

Supporting information

Dehydrogenation of formic acid catalysed by M-embedded nitrogen-doped graphene (M= Fe, Ru, Os): A DFT study

*Thayalaraj Christopher Jeyakumar and Chinnappan Sivasankar**

Catalysis and Energy Laboratory, Department of Chemistry, Pondicherry University (A Central University), Puducherry 605 014, India

Table S1. List of all electronic energies of all the systems calculated at the B3LYP/6-31G*/LANL2DZ level of theory and basis sets.

System	E (Hartree)	ZPE (Hartree)	Thermal correction to energy (Hartree)	Thermal correction to Gibbs free energy (Hartree)	Total energy including ZPE and thermal corrections (Hartree)
Fe-1	-1554.300464	0.384983	0.407658	0.336307	-1553.171516
Fe-2	-1744.077533	0.420357	0.447572	0.365326	-1742.844278
Fe-2a	-1744.071586	0.419609	0.446833	0.364334	-1742.8408098
Fe-3	-1744.059017	0.417118	0.443917	0.362096	-1742.835886
Fe-3a	-1744.082247	0.418914	0.445457	0.364824	-1742.853052
Fe-4	-1744.072618	0.413419	0.441185	0.357655	-1742.860359
Fe-5	-1742.888982	0.397268	0.424116	0.341409	-1741.726189
Fe-6	-1555.484874	0.401170	0.424706	0.352146	-1554.306852
Fe-TS-I	-1744.049056	0.417455	0.443349	0.365199	-1742.823053
Fe-TS-Ia	-1744.021207	0.414325	0.441172	0.359768	-1742.805942
Fe-TS-II	-1744.027679	0.413648	0.439587	0.361072	-1742.813372
Fe-TS-IIa	-1744.029508	0.409987	0.436658	0.356320	-1742.826543
Ru-1	-1524.731467	0.384028	0.406964	0.334843	-1523.605632
Ru-2	-1714.506518	0.419442	0.446973	0.36382	-1713.276283
Ru-2a	-1714.502181	0.418869	0.44639	0.362667	-1713.2742549
Ru-3	-1714.503294	0.417188	0.444026	0.363125	-1713.278955
Ru-3a	-1714.526364	0.417504	0.444443	0.362509	-1713.301908
Ru-4	-1714.514443	0.41291	0.440746	0.356269	-1713.304518
Ru-5	-1713.320757	0.396507	0.423613	0.34007	-1712.160567
Ru-6	-1525.925962	0.400388	0.424031	0.350948	-1524.750595
Ru-TS-I	-1714.492199	0.415902	0.442273	0.362617	-1713.271407
Ru-TS-Ia	-1714.462165	0.413358	0.440496	0.358088	-1713.250223
Ru-TS-II	-1714.471842	0.411826	0.438247	0.358206	-1713.263563
Ru-TS-IIa	-1714.462291	0.409004	0.435985	0.354593	-1713.262709
Os-1	-1521.855386	0.383815	0.406802	0.334213	-1520.730556
Os-2	-1711.665826	0.420413	0.446968	0.3668	-1710.431645
Os-2a	-1711.624496	0.418513	0.446075	0.362035	-1710.397873
Os-3	-1711.667732	0.417124	0.444139	0.361928	-1710.444541
Os-3a	-1711.695762	0.417768	0.444697	0.362231	-1710.471066
Os-4a	-1711.679436	0.413104	0.440509	0.356649	-1710.469174
Os-5a	-1523.086700	0.400162	0.423858	0.35012	-1521.912560
Os-TS-I	-1711.641783	0.417006	0.443232	0.36409	-1710.417455
Os-TS-Ia	-1711.610542	0.413766	0.4408460	0.358550	-1710.397380
Os-TS-II	-1711.623452	0.411269	0.437747	0.357646	-1710.416790
Os-TS-IIa	-1711.602727	0.409128	0.436442	0.353014	-1710.404143

