0.41831800
C	3.67215700	4.68375400	-0.80750800
H	4.26323100	2.63218100	-0.59369500
C	1.31102400	5.14199900	-0.62289400
H	0.04037900	3.43662400	-0.30398200
C	2.61731000	5.59623400	-0.81664900
H	4.69099100	5.02576000	-0.96617500
H	0.48171700	5.84403200	-0.63997200
H	2.81030500	6.65260500	-0.97987500
C	-2.18426000	-2.45721300	0.17407200
C	-3.53891100	-2.21136400	0.43902500
C	-1.81126700	-3.69448200	-0.37573500
C	-4.49862300	-3.19068400	0.17515300
H	-3.85923800	-1.26090900	0.85385800
C	-2.77365800	-4.66660800	-0.64596200
H	-0.76588500	-3.90950800	-0.57749600
C	-4.11950800	-4.41866400	-0.36698800
H	-5.54321300	-2.99047500	0.39481200
H	-2.46960100	-5.62166600	-1.06464600
H	-4.86759600	-5.17926300	-0.57024700
C	0.38833200	-2.26661100	1.35419200
C	0.09089900	-2.84836300	2.60132900
C	1.60142400	-2.58404300	0.73052900
C	1.00218800	-3.70376400	3.21685600
H	-0.85827000	-2.64810400	3.09024300
C	2.51240200	-3.44586700	1.34879800
H	1.83762900	-2.16007500	-0.23756400
C	2.21762500	-4.00185200	2.59262100
H	0.76123500	-4.14247400	4.18078800
H	3.45087500	-3.67620000	0.85312400

H	2.92572100	-4.67025000	3.07393100
C	1.60184000	1.13985800	1.82162200
H	1.85688900	0.15525000	2.22705200
H	2.35044100	1.85103000	2.18163500
C	-1.63691100	-0.17983100	1.87958300
H	-2.23953100	0.58587300	1.38176500
H	-2.31539700	-0.81638100	2.45558400
C	0.23807300	1.60445800	2.34572600
H	-0.29806600	2.21104400	1.60291100
C	-0.68850600	0.49792400	2.86495500
H	-0.07814400	-0.25527900	3.38493100
O	0.45847600	2.36525300	3.53140500
O	-1.49764900	1.20073800	3.80146600
C	-0.70880700	2.26517600	4.36280000
C	-0.25657200	1.91253900	5.77578100
H	0.41024100	2.68816400	6.16509600
H	-1.12133500	1.82623700	6.44057500
H	0.28354200	0.96107700	5.77255500
C	-1.53123500	3.54804600	4.29558200
H	-2.45909800	3.43452500	4.86481500
H	-0.96282800	4.38477400	4.71258200
H	-1.78781400	3.77696700	3.25663800
Ir	-0.18519600	0.11159500	-1.30496900
C	-4.22320900	3.46022700	-2.42282000
C	-3.21245100	3.46554700	-1.45912900
C	-2.91897300	4.60391600	-0.70656700
C	-3.67074600	5.75286000	-0.94967200
C	-4.68108500	5.75363000	-1.92382500
C	-4.96987500	4.60716200	-2.67131900
C	-4.30237800	2.09049600	-3.03392200
H	-2.13997200	4.58811800	0.04927200
H	-3.47660500	6.65683100	-0.38036100
H	-5.25221800	6.66089300	-2.09753600
H	-5.75751300	4.61968600	-3.41935300
H	-5.28510400	1.62965100	-2.90964800
N	-3.26622100	1.32909100	-2.29909600
C	-2.58557800	2.13550400	-1.43838200
O	-1.57753800	1.82956600	-0.75058000
H	-4.07226800	2.08307900	-4.10678600
C	-1.84892400	-0.67064600	-2.25204200
C	-3.01552600	-0.06351600	-2.55526800
H	-1.83975300	-1.73155200	-2.49042900
C	-4.15658800	-0.81280900	-3.16440200
C	-3.97537900	-1.52599800	-4.35932500

C	-5.41870600	-0.85902600	-2.54490000
C	-5.01926300	-2.26544700	-4.91804600
H	-3.00892900	-1.49324500	-4.85469600
C	-6.46473500	-1.58984700	-3.10697300
H	-5.57455100	-0.33463000	-1.60504000
C	-6.26855500	-2.29570400	-4.29693500
H	-4.85804700	-2.80884000	-5.84491600
H	-7.43167400	-1.61538900	-2.61180500
H	-7.08378400	-2.86403400	-4.73534000
C	0.75644600	1.56913300	-2.92857200
C	0.01510600	0.69694000	-3.68959600
H	0.34875400	2.52772900	-2.62952400
H	1.83767700	1.48507700	-2.89302500
H	-1.00614600	0.97623800	-3.92447700
C	0.58044600	-0.42053700	-4.52029500
H	0.61986100	-0.09226300	-5.56814400
H	1.59361900	-0.69284500	-4.21303800
H	-0.05171800	-1.31225700	-4.47979700
H	0.70726300	-1.10320600	-1.76179300

TS4a

P	1.79588600	1.06198400	0.07284900
P	-0.79338300	-1.28250200	0.53194700
C	3.42319200	0.20056100	-0.07500900
C	4.38789000	0.31411600	0.94017000
C	3.74847900	-0.52059800	-1.23429200
C	5.63522800	-0.29623000	0.80620600
H	4.17840200	0.88313900	1.84004800
C	5.00127300	-1.12259700	-1.37167800
H	3.01607900	-0.62187600	-2.02867700
C	5.94538200	-1.01651500	-0.34922300
H	6.36596500	-0.20420500	1.60462700
H	5.23594200	-1.67590000	-2.27675500
H	6.91840700	-1.48799000	-0.45323200
C	2.28012000	2.81297200	-0.28159700
C	3.24307100	3.08785400	-1.26658800
C	1.68954600	3.88843700	0.40364800
C	3.60106100	4.40278700	-1.56503200
H	3.73397100	2.27438100	-1.79152000
C	2.05325100	5.20320100	0.10347600
H	0.96753900	3.71757100	1.19482800
C	3.00461500	5.46503000	-0.88352000
H	4.35431000	4.59484900	-2.32393500
H	1.59840100	6.02271100	0.65304600

H	3.28792000	6.48853500	-1.11155400
C	-2.02706300	-2.54439000	-0.01378000
C	-3.39046700	-2.46981900	0.29989400
C	-1.56654200	-3.63090800	-0.77797600
C	-4.27153400	-3.46747000	-0.12682300
H	-3.78175000	-1.64151200	0.88166000
C	-2.44780300	-4.62149800	-1.20677500
H	-0.51065700	-3.71620100	-1.02093700
C	-3.80446500	-4.54345400	-0.87947100
H	-5.32416500	-3.39814800	0.13136500
H	-2.07370600	-5.45986600	-1.78772500
H	-4.49049800	-5.31886800	-1.20762800
C	0.41680600	-2.36751600	1.41112400
C	0.07430900	-2.97472200	2.63351600
C	1.65648800	-2.66968800	0.83229300
C	0.96277700	-3.84149700	3.26732500
H	-0.89208900	-2.78518800	3.09145000
C	2.54475300	-3.54261100	1.46707100
H	1.93268300	-2.22163300	-0.11445500
C	2.20230900	-4.12550400	2.68630200
H	0.68516300	-4.29957000	4.21236200
H	3.50387700	-3.75882400	1.00544100
H	2.89271800	-4.80201000	3.18189400
C	1.49805500	1.10443600	1.91174500
H	1.74728300	0.11549000	2.31018800
H	2.19222500	1.81979400	2.36079700
C	-1.68740700	-0.38187000	1.89356700
H	-2.36646000	0.32563400	1.40676700
H	-2.30114000	-1.08784600	2.46153000
C	0.07219300	1.51350500	2.32325500
H	-0.46080600	2.01559900	1.50553700
C	-0.81468200	0.39133800	2.88189100
H	-0.19025500	-0.30505900	3.46127200
O	0.17779000	2.39053300	3.44642300
O	-1.69302200	1.10037400	3.74988800
C	-1.01101800	2.26442500	4.24357200
C	-0.58960300	2.06639600	5.69572300
H	-0.00552500	2.92443200	6.04286300
H	-1.47099500	1.95916700	6.33514000
H	0.02609900	1.16700200	5.78898800
C	-1.92547400	3.46880400	4.03976500
H	-2.86219600	3.33192000	4.58897400
H	-1.43838600	4.38060200	4.39872500
H	-2.16162300	3.58529700	2.97720800

Ir	-0.00737500	0.18495200	-1.20656700
C	-3.99796200	3.58792900	-2.31902400
C	-2.99730600	3.54724200	-1.34602100
C	-2.67217000	4.66183800	-0.57114900
C	-3.39314000	5.83365100	-0.79218100
C	-4.40150900	5.87909800	-1.76833400
C	-4.71413300	4.75900900	-2.54537700
C	-4.09576200	2.24180500	-2.97918700
H	-1.88041300	4.61045300	0.16938000
H	-3.17383400	6.72272200	-0.20893600
H	-4.94887100	6.80409700	-1.92429900
H	-5.49413000	4.81063800	-3.29961800
H	-5.08648500	1.79219400	-2.88342100
N	-3.07647700	1.43733600	-2.25923900
C	-2.39609400	2.20853700	-1.34291000
O	-1.43548200	1.85345700	-0.63040600
H	-3.85078600	2.27334100	-4.04821400
C	-1.60509900	-0.49238100	-2.49796000
C	-2.85365300	0.06181600	-2.54585600
H	-1.57817900	-1.55272300	-2.72910400
C	-4.05548900	-0.71623700	-2.93565600
C	-4.00139300	-1.60566100	-4.02297100
C	-5.26730600	-0.59902300	-2.22719200
C	-5.12103300	-2.35029300	-4.39202400
H	-3.08099400	-1.69947100	-4.59203400
C	-6.38540500	-1.34234200	-2.59825900
H	-5.32252000	0.05915500	-1.36362000
C	-6.31762100	-2.21886600	-3.68488600
H	-5.06118300	-3.02472000	-5.24140600
H	-7.30958300	-1.24188600	-2.03593100
H	-7.19153900	-2.79322200	-3.97801800
C	-0.30422700	0.42294800	-3.65402200
C	0.60160400	1.33719600	-3.00415600
H	0.11018300	-0.48784600	-4.07772100
H	-1.08849100	0.87051700	-4.25752300
H	1.65377900	1.08063000	-3.11231400
C	0.31490900	2.82565100	-3.11495900
H	0.90243500	3.26420700	-3.93243400
H	-0.74050500	3.01511000	-3.33996800
H	0.56503800	3.37558800	-2.20582300
H	0.93452500	-0.98922100	-1.68031300
TS4b			
P	1.78246400	1.10407200	0.00548400

P	-0.83623400	-1.19935700	0.53662000
C	3.40327200	0.24084100	-0.18619200
C	4.34751100	0.19720600	0.85368600
C	3.73371800	-0.35362000	-1.41514200
C	5.58078300	-0.43185600	0.67051500
H	4.13632300	0.65466500	1.81406300
C	4.96821000	-0.97732700	-1.59887500
H	3.01687100	-0.34050200	-2.22862500
C	5.89457600	-1.02106900	-0.55493500
H	6.29504100	-0.45842200	1.48851800
H	5.20416100	-1.43148900	-2.55718100
H	6.85462100	-1.50914600	-0.69625400
C	2.17829900	2.86421000	-0.41058000
C	3.49908900	3.31902100	-0.54550700
C	1.12723900	3.78610700	-0.55050700
C	3.76045000	4.66609200	-0.80654100
H	4.32972000	2.62833300	-0.44991600
C	1.39318000	5.13191400	-0.80466900
H	0.10054100	3.44427000	-0.47709500
C	2.71078600	5.57610100	-0.93352500
H	4.78859600	5.00076400	-0.91192900
H	0.56906200	5.83252700	-0.91001600
H	2.91747300	6.62303600	-1.13648700
C	-2.14349500	-2.41664300	0.06798200
C	-3.48471800	-2.29751500	0.45618500
C	-1.75998400	-3.52397600	-0.70861200
C	-4.41665800	-3.27433800	0.09428300
H	-3.81811700	-1.45249200	1.04997000
C	-2.69194300	-4.49379700	-1.07280500
H	-0.72209000	-3.64218300	-1.00906200
C	-4.02427400	-4.37314200	-0.66835900
H	-5.44985900	-3.17341200	0.41424700
H	-2.37614300	-5.34937100	-1.66321100
H	-4.74944000	-5.13287400	-0.94500400
C	0.35610300	-2.31134000	1.40539300
C	-0.01151200	-2.94027800	2.60956000
C	1.60844200	-2.60059300	0.84749100
C	0.86422800	-3.81682500	3.24696300
H	-0.98824300	-2.75880000	3.04929100
C	2.48406500	-3.48401900	1.48628900
H	1.90387300	-2.13648200	-0.08620700
C	2.11635800	-4.08899900	2.68711700
H	0.56764100	-4.29190200	4.17774900
H	3.45276300	-3.69231900	1.04128100

H	2.79682800	-4.77402900	3.18483200
C	1.58449500	1.19488800	1.85967600
H	1.84926900	0.21952600	2.28193600
H	2.30487500	1.92690600	2.23600200
C	-1.64125200	-0.22263100	1.90335800
H	-2.28750500	0.51839200	1.42221100
H	-2.28206500	-0.88302900	2.49567800
C	0.19202100	1.62496400	2.34242000
H	-0.34805700	2.19546400	1.57401100
C	-0.70832300	0.49782600	2.87472200
H	-0.07948700	-0.23371400	3.40465600
O	0.36979700	2.42356700	3.51181200
O	-1.53844700	1.19010000	3.80254900
C	-0.78633700	2.28360900	4.35133800
C	-0.31187400	1.95777200	5.76421100
H	0.32963600	2.75936300	6.14340600
H	-1.16834500	1.84536200	6.43589600
H	0.26176600	1.02611200	5.76384800
C	-1.65573200	3.53553000	4.28322800
H	-2.57233300	3.39373700	4.86431800
H	-1.11336800	4.39620800	4.68602600
H	-1.93165100	3.74457200	3.24498100
Ir	-0.03445500	0.20155800	-1.22880800
C	-4.15728900	3.47709200	-2.43854000
C	-3.17061000	3.48310400	-1.45071100
C	-2.91182400	4.61279400	-0.67155400
C	-3.67486400	5.75343000	-0.91388700
C	-4.66286700	5.75368400	-1.91167900
C	-4.91642100	4.61661900	-2.68531800
C	-4.20152400	2.12013400	-3.08075600
H	-2.14741900	4.59464300	0.09896800
H	-3.50773100	6.65129100	-0.32687700
H	-5.24424100	6.65472800	-2.08372900
H	-5.68628700	4.63055400	-3.45148700
H	-5.17752200	1.63942500	-2.98530400
N	-3.16149900	1.36052900	-2.34099800
C	-2.51426100	2.16934000	-1.42949900
O	-1.54576400	1.86176000	-0.70565700
H	-3.95004700	2.14293500	-4.14850300
C	-1.59148000	-0.48579500	-2.56340400
C	-2.86700400	-0.00018600	-2.63512600
H	-1.50128900	-1.53490100	-2.83115100
C	-4.02476600	-0.82444400	-3.06519600
C	-3.91077400	-1.69542500	-4.16237200

C	-5.25501300	-0.76887200	-2.38179100
C	-4.99078600	-2.47770600	-4.56892000
H	-2.97491700	-1.74588900	-4.71049800
C	-6.33348400	-1.55072700	-2.78916500
H	-5.35521500	-0.13064000	-1.50772100
C	-6.20732600	-2.40494500	-3.88786900
H	-4.88433100	-3.13603200	-5.42630700
H	-7.27216600	-1.49809900	-2.24477200
H	-7.05062500	-3.00903500	-4.20944600
C	0.59196200	1.34448600	-2.96860100
C	-0.40099000	0.65449800	-3.75113400
H	0.42292200	2.40653700	-2.80130000
H	1.62991300	1.11447900	-3.20405400
H	-1.24144900	1.27035300	-4.06018500
C	0.03143200	-0.37699000	-4.76682000
H	0.51173200	0.15517000	-5.59950200
H	0.76389700	-1.07026700	-4.34379600
H	-0.80508500	-0.94926500	-5.17533300
H	0.91664400	-0.96238900	-1.69425600