H ₂	-1.1754824	0.010145	0.012505	-0.00134	-1.1541744
CO ₂	-188.5809402	0.011593	0.01424	-0.00913	-188.5642332
HCOOH	-189.7471678	0.03354	0.036776	0.009453	-189.6673988

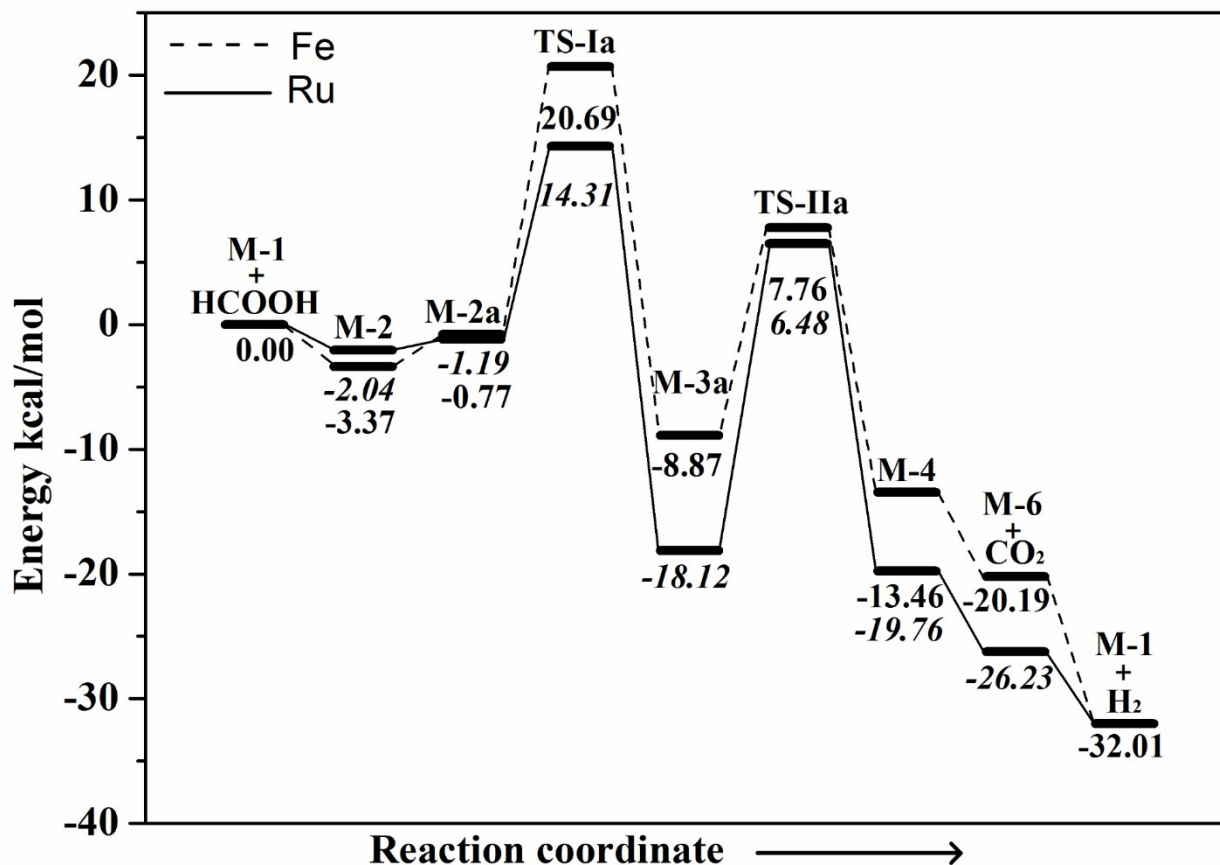


Figure S1. The energy profile for the formation of **M-1** from **M-4** (obtained from pathway B) via pathway A-1.

Table S2. Cartesian coordinates of all the systems.

Fe-1

C	2.29841200	4.53565300	-0.26955900
C	0.94378100	4.13128600	-0.15180300
C	0.62506500	2.73601200	0.01838900
C	1.72306600	1.79938400	0.04576000
C	3.07345200	2.23529700	-0.16117600
C	-0.77076900	2.36916800	0.04541700
C	0.69694200	-2.39180200	0.04526000
H	2.50607500	5.59725400	-0.38058400

C	-0.10085000	5.08375400	-0.26929500
C	-1.42122300	4.71735400	-0.28823200
C	-1.79804800	3.34812700	-0.16143900
H	0.17316000	6.13022900	-0.37994800
H	-2.20366500	5.46153700	-0.40834900
C	-3.12960300	2.90477600	-0.21366400
C	-3.47274800	1.54396300	-0.16113800
C	-2.42000500	0.59244100	0.04562200
H	-3.92058800	3.63898200	-0.34478000
C	-4.81020000	1.06633100	-0.28745400
C	-2.68200700	-0.82679700	0.01881600
C	-4.04982100	-1.24850000	-0.15037300
C	-1.66628400	-1.85202300	0.04523000
C	-4.35235600	-2.62943600	-0.26793800
H	-5.39566300	-2.91547100	-0.37806800
C	3.79880900	-0.11697800	-0.16027000
C	0.39917300	-3.77915000	-0.16207300
C	-2.00056700	-3.23102600	-0.16209300
C	-3.37476600	-3.58952400	-0.28827800
H	-3.62787000	-4.63924000	-0.40864500
C	-0.95088100	-4.16246000	-0.21494400
H	-1.19129000	-5.21450300	-0.34655600
C	1.48144700	-4.69860600	-0.28888600
H	1.25363600	-5.75408000	-0.40949000
C	2.43733500	-0.51707900	0.04641200
C	4.08055600	1.25785600	-0.21296500
H	5.11182200	1.57588400	-0.34429900
N	-0.35160200	-1.53915800	0.26671500
C	-5.07740700	-0.27760500	-0.26764900
H	-6.10064100	-0.62870800	-0.37786800
H	-5.61054900	1.79122800	-0.40755500
N	-1.15730300	1.07420900	0.26699000
C	3.32861800	3.63223800	-0.28860700
H	4.35659700	3.96267300	-0.40912100
N	1.50910700	0.46512400	0.26790300
C	4.79629400	-1.12787500	-0.28671100
H	5.83196700	-0.82218200	-0.40666700
C	2.05719300	-1.90934000	0.01891000
C	3.10620800	-2.88298500	-0.15108400
C	4.45348700	-2.45454100	-0.26788500
C	2.77899300	-4.25824200	-0.26911900
H	3.59453900	-4.96896100	-0.37960800
H	5.22282900	-3.21501700	-0.37845500
Fe	-0.00036800	0.00004300	1.17637100