INT7a

P	1.87175800	1.43714600	0.02571600
P	-1.49710300	0.57522000	1.00753800
C	3.36678300	1.18577100	-1.02793600
C	3.72075900	-0.12504200	-1.39156700
C	4.14357800	2.25395200	-1.49672500
C	4.83740500	-0.36039100	-2.19206100
H	3.12399300	-0.96923200	-1.05602000
C	5.25979800	2.01475800	-2.30295600
H	3.88655000	3.27468400	-1.23431700
C	5.61066900	0.71034100	-2.64934100
H	5.10466600	-1.37933000	-2.45751500
H	5.85377700	2.85231700	-2.65735400
H	6.48091200	0.52652400	-3.27267600
C	2.04156200	3.14025100	0.70147200
C	3.17267900	3.51986600	1.44592900
C	1.02297000	4.08162000	0.49311500
C	3.27492300	4.80869600	1.96876900
H	3.98032300	2.81353700	1.61622900
C	1.12691600	5.37334700	1.01481000
H	0.14580500	3.81075700	-0.08882100
C	2.25238800	5.73723000	1.75473800
H	4.15388500	5.08801200	2.54231300
H	0.33248000	6.09281500	0.83851300

H	2.33569700	6.74079200	2.16153300
C	-2.99917400	1.65274100	0.98748200
C	-2.83653900	3.03452200	1.19188800
C	-4.28695800	1.15683800	0.73895500
C	-3.93598600	3.89295900	1.16938700
H	-1.85006800	3.44979500	1.38282500
C	-5.38743800	2.01771000	0.72055600
H	-4.43972400	0.09599500	0.57137400
C	-5.21697300	3.38570500	0.93742600
H	-3.79302700	4.95612100	1.34153000
H	-6.37940200	1.61364900	0.53852400
H	-6.07464400	4.05225800	0.93016200
C	-2.12720000	-1.14038900	1.25291300
C	-3.00873900	-1.44935600	2.30586000
C	-1.66101500	-2.18095000	0.43718300
C	-3.40880800	-2.76475300	2.53366000
H	-3.39261800	-0.66338700	2.94958600
C	-2.05739500	-3.50084600	0.67122600
H	-0.98163100	-1.96134600	-0.37986200
C	-2.92980100	-3.79447100	1.71877900
H	-4.08934600	-2.98632900	3.35079400
H	-1.68145100	-4.29299100	0.03088600
H	-3.23558900	-4.82039600	1.90357900
C	2.33346600	0.33345400	1.46510400
H	2.12119400	-0.70217100	1.17790800
H	3.42028200	0.41457200	1.56981700
C	-0.85846700	0.95040300	2.72426300
H	-0.60827700	2.01445000	2.79136300
H	-1.67691500	0.77041200	3.42760100
C	1.72316400	0.64062400	2.83076400
H	1.72938300	1.72452200	3.01898600
C	0.32983200	0.09014100	3.14400400
H	0.23803900	-0.92912100	2.73516800
O	2.52228400	-0.02393500	3.80558300
O	0.36047800	0.03963700	4.56708500
C	1.71002800	-0.24172100	4.97490500
C	1.85671300	-1.70216100	5.38825700
H	2.90390700	-1.92984700	5.61046700
H	1.25590000	-1.90534800	6.27982800
H	1.52251800	-2.35943600	4.57991800
C	2.08500900	0.74074800	6.07875400
H	1.40737800	0.62970800	6.93096900
H	3.10899200	0.55753700	6.41798200
H	2.01247200	1.76810900	5.70963300

Ir	-0.12104600	1.04352200	-1.01601600
C	-4.48414900	0.05205800	-4.40618500
C	-4.03308000	0.86888900	-3.36600400
C	-4.79065300	1.93619600	-2.88263100
C	-6.03272800	2.16448500	-3.47375600
C	-6.49404200	1.34182200	-4.51296700
C	-5.72617900	0.27493700	-4.99111500
C	-3.43188700	-0.97790000	-4.70520600
H	-4.42194800	2.55902100	-2.07514000
H	-6.65151300	2.98736600	-3.12887300
H	-7.46514100	1.53957600	-4.95749000
H	-6.09297100	-0.35125700	-5.79938200
H	-3.78041000	-2.00759800	-4.57288400
N	-2.36865200	-0.66422600	-3.72518000
C	-2.69828500	0.40814000	-2.95053400
O	-2.02866700	0.94088100	-2.03363500
H	-3.02572100	-0.89000000	-5.72040700
C	0.02621900	-0.60750200	-3.94227500
C	-1.10132400	-1.32866700	-3.79191600
H	0.96735000	-1.15294700	-3.91888900
C	-1.14413500	-2.81166100	-3.73265300
C	-0.21232400	-3.58301100	-4.44993200
C	-2.11974900	-3.48112700	-2.97302200
C	-0.23739200	-4.97495700	-4.38594000
H	0.51911500	-3.08757900	-5.08154400
C	-2.15142200	-4.87508600	-2.91997200
H	-2.84606100	-2.90615900	-2.40557800
C	-1.20810400	-5.62784200	-3.62232800
H	0.48988400	-5.55144800	-4.95052200
H	-2.91574700	-5.37260700	-2.32913700
H	-1.23616100	-6.71292600	-3.58520200
C	0.12041400	0.87819400	-4.10881000
C	0.73664300	1.60374300	-2.88968200
H	0.76041100	1.08451700	-4.98214200
H	-0.85947000	1.30147100	-4.35245100
H	1.80190300	1.36638500	-2.89348100
C	0.57546600	3.12284400	-3.06457300
H	0.89404600	3.44119500	-4.06916000
H	-0.47200300	3.43961400	-2.95414900
H	1.17577100	3.69062100	-2.34554500
H	0.42230500	-0.40134400	-1.16706400
INT7b			
P	-1.47023000	-0.44398800	0.67174600

P	1.38502900	-2.05319300	-0.81655300
C	-2.53705300	1.04142400	0.93963800
C	-1.96344100	2.21153400	1.46524700
C	-3.90119300	1.04649800	0.61241300
C	-2.74237000	3.34825300	1.68038500
H	-0.90541500	2.24161100	1.70895200
C	-4.67652500	2.19128600	0.81757500
H	-4.36909200	0.15020100	0.21815400
C	-4.10148600	3.34218800	1.35618400
H	-2.28739000	4.23856200	2.10576800
H	-5.73422800	2.17489600	0.56907700
H	-4.70732800	4.22744600	1.52667600
C	-2.67974300	-1.83604900	0.60328600
C	-3.49304500	-2.16283400	1.70418200
C	-2.79685100	-2.59418400	-0.56935400
C	-4.38416300	-3.23277200	1.63429200
H	-3.43815900	-1.57972900	2.61901500
C	-3.69409600	-3.66408700	-0.64109800
H	-2.19375700	-2.33953500	-1.43500300
C	-4.48355100	-3.98830100	0.46188700
H	-5.00110500	-3.47684700	2.49437900
H	-3.77856900	-4.23363300	-1.56197500
H	-5.17768900	-4.82232800	0.41043400
C	1.22082700	-3.20632000	-2.24806300
C	0.13289900	-4.09117400	-2.33344300
C	2.14782900	-3.17303400	-3.30428600
C	-0.02050400	-4.92337000	-3.44425200
H	-0.59840900	-4.14577500	-1.53412200
C	1.98966200	-4.00399400	-4.41462700
H	3.00766800	-2.51335700	-3.25290600
C	0.90533100	-4.88105300	-4.48798900
H	-0.85997900	-5.61161500	-3.48693600
H	2.72150200	-3.97237700	-5.21681200
H	0.78849000	-5.53324000	-5.34869700
C	3.20799400	-1.89449400	-0.56499600
C	4.00834000	-3.05150200	-0.57955100
C	3.80983800	-0.66135800	-0.27606900
C	5.37491300	-2.97236600	-0.31704100
H	3.57052500	-4.01950300	-0.80630900
C	5.17900500	-0.58507300	-0.01013400
H	3.21065500	0.24208400	-0.26745500
C	5.96347800	-1.73803800	-0.03071200
H	5.97877800	-3.87499200	-0.33459200
H	5.62944100	0.37851900	0.21013700

H	7.02834000	-1.67743700	0.17481000
C	-0.72697600	-0.62025800	2.38369500
H	0.04872600	0.14618000	2.48232000
H	-1.50073900	-0.38928500	3.12288100
C	0.93988300	-3.12346300	0.63832500
H	-0.08803100	-3.48501400	0.53578700
H	1.59782300	-3.99700200	0.60632000
C	-0.13738800	-1.98602500	2.71959600
H	-0.90167900	-2.76766600	2.59074300
C	1.13790300	-2.42506100	1.99092700
H	1.82324900	-1.56744500	1.90097400
O	0.29835000	-1.95188700	4.07393700
O	1.67203900	-3.37327300	2.90986600
C	1.31374100	-2.95862800	4.24015400
C	2.50436400	-2.31781700	4.94505500
H	2.20041900	-1.92516400	5.92037900
H	3.29840500	-3.05555500	5.09469300
H	2.89813900	-1.49150500	4.34572000
C	0.75412600	-4.17016900	4.97763900
H	1.50454600	-4.96548300	5.02491900
H	0.46961500	-3.89461600	5.99757500
H	-0.12714600	-4.55543500	4.45624700
Ir	0.23367500	-0.09875800	-1.07900100
C	-2.65107700	3.74618300	-3.57937800
C	-1.82657800	3.68729400	-2.45182600
C	-1.53555500	4.81751000	-1.68772300
C	-2.09951800	6.02835900	-2.08649900
C	-2.93024400	6.09266300	-3.21588300
C	-3.21712900	4.95333100	-3.97517800
C	-2.75916000	2.37233700	-4.18594200
H	-0.89258900	4.74598500	-0.81695200
H	-1.89515100	6.93252500	-1.52128600
H	-3.35792100	7.04741700	-3.50773900
H	-3.86031900	5.01934900	-4.84805700
H	-3.78631300	1.99490700	-4.22088300
N	-1.93208800	1.55123100	-3.27623700
C	-1.36930500	2.30257900	-2.28076900
O	-0.61063000	1.89029200	-1.37852700
H	-2.34843000	2.32314300	-5.20221400
C	-0.36757500	-0.23267700	-3.71318800
C	-1.65533000	0.17298400	-3.52928100
H	-0.20214700	-1.29592100	-3.87108000
C	-2.84597800	-0.69645100	-3.70532100
C	-2.80520100	-1.79329000	-4.58496400

C	-4.05280300	-0.41647900	-3.03830100
C	-3.92963100	-2.59530500	-4.77473500
H	-1.89947000	-2.00050600	-5.14611300
C	-5.17855600	-1.21340800	-3.23759100
H	-4.10134200	0.41950600	-2.34645900
C	-5.12141600	-2.30675000	-4.10513700
H	-3.88152800	-3.43139500	-5.46655800
H	-6.10097100	-0.98304100	-2.71229000
H	-6.00184400	-2.92173900	-4.26736100
C	1.65849200	0.52245700	-2.54059900
C	0.85148200	0.66379700	-3.84732200
H	2.48240400	-0.18203500	-2.68104600
H	2.09657800	1.47812500	-2.23234900
H	1.13899300	0.43438500	0.07929900
H	0.50651100	1.69896700	-3.94435400
C	1.64845000	0.31720200	-5.11590900
H	2.53129800	0.96158800	-5.19161700
H	1.99205100	-0.72336800	-5.09263300
H	1.04753100	0.45501300	-6.02333400

TS5a

P	1.83860400	1.42443600	0.12550400
P	-1.47269900	0.74304900	1.01131400
C	3.31944000	1.16158700	-0.95160000
C	3.65114200	-0.15074900	-1.33282100
C	4.10413300	2.22286600	-1.42345500
C	4.75174300	-0.39338000	-2.15379300
H	3.04742400	-0.98889300	-0.99433500
C	5.20317300	1.97678800	-2.25185300
H	3.86759600	3.24413700	-1.14405900
C	5.53119900	0.67118200	-2.61570200
H	5.00233600	-1.41355600	-2.43089900
H	5.80252500	2.80978000	-2.60823300
H	6.38879600	0.48161100	-3.25473400
C	2.05209200	3.13307700	0.78699800
C	3.17495600	3.48954800	1.55535400
C	1.07787500	4.10707700	0.52193700
C	3.31101700	4.78626000	2.05043600
H	3.95161700	2.75969400	1.76624200
C	1.21648800	5.40675400	1.01665400
H	0.21520500	3.84097000	-0.08250600
C	2.33132500	5.74691300	1.78338500
H	4.18282500	5.04687400	2.64358700
H	0.45625600	6.15163600	0.79857200

H	2.44064700	6.75627800	2.16941500
C	-2.95977800	1.83878600	0.99629800
C	-2.77239700	3.22048400	1.17620800
C	-4.26174700	1.35103100	0.81750200
C	-3.86357100	4.08863400	1.19734100
H	-1.77315400	3.62625300	1.30916300
C	-5.35398100	2.22279800	0.84505000
H	-4.43212600	0.29100400	0.66455600
C	-5.15939200	3.59093300	1.03655600
H	-3.70238400	5.15261400	1.34607000
H	-6.35743000	1.82645200	0.71691800
H	-6.00990200	4.26608300	1.06329100
C	-2.09556500	-0.97990700	1.19358000
C	-2.98025300	-1.32609900	2.23141700
C	-1.60762100	-1.98935000	0.35082400
C	-3.36910400	-2.65213900	2.41572800
H	-3.37284500	-0.56448400	2.89869400
C	-1.99228500	-3.31885800	0.54453900
H	-0.91418600	-1.72692600	-0.44356400
C	-2.87244200	-3.65155800	1.57465500
H	-4.05281000	-2.90526000	3.22088700
H	-1.59803700	-4.09025100	-0.11021100
H	-3.16801900	-4.68574500	1.72754900
C	2.33345200	0.33549800	1.56899700
H	2.13104100	-0.70317700	1.28703100
H	3.41934600	0.43081400	1.67239200
C	-0.84466700	1.07973600	2.73560800
H	-0.54776500	2.13082900	2.81536700
H	-1.69360800	0.93682400	3.41122500
C	1.71086600	0.64360700	2.92592200
H	1.76485500	1.72250000	3.13458700
C	0.28515000	0.15772200	3.18630900
H	0.15861000	-0.85061700	2.76178500
O	2.44445900	-0.07687600	3.91210000
O	0.26480600	0.08940700	4.60899600
C	1.58828800	-0.25769800	5.05543700
C	1.65095200	-1.72476700	5.46623400
H	2.67856600	-2.00353400	5.71953400
H	1.01359600	-1.90152400	6.33784400
H	1.31089900	-2.36208600	4.64451300
C	1.97662600	0.70169100	6.17498500
H	1.26817800	0.62198500	7.00539100
H	2.97919900	0.46645300	6.54469300
H	1.96714100	1.73265400	5.80889900

Ir	-0.12041800	1.02328200	-0.93468300
C	-4.52433300	-0.11308600	-4.32627400
C	-4.06097200	0.68250700	-3.27598700
C	-4.83137200	1.71260000	-2.73576600
C	-6.10053900	1.92032200	-3.27478900
C	-6.57529200	1.11498500	-4.32137200
C	-5.79278500	0.08857200	-4.86025700
C	-3.45206100	-1.09610400	-4.70026200
H	-4.45054700	2.32438200	-1.92595200
H	-6.72953700	2.71421600	-2.88345300
H	-7.56752300	1.29552100	-4.72468500
H	-6.16874800	-0.52307100	-5.67546800
H	-3.75952900	-2.14068200	-4.58230900
N	-2.35780400	-0.77290700	-3.75825800
C	-2.69547700	0.25577500	-2.91918000
O	-2.01719400	0.77180900	-2.00578000
H	-3.09669400	-0.96662600	-5.73005100
C	0.02577100	-0.66232200	-4.10368800
C	-1.08215500	-1.40263100	-3.90989000
H	0.97244100	-1.19583800	-4.15754400
C	-1.08927000	-2.88779800	-3.89584700
C	-0.19711500	-3.61664200	-4.70140800
C	-1.99103900	-3.59817100	-3.08421100
C	-0.18710700	-5.01015800	-4.67381700
H	0.47448600	-3.08802900	-5.37154000
C	-1.98559200	-4.99298800	-3.06434600
H	-2.68669200	-3.05386800	-2.45185300
C	-1.08120800	-5.70458100	-3.85577300
H	0.50755600	-5.55466100	-5.30697000
H	-2.69075000	-5.52426800	-2.43089200
H	-1.08114600	-6.79056800	-3.84434100
C	0.09270800	0.83082800	-4.21000400
C	0.79559300	1.50782800	-3.01322000
H	0.66530800	1.09631400	-5.11182800
H	-0.90408100	1.25789500	-4.34703700
H	1.87089700	1.32797500	-3.09351400
C	0.57093500	3.02558300	-3.04135300
H	0.86363800	3.40186200	-4.03465500
H	-0.47906800	3.29362400	-2.88477200
H	1.17881900	3.55258300	-2.30278000
H	0.78981100	0.31859100	-2.06640600
TS5b			
P	-1.24993500	-0.38545800	0.74069500