Fe-2

C	-4.65531500	1.23034300	-1.07928000
C	-3.97776900	-0.00028000	-0.88613600
C	-2.56729000	-0.00018100	-0.55962600
C	-1.89927100	1.27706900	-0.46273000
C	-2.60208100	2.49537200	-0.75951600
C	-1.89911700	-1.27735800	-0.46270200
C	2.37004900	1.20350800	-0.02304900
H	-5.71810600	1.19780700	-1.30944400
C	-4.65517800	-1.23100400	-1.07912400
C	-4.00131000	-2.43525300	-1.03321900
C	-2.60178400	-2.49575500	-0.75933600
H	-5.71798000	-1.19860800	-1.30925800
H	-4.53364600	-3.36513000	-1.21470800
C	-1.87576600	-3.69439400	-0.73393700
C	-0.48709200	-3.72285700	-0.52304200
C	0.17454300	-2.48248600	-0.23318400
H	-2.39666700	-4.62922100	-0.92709000
C	0.28230600	-4.92031200	-0.56366600
C	1.60985400	-2.42834800	-0.10552000
C	2.34072900	-3.66699200	-0.20257100
C	2.37022000	-1.20321300	-0.02306800
C	3.75973800	-3.65421700	-0.18487200
H	4.28015000	-4.60751900	-0.24033100
C	-0.48756900	3.72276300	-0.52315800
C	3.80319500	1.22763800	-0.10008900
C	3.80335200	-1.22714800	-0.10014700
C	4.47253400	-2.48546600	-0.15061400
H	5.55895200	-2.49392700	-0.17269400
C	4.48133900	0.00029200	-0.09490400
H	5.56850900	0.00036100	-0.12046800
C	4.47220900	2.48605000	-0.15046800
H	5.55862800	2.49465400	-0.17246500
C	0.17421400	2.48249400	-0.23318900
C	-1.87623100	3.69410300	-0.73413400
H	-2.39724000	4.62885000	-0.92738800
N	1.74302900	0.00010100	0.13250400
C	1.64267200	-4.88507900	-0.39340700
H	2.22097400	-5.80477100	-0.44231100
H	-0.23176700	-5.86066700	-0.74403000
N	-0.59100200	-1.35886300	-0.08434700
C	-4.00157800	2.43466800	-1.03349100
H	-4.53400800	3.36446200	-1.21513200
N	-0.59121700	1.35880100	-0.08420600
C	0.28167200	4.92030900	-0.56379600
H	-0.23250700	5.86059300	-0.74423200

C	1.60952600	2.42853800	-0.10552000
C	2.34025200	3.66729700	-0.20255100
C	1.64203900	4.88526900	-0.39345600
C	3.75926000	3.65470500	-0.18475500
H	4.27954800	4.60807900	-0.24015200
H	2.22020200	5.80505000	-0.44234200
Fe	0.08333500	-0.00002900	1.00078300
O	-3.02653300	0.00025600	3.86368100
C	-2.50714100	0.00008400	2.64115500
O	-1.29632200	-0.00044400	2.49008200
H	-3.99819800	0.00061000	3.81094500
H	-3.20763300	0.00039800	1.79557700

Fe-2a

C	0.53409600	5.00926200	-0.68552000
C	-0.60089000	4.18871300	-0.46866200
C	-0.43530200	2.76989600	-0.27974200
C	0.90243400	2.23606700	-0.34591000
C	2.01662700	3.08510000	-0.65786300
C	-1.62860200	1.96290200	-0.16925000
C	1.29143400	-2.05001600	-0.30562500
H	0.37734700	6.07871800	-0.80458000
C	-1.90388200	4.74973800	-0.51276000
C	-3.02906900	3.97179200	-0.45425500
C	-2.92715800	2.55629500	-0.31475000
H	-1.99265300	5.82651800	-0.63584300
H	-4.01831300	4.41557600	-0.52604400
C	-4.04311800	1.70724300	-0.29252200
C	-3.91874100	0.31219300	-0.22552200
C	-2.60139500	-0.23862900	-0.08093200
H	-5.03637800	2.14296100	-0.37001600
C	-5.03665400	-0.57214500	-0.27211900
C	-2.39618300	-1.66816900	-0.09748700
C	-3.56105600	-2.51142700	-0.19418000
C	-1.10193000	-2.30111200	-0.15538600
C	-3.40831300	-3.91448300	-0.31834100
H	-4.30672000	-4.52485800	-0.37086800
C	3.46677900	1.10108000	-0.71986500
C	1.45243600	-3.46142300	-0.51883500
C	-0.98741700	-3.71549000	-0.37123900
C	-2.17324600	-4.50206700	-0.41872400
H	-2.07734500	-5.57703400	-0.54574700
C	0.30118400	-4.26067500	-0.50253800
H	0.40511300	-5.33479300	-0.63579900
C	2.76821100	-3.98301200	-0.70449200
H	2.88690000	-5.05688500	-0.82053900

C	2.32360200	0.28878500	-0.41016400
C	3.28188600	2.48928600	-0.79315700
H	4.14059600	3.12336400	-1.00038500
N	0.04766700	-1.57474800	-0.00396800
C	-4.85459700	-1.92873800	-0.24201100
H	-5.71301700	-2.59421600	-0.29471900
H	-6.03294100	-0.14454100	-0.34483500
N	-1.54892600	0.61969300	0.06969700
C	1.79677500	4.48572500	-0.79207700
H	2.65063400	5.12800200	-0.99032700
N	1.14560500	0.91008500	-0.11342300
C	4.73253400	0.46695600	-0.90224300
H	5.60087400	1.09150200	-1.09383300
C	2.42657600	-1.15568700	-0.39589500
C	3.72880100	-1.74111200	-0.63805500
C	4.84919200	-0.89841700	-0.84671300
C	3.85573500	-3.14905700	-0.74569100
H	4.84930400	-3.56129400	-0.90671600
H	5.81775600	-1.36688900	-1.00631700
O	1.00879200	1.09954800	3.70466300
C	1.79311300	0.27428600	3.33559700
O	1.45885700	-0.59879000	2.33696100
H	2.80332000	0.11286800	3.74044800
H	2.21914100	-1.06492100	1.92635900
Fe	-0.05032300	-0.00028200	0.98700700

Fe-3

C	1.55561400	-4.86735200	-0.49610300
C	2.24970500	-3.63406900	-0.33559500
C	1.52258000	-2.40915900	-0.17196400
C	0.07545800	-2.47431400	-0.22592500
C	-0.58043800	-3.71914400	-0.50929100
C	2.28212100	-1.17468800	-0.13691300
C	-2.01164100	1.25791600	-0.31616200
H	2.14239100	-5.77805800	-0.58293600
C	3.67102400	-3.62238500	-0.41815000
C	4.37748100	-2.45169300	-0.43976800
C	3.70408700	-1.19888100	-0.33713900
H	4.18680900	-4.57439200	-0.51239800
H	5.45885700	-2.45487400	-0.54817000
C	4.37592700	0.03002500	-0.39974800
C	3.68897600	1.25160200	-0.35195600
C	2.27096800	1.21199000	-0.13986100
H	5.45735800	0.03545100	-0.51665600
C	4.34482700	2.51247000	-0.46814500
C	1.49360800	2.43134500	-0.16582000

C	2.19916600	3.66369900	-0.34814400
C	0.04599300	2.47140000	-0.19111100
C	1.48469000	4.88709800	-0.50155300
H	2.05568400	5.80673200	-0.59908200
C	-2.70599200	-2.50904300	-0.64822200
C	-2.73479400	2.46222000	-0.60765300
C	-0.63151900	3.70236400	-0.47819100
C	0.12160800	4.91046300	-0.58392700
H	-0.41243500	5.84311500	-0.74477400
C	-2.02333000	3.66780700	-0.62813600
H	-2.56038800	4.59683000	-0.80469500
C	-4.14021900	2.39847200	-0.84538500
H	-4.68085900	3.32573700	-1.01466800
C	-1.99974800	-1.29704900	-0.35052900
C	-1.97238100	-3.70342100	-0.67276300
H	-2.49320600	-4.64024900	-0.85719200
N	-0.69712100	1.35269400	0.01396700
C	3.61994700	3.67175100	-0.44921400
H	4.12022800	4.63089300	-0.55486000
H	5.42546500	2.53133100	-0.58204700
N	1.66799800	0.01705400	0.07291000
C	0.19322600	-4.91425100	-0.59885400
H	-0.32148500	-5.85689200	-0.76472800
N	-0.68139400	-1.36260300	-0.03450500
C	-4.11144500	-2.46045900	-0.88279900
H	-4.64400600	-3.39046200	-1.06260600
C	-2.67962700	-0.02325500	-0.40252300
C	-4.07714700	-0.03002500	-0.69907400
C	-4.76717300	-1.26151500	-0.89184900
C	-4.78451000	1.19504400	-0.87002400
H	-5.85311100	1.14868300	-1.06203800
H	-5.83606400	-1.22429600	-1.08462400
Fe	0.02282100	0.01063900	1.15042900
O	-0.56792700	-0.30830700	3.90951500
C	-1.13420500	0.02566300	2.69616700
O	-2.33700400	0.14825700	2.62838300
H	0.38377300	-0.12526300	3.82511800
H	0.65367200	1.07573400	2.08335200