P	1.49657600	-2.04680300	-0.67247500
C	-2.19321600	1.17186400	1.05164100
C	-1.54486100	2.26503200	1.64935600
C	-3.54808900	1.28980700	0.71035900
C	-2.24590100	3.43965200	1.92292500
H	-0.49181900	2.20555700	1.90935300
C	-4.24438500	2.47176800	0.97553800
H	-4.07059600	0.45294900	0.25757000
C	-3.59803400	3.54586500	1.58741500
H	-1.73601300	4.26997500	2.40379700
H	-5.29657300	2.54523300	0.71485800
H	-4.14393900	4.45928000	1.80521700
C	-2.55560100	-1.67970700	0.63946900
C	-3.39912600	-1.97518400	1.72562600
C	-2.72103700	-2.38618700	-0.56007600
C	-4.37229300	-2.96699400	1.61304700
H	-3.30359500	-1.42919400	2.65999200
C	-3.70308400	-3.37427800	-0.67499100
H	-2.08399300	-2.15271900	-1.40898500
C	-4.52419700	-3.66943300	0.41323600
H	-5.01371200	-3.19075700	2.46061600
H	-3.82921800	-3.90122700	-1.61611600
H	-5.28468600	-4.44054100	0.32905800
C	1.45362400	-3.21759400	-2.10694300
C	0.30249000	-3.99811700	-2.31240900
C	2.49518900	-3.29973200	-3.04546300
C	0.20098700	-4.84167400	-3.41923400
H	-0.52433400	-3.95490600	-1.60996600
C	2.38923200	-4.14137300	-4.15566900
H	3.40174700	-2.71914000	-2.90886600
C	1.24341700	-4.91447000	-4.34597600
H	-0.69223800	-5.44519100	-3.55433400
H	3.20911600	-4.19578700	-4.86634000
H	1.16482100	-5.57301000	-5.20615500
C	3.28783400	-1.74791200	-0.33842300
C	4.20119700	-2.81816300	-0.32789500
C	3.74696500	-0.46676300	0.00297600
C	5.54100600	-2.60409300	-0.00711300
H	3.87285900	-3.82252500	-0.57935100
C	5.08932700	-0.25485900	0.32629500
H	3.04668200	0.36236600	0.03165500
C	5.98875300	-1.32097300	0.31763500
H	6.23431000	-3.44021900	-0.00873300
H	5.42795800	0.74354600	0.58812700

H	7.03284700	-1.15625300	0.56779000
C	-0.49441400	-0.64198000	2.43343000
H	0.35427300	0.04291300	2.52720100
H	-1.24170700	-0.33118800	3.17100600
C	1.07964900	-3.20000900	0.73042200
H	0.07326500	-3.60728600	0.58848300
H	1.78041300	-4.03721300	0.65347700
C	-0.05471600	-2.06069800	2.77087300
H	-0.87032300	-2.77045200	2.56643300
C	1.22726000	-2.58143800	2.12035500
H	1.98760400	-1.78472100	2.11909500
O	0.28549500	-2.09916800	4.15239200
O	1.60532000	-3.60731600	3.03334800
C	1.19224400	-3.20157600	4.35087100
C	2.38258500	-2.69543600	5.15811000
H	2.04661100	-2.30311500	6.12302900
H	3.09215900	-3.50882100	5.33733800
H	2.89408400	-1.89381700	4.61697700
C	0.47372500	-4.37698300	5.00367100
H	1.14315800	-5.24025900	5.07051100
H	0.14586800	-4.10777700	6.01221900
H	-0.40094600	-4.66164100	4.41116600
Ir	0.23918800	-0.20245200	-1.10495600
C	-2.88821600	3.67653300	-3.59413500
C	-2.03628700	3.52087400	-2.49730400
C	-1.71694900	4.58382200	-1.65272400
C	-2.28251900	5.82621700	-1.93636200
C	-3.14256000	5.98706400	-3.03354300
C	-3.45714600	4.91442600	-3.87462500
C	-3.01333000	2.35783500	-4.30743300
H	-1.05620200	4.43679900	-0.80527400
H	-2.05649900	6.68025300	-1.30505200
H	-3.57079400	6.96464000	-3.23534700
H	-4.12206600	5.05407700	-4.72225600
H	-4.04073000	1.97961300	-4.34264700
N	-2.16078300	1.46382000	-3.49718800
C	-1.57961900	2.12260200	-2.44940900
O	-0.79694900	1.65943800	-1.59246800
H	-2.63452700	2.39248300	-5.33656700
C	-0.64425000	-0.31653300	-4.05152900
C	-1.91348100	0.10950500	-3.87725500
H	-0.49503800	-1.37641600	-4.24783100
C	-3.11375000	-0.74613100	-4.04986600
C	-3.12425100	-1.78019300	-5.00286900

C	-4.27153600	-0.53616700	-3.27910300
C	-4.24618300	-2.59187100	-5.16224200
H	-2.25762200	-1.92861000	-5.64018400
C	-5.39676900	-1.34256400	-3.44634900
H	-4.28224600	0.25430800	-2.53341400
C	-5.38831000	-2.37520800	-4.38670200
H	-4.23703700	-3.37986100	-5.91005200
H	-6.28003400	-1.16612200	-2.83897600
H	-6.26804100	-2.99741600	-4.52344500
C	1.55960600	0.21245200	-2.92851100
C	0.59757800	0.54085800	-4.08433300
H	2.04830500	-0.74613900	-3.09581700
H	2.36127200	0.96347200	-2.93180500
H	1.57956800	0.61929400	-1.43110500
H	0.31111700	1.59356700	-4.01045500
C	1.32504400	0.35432100	-5.43488800
H	2.22369900	0.97993600	-5.47871900
H	1.63119700	-0.68881400	-5.57655400
H	0.67529000	0.63399200	-6.27217300

4a

C	-1.85738100	3.20441700	-0.63701700
C	-1.96804100	1.81528200	-0.68280100
C	-1.31903000	0.99430700	0.23585500
C	-0.53951500	1.60459900	1.21944400
C	-0.42214500	3.00159200	1.26897400
C	-1.07941700	3.81721600	0.34147800
C	-2.67666000	3.80000900	-1.75498900
H	-1.42675200	-0.08453300	0.17410700
H	-0.01782200	0.99687800	1.95355800
H	0.18949200	3.45870200	2.04230000
H	-0.98128200	4.89877900	0.39192700
H	-3.47472700	4.45826000	-1.38781300
N	-3.23535200	2.61713800	-2.42040500
C	-2.85155600	1.42078900	-1.81306900
O	-3.18397400	0.29366900	-2.14472400
H	-2.06556400	4.38303200	-2.45802700
C	-3.93113000	2.15994900	-4.69665500
C	-4.16041900	2.73087900	-3.49930200
C	-2.70445400	1.42690700	-5.16810300
H	-1.94005300	1.46843600	-4.38477100
C	-3.03133200	-0.05451900	-5.44021800
C	-2.14132300	2.10969300	-6.43113500
H	-2.13923200	-0.58537800	-5.79470800

H	-3.38581300	-0.53620200	-4.52593200
H	-3.80543000	-0.14914500	-6.21301500
H	-1.24622300	1.58453300	-6.78513500
H	-2.87703800	2.09899000	-7.24572400
H	-1.87010600	3.15388500	-6.23753000
H	-4.73966500	2.22138000	-5.42523000
C	-5.40908500	3.48718300	-3.20397100
C	-6.01307900	4.29928900	-4.17868400
C	-6.01827800	3.39986700	-1.93998000
C	-7.20070400	4.97837100	-3.90914100
H	-5.53476600	4.40962800	-5.14785800
C	-7.20301800	4.08330200	-1.66872200
H	-5.56831700	2.77288200	-1.17518000
C	-7.80133900	4.87369500	-2.65267000
H	-7.64985400	5.60195900	-4.67780000
H	-7.66316600	3.99280100	-0.68816900
H	-8.72304700	5.40845800	-2.43995700

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C	-1.85195700	3.22263500	-0.60193600
C	-1.92746800	1.83056400	-0.62983700
C	-1.23186100	1.03762800	0.27936100
C	-0.44135700	1.67910700	1.23393800
C	-0.35974700	3.07912600	1.26549500
C	-1.06439000	3.86655600	0.34840400
C	-2.71478500	3.78581500	-1.70415300
H	-1.31291700	-0.04430300	0.23240000
H	0.11665200	1.09348500	1.95927400
H	0.26110600	3.56089800	2.01617400
H	-0.99362900	4.95084600	0.38454800
H	-3.51546100	4.43298600	-1.32405100
N	-3.26482800	2.58171000	-2.33873200
C	-2.83114100	1.40035100	-1.73073900
O	-3.14658500	0.26388100	-2.04390000
H	-2.13503200	4.37170300	-2.43084300
C	-3.96681600	1.98181100	-4.57057300
C	-4.18648800	2.64678400	-3.41969800
H	-4.77682400	1.98970100	-5.29854000
C	-5.42002300	3.44439900	-3.18145200
C	-5.99679700	4.20874300	-4.20955800
C	-6.04429900	3.44321100	-1.92173700
C	-7.17276800	4.92647200	-3.99403800
H	-5.50570000	4.25004300	-5.17774600
C	-7.21660000	4.16613900	-1.70446700

H	-5.61635900	2.85060900	-1.11769400
C	-7.78775000	4.90920900	-2.74025900
H	-7.60153500	5.51191400	-4.80327500
H	-7.68899700	4.14284200	-0.72583700
H	-8.69999000	5.47454000	-2.57001100
C	-2.74365800	1.20197000	-4.95368800
C	-2.40732600	1.32513700	-6.45031200
H	-2.89621700	0.14356700	-4.69648600
H	-1.88658000	1.52841400	-4.35132500
C	-1.17234200	0.51048900	-6.84715300
H	-3.27125600	0.99395900	-7.04392600
H	-2.24986800	2.38272200	-6.70374300
H	-0.95766000	0.60637800	-7.91764700
H	-0.28367800	0.84426300	-6.29735800
H	-1.31507600	-0.55460800	-6.62752800

TS1a

P	-1.00089500	1.77845700	1.50137600
P	2.50969500	1.42594300	1.82444300
C	-2.54953600	1.73573100	0.49564400
C	-3.80818400	1.46199900	1.05024900
C	-2.45613500	2.01916300	-0.87806900
C	-4.95035600	1.47073200	0.24427000
H	-3.90467000	1.23931800	2.10769300
C	-3.59872600	2.03362700	-1.67703800
H	-1.48842900	2.22669700	-1.32803200
C	-4.84896400	1.75703900	-1.11732000
H	-5.91901500	1.25423900	0.68575700
H	-3.51255300	2.25942700	-2.73605000
H	-5.73848000	1.76562700	-1.74049000
C	-1.51791600	1.46396500	3.23568400
C	-2.28485200	2.39011900	3.96565800
C	-1.14271800	0.25745800	3.84782300
C	-2.66177300	2.11339200	5.27986400
H	-2.59586300	3.32739400	3.51302300
C	-1.52367500	-0.01699400	5.16346000
H	-0.55330200	-0.46280700	3.28660500
C	-2.28069700	0.91044400	5.88085800
H	-3.25241100	2.83712700	5.83397800
H	-1.22989700	-0.95558800	5.62474700
H	-2.57573100	0.69820900	6.90446600
C	3.23925100	0.11602000	2.89224100
C	2.75284600	-0.08499500	4.19528100
C	4.23085900	-0.74454000	2.39338100

C	3.26674300	-1.10963600	4.99060900
H	1.96796000	0.54713400	4.59914900
C	4.73931200	-1.76915400	3.19317300
H	4.60342300	-0.61895800	1.38318200
C	4.26268200	-1.95197000	4.49286800
H	2.88977000	-1.24594700	6.00024000
H	5.51027300	-2.42403500	2.79726800
H	4.66542900	-2.74602200	5.11517000
C	3.81460100	1.94750400	0.64654800
C	5.10961000	2.25205200	1.09974300
C	3.50603800	2.10816400	-0.71232300
C	6.07731500	2.70636300	0.20489400
H	5.36989200	2.12662900	2.14727800
C	4.47717200	2.56824400	-1.60387600
H	2.50675800	1.86891000	-1.06493400
C	5.76167400	2.86673700	-1.14720400
H	7.07618600	2.93730700	0.56349800
H	4.22851200	2.69302200	-2.65395200
H	6.51664100	3.22465900	-1.84141100
C	-0.66771800	3.61771200	1.41528700
H	-0.28201100	3.81717800	0.40958900
H	-1.64224500	4.11359700	1.47940400
C	2.38777700	2.88723400	2.96316900
H	1.83621800	2.61034000	3.86697200
H	3.40802100	3.13992500	3.26947600
C	0.23679400	4.25747700	2.46583900
H	-0.04908000	3.91847100	3.47342000
C	1.75626500	4.11739500	2.31356400
H	2.03257700	4.18662800	1.24879800
O	0.06065000	5.66668200	2.35927700
O	2.22002200	5.26499400	3.01453400
C	1.24802800	6.31230900	2.85618100
C	1.70957800	7.32487900	1.81344700
H	0.92638800	8.06801900	1.63419200
H	2.61083100	7.84007200	2.15893600
H	1.93167000	6.82097900	0.86795200
C	0.99025900	6.92865800	4.22620200
H	1.91604400	7.34645600	4.63378100
H	0.24850500	7.72907300	4.14782400
H	0.61858500	6.16742000	4.91853600
Ir	0.63494300	0.41757200	0.71810800
C	0.00206100	-3.50871400	-0.69648100
C	0.32071100	-2.19876800	-0.37809700
C	-0.56015100	-1.19072100	0.03463100

C	-1.90570700	-1.59343500	0.07846900
C	-2.26220900	-2.91906800	-0.23409300
C	-1.33408700	-3.89681500	-0.62636600
C	1.29539300	-4.21294100	-1.04802800
H	-0.30208400	0.14639100	-0.60780000
H	-2.68924000	-0.89445600	0.34637500
H	-3.31169100	-3.19469700	-0.17480800
H	-1.66270500	-4.90330400	-0.86694100
H	1.50696200	-5.07950500	-0.41433500
N	2.32923200	-3.15813500	-0.83024500
C	1.74263000	-1.99538900	-0.44732500
O	2.26613100	-0.88796300	-0.14702600
H	1.32858800	-4.54308500	-2.09328800
C	4.43567900	-2.46580900	-1.74638200
C	3.72270000	-3.37495500	-1.06557300
H	5.50795800	-2.58322400	-1.85450900
C	4.29715800	-4.61918700	-0.49272300
C	3.93948300	-5.05161200	0.79636700
C	5.23148700	-5.36948900	-1.22394100
C	4.51191800	-6.20007000	1.34170300
H	3.23132400	-4.47000400	1.38138100
C	5.80500800	-6.51610000	-0.67496300
C	5.44620900	-6.93548300	0.60776400
H	4.23237000	-6.51893000	2.34196200
H	6.52316500	-7.08875800	-1.25468200
H	5.88804600	-7.83257400	1.03163700
H	3.98015700	-1.58144100	-2.17641300
H	5.49204200	-5.05985900	-2.23192300

TS1b

P	-0.78090000	1.58069500	-0.34117700
P	1.08979400	-1.18281000	0.64053800
C	-1.93883500	2.42111400	-1.51172300
C	-3.15156100	2.98205000	-1.08957500
C	-1.57938900	2.51907200	-2.86697900
C	-3.97946100	3.64413000	-2.00044800
H	-3.44962300	2.91715300	-0.04844600
C	-2.40574800	3.18501900	-3.77206100
H	-0.65194300	2.07655100	-3.22047400
C	-3.60724900	3.75287700	-3.34012300
H	-4.91232700	4.08174600	-1.65626000
H	-2.10604400	3.26967500	-4.81323100
H	-4.24691700	4.27752200	-4.04394700
C	-1.35452500	2.10420200	1.32625900

C	-1.30745700	3.44696800	1.74370700
C	-1.87085300	1.13835500	2.20216200
C	-1.75798300	3.80716000	3.01289200
H	-0.92849000	4.21697000	1.07765400
C	-2.32543100	1.50188000	3.47225600
H	-1.91196000	0.09852500	1.89239700
C	-2.26614400	2.83465400	3.87975000
H	-1.71330100	4.84650300	3.32532200
H	-2.71988700	0.74175500	4.14035600
H	-2.61500600	3.11828900	4.86855500
C	0.35985400	-2.00964700	2.12509000
C	1.04731300	-2.07260600	3.35084500
C	-0.93025700	-2.56205900	2.05009300
C	0.46336400	-2.68055600	4.46299800
H	2.04202200	-1.65046300	3.44998500
C	-1.51368300	-3.16723300	3.16499600
H	-1.47965800	-2.51380500	1.11424000
C	-0.81743800	-3.22983700	4.37286600
H	1.01069300	-2.72216400	5.40030300
H	-2.51157300	-3.58937900	3.08664200
H	-1.26969800	-3.70177300	5.24040100
C	2.46216600	-2.27472900	0.05231900
C	2.94534200	-3.34690200	0.81728600
C	3.08025100	-1.98675000	-1.17617500
C	4.02315900	-4.11069300	0.36420300
H	2.47851000	-3.59929000	1.76337000
C	4.16294700	-2.74518200	-1.62120200
H	2.71137800	-1.17244300	-1.79381800
C	4.63619800	-3.81054500	-0.85246500
H	4.38009500	-4.94257000	0.96472000
H	4.63286600	-2.50645500	-2.57109100
H	5.47528500	-4.40486500	-1.20231700
C	0.74846600	2.60754300	-0.66184600
H	1.13986900	2.29628400	-1.63544000
H	0.43093700	3.65079400	-0.76189900
C	2.05765900	0.19372400	1.44648600
H	1.42110000	0.66807000	2.20152800
H	2.89125600	-0.28125200	1.97195400
C	1.85756800	2.54251400	0.37778400
H	1.46184200	2.80871800	1.37015800
C	2.64804800	1.23673700	0.49780300
H	2.82295900	0.81620900	-0.50455300
O	2.86850500	3.46589400	-0.00866500
O	3.87572200	1.69844900	1.05205700

C	4.10867900	3.03950100	0.58474000
C	5.18094600	3.05323600	-0.49916800
H	5.29267900	4.06192800	-0.90889600
H	6.14188800	2.73326700	-0.08536000
H	4.90431700	2.37669200	-1.31333000
C	4.45581600	3.90650100	1.78998800
H	5.35193600	3.52221500	2.28696400
H	4.64353800	4.93709500	1.47423700
H	3.63131000	3.90108900	2.50914200
Ir	-0.54739500	-0.74229600	-0.88787300
C	-4.60499700	-0.45579100	-4.62289700
C	-4.42120300	-0.29119900	-3.24624800
C	-5.45706300	0.11451900	-2.40536600
C	-6.70371200	0.34874600	-2.98377500
C	-6.89267000	0.18895400	-4.36521800
C	-5.84521600	-0.21036000	-5.20216100
C	-3.30444700	-0.89603000	-5.24319800
H	-5.28973600	0.23985100	-1.34075100
H	-7.53871500	0.65832900	-2.36263500
H	-7.87302700	0.37707800	-4.79323100
H	-6.00689300	-0.32930500	-6.26976700
H	-3.36730600	-1.87782900	-5.72706400
N	-2.40045200	-0.96975200	-4.07970000
C	-3.02270100	-0.60542900	-2.92871100
O	-2.49257400	-0.52156000	-1.79783600
H	-2.92498500	-0.17945700	-5.98161900
C	-0.22216300	-1.21696200	-5.05531500
C	-1.11342500	-1.59300400	-4.13226100
H	0.45810500	-1.48311900	-1.92923600
H	0.71559200	-1.75082300	-5.16198800
C	-0.92654200	-2.77628600	-3.22988400
C	-1.17857600	-4.03998500	-3.78391900
C	-0.49067700	-2.65579200	-1.88678300
C	-0.99201100	-5.20090900	-3.03621000
H	-1.50614900	-4.10986600	-4.81776200
C	-0.25418600	-3.84709100	-1.17492300
C	-0.52228700	-5.09900600	-1.72757900
H	-1.18712800	-6.17253600	-3.48042200
H	0.13415300	-3.81066400	-0.16520600
H	-0.35288100	-5.99434400	-1.13574000
H	-0.40386700	-0.38506500	-5.72943800
[Rh(cod)DIOP] ⁺			
P	-0.42075500	1.70675900	-0.19854600

P	1.48379600	-1.21986700	0.42119700
C	-1.67216400	2.78145200	-1.03989300
C	-3.03786400	2.60546700	-0.75933300
C	-1.29605100	3.75293500	-1.98281400
C	-4.00063200	3.38345000	-1.40355900
H	-3.35284900	1.87669900	-0.01775800
C	-2.26243800	4.53222300	-2.62284000
H	-0.24944300	3.91934800	-2.22022200
C	-3.61583700	4.34830300	-2.33681500
H	-5.05129100	3.24057000	-1.16787900
H	-1.95336700	5.28609200	-3.34117800
H	-4.36572100	4.95674100	-2.83359200
C	-1.08094700	1.65608100	1.51962500
C	-1.07868900	2.80135400	2.33671800
C	-1.67078000	0.47934900	2.00028000
C	-1.63341200	2.75539700	3.61448900
H	-0.65661300	3.73505000	1.97629000
C	-2.23211400	0.43717300	3.27948600
H	-1.68943300	-0.40741700	1.37642900
C	-2.20891800	1.57239200	4.08910200
H	-1.62195900	3.64457000	4.23816200
H	-2.68073100	-0.48440000	3.63853200
H	-2.64123300	1.54105000	5.08501000
C	0.51354400	-2.28347200	1.56825000
C	0.98179300	-2.57653900	2.85978600
C	-0.69359000	-2.85453500	1.13631900
C	0.24767100	-3.41075500	3.70311800
H	1.92170700	-2.16334500	3.21297600
C	-1.42285600	-3.69638400	1.97906500
H	-1.06391500	-2.62831700	0.13985400
C	-0.95435100	-3.97237100	3.26491900
H	0.61813700	-3.62638200	4.70110100
H	-2.35476500	-4.13385600	1.63204400
H	-1.52069800	-4.62546600	3.92255000
C	2.89642000	-2.32089800	-0.04799400
C	2.69135800	-3.70218800	-0.20591600
C	4.18133000	-1.79734100	-0.28139400
C	3.73954000	-4.53710700	-0.59664800
H	1.71951500	-4.13811700	0.00484100
C	5.22636800	-2.63785400	-0.66910700
H	4.39247700	-0.74284700	-0.13698600
C	5.00837600	-4.00699800	-0.83373300
H	3.56396500	-5.60368500	-0.70377700
H	6.21505400	-2.21911700	-0.83353000

H	5.82483000	-4.65741900	-1.13336000
C	1.04874200	2.86061300	-0.12223700
H	1.51493800	2.85015000	-1.11318000
H	0.68347300	3.87844200	0.05031100
C	2.30296000	0.02820800	1.52979600
H	1.56518000	0.35456100	2.27036400
H	3.11840000	-0.45797300	2.07232300
C	2.12678200	2.55543000	0.91458400
H	1.71135800	2.62594500	1.93109000
C	2.88735100	1.23100500	0.76804900
H	2.99539400	1.00751300	-0.30654100
O	3.15794100	3.51674000	0.73155900
O	4.15591700	1.54147400	1.32978700
C	4.39347100	2.95857900	1.20494400
C	5.46745000	3.22895300	0.15840800
H	5.59210000	4.30634400	0.01322700
H	6.42402000	2.80568600	0.47894000
H	5.18325400	2.78012200	-0.79825100
C	4.74108300	3.50432300	2.58576500
H	5.63817500	3.01191500	2.97344000
H	4.92696500	4.58110800	2.53127900
H	3.91783300	3.32277000	3.28320400
C	0.33466400	-2.31264200	-2.53982300
H	0.59373500	-3.04824100	-1.78305900
C	-0.93652500	-2.61359800	-3.32089800
H	-0.72740200	-2.58238000	-4.39411200
H	-1.24084400	-3.64382000	-3.10752000
C	-2.10892900	-1.67149900	-2.96841600
H	-2.86433600	-1.69182200	-3.76899800
H	-2.61528300	-2.04860900	-2.07229500
C	-1.69879200	-0.24171100	-2.69430100
H	-2.40205400	0.31986000	-2.08276600
C	-0.73748600	0.49114900	-3.36989900
H	-0.74478900	1.56486000	-3.20959500
C	0.06186700	0.01841700	-4.57156700
H	0.24521300	0.87485000	-5.22925800
H	-0.52819200	-0.69058600	-5.15873100
C	1.41567000	-0.60028200	-4.17225700
H	2.13844500	0.20331400	-3.98762200
H	1.82824100	-1.18928500	-5.00628300
C	1.35921300	-1.45924200	-2.93059900
H	2.32404100	-1.60910600	-2.45199700
Rh	0.15686000	-0.33881100	-1.38427600

INT8

P	0.92380100	1.92764200	0.75341200
P	2.45801900	-1.30751300	1.10923200
C	1.36190200	2.90306700	-0.75059400
C	0.62988400	2.66371100	-1.92890400
C	2.39367300	3.85591200	-0.77964400
C	0.92325700	3.36094100	-3.10068500
H	-0.17862200	1.93956500	-1.92123100
C	2.68540100	4.54976800	-1.95669400
H	2.97504800	4.07445100	0.10944900
C	1.95354900	4.30396300	-3.11886000
H	0.34559100	3.16747100	-4.00032800
H	3.48436200	5.28587800	-1.96000200
H	2.18231300	4.84570300	-4.03213200
C	-0.58330900	2.75040700	1.42298300
C	-0.78908200	4.13096700	1.26840000
C	-1.52245200	1.99783800	2.14417400
C	-1.90838000	4.74450300	1.83135800
H	-0.07928600	4.72778200	0.70271300
C	-2.63873300	2.61532700	2.71222500
H	-1.38575500	0.92632200	2.25431600
C	-2.83349200	3.98864800	2.55608900
H	-2.05710000	5.81312600	1.70450500
H	-3.35646700	2.02212500	3.27196900
H	-3.70296400	4.46904400	2.99583800
C	2.60429900	-3.14319300	1.11366100
C	1.84484200	-3.89575800	2.02538900
C	3.42005300	-3.81296900	0.18987100
C	1.92249500	-5.28821900	2.02886800
H	1.18965100	-3.40258600	2.73789800
C	3.48954900	-5.20814300	0.19218200
H	4.00881700	-3.25176100	-0.52854200
C	2.74620900	-5.94740000	1.11266600
H	1.34158300	-5.85714900	2.74922700
H	4.12970100	-5.71368900	-0.52498000
H	2.80725200	-7.03180300	1.11715600
C	4.01141800	-0.71983600	0.33099700
C	5.26455900	-1.00718300	0.90232700
C	3.95847000	0.01298400	-0.86385000
C	6.43481100	-0.55853200	0.29226100
H	5.33084100	-1.58804300	1.81814700
C	5.13325000	0.45879100	-1.47482900
H	2.99970700	0.24077500	-1.32224000
C	6.37055900	0.17569000	-0.89623800

H	7.39708600	-0.78370800	0.74272300
H	5.07689300	1.02644800	-2.39884700
H	7.28466500	0.52261700	-1.36927500
C	2.22584300	2.44216800	1.98135500
H	3.21144200	2.35729000	1.51104700
H	2.06349300	3.49643800	2.22757200
C	2.62737400	-0.93918600	2.93341100
H	1.65145900	-1.12125300	3.39487700
H	3.31636400	-1.68516000	3.34347900
C	2.20077100	1.64550600	3.28705100
H	1.17498700	1.33882400	3.55026900
C	3.14364800	0.43369200	3.36352600
H	4.07442400	0.67573900	2.82802000
O	2.73580800	2.48276600	4.30669500
O	3.39511600	0.33806200	4.76152600
C	3.28728300	1.65259700	5.33900600
C	4.66678400	2.19361200	5.69651300
H	4.58769000	3.22256100	6.06082400
H	5.12386200	1.57877300	6.47756600
H	5.31490600	2.18608300	4.81511600
C	2.34170200	1.57055700	6.53311000
H	2.72726300	0.86300500	7.27369500
H	2.24066200	2.55274100	7.00450300
H	1.35252900	1.23098100	6.21122900
C	-4.38945900	-1.02419300	-1.70616700
C	-3.59471200	0.05140600	-1.29993700
C	-4.11935500	1.32986200	-1.10400900
C	-5.48196500	1.50757700	-1.33987600
C	-6.28415500	0.43242100	-1.75327300
C	-5.74856200	-0.84665100	-1.94005000
C	-3.53000400	-2.25354000	-1.81177000
H	-3.48610700	2.14735000	-0.77468800
H	-5.93075200	2.48644500	-1.20116800
H	-7.34328200	0.59612900	-1.92947800
H	-6.38260300	-1.67006700	-2.25620200
H	-3.82609900	-3.04817200	-1.11710800
N	-2.18369700	-1.75338400	-1.44587200
C	-2.22530500	-0.43558900	-1.11948300
O	-1.25601500	0.26262700	-0.72206200
H	-3.51989700	-2.68136600	-2.81747000
C	0.08284000	-2.25730100	-0.67169900
C	-1.04493500	-2.59685100	-1.34304500
H	-0.12479700	-0.89132300	1.43641900
H	0.83599800	-3.04083100	-0.67615200

C	-1.15011800	-3.90648500	-2.05604300
C	-1.33996100	-3.95984400	-3.44826700
C	-1.00622800	-5.10816900	-1.34645900
C	-1.39206500	-5.18575600	-4.11028000
H	-1.42040200	-3.03582800	-4.01630900
C	-1.05977800	-6.33464100	-2.01092000
H	-0.85211000	-5.07450500	-0.27170600
C	-1.25624500	-6.37705700	-3.39214300
H	-1.52911300	-5.21133100	-5.18766900
H	-0.95193600	-7.25721300	-1.44753300
H	-1.29922900	-7.33169700	-3.90844800
Rh	0.53648200	-0.47034300	0.12804800

TS6a

P	0.97024000	0.49102100	-3.25778300
P	2.01345000	-1.35081200	-0.40179400
C	0.55438900	-0.32489400	-4.86025500
C	-0.73556200	-0.15165300	-5.39208800
C	1.46480300	-1.13349100	-5.55873100
C	-1.10428800	-0.77392300	-6.58406300
H	-1.44540700	0.49750500	-4.88989700
C	1.09296100	-1.75676700	-6.75287600
H	2.47568300	-1.27655300	-5.19272300
C	-0.19197200	-1.58259900	-7.26746000
H	-2.10057200	-0.61416500	-6.98729200
H	1.81597400	-2.36811200	-7.28559700
H	-0.47609100	-2.05951500	-8.20114000
C	0.38254400	2.22263800	-3.53483800
C	0.64835000	2.84726400	-4.76723900
C	-0.27298400	2.95265200	-2.53534100
C	0.27398800	4.17170400	-4.98639600
H	1.14267300	2.29912600	-5.56411000
C	-0.64779600	4.28032600	-2.75729000
H	-0.49137900	2.48005000	-1.58545100
C	-0.37514600	4.89230700	-3.98049400
H	0.49016300	4.64024000	-5.94220300
H	-1.15261300	4.83465800	-1.97077800
H	-0.66627100	5.92476100	-4.15178500
C	1.80175300	-2.23930000	1.20008300
C	1.98367600	-1.60315700	2.43803300
C	1.39755800	-3.58605400	1.18112900
C	1.77367200	-2.30105400	3.63053200
H	2.30229100	-0.56665200	2.48893000
C	1.18847300	-4.27840100	2.37284000