Fe-3a

C	4.59036000	-1.57919100	-0.99379200
C	3.98199500	-0.29569200	-0.81333800
C	2.61115000	-0.18772200	-0.48292500
C	1.83416300	-1.41486700	-0.38103900
C	2.44866700	-2.67167800	-0.69766900
C	2.03784200	1.14918200	-0.44123000

C	-2.41119900	-1.01777200	-0.04086600
H	5.65602100	-1.61697600	-1.20244400
C	4.77570100	0.87871500	-1.03292800
C	4.23118700	2.12561500	-1.02532900
C	2.83484400	2.29499000	-0.76581200
H	5.83386000	0.74449800	-1.24045900
H	4.83918000	3.00429700	-1.22242800
C	2.20454700	3.54263800	-0.78577800
C	0.82669500	3.66804500	-0.57241400
C	0.08772200	2.47892800	-0.26236500
H	2.79439200	4.43410100	-0.98625100
C	0.14463200	4.92242600	-0.62851600
C	-1.36250900	2.52703400	-0.11808100
C	-1.98655200	3.79347400	-0.24651600
C	-2.21827600	1.35184000	-0.02256600
C	-3.41442200	3.90487100	-0.23942800
H	-3.85053200	4.89825700	-0.30141600
C	0.26362700	-3.73338300	-0.54658800
C	-3.83238500	-0.93327800	-0.18756600
C	-3.64054400	1.49352000	-0.14424300
C	-4.21253300	2.80312900	-0.21175200
H	-5.29457900	2.89566200	-0.25052200
C	-4.42271600	0.33537300	-0.17931500
H	-5.50489800	0.42284600	-0.23610900
C	-4.59636500	-2.13641800	-0.30533400
H	-5.67894000	-2.06309000	-0.36393200
C	-0.30009200	-2.45904600	-0.21712600
C	1.64765600	-3.81678500	-0.72323800
H	2.10496000	-4.78370000	-0.91809000
N	-1.68859500	0.11241700	0.17201500
C	-1.20533700	4.97578600	-0.45523100
H	-1.72745500	5.92724500	-0.51035500
H	0.72039200	5.82401100	-0.81936500
N	0.74143100	1.30941000	-0.12119200
C	3.85404000	-2.72240300	-0.95998100
H	4.31280600	-3.69015800	-1.14303500
N	0.52404300	-1.39994000	-0.01035900
C	-0.59372300	-4.87354700	-0.65578100
H	-0.14605200	-5.84380900	-0.85274100
C	-1.74141400	-2.30138000	-0.13242600
C	-2.54455800	-3.45369400	-0.31669200
C	-1.94150700	-4.73530000	-0.52774500
C	-3.97166600	-3.34530800	-0.35317700
H	-4.55116900	-4.25893200	-0.45572500
H	-2.59427600	-5.59885400	-0.62318300
Fe	-0.04641500	-0.01466700	1.07720300

O	2.70612300	-0.14744100	4.00635200
C	1.72065500	-0.38330000	3.32930300
O	1.38550500	0.27154900	2.23840200
H	1.01089800	-1.19368400	3.59746600
H	-0.68711100	-0.97527400	2.10495200