H	1.25706200	-4.09907600	0.23428400
C	1.37584700	-3.63739000	3.60076500
H	1.92749500	-1.79739400	4.58046400
H	0.88491300	-5.32085900	2.34232700
H	1.21627700	-4.17929800	4.52830300
C	3.04264200	-2.54361200	-1.36313600
C	4.20012600	-3.07357500	-0.76254900
C	2.72773100	-2.91925500	-2.67549100
C	5.02558000	-3.94781600	-1.46703400
H	4.45565400	-2.81241800	0.26032900
C	3.55433100	-3.80212900	-3.37686700
H	1.82811100	-2.54265200	-3.14707800
C	4.70420200	-4.31437700	-2.77722300
H	5.91666800	-4.34660300	-0.99108000
H	3.28965600	-4.09275800	-4.38959300
H	5.34532400	-5.00076600	-3.32268600
C	2.81534400	0.72496000	-3.36089900
H	3.30771900	-0.24272400	-3.49551800
H	3.01814300	1.32590000	-4.25271100
C	3.21724100	0.00300300	0.04701300
H	2.65107600	0.81457100	0.51415600
H	3.90502300	-0.39884800	0.79861400
C	3.40742100	1.45261000	-2.14939700
H	2.66238000	2.10977300	-1.67427200
C	4.07192000	0.56707300	-1.08605200
H	4.61019200	-0.24958700	-1.59070100
O	4.51796300	2.22142300	-2.60182900
O	4.99973200	1.46709100	-0.49158000
C	5.41858800	2.40899100	-1.49782100
C	6.82941300	2.08773500	-1.97777400
H	7.11107900	2.75361900	-2.79937700
H	7.54567700	2.21554400	-1.16070400
H	6.88037500	1.05496500	-2.33512700
C	5.28090400	3.81302300	-0.91898100
H	5.90314900	3.91674000	-0.02464200
H	5.59649000	4.55849300	-1.65499900
H	4.24030800	4.00863000	-0.64304900
C	-4.79364900	-0.92726900	-3.65065100
C	-4.02686900	0.09757300	-3.09123500
C	-4.48701600	1.41328600	-3.02153300
C	-5.75831900	1.67891400	-3.52950100
C	-6.53542500	0.65177500	-4.08701100
C	-6.06205000	-0.66317000	-4.15598000
C	-4.00739400	-2.20541600	-3.58624200

H	-3.86860200	2.19687500	-2.59518400
H	-6.15375600	2.68956200	-3.49526400
H	-7.52348500	0.88277600	-4.47430400
H	-6.67351800	-1.44770300	-4.59279900
H	-4.49720100	-2.98444400	-2.99200400
N	-2.74230600	-1.79577100	-2.93741900
C	-2.75112500	-0.47428200	-2.64073700
O	-1.84694000	0.20012900	-2.07633600
H	-3.80156400	-2.62914700	-4.57461100
C	-0.53107100	-2.40040800	-2.07324100
C	-1.68331600	-2.73153900	-2.68122200
H	0.32309100	0.91338500	-0.50812100
H	0.12698000	-3.25837200	-1.95232900
C	-1.96333700	-4.13139800	-3.14579600
C	-1.70712500	-4.51242600	-4.47319800
C	-2.45574500	-5.09300300	-2.25009200
C	-1.94067700	-5.82331000	-4.89242800
H	-1.31237300	-3.77902400	-5.17214900
C	-2.68805800	-6.40447300	-2.66978000
H	-2.65079900	-4.80904000	-1.21899500
C	-2.43291900	-6.77153600	-3.99250700
H	-1.73318100	-6.10631300	-5.92090900
H	-3.06693000	-7.13839800	-1.96382200
H	-2.61297000	-7.79164400	-4.31972500
C	-1.17569500	-1.04370700	0.51428600
C	-0.74064800	0.25157000	0.85547700
H	-0.72466000	-1.90840500	0.98355600
H	-2.19479300	-1.17568200	0.16240800
H	0.11753800	0.32101500	1.51893500
C	-1.67286100	1.43859800	0.87359900
H	-1.13094800	2.38870200	0.88296600
H	-2.35100200	1.42093900	0.01731500
H	-2.27774100	1.38880600	1.78936900
Rh	0.00826600	-0.54027100	-1.29133400

TS6b

P	0.87666700	0.41225000	-3.13804800
P	2.17092700	-1.43171400	-0.36953300
C	0.36600700	-0.38282800	-4.72618800
C	-0.90358500	-0.10337000	-5.26093700
C	1.19590300	-1.28573700	-5.41065900
C	-1.33266700	-0.71519600	-6.43916500
H	-1.55191500	0.61819900	-4.77478800
C	0.76493200	-1.89584600	-6.59140300

H	2.19046600	-1.51380100	-5.04358100
C	-0.50131800	-1.61719600	-7.10707800
H	-2.31177800	-0.47189400	-6.84267200
H	1.42866400	-2.57884500	-7.11437800
H	-0.83144600	-2.08687600	-8.02912800
C	0.27018200	2.14781900	-3.35086200
C	0.52130300	2.81692000	-4.56310500
C	-0.39049400	2.83640300	-2.32509400
C	0.12970700	4.14301200	-4.73648800
H	1.01757800	2.30247600	-5.38083300
C	-0.78291400	4.16611200	-2.50113400
H	-0.60196600	2.33031300	-1.39139500
C	-0.52293600	4.82192200	-3.70411300
H	0.33611300	4.64581700	-5.67690800
H	-1.29043800	4.68732700	-1.69407000
H	-0.82643700	5.85614300	-3.83939300
C	2.11595600	-2.32517600	1.24381700
C	2.36233700	-1.67500500	2.46359100
C	1.76855600	-3.68769700	1.25903900
C	2.26915200	-2.37327200	3.67010500
H	2.63992500	-0.62581200	2.48872200
C	1.67515200	-4.38048200	2.46525000
H	1.58257500	-4.21399400	0.32752600
C	1.92486500	-3.72492700	3.67400800
H	2.47116200	-1.85775100	4.60452200
H	1.41318500	-5.43455900	2.46003000
H	1.85530200	-4.26687100	4.61256100
C	3.14236600	-2.60198000	-1.41282400
C	4.38586100	-3.06053100	-0.93814700
C	2.68988100	-3.04231100	-2.66290100
C	5.16129400	-3.92519300	-1.70796100
H	4.74957700	-2.75146100	0.03770100
C	3.46739200	-3.91612000	-3.42925600
H	1.72203000	-2.72225100	-3.03011200
C	4.70366900	-4.35489200	-2.95713000
H	6.12020300	-4.26763500	-1.33005400
H	3.09812600	-4.25739000	-4.39233800
H	5.30684700	-5.03357500	-3.55315100
C	2.70988800	0.65327500	-3.37213000
H	3.19276100	-0.31499000	-3.53344000
H	2.84801800	1.24412600	-4.28245500
C	3.37619400	-0.05253700	-0.01063000
H	2.82915900	0.75045500	0.49295800
H	4.12158100	-0.43603000	0.69395700

C	3.38421100	1.39507000	-2.21381600
H	2.66947700	2.04554800	-1.68563400
C	4.13895400	0.52333700	-1.20165200
H	4.65084900	-0.28578400	-1.74436800
O	4.44745800	2.17599500	-2.75095300
O	5.09335500	1.43917400	-0.67835500
C	5.42155700	2.38482900	-1.71496100
C	6.79974800	2.08745500	-2.29436300
H	7.00743600	2.75329000	-3.13771200
H	7.57093500	2.23461600	-1.53237800
H	6.84500000	1.05350200	-2.64902500
C	5.29980500	3.78842200	-1.13150700
H	5.98025200	3.90597600	-0.28241200
H	5.55106800	4.53656600	-1.88928500
H	4.27761800	3.96764800	-0.78468900
C	-4.53676500	-0.92789700	-3.77606400
C	-3.87201100	0.04031600	-3.01958200
C	-4.34866800	1.34708700	-2.90630700
C	-5.53205800	1.66162400	-3.57400700
C	-6.20663100	0.69148900	-4.33120900
C	-5.71621500	-0.61426600	-4.44311900
C	-3.76259400	-2.21270400	-3.70011300
H	-3.80964100	2.08736100	-2.32384600
H	-5.93801700	2.66661600	-3.50966800
H	-7.12726800	0.96002400	-4.84108700
H	-6.24790200	-1.35496700	-5.03383800
H	-4.34398500	-3.03840800	-3.27958000
N	-2.62863000	-1.87541900	-2.81250000
C	-2.66684200	-0.57176200	-2.44395300
O	-1.83334900	0.05864100	-1.73922700
H	-3.37931000	-2.53854800	-4.67408400
C	-0.48314000	-2.52518900	-1.82470800
C	-1.62384600	-2.83990400	-2.46529500
H	0.41919100	0.83223500	-0.40429200
H	0.12243900	-3.40472500	-1.61352100
C	-1.95364400	-4.25253700	-2.84950700
C	-1.29906100	-4.86328100	-3.92960200
C	-2.89008600	-5.00227100	-2.11784500
C	-1.56994500	-6.19115800	-4.26762500
H	-0.57929400	-4.28826000	-4.50607700
C	-3.16300500	-6.32772400	-2.45723300
H	-3.39537500	-4.54735400	-1.26881400
C	-2.50308000	-6.92557500	-3.53402300
H	-1.05350300	-6.65086400	-5.10594400

H	-3.88446700	-6.89609500	-1.87672400
H	-2.71394500	-7.95823000	-3.79698500
C	-0.42045800	0.16052900	1.02871800
C	-0.92892500	-1.14690800	0.88700800
H	0.47586700	0.33164300	1.61573400
H	-1.10784400	1.00207400	0.98776500
H	-0.33522500	-1.95392800	1.30175000
C	-2.40951900	-1.42888500	0.81663600
H	-2.77816400	-1.63744900	1.83085300
H	-2.97337800	-0.57931700	0.42449400
H	-2.62202300	-2.31115500	0.20594900
Rh	0.08210700	-0.65374700	-1.09524000

INT9a

P	1.13443500	0.65372600	-3.49754500
P	1.95905400	-1.83974300	-0.98911000
C	1.11403700	-0.00979800	-5.22434300
C	-0.10851700	-0.47704700	-5.74256400
C	2.25639500	-0.07779400	-6.03917400
C	-0.18185300	-0.99970300	-7.03357500
H	-1.00419500	-0.42279800	-5.13354800
C	2.17927600	-0.60500800	-7.33105300
H	3.21452700	0.28662300	-5.68674700
C	0.96274400	-1.06970700	-7.83104700
H	-1.13572300	-1.35108400	-7.41744400
H	3.07362100	-0.64406400	-7.94665900
H	0.90528600	-1.47729300	-8.83629600
C	0.34029800	2.31283800	-3.66158100
C	0.36772200	3.02353900	-4.87301600
C	-0.25782500	2.90831100	-2.54084700
C	-0.18731800	4.30087600	-4.95572000
H	0.81860600	2.58001300	-5.75551100
C	-0.80723300	4.18946300	-2.62400100
H	-0.29997600	2.37217900	-1.59930000
C	-0.77420300	4.88738400	-3.83189600
H	-0.15938300	4.83838200	-5.89943200
H	-1.26289100	4.63856800	-1.74589600
H	-1.20392300	5.88282700	-3.89849700
C	1.77062400	-3.08447600	0.35934200
C	1.61558900	-2.68727600	1.69803200
C	1.72495200	-4.45377400	0.04918500
C	1.42974400	-3.63936800	2.70215500
H	1.65181700	-1.63777700	1.97356700
C	1.53640200	-5.40197800	1.05536700

H	1.84722000	-4.78505200	-0.97770900
C	1.38929900	-4.99764800	2.38358100
H	1.32378200	-3.31658100	3.73391600
H	1.50971600	-6.45717400	0.79934300
H	1.24903100	-5.73719200	3.16654500
C	3.09104500	-2.66909800	-2.17552100
C	4.37224600	-3.09023400	-1.77478100
C	2.67332700	-2.91467700	-3.49117000
C	5.21746200	-3.72977400	-2.67954500
H	4.70888300	-2.93003100	-0.75414200
C	3.52151200	-3.55977400	-4.39558200
H	1.68547000	-2.60205300	-3.81736000
C	4.79364200	-3.96431200	-3.99165500
H	6.20543200	-4.04869600	-2.36036700
H	3.18466300	-3.74010500	-5.41204500
H	5.45433900	-4.46494100	-4.69355700
C	2.92800700	1.11024700	-3.25914200
H	3.55315000	0.27380800	-3.58872100
H	3.15421600	1.96788400	-3.90017800
C	2.99472800	-0.54178600	-0.13124200
H	2.32164700	0.08389400	0.46364200
H	3.63933400	-1.07094500	0.57820000
C	3.29139000	1.48104000	-1.81950400
H	2.43452400	1.92907000	-1.28932100
C	3.90485500	0.35533100	-0.96902800
H	4.55018200	-0.26001900	-1.61438000
O	4.36783400	2.41080700	-1.87471500
O	4.69701400	1.08479300	-0.03754900
C	5.14213900	2.29740000	-0.67074200
C	6.61217700	2.18996300	-1.06116900
H	6.92349700	3.08125500	-1.61464900
H	7.23617300	2.09532900	-0.16743700
H	6.76993500	1.31393900	-1.69742600
C	4.84952900	3.45987300	0.27173200
H	5.37832600	3.32229600	1.22003300
H	5.17440100	4.40263500	-0.17837900
H	3.77643800	3.51876100	0.47742800
C	-5.23435000	-1.18797300	-3.02121400
C	-4.15818700	-0.37377700	-3.38364600
C	-4.33138000	0.80802700	-4.10531600
C	-5.63237700	1.15487400	-4.46780400
C	-6.71693800	0.33849700	-4.11081700
C	-6.53172800	-0.84197200	-3.38263100
C	-4.71318500	-2.36857000	-2.24932600

H	-3.48083100	1.43019700	-4.36588800
H	-5.81184500	2.06609200	-5.03022100
H	-7.72119800	0.63045200	-4.40371100
H	-7.38140700	-1.46169700	-3.11058700
H	-5.09139300	-2.41382800	-1.22168600
N	-3.24896100	-2.13902600	-2.23148800
C	-2.92993500	-0.97859400	-2.86281700
O	-1.77778600	-0.48925900	-2.98530400
H	-4.94406300	-3.32466900	-2.72677400
C	-1.05062200	-2.66107700	-1.27563200
C	-2.34175900	-2.98291200	-1.53324800
H	-2.55573500	-0.38287100	-0.06447700
H	-0.53197100	-3.41763800	-0.69274300
C	-2.90384300	-4.29927800	-1.09459700
C	-3.29581000	-5.26707300	-2.03586400
C	-3.00498800	-4.60467900	0.27074000
C	-3.78380600	-6.50520100	-1.61925700
H	-3.19654100	-5.05503100	-3.09807600
C	-3.49342300	-5.84490600	0.68658100
H	-2.69965500	-3.86393400	1.00456100
C	-3.88696100	-6.79586300	-0.25615900
H	-4.07520100	-7.24642600	-2.35815200
H	-3.56935200	-6.06533600	1.74765500
H	-4.26833400	-7.76002300	0.06753500
C	-0.42574400	-0.06412200	-0.18867300
C	-1.85061400	0.45566800	-0.05613600
H	0.29644200	0.75924700	-0.19172500
H	-0.19677500	-0.73785400	0.64136200
H	-2.10937600	1.10104700	-0.90176800
C	-2.02280400	1.24336900	1.25701900
H	-3.05050100	1.61113500	1.35390000
H	-1.80748900	0.61652700	2.13020000
H	-1.35326100	2.11110200	1.29624000
Rh	-0.02082900	-1.09293900	-1.96958400

INT9b

P	1.05084800	0.70454100	-3.20386700
P	2.19916200	-1.88427800	-0.89332000
C	0.93508800	0.15705900	-4.96660000
C	-0.01461600	-0.81166400	-5.33041400
C	1.76196500	0.69906700	-5.96482900
C	-0.12767700	-1.23460700	-6.65728500
H	-0.67928600	-1.22375600	-4.57755700
C	1.65105300	0.27148400	-7.28803800

H	2.49443000	1.46192700	-5.72095800
C	0.70809200	-0.69795800	-7.63753300
H	-0.87000800	-1.98247800	-6.92272200
H	2.29988600	0.69975000	-8.04679500
H	0.62259900	-1.02793300	-8.66894300
C	0.18835300	2.34081400	-3.23962700
C	-1.04243500	2.44826700	-3.90951300
C	0.70355200	3.47534100	-2.59089000
C	-1.73884800	3.65621300	-3.92867100
H	-1.44350400	1.59017600	-4.43911000
C	-0.00064400	4.68201500	-2.60852000
H	1.66442000	3.44736600	-2.08797500
C	-1.22322300	4.77643200	-3.27271500
H	-2.68058500	3.72666000	-4.46635600
H	0.41749300	5.55119800	-2.10865900
H	-1.76509900	5.71755600	-3.28936300
C	2.24613300	-3.29212400	0.30629100
C	2.51079100	-3.10910300	1.67285200
C	1.99141500	-4.59236300	-0.16320200
C	2.52440400	-4.19943100	2.54595800
H	2.72202800	-2.12289000	2.07296600
C	2.00383200	-5.67839900	0.71098000
H	1.79472400	-4.76187200	-1.21774400
C	2.27008500	-5.48496400	2.06843600
H	2.74034600	-4.03931800	3.59836200
H	1.80981900	-6.67647800	0.32910100
H	2.28386400	-6.33208100	2.74795600
C	3.14123100	-2.58646200	-2.31257500
C	4.48286900	-2.98172700	-2.16138800
C	2.51128900	-2.78628700	-3.54818400
C	5.17819500	-3.54012000	-3.23234600
H	4.98564300	-2.86777400	-1.20497500
C	3.20836700	-3.34969000	-4.62052300
H	1.47276100	-2.50055500	-3.68304300
C	4.54289600	-3.72237600	-4.46501000
H	6.21492700	-3.83753700	-3.10396800
H	2.70513800	-3.48987100	-5.57263200
H	5.08789700	-4.15836100	-5.29726400
C	2.84368400	1.19429200	-3.06451100
H	3.43940300	0.40966400	-3.54305100
H	3.00321700	2.11308900	-3.63601000
C	3.37655600	-0.67968500	-0.08858500
H	2.81676000	-0.12267100	0.66895500
H	4.12848400	-1.26789400	0.44665600