Fe-4

C	-0.83500000	5.06280800	-0.43066300
C	-1.72540900	3.97773000	-0.23730400
C	-1.20744700	2.63817000	-0.10959800
C	0.21668500	2.45103300	-0.21326600
C	1.07533500	3.56323400	-0.50756800
C	-2.15400100	1.55502200	-0.02323900
C	1.65686800	-1.59005300	-0.38017400
H	-1.25395600	6.06355900	-0.50397000
C	-3.12645100	4.19535500	-0.25217100
C	-4.01818400	3.15626800	-0.22098600
C	-3.56247900	1.80851900	-0.13595500
H	-3.48477200	5.21894000	-0.33153300
H	-5.08836500	3.33794500	-0.27028800
C	-4.43174600	0.70817100	-0.12951600
C	-3.96130100	-0.61144400	-0.10634200
C	-2.54472300	-0.81879300	0.00460100
H	-5.50362500	0.88404500	-0.17883900
C	-4.82533900	-1.74529200	-0.15331600
C	-1.99335800	-2.15381700	-0.04853300
C	-2.91495500	-3.25891200	-0.15150900
C	-0.58275600	-2.44121600	-0.16767700
C	-2.42021700	-4.57651900	-0.32316000
H	-3.13989100	-5.39056700	-0.36939300
C	2.96170400	2.00832200	-0.70504500
C	2.15389500	-2.90656500	-0.66927400
C	-0.12994200	-3.77528800	-0.44598100
C	-1.08383800	-4.83469400	-0.47858700
H	-0.72676900	-5.84806900	-0.64060000
C	1.24273600	-3.97294700	-0.64803000
H	1.60793000	-4.98020000	-0.83344100
C	3.54342200	-3.07778100	-0.93670900
H	3.91673700	-4.08349200	-1.10967500
C	2.06948000	0.92419000	-0.40111900
C	2.44281100	3.30979800	-0.69516800
H	3.11140400	4.14520200	-0.88811200
N	0.34827200	-1.45447900	-0.01519900
C	-4.31196100	-3.01479800	-0.15961700
H	-4.98010800	-3.87120500	-0.21361400
H	-5.89800800	-1.57693800	-0.19398800

N	-1.73552900	0.26806500	0.17285900
C	0.51379300	4.87055000	-0.57731400
H	1.17889100	5.70920800	-0.76480100
N	0.78495300	1.21671600	-0.03038900
C	4.33309500	1.72068700	-0.97342300
H	5.00740600	2.55131700	-1.16322000
C	2.52724200	-0.44237800	-0.47743200
C	3.91514000	-0.67372800	-0.80148600
C	4.78464400	0.42828800	-1.00358800
C	4.38558100	-1.99762700	-0.98521700
H	5.44086900	-2.13979100	-1.20588600
H	5.82904200	0.22172500	-1.22516800
Fe	-0.11361000	0.00424400	1.07823100
O	1.61593200	-0.16336800	2.51451200
C	2.78638000	-0.06281200	2.59552700
O	3.93456900	0.03355900	2.73662200
H	-0.88501600	-0.75023400	2.57556000
H	-1.04398800	-1.31631500	2.07602700

Fe-5

C	-1.64711200	4.88662400	-0.36819200
C	-2.34877400	3.66901400	-0.18241700
C	-1.61933100	2.42991700	-0.07610600
C	-0.18199000	2.48622400	-0.18382200
C	0.48514000	3.72529400	-0.46506000
C	-2.38183100	1.20765900	0.00765100
C	1.90049700	-1.27845500	-0.37769600
H	-2.22492200	5.80602700	-0.42634500
C	-3.76714700	3.65571800	-0.17618900
C	-4.48120600	2.48705000	-0.14009200
C	-3.81396100	1.22860200	-0.07777900
H	-4.28731300	4.60854900	-0.24018100
H	-5.56734600	2.49649100	-0.16942300
C	-4.49112900	-0.00041500	-0.07387000
C	-3.81374100	-1.22926000	-0.07761500
C	-2.38161100	-1.20798700	0.00763900
H	-5.57786800	-0.00049500	-0.10876600
C	-4.48069000	-2.48792800	-0.13962100
C	-1.61883600	-2.43009200	-0.07620600
C	-2.34794800	-3.66935800	-0.18220500
C	-0.18148700	-2.48606400	-0.18448600
C	-1.64605400	-4.88680200	-0.36806600
H	-2.22366000	-5.80634700	-0.42601400
C	2.60480000	2.49660200	-0.66602100
C	2.60529300	-2.49577300	-0.66680000
C	0.48589000	-3.72500400	-0.46565400