C	3.34493000	1.44995800	-1.63594200
H	2.52373000	1.75430200	-0.96764000
C	4.13477800	0.31517700	-0.96743100
H	4.72159500	-0.21750100	-1.73026900
O	4.31490000	2.48995600	-1.70789000
O	4.99926700	1.02603600	-0.08681400
C	5.27287800	2.31848900	-0.64908200
C	6.66903400	2.35603000	-1.26188300
H	6.83680500	3.31360400	-1.76443300
H	7.42790700	2.23000000	-0.48388900
H	6.78028800	1.55412400	-1.99786700
C	5.06292200	3.36484700	0.43982400
H	5.74229400	3.18109600	1.27786100
H	5.25660800	4.36659200	0.04480800
H	4.03434000	3.32334500	0.81101400
C	-5.18271500	-1.57540700	-2.30282200
C	-4.18218500	-0.73837200	-2.80440500
C	-4.47573600	0.33956000	-3.64041500
C	-5.81222900	0.55566200	-3.97302200
C	-6.81893900	-0.28631200	-3.47624400
C	-6.51612700	-1.36114900	-2.63371700
C	-4.54962000	-2.62376600	-1.43290100
H	-3.68772400	0.98872900	-4.00588200
H	-6.08071400	1.38424800	-4.62132800
H	-7.85324800	-0.09782800	-3.74857900
H	-7.30511800	-2.00284900	-2.25193400
H	-4.88465100	-2.58008900	-0.39051000
N	-3.10744700	-2.29708800	-1.50874800
C	-2.89064700	-1.20235700	-2.28421000
O	-1.77612200	-0.66809300	-2.52185200
H	-4.72921400	-3.64071100	-1.79310600
C	-0.82880700	-2.61240600	-0.65368200
C	-2.11931600	-3.00654600	-0.77338900
H	-1.43375800	1.54038000	-1.11564200
H	-0.24736100	-3.27064700	-0.01431700
C	-2.59835600	-4.26635000	-0.11759300
C	-2.93985800	-5.39268200	-0.88571700
C	-2.67132700	-4.35513600	1.28016700
C	-3.35092000	-6.57444500	-0.26949700
H	-2.86263300	-5.34673900	-1.96972100
C	-3.08233500	-5.53886400	1.89662700
H	-2.40384000	-3.49189800	1.88348400
C	-3.42593200	-6.64923800	1.12396700
H	-3.60461500	-7.43926400	-0.87624300

H	-3.13574700	-5.59111300	2.98044500
H	-3.74650600	-7.56966400	1.60344800
C	-1.38290300	1.06433100	-0.13570700
C	-0.12425500	0.23252300	0.06610200
H	-1.39315700	1.86256000	0.62331400
H	-2.28928700	0.46807100	0.01448600
H	0.76160900	0.86257600	-0.06414000
C	-0.10907500	-0.41962000	1.44028400
H	-0.08131200	0.36915800	2.20887900
H	-1.01034000	-1.01527300	1.60947100
H	0.75138000	-1.06967700	1.61009000
Rh	0.09206900	-1.09502000	-1.58221800

TS7a

P	1.07372400	0.60667300	-3.38869800
P	1.95767900	-1.42188000	-0.63631400
C	0.62416700	-0.07684500	-5.03970900
C	-0.56875600	0.31825300	-5.66829500
C	1.42560900	-1.04847400	-5.66244700
C	-0.94231700	-0.23659100	-6.89283600
H	-1.20145500	1.06853700	-5.20727200
C	1.04885900	-1.59933200	-6.88836200
H	2.34818500	-1.38596500	-5.20148700
C	-0.13507800	-1.19575400	-7.50744800
H	-1.86306400	0.08813900	-7.36955200
H	1.68724100	-2.34017800	-7.36168800
H	-0.42360100	-1.62156300	-8.46417800
C	0.46705000	2.34599900	-3.41077300
C	0.74873700	3.19458600	-4.49559400
C	-0.23593700	2.85824700	-2.31060300
C	0.33579200	4.52613900	-4.47569600
H	1.28233600	2.81661800	-5.36340200
C	-0.64694600	4.19325400	-2.29189900
H	-0.46544300	2.20775100	-1.47154500
C	-0.36138600	5.02795100	-3.37312200
H	0.55988900	5.17206900	-5.31977300
H	-1.18812600	4.57896200	-1.43241900
H	-0.67934900	6.06659100	-3.35845200
C	1.76154600	-2.29211800	0.98087500
C	1.70035000	-1.56473500	2.18180100
C	1.61642600	-3.68859700	1.02845900
C	1.50990200	-2.21923900	3.39942500
H	1.80706700	-0.48382900	2.17861400
C	1.42128500	-4.33994300	2.24817700

H	1.67856900	-4.27531600	0.11696000
C	1.36855100	-3.60810900	3.43562400
H	1.47618500	-1.64272300	4.31944800
H	1.32224700	-5.42156100	2.26852300
H	1.22433700	-4.11661100	4.38445500
C	2.91756600	-2.63597700	-1.63359500
C	4.19817300	-3.05641300	-1.23040600
C	2.35181100	-3.18865700	-2.79156800
C	4.90108000	-3.99565300	-1.98299900
H	4.64733100	-2.66021200	-0.32371600
C	3.05676700	-4.13609000	-3.54032000
H	1.35579100	-2.88187400	-3.09766500
C	4.33175500	-4.53630200	-3.14031600
H	5.89075800	-4.30975500	-1.66417800
H	2.60486500	-4.56134800	-4.43203900
H	4.88040200	-5.27124000	-3.72237400
C	2.91526200	0.84932000	-3.53700700
H	3.39551600	-0.10011300	-3.79246900
H	3.09115400	1.53641400	-4.37067800
C	3.18767800	-0.09021500	-0.16644200
H	2.62319500	0.73888400	0.27357900
H	3.82404900	-0.49997100	0.62469600
C	3.55442400	1.44194500	-2.28094900
H	2.86532900	2.14043600	-1.77858500
C	4.11357800	0.44450800	-1.25774700
H	4.58503400	-0.39037200	-1.79739900
O	4.73682300	2.12881200	-2.67708400
O	5.10939100	1.22537900	-0.60428000
C	5.62691400	2.18005200	-1.55029600
C	7.01541100	1.76589300	-2.02414300
H	7.36910400	2.44812500	-2.80337500
H	7.72280400	1.78874300	-1.18974100
H	6.98721100	0.75295500	-2.43659100
C	5.59622800	3.55858700	-0.89867500
H	6.20493800	3.56186700	0.01088700
H	5.98992900	4.31169700	-1.58779600
H	4.57038000	3.82833200	-0.63013700
C	-5.04721400	-1.07525800	-3.29605600
C	-4.06452100	-0.08288000	-3.32060600
C	-4.32620100	1.20841400	-3.78065400
C	-5.61680800	1.48213600	-4.23208900
C	-6.60610500	0.48660100	-4.21694200
C	-6.33369700	-0.80365700	-3.74883100
C	-4.45240200	-2.33752400	-2.73522100

H	-3.55033900	1.96786600	-3.77588900
H	-5.86284800	2.47461400	-4.59727000
H	-7.60457500	0.72353300	-4.57257400
H	-7.11102900	-1.56243100	-3.73910700
H	-4.92627600	-2.65519400	-1.79895300
N	-3.04287000	-1.95903700	-2.47527300
C	-2.82173400	-0.64861200	-2.78784100
O	-1.74738000	-0.01979000	-2.64630300
H	-4.50335900	-3.17796300	-3.43231700
C	-1.01845400	-2.40570100	-1.16329100
C	-2.13446100	-2.82803000	-1.81877300
H	-3.29384000	-1.33553700	0.15704500
H	-0.45994100	-3.19937000	-0.67813300
C	-2.43204700	-4.28525000	-1.92233600
C	-2.56230600	-4.90824500	-3.17728600
C	-2.54439300	-5.07233800	-0.76504200
C	-2.80324500	-6.27814900	-3.26802000
H	-2.44941100	-4.31797000	-4.08364900
C	-2.78219000	-6.44455100	-0.85824600
H	-2.45417400	-4.60094900	0.20977300
C	-2.91556900	-7.05063300	-2.10846900
H	-2.89390800	-6.74558200	-4.24455600
H	-2.87251500	-7.03763400	0.04743600
H	-3.10475800	-8.11767900	-2.18072600
C	-1.16598400	-0.95425100	0.30509900
C	-2.61881100	-0.51725800	0.43013900
H	-0.50357700	-0.11570900	0.57056000
H	-0.92256300	-1.76904100	0.98581200
H	-2.82774700	0.31914400	-0.24523500
C	-2.92436000	-0.08025900	1.87456600
H	-3.97157600	0.22764800	1.96958300
H	-2.74906800	-0.89754400	2.58361300
H	-2.29831200	0.76702300	2.17803700
Rh	-0.01221800	-0.70712900	-1.62363800

TS7b

P	0.98151800	0.59979800	-3.12029700
P	2.24533400	-1.41246000	-0.52781400
C	0.37893400	-0.09177300	-4.72064200
C	-0.88188100	0.26627900	-5.22602500
C	1.14611600	-1.03218400	-5.42879800
C	-1.35590700	-0.29330300	-6.41310000
H	-1.48993500	0.99167000	-4.69814900
C	0.66897700	-1.58878900	-6.61655200

H	2.11960000	-1.34219500	-5.06352000
C	-0.58262100	-1.22133400	-7.11287000
H	-2.32944300	0.00310700	-6.79373500
H	1.28168300	-2.30543300	-7.15636800
H	-0.95009100	-1.65098600	-8.04038100
C	0.30290100	2.31122500	-3.04607200
C	0.35465000	3.16312000	-4.16264300
C	-0.21432600	2.80239600	-1.83898200
C	-0.10630800	4.47598200	-4.06989200
H	0.74482000	2.80149000	-5.10991200
C	-0.67224200	4.11868700	-1.74665600
H	-0.25659400	2.14836300	-0.97251200
C	-0.61991700	4.95593200	-2.86191300
H	-0.06197500	5.12470800	-4.94004600
H	-1.06809900	4.48801800	-0.80471900
H	-0.97555600	5.97994800	-2.79151600
C	2.33775300	-2.30843500	1.08568600
C	2.45963100	-1.60231200	2.29443500
C	2.24841800	-3.70968400	1.12751400
C	2.49971800	-2.28166500	3.51285100
H	2.53013300	-0.51854200	2.29729000
C	2.28357000	-4.38623300	2.34874800
H	2.17179000	-4.27889400	0.20614300
C	2.40982000	-3.67477900	3.54337400
H	2.60485200	-1.72101900	4.43730300
H	2.22233700	-5.47073900	2.36308900
H	2.44447800	-4.20260100	4.49196300
C	3.10293200	-2.57801600	-1.66766600
C	4.44681700	-2.94033400	-1.46249400
C	2.39596700	-3.15861600	-2.73041800
C	5.07027300	-3.84954200	-2.31536500
H	5.00837300	-2.52245000	-0.63144500
C	3.02192300	-4.07660400	-3.57946900
H	1.35338500	-2.89509100	-2.88441200
C	4.35878900	-4.41882100	-3.37624300
H	6.10948400	-4.11831400	-2.14923600
H	2.46072000	-4.52379100	-4.39511900
H	4.84610000	-5.13079200	-4.03622400
C	2.77641400	0.93590400	-3.49446700
H	3.26692800	0.01721000	-3.83011700
H	2.80772600	1.64518300	-4.32756900
C	3.49030200	-0.04504900	-0.20642900
H	2.97046600	0.76104900	0.32302300
H	4.23811300	-0.44852200	0.48402800

C	3.53836800	1.53647800	-2.31537500
H	2.88581600	2.19538400	-1.71952300
C	4.25259300	0.54020300	-1.39383200
H	4.67702700	-0.26735300	-2.00880600
O	4.63618800	2.27911600	-2.83472300
O	5.29903600	1.34020500	-0.85184100
C	5.66344100	2.33066300	-1.83103200
C	6.98932200	1.96977500	-2.49145200
H	7.21939800	2.67990600	-3.29175300
H	7.79845500	1.99576600	-1.75543300
H	6.93529300	0.96597800	-2.92319300
C	5.68082900	3.69243200	-1.14470900
H	6.40619100	3.69476900	-0.32514300
H	5.95620800	4.47323500	-1.85997800
H	4.69279000	3.92235300	-0.73471700
C	-5.02756200	-1.29614000	-2.47561300
C	-4.06683600	-0.29609000	-2.64544700
C	-4.39229100	0.96523800	-3.14608200
C	-5.72340500	1.19934100	-3.48934100
C	-6.69054000	0.19484800	-3.32985600
C	-6.35468600	-1.06439400	-2.82048800
C	-4.36462300	-2.51841500	-1.90220200
H	-3.63313400	1.73416400	-3.25101300
H	-6.01851200	2.16806200	-3.88103600
H	-7.72134500	0.40057800	-3.60311200
H	-7.11517000	-1.83024700	-2.69703000
H	-4.74802800	-2.78850200	-0.91107100
N	-2.94481900	-2.10866800	-1.79091800
C	-2.77181000	-0.81760100	-2.19718500
O	-1.69810000	-0.17374500	-2.17982500
H	-4.46425200	-3.39739300	-2.54439700
C	-0.80298200	-2.45319500	-0.64266500
C	-1.96212300	-2.92780600	-1.17655500
H	-2.07410900	0.78014700	0.08977600
H	-0.19089300	-3.21387900	-0.16891700
C	-2.22378400	-4.39621000	-1.22294700
C	-2.45212000	-5.04183100	-2.45278200
C	-2.20043100	-5.17130100	-0.05268400
C	-2.65786400	-6.41934700	-2.50596200
H	-2.44291700	-4.46126800	-3.37236800
C	-2.40435400	-6.55106000	-0.10827100
H	-2.02960700	-4.68800400	0.90455900
C	-2.63697000	-7.17889600	-1.33280100
H	-2.82487600	-6.90228000	-3.46474500

H	-2.38966200	-7.13364400	0.80860900
H	-2.79881500	-8.25203900	-1.37477100
C	-2.14191400	-0.04876900	0.79523700
C	-0.87594300	-0.88847700	0.86839500
H	-2.32330400	0.37461200	1.79453700
H	-3.02029400	-0.65393400	0.54849500
H	-0.00779400	-0.25520100	1.07437100
C	-0.98532400	-1.94362900	1.96601300
H	-1.00869900	-1.42047700	2.93332400
H	-1.91338100	-2.51712600	1.87943600
H	-0.14629800	-2.63807700	1.99920100
Rh	0.14179800	-0.77357200	-1.26319100

TS8a

P	1.80458200	1.08220700	0.06379900
P	-0.79844400	-1.34535200	0.51597300
C	3.44399900	0.24800300	-0.09064200
C	4.43372900	0.43415600	0.88972200
C	3.75005200	-0.53109600	-1.21645900
C	5.68751500	-0.16140200	0.75451700
H	4.23644500	1.05007700	1.76154200
C	5.00982200	-1.11887200	-1.35630800
H	2.99711400	-0.69004000	-1.98243800
C	5.97904700	-0.93932300	-0.36859000
H	6.43845400	-0.01281200	1.52518400
H	5.22994000	-1.71767300	-2.23570000
H	6.95767000	-1.39868100	-0.47419200
C	2.26293500	2.84877900	-0.23266700
C	3.22885700	3.16632200	-1.20235600
C	1.64857200	3.89487200	0.47705400
C	3.56862900	4.49441500	-1.46023200
H	3.73520300	2.37525300	-1.74715900
C	1.99397800	5.22303400	0.21629800
H	0.92406400	3.69048100	1.25794600
C	2.94947600	5.52754500	-0.75419300
H	4.32503600	4.71974600	-2.20675000
H	1.52189500	6.01948500	0.78493100
H	3.21834500	6.56137700	-0.95089200
C	-2.01413100	-2.61875100	-0.03730100
C	-3.38409100	-2.54115000	0.24637000
C	-1.53666000	-3.71237100	-0.78079100
C	-4.25488400	-3.54441700	-0.18728600
H	-3.78796400	-1.70562800	0.80876700
C	-2.40821100	-4.70862500	-1.21662600

H	-0.47595400	-3.80006200	-1.00091300
C	-3.77123000	-4.62841100	-0.91800200
H	-5.31301400	-3.47172100	0.04561500
H	-2.02137700	-5.55268200	-1.78075400
H	-4.44983700	-5.40788200	-1.25192300
C	0.42686400	-2.41395500	1.39338800
C	0.09506300	-3.03268800	2.61292900
C	1.67348100	-2.68818400	0.81544600
C	1.00027900	-3.88402800	3.24401300
H	-0.87567500	-2.86403400	3.06991200
C	2.57868400	-3.54563600	1.44733900
H	1.94262900	-2.23072300	-0.12935600
C	2.24618900	-4.14041900	2.66360000
H	0.73077800	-4.35197300	4.18655300
H	3.54277200	-3.74002700	0.98634700
H	2.94953500	-4.80472300	3.15744300
C	1.47885900	1.05788500	1.89935700
H	1.72254400	0.05355200	2.26052700
H	2.16680400	1.75348600	2.38776500
C	-1.70276400	-0.45090000	1.87527200
H	-2.38332700	0.25441500	1.38733300
H	-2.31462100	-1.16076000	2.44103600
C	0.04583900	1.45478900	2.30403400
H	-0.48834500	1.94754900	1.48164700
C	-0.83389800	0.32686000	2.86472100
H	-0.20597000	-0.36597300	3.44456800
O	0.13895300	2.33874000	3.42317300
O	-1.71780300	1.02982100	3.73135700
C	-1.05098900	2.20585500	4.21736200
C	-0.63200800	2.02369600	5.67225400
H	-0.05976500	2.89135900	6.01515200
H	-1.51425800	1.91033300	6.30940900
H	-0.00580600	1.13249000	5.77398100
C	-1.97876400	3.39773100	4.00093100
H	-2.91604700	3.25332800	4.54724300
H	-1.50433900	4.31778600	4.35583600
H	-2.21155500	3.50398000	2.93662300
C	-3.93191500	3.64525600	-2.42063100
C	-2.94498900	3.60658500	-1.43346900
C	-2.59934800	4.73455400	-0.68812300
C	-3.28436400	5.91900000	-0.95381500
C	-4.27889500	5.96248700	-1.94381200
C	-4.61267200	4.82811300	-2.69096000
C	-4.05982400	2.28171200	-3.04080500

H	-1.81892400	4.68348800	0.06447600
H	-3.04770300	6.81898000	-0.39446900
H	-4.79875000	6.89684900	-2.13444600
H	-5.38204300	4.87803800	-3.45623400
H	-5.06376300	1.86163900	-2.94164400
N	-3.07202500	1.47556500	-2.28488100
C	-2.38519800	2.24856100	-1.37617500
O	-1.45463200	1.87430200	-0.63779600
H	-3.80464300	2.27454300	-4.10811500
C	-1.65124600	-0.49335100	-2.47677600
C	-2.88219200	0.08351700	-2.52291700
H	-1.62591900	-1.56089000	-2.67056900
C	-4.11219900	-0.68495600	-2.84631700
C	-4.11018600	-1.62857700	-3.88748000
C	-5.30083600	-0.49843600	-2.11436200
C	-5.25699600	-2.36352200	-4.18625100
H	-3.20863100	-1.77340300	-4.47578700
C	-6.44708500	-1.23073400	-2.41649900
H	-5.31672500	0.20946000	-1.28925800
C	-6.43013800	-2.16533500	-3.45558700
H	-5.23721800	-3.08210700	-5.00065000
H	-7.35363300	-1.07495200	-1.83818200
H	-7.32564800	-2.73115500	-3.69545000
C	-0.29057100	0.40365600	-3.64721000
C	0.63386300	1.30945100	-3.04561300
H	0.09235300	-0.52737300	-4.05567200
H	-1.08582700	0.85277700	-4.23294000
H	1.67930300	1.01358700	-3.07748000
C	0.37836300	2.79935000	-3.13333700
H	1.02802600	3.24615400	-3.89772700
H	-0.65713100	3.00810500	-3.42243600
H	0.57812200	3.32466800	-2.19708000
H	0.88243400	-0.97853800	-1.66301700
Rh	-0.03842200	0.19051600	-1.23471800

TS8b

P	1.79571000	1.12141700	0.00022900
P	-0.83595800	-1.24947900	0.52448500
C	3.42191600	0.26702600	-0.17434600
C	4.38400300	0.29723400	0.85012100
C	3.73613500	-0.40318500	-1.36769900
C	5.61872400	-0.33346600	0.68631000
H	4.18410100	0.81580500	1.78168100
C	4.97255800	-1.02893000	-1.53276500

H	3.00445700	-0.44960200	-2.16712800
C	5.91642600	-0.99826700	-0.50438700
H	6.34722000	-0.30239700	1.49146600
H	5.19577300	-1.54276900	-2.46356000
H	6.87787300	-1.48771300	-0.63048700
C	2.17495900	2.88666100	-0.40375700
C	3.48793400	3.34981600	-0.57883900
C	1.11305500	3.80161000	-0.50966300
C	3.73219000	4.69971200	-0.84234100
H	4.32519400	2.66381900	-0.51188300
C	1.36289600	5.14991700	-0.76647700
H	0.09039600	3.45323800	-0.40895000
C	2.67327700	5.60326200	-0.93303900
H	4.75439200	5.04168000	-0.97781500
H	0.53138200	5.84524300	-0.84471900
H	2.86691400	6.65232900	-1.13770400
C	-2.12842200	-2.47646600	0.05007000
C	-3.47652300	-2.35258200	0.41203700
C	-1.73045500	-3.59030200	-0.70988100
C	-4.40191900	-3.33151400	0.04018500
H	-3.82014300	-1.50134100	0.99090600
C	-2.65636500	-4.56232200	-1.08355600
H	-0.68713400	-3.71278400	-0.98932400
C	-3.99611800	-4.43667900	-0.70623500
H	-5.44122300	-3.22619200	0.33765400
H	-2.33009900	-5.42295500	-1.66076400
H	-4.71698500	-5.19727100	-0.99149400
C	0.37350800	-2.34319400	1.39040500
C	0.02548100	-2.97356200	2.59967000
C	1.62533500	-2.61539700	0.82277100
C	0.91988100	-3.83535900	3.23133600
H	-0.94991100	-2.80456100	3.04726200
C	2.51976900	-3.48395100	1.45568200
H	1.90629800	-2.14950500	-0.11494700
C	2.17108600	-4.09067000	2.66131700
H	0.63847600	-4.31255500	4.16573700
H	3.48762400	-3.67890800	1.00287200
H	2.86583400	-4.76409000	3.15508400
C	1.57050900	1.19099100	1.85471700
H	1.84925900	0.21492300	2.26631100
H	2.27450100	1.93019100	2.24765000
C	-1.64822100	-0.27196100	1.88596400
H	-2.29416900	0.46658300	1.40086400
H	-2.28921600	-0.93382500	2.47708700

C	0.16757100	1.59488300	2.33323300
H	-0.37896100	2.16162800	1.56698100
C	-0.71945200	0.45283800	2.85953600
H	-0.08203700	-0.27446600	3.38496500
O	0.33258600	2.39041000	3.50681300
O	-1.55761900	1.12911200	3.79159500
C	-0.82312000	2.23296800	4.34343700
C	-0.34722500	1.91193100	5.75689200
H	0.28073600	2.72268000	6.13927600
H	-1.20366500	1.78518600	6.42602300
H	0.24066100	0.98919100	5.75634000
C	-1.71074600	3.47198300	4.27496800
H	-2.62609000	3.31594000	4.85435800
H	-1.18187300	4.34007700	4.67982500
H	-1.98809200	3.67802000	3.23652000
C	-4.10912900	3.52783900	-2.50472300
C	-3.14592700	3.52586600	-1.49383600
C	-2.88769600	4.65769700	-0.71833400
C	-3.62462300	5.80954300	-0.98874000
C	-4.58786100	5.81785700	-2.01007500
C	-4.84233700	4.67796900	-2.77936500
C	-4.16330200	2.16452400	-3.13470700
H	-2.14464300	4.63285600	0.07272600
H	-3.45677600	6.70934100	-0.40479900
H	-5.14957500	6.72696800	-2.20379600
H	-5.59393100	4.69777400	-3.56341800
H	-5.15058500	1.70262000	-3.05905900
N	-3.15811100	1.39627700	-2.36136300
C	-2.51699900	2.19680000	-1.44057300
O	-1.57612600	1.86589100	-0.69397600
H	-3.88559500	2.17266700	-4.19640500
C	-1.62138000	-0.47806400	-2.55489700
C	-2.88397100	0.02231300	-2.62603900
H	-1.52485800	-1.53362900	-2.79228700
C	-4.06231000	-0.79787500	-3.01275600
C	-3.97895800	-1.71477700	-4.07404800
C	-5.28405900	-0.68580000	-2.32171700
C	-5.07917300	-2.49135700	-4.43553300
H	-3.05070100	-1.80714100	-4.62998200
C	-6.38383400	-1.45980000	-2.68570800
H	-5.36233900	-0.00506300	-1.47781000
C	-6.28688100	-2.36374000	-3.74690100
H	-4.99577900	-3.18726600	-5.26543800
H	-7.31648800	-1.36118100	-2.13719800

H	-7.14631300	-2.96202500	-4.03498900
C	0.65195900	1.32941000	-2.97687500
C	-0.36796600	0.67321900	-3.72710400
H	0.51770800	2.38401900	-2.75225500
H	1.68250900	1.04114600	-3.16954900
H	-1.20644300	1.30889700	-3.99707400
C	0.00642000	-0.36231500	-4.76384600
H	0.45756700	0.16125500	-5.61753200
H	0.74464100	-1.06974200	-4.37523700
H	-0.85665100	-0.92056300	-5.13466000
H	0.87401500	-0.94168600	-1.68326100
Rh	-0.05452800	0.21229300	-1.25222700

INT10a

P	1.87408700	1.45189700	-0.00666500
P	-1.53981000	0.72966000	1.06250100
C	3.37952000	1.24119800	-1.05102900
C	3.77345900	-0.05730900	-1.41775200
C	4.12058800	2.33456500	-1.52118800
C	4.89553800	-0.25582900	-2.22072400
H	3.20486500	-0.92048800	-1.08188900
C	5.24193000	2.13176300	-2.33003400
H	3.83329900	3.34632400	-1.25505700
C	5.63324700	0.83940600	-2.67866800
H	5.19445300	-1.26549700	-2.48764900
H	5.80879500	2.98809800	-2.68391500
H	6.50746500	0.68402200	-3.30411300
C	2.03366700	3.13257600	0.72075700
C	3.16668800	3.49956800	1.46917100
C	1.00545300	4.06976300	0.54326600
C	3.26109400	4.77431300	2.02639500
H	3.98059500	2.79471200	1.61455200
C	1.10304800	5.34802500	1.09908200
H	0.12553000	3.80541800	-0.03685900
C	2.22997700	5.70024500	1.84232000
H	4.14071900	5.04536500	2.60288300
H	0.30215600	6.06579900	0.94662900
H	2.30812900	6.69321100	2.27530500
C	-2.95891200	1.91218800	1.09014400
C	-2.72291300	3.25801500	1.42350100
C	-4.26113900	1.52813300	0.73615100
C	-3.76342700	4.18728800	1.42264400
H	-1.72528400	3.59101700	1.69632500
C	-5.30247500	2.45971900	0.74069800

H	-4.47175400	0.49833300	0.46769600
C	-5.05873600	3.79025400	1.08404000
H	-3.56296300	5.21976800	1.69503800
H	-6.30713200	2.13914300	0.47867100
H	-5.87084500	4.51147600	1.09218200
C	-2.28953600	-0.94264400	1.25480300
C	-3.23607500	-1.21459700	2.25947200
C	-1.83698200	-1.99682100	0.44823300
C	-3.71577300	-2.50946300	2.44928400
H	-3.60668800	-0.41464500	2.89411000
C	-2.31009300	-3.29697300	0.64802900
H	-1.10750600	-1.80091400	-0.33228600
C	-3.24925500	-3.55439300	1.64667600
H	-4.44744100	-2.70407500	3.22826000
H	-1.93984700	-4.10310700	0.02183000
H	-3.61598200	-4.56491500	1.80351000
C	2.28963700	0.28354600	1.39738700
H	2.01414400	-0.72845800	1.08243900
H	3.38024100	0.30198300	1.49149200
C	-0.85662400	0.98613100	2.78694600
H	-0.56395900	2.03352200	2.91494600
H	-1.66438800	0.78922000	3.49856900
C	1.71824600	0.57655100	2.78535900
H	1.76928900	1.65332000	3.00431800
C	0.31310200	0.06590200	3.12534700
H	0.16835700	-0.93247400	2.68142800
O	2.52252100	-0.14501600	3.71471900
O	0.38896900	-0.04083900	4.54362600
C	1.73546200	-0.39458400	4.89519100
C	1.83722900	-1.87973700	5.22768200
H	2.88091600	-2.15821100	5.40385700
H	1.25624600	-2.10709100	6.12654800
H	1.45307900	-2.48110500	4.39819100
C	2.18102600	0.51249800	6.03652300
H	1.52487800	0.38134000	6.90257000
H	3.20645200	0.27262100	6.33327800
H	2.13819700	1.56013500	5.72402700
C	-4.49130200	-0.19691700	-4.40421100
C	-4.07842100	0.64928500	-3.37228600
C	-4.89278600	1.67367800	-2.88893700
C	-6.15280800	1.82508600	-3.46703500
C	-6.57569000	0.97100000	-4.49702700
C	-5.74995300	-0.05025000	-4.97803400
C	-3.38384800	-1.16429300	-4.71255200

H	-4.55250400	2.32251300	-2.08943100
H	-6.81498100	2.61285100	-3.12039400
H	-7.56139200	1.10815600	-4.93217000
H	-6.08649100	-0.70106000	-5.78008800
H	-3.67068500	-2.21196100	-4.57282600
N	-2.33039200	-0.78372500	-3.74760400
C	-2.71126400	0.27304900	-2.96601200
O	-2.05611900	0.84243900	-2.06781700
H	-2.99864700	-1.05701100	-5.73427300
C	0.06550900	-0.63626000	-3.94316100
C	-1.03832400	-1.39508400	-3.80412300
H	1.02453600	-1.14877700	-3.90886500
C	-1.01937000	-2.87893800	-3.73816900
C	-0.06215200	-3.61456600	-4.45867200
C	-1.95942400	-3.58343400	-2.96549100
C	-0.02718100	-5.00608800	-4.38488100
H	0.64158900	-3.09255600	-5.10032600
C	-1.93018600	-4.97679900	-2.90151300
H	-2.70567000	-3.03499300	-2.39763800
C	-0.96146700	-5.69381500	-3.60704800
H	0.71867300	-5.55525900	-4.95247800
H	-2.66771100	-5.50299800	-2.30138100
H	-0.94242800	-6.77875300	-3.56134300
C	0.11109400	0.85087800	-4.11782200
C	0.73143100	1.60492700	-2.92696200
H	0.73237300	1.06997100	-5.00291300
H	-0.88300700	1.24629300	-4.34607000
H	1.79831200	1.38064300	-2.90843700
C	0.51794700	3.11355700	-3.06589000
H	0.79621700	3.45620300	-4.07515600
H	-0.53612000	3.39333700	-2.92438600
H	1.12236500	3.68981500	-2.35716100
H	0.45808200	-0.30407900	-1.27744700
Rh	-0.12896800	1.08901500	-1.06665100

INT10b

P	-1.49030600	-0.47788400	0.70941300
P	1.44627900	-2.06152000	-0.80653800
C	-2.54206900	1.01802800	0.97032300
C	-1.95408100	2.19235000	1.46983500
C	-3.90948200	1.02808500	0.65638700
C	-2.72272300	3.33762800	1.67618400
H	-0.89295900	2.21943300	1.70035900
C	-4.67394400	2.18166000	0.85175600

H	-4.38802300	0.12991000	0.27925900
C	-4.08522000	3.33648100	1.36686300
H	-2.25664300	4.23127100	2.08215700
H	-5.73414700	2.16942200	0.61389100
H	-4.68280900	4.22875900	1.52961600
C	-2.71132300	-1.86064400	0.66128300
C	-3.48757200	-2.21215600	1.78087600
C	-2.88302600	-2.58113000	-0.52954100
C	-4.39488300	-3.26863200	1.71135300
H	-3.39264200	-1.65795400	2.71023000
C	-3.79799100	-3.63584900	-0.60129200
H	-2.31297900	-2.30757900	-1.41219200
C	-4.54956800	-3.98485100	0.52049200
H	-4.98301300	-3.53156200	2.58597400
H	-3.92579200	-4.17377800	-1.53612100
H	-5.25734600	-4.80732800	0.46931800
C	1.27442100	-3.21342000	-2.23369200
C	0.13342400	-4.02596900	-2.34916500
C	2.23668400	-3.24947100	-3.25745500
C	-0.03512700	-4.85900800	-3.45638900
H	-0.62839700	-4.02118400	-1.57646500
C	2.06324800	-4.08268300	-4.36404800
H	3.13334900	-2.64303700	-3.18436900
C	0.92783300	-4.88894700	-4.46690500
H	-0.91648100	-5.49051400	-3.52339400
H	2.82201700	-4.10644800	-5.14102800
H	0.79832300	-5.54165100	-5.32534800
C	3.26219000	-1.88717000	-0.54527400
C	4.06858200	-3.04013700	-0.51821300
C	3.85469400	-0.64129600	-0.29517600
C	5.43337400	-2.94337900	-0.25294700
H	3.63681900	-4.01756900	-0.71372200
C	5.22210000	-0.54768100	-0.02633300
H	3.24863400	0.25778500	-0.31646200
C	6.01303400	-1.69628900	-0.00570700
H	6.04280900	-3.84222700	-0.23701800
H	5.66595400	0.42515800	0.16434800
H	7.07659100	-1.62244700	0.20205200
C	-0.72620400	-0.64145400	2.41407000
H	0.04211600	0.13408000	2.50122400
H	-1.49050400	-0.41853400	3.16548300
C	0.97744100	-3.11744300	0.65252400
H	-0.05242900	-3.47036200	0.53671800
H	1.62712300	-3.99777200	0.63433800

C	-0.11261100	-1.99895500	2.74147700
H	-0.86373700	-2.79380900	2.61461300
C	1.16724500	-2.41161000	2.00377100
H	1.83153200	-1.53783700	1.90821100
O	0.33134300	-1.96066900	4.09296300
O	1.73081300	-3.34669100	2.91785300
C	1.36531100	-2.94836800	4.25178700
C	2.54422400	-2.28991600	4.95978500
H	2.23408000	-1.91049400	5.93836200
H	3.35246700	-3.01333800	5.10304000
H	2.92094500	-1.45172600	4.36600400
C	0.83028700	-4.17599500	4.98109400
H	1.59597600	-4.95698500	5.02162600
H	0.54206000	-3.91332200	6.00337200
H	-0.04421000	-4.57472300	4.45837500
C	-2.66745700	3.76930600	-3.58722000
C	-1.83862100	3.67966700	-2.46571400
C	-1.53734200	4.79071700	-1.67827800
C	-2.09550700	6.01405400	-2.04642000
C	-2.93117200	6.10897500	-3.16988900
C	-3.22812900	4.98860000	-3.95305700
C	-2.78532700	2.41040800	-4.22474500
H	-0.89049700	4.69514800	-0.81260900
H	-1.88263100	6.90403000	-1.46200600
H	-3.35440800	7.07261700	-3.43820100
H	-3.87472300	5.07795000	-4.82142000
H	-3.81465900	2.03772300	-4.25755300
N	-1.95258400	1.56557600	-3.34428800
C	-1.38373500	2.28747400	-2.32497300
O	-0.62778400	1.85091300	-1.43777500
H	-2.38694300	2.38505200	-5.24689800
C	-0.42813000	-0.24945300	-3.79782500
C	-1.70139300	0.18990300	-3.62844100
H	-0.29174300	-1.31604000	-3.96529900
C	-2.90735200	-0.66001900	-3.80473900
C	-2.90225400	-1.72741600	-4.72023300
C	-4.08860400	-0.39740600	-3.08720100
C	-4.03589100	-2.51978500	-4.89617600
H	-2.01649100	-1.91690900	-5.31871700
C	-5.22352800	-1.18562700	-3.27076500
H	-4.10945900	0.41780600	-2.36923500
C	-5.20154500	-2.25064900	-4.17450100
H	-4.01614400	-3.33285700	-5.61633200
H	-6.12580100	-0.96992100	-2.70565500

H	-6.08951100	-2.85787300	-4.32471300
C	1.64236300	0.43455200	-2.58728800
C	0.82012900	0.60888900	-3.87862500
H	2.44227900	-0.29515500	-2.73273900
H	2.09523800	1.37504300	-2.26017700
H	1.16917200	0.39779600	-0.01983100
H	0.50857300	1.65568500	-3.95649500
C	1.62352600	0.26330200	-5.14657100
H	2.52432700	0.88427100	-5.20413600
H	1.93707800	-0.78713100	-5.13793500
H	1.03308200	0.43393200	-6.05499900
Rh	0.24473500	-0.14042700	-1.11752000

TS9a

P	1.85839300	1.42485700	0.08796500
P	-1.48890000	0.80487900	1.04094000
C	3.35198300	1.20432000	-0.97737600
C	3.73678600	-0.09728500	-1.34424700
C	4.09437400	2.29180000	-1.45867000
C	4.84894300	-0.30388900	-2.15916000
H	3.16798800	-0.95658800	-0.99849100
C	5.20526800	2.08125800	-2.28072700
H	3.81662300	3.30576000	-1.19063700
C	5.58655700	0.78622500	-2.62994500
H	5.14080200	-1.31602600	-2.42484600
H	5.77206300	2.93394700	-2.64361400
H	6.45306300	0.62459200	-3.26452500
C	2.03527500	3.12390100	0.77668000
C	3.15680900	3.49118700	1.54221000
C	1.03619600	4.07913500	0.53774000
C	3.26709300	4.78131300	2.05994600
H	3.95128200	2.77483300	1.73213600
C	1.14993300	5.37278800	1.05446200
H	0.17210000	3.80936200	-0.06267700
C	2.26345900	5.72395300	1.81803200
H	4.13767800	5.05127000	2.65062700
H	0.37146700	6.10395400	0.85542400
H	2.35335200	6.72857400	2.22097300
C	-2.93204600	1.95613600	1.05958400
C	-2.71407700	3.31223200	1.36091200
C	-4.23675300	1.53215400	0.76827100
C	-3.77659700	4.21522800	1.38807200
H	-1.71401000	3.67215500	1.58603300
C	-5.30012800	2.43837200	0.80199700

H	-4.43193600	0.49319100	0.52515200
C	-5.07481700	3.77997400	1.11198600
H	-3.59096800	5.25729500	1.63271900
H	-6.30645500	2.08918400	0.58750900
H	-5.90361000	4.48136500	1.14230500
C	-2.18570900	-0.89161500	1.20469000
C	-3.10960700	-1.20594900	2.21781400
C	-1.71191800	-1.91853000	0.37493300
C	-3.54852900	-2.51747800	2.39284000
H	-3.49350000	-0.42858600	2.87203300
C	-2.14475100	-3.23447900	0.56062500
H	-0.99570500	-1.68554300	-0.40838800
C	-3.06269600	-3.53506700	1.56732500
H	-4.26287300	-2.74566900	3.17866700
H	-1.75911400	-4.02014700	-0.08215500
H	-3.39695400	-4.55840400	1.71331100
C	2.33390900	0.30588700	1.51560200
H	2.11205000	-0.72561900	1.22224300
H	3.42174400	0.37946100	1.61750200
C	-0.83196700	1.07594400	2.76953400
H	-0.51759700	2.11875800	2.88241900
H	-1.66719200	0.91768400	3.45876600
C	1.72638300	0.60189800	2.88435100
H	1.79695900	1.67637600	3.10968900
C	0.29785000	0.12798600	3.16428900
H	0.14745300	-0.86786600	2.71804500
O	2.47167700	-0.14361700	3.84261000
O	0.30897400	0.02504800	4.58511000
C	1.63441400	-0.35116800	4.99575000
C	1.68788900	-1.83109600	5.35977100
H	2.71671800	-2.12909900	5.58462400
H	1.06504900	-2.02760400	6.23761500
H	1.32475100	-2.43927700	4.52588400
C	2.05545300	0.56809700	6.13688300
H	1.36172500	0.47039800	6.97771900
H	3.06177800	0.30977800	6.47995900
H	2.05148100	1.61007600	5.80323000
C	-4.52104500	-0.21191000	-4.36353100
C	-4.08435500	0.60047200	-3.31490100
C	-4.88291200	1.61688400	-2.79033600
C	-6.15181000	1.79287300	-3.34153900
C	-6.59928000	0.97013700	-4.38646600
C	-5.78869600	-0.04187500	-4.91057300
C	-3.42488200	-1.17396300	-4.72296100

H	-4.52312600	2.24262500	-1.98138200
H	-6.80152700	2.57584300	-2.96197200
H	-7.59158800	1.12553100	-4.79995700
H	-6.14306700	-0.66742500	-5.72498300
H	-3.71255200	-2.22407500	-4.60336300
N	-2.34749700	-0.82246700	-3.77357300
C	-2.71087400	0.20709000	-2.94130600
O	-2.04178600	0.73696800	-2.03342500
H	-3.06474800	-1.04168900	-5.75090100
C	0.04223200	-0.68325500	-4.07179300
C	-1.06156500	-1.43513400	-3.89681700
H	0.99588800	-1.20622000	-4.10313300
C	-1.04720400	-2.92038300	-3.86673400
C	-0.13028700	-3.64544100	-4.64739200
C	-1.95227100	-3.63475800	-3.06217000
C	-0.09930100	-5.03828400	-4.60169900
H	0.54450200	-3.11472300	-5.31264500
C	-1.92572200	-5.02892900	-3.02410200
H	-2.66786500	-3.09295700	-2.45019100
C	-0.99654100	-5.73629800	-3.79024400
H	0.61450900	-5.57983900	-5.21584800
H	-2.63408900	-5.56341900	-2.39686500
H	-0.97988200	-6.82192900	-3.76474600
C	0.09462200	0.80933400	-4.18838600
C	0.77544300	1.50577200	-2.99241800
H	0.67516400	1.07296700	-5.08672800
H	-0.90526200	1.22305600	-4.34171800
H	1.85238000	1.33630700	-3.05054800
C	0.51710400	3.01556900	-3.02158000
H	0.77923300	3.40019800	-4.02057000
H	-0.53659500	3.26166100	-2.84763800
H	1.12767300	3.56129100	-2.29763200
H	0.76737400	0.20618800	-1.98437400
Rh	-0.11654000	1.03215200	-0.98882000

TS9b

P	-1.23551400	-0.25431600	0.89947800
P	1.47235900	-1.98187800	-0.65527000
C	-1.84808900	1.43591500	1.32093900
C	-0.89602600	2.42560500	1.61904200
C	-3.20942300	1.75731900	1.40094500
C	-1.29947900	3.69695400	2.02607500
H	0.16459900	2.20524800	1.53093300
C	-3.61110000	3.03543500	1.79965600

H	-3.96263300	1.01206100	1.16741100
C	-2.66021600	4.00347500	2.12307600
H	-0.55179600	4.44678100	2.26971400
H	-4.67035600	3.26787900	1.86462200
H	-2.97487700	4.99132400	2.44762800
C	-2.72506200	-1.33752700	0.86991300
C	-3.52624400	-1.55969300	2.00490400
C	-3.05321700	-1.99356100	-0.32588500
C	-4.62090700	-2.42128200	1.94100300
H	-3.30236900	-1.05934800	2.94261700
C	-4.15184900	-2.85460600	-0.39042000
H	-2.44871600	-1.82738200	-1.21423900
C	-4.93378500	-3.07243100	0.74417600
H	-5.22862900	-2.58558900	2.82621800
H	-4.39310200	-3.34746900	-1.32746300
H	-5.78513500	-3.74562500	0.69902000
C	1.33793600	-3.06913100	-2.14128100
C	0.12353900	-3.73905700	-2.37382000
C	2.37006400	-3.19546600	-3.08477200
C	-0.04855200	-4.52386700	-3.51432700
H	-0.69825600	-3.65093000	-1.66878900
C	2.19377400	-3.98043400	-4.22683700
H	3.31962300	-2.69414800	-2.92835700
C	0.98677500	-4.64691100	-4.44407900
H	-0.99189800	-5.03738100	-3.67545700
H	3.00578300	-4.07442400	-4.94232500
H	0.85468400	-5.26164000	-5.32976800
C	3.27327000	-1.75066600	-0.34534500
C	4.13693600	-2.86209700	-0.33900000
C	3.79754400	-0.48729700	-0.03537300
C	5.49090300	-2.70532900	-0.04710300
H	3.75897300	-3.85325800	-0.57238700
C	5.15382200	-0.33300900	0.26026300
H	3.14296200	0.37833700	-0.01595400
C	6.00253400	-1.43988700	0.25182600
H	6.14531800	-3.57212400	-0.05128400
H	5.54329100	0.65264100	0.49805100
H	7.05757200	-1.31985500	0.48022300
C	-0.45066700	-0.66560400	2.55102900
H	0.43729100	-0.03379500	2.66099400
H	-1.15355700	-0.35664100	3.33170900
C	1.02339500	-3.18779700	0.69305300
H	0.00683500	-3.55801800	0.52503800
H	1.69849700	-4.04114800	0.57327100

C	-0.08777600	-2.12487100	2.78875400
H	-0.93387500	-2.77773000	2.52247700
C	1.18017900	-2.65642900	2.11712800
H	1.97181300	-1.89175900	2.16885600
O	0.22957900	-2.28005900	4.16770200
O	1.51154500	-3.75270000	2.96279900
C	1.08518100	-3.42995700	4.29992100
C	2.27778500	-3.03664500	5.16436200
H	1.93830700	-2.71037000	6.15230600
H	2.95277600	-3.88877600	5.28816200
H	2.82793600	-2.21427600	4.69741000
C	0.30651800	-4.62085900	4.84788400
H	0.93923500	-5.51380100	4.86153900
H	-0.03229300	-4.41479700	5.86763000
H	-0.56597100	-4.82388000	4.21974600
C	-3.27557800	3.31305700	-3.78439400
C	-2.52197000	3.24705800	-2.60972600
C	-2.48107500	4.30010700	-1.69652300
C	-3.22454800	5.44138500	-1.99542900
C	-3.98279200	5.51398800	-3.17395300
C	-4.01891300	4.45043900	-4.08204600
C	-3.10628500	2.02741800	-4.54740900
H	-1.89412000	4.22167800	-0.78771600
H	-3.21880700	6.28432100	-1.31092900
H	-4.55332200	6.41373700	-3.38562800
H	-4.61052500	4.52000600	-4.99053300
H	-4.04888000	1.49263400	-4.70638700
N	-2.20507300	1.24489300	-3.67731000
C	-1.83842600	1.94289100	-2.55562500
O	-1.07365100	1.57107700	-1.64468200
H	-2.63561100	2.17288800	-5.52800800
C	-0.40680400	-0.30161100	-4.10749900
C	-1.73087700	-0.04742800	-4.05611900
H	-0.10751300	-1.32642400	-4.31760600
C	-2.77655200	-1.05031400	-4.38802300
C	-2.55390200	-2.01039600	-5.39098300
C	-4.01566000	-1.05510200	-3.72292100
C	-3.52750100	-2.95887100	-5.70025800
H	-1.62192200	-1.99397800	-5.94786800
C	-4.99361400	-1.99821500	-4.04063600
H	-4.20834100	-0.32402400	-2.94247500
C	-4.75234900	-2.95627000	-5.02807800
H	-3.33863900	-3.68644100	-6.48465400
H	-5.94558500	-1.98212500	-3.51706100

H	-5.51690000	-3.68486500	-5.28173100
C	1.59454300	0.40539100	-2.74049100
C	0.71549100	0.69529800	-3.96828300
H	2.20255800	-0.48597300	-2.89988900
H	2.29933600	1.23761500	-2.62131500
H	1.46970700	0.72615900	-1.11244400
H	0.29745700	1.70023700	-3.86517100
C	1.58259300	0.68279700	-5.24851200
H	2.40453000	1.40251200	-5.16360200
H	2.01719000	-0.30916900	-5.41950600
H	0.98716900	0.94860600	-6.12977900
Rh	0.18360900	-0.14505200	-1.08109800