C	-0.28410900	-4.92269400	-0.52029000
H	0.23199300	-5.86280700	-0.69514200
C	1.87693100	-3.69480800	-0.65538200
H	2.40094700	-4.62874900	-0.84345000
C	4.00673100	-2.43386600	-0.92525800
H	4.54231600	-3.36275000	-1.10112400
C	1.90025000	1.27911800	-0.37697700
C	1.87620200	3.69550200	-0.65450700
H	2.40001300	4.62956200	-0.84253600
N	0.58372600	-1.36344400	-0.02315100
C	-3.76636700	-3.65640600	-0.17566800
H	-4.28629400	-4.60938200	-0.23941800
H	-5.56683400	-2.49761600	-0.16875600
N	-1.75997100	-0.00010400	0.17197600
C	-0.28515500	4.92279300	-0.52007300
H	0.23079500	5.86298900	-0.69494100
N	0.58357800	1.36390800	-0.02177800
C	4.00619800	2.43503500	-0.92467200
H	4.54154700	3.36406500	-1.10049000
C	2.56877100	0.00042300	-0.46059800
C	3.97887500	0.00058700	-0.77345400
C	4.65892700	1.23047600	-0.96096500
C	4.65916900	-1.22914900	-0.96124500
H	5.72486800	-1.19528100	-1.17516700
H	5.72462000	1.19691100	-1.17495900
Fe	-0.11686700	-0.00034200	1.01534400
O	1.50397400	-0.00064300	2.54812100
C	2.67621200	-0.00046300	2.66903900
O	3.82301400	-0.00029400	2.84617800

Fe-6

C	-1.35282300	4.89723000	-0.32444800
C	-2.08330500	3.69097800	-0.17814400
C	-1.38351600	2.44475800	0.00295600
C	0.05836200	2.48005000	0.00966800
C	0.76278800	3.70788300	-0.22590200
C	-2.16451000	1.23452000	0.04546600
C	2.10222100	-1.30586400	0.01784900
H	-1.91164500	5.82251800	-0.44227100
C	-3.49814400	3.69668100	-0.28493100
C	-4.22699900	2.53771800	-0.29099200
C	-3.58405700	1.27202500	-0.15731300
H	-3.99826700	4.65482800	-0.40401400
H	-5.30666200	2.55901600	-0.41141300
C	-4.27820100	0.05370200	-0.19688200
C	-3.61509100	-1.18167800	-0.15697200

C	-2.19501600	-1.17993400	0.04581000
H	-5.35872400	0.06737300	-0.31565800
C	-4.28971300	-2.43088400	-0.29034200
C	-1.44477700	-2.40935300	0.00334700
C	-2.17566000	-3.63761100	-0.17762200
C	-0.00422700	-2.48062900	0.00963700
C	-1.47575700	-4.86177900	-0.32407500
H	-2.05758500	-5.77280300	-0.44163700
C	2.87783600	2.45908500	-0.21123500
C	2.81481300	-2.53047600	-0.21205500
C	0.66903600	-3.72578200	-0.22621900
C	-0.10704300	-4.91264200	-0.36325400
H	0.41157600	-5.85682200	-0.50528800
C	2.07191500	-3.71610500	-0.28808600
H	2.59682500	-4.65684600	-0.43500800
C	4.23697100	-2.48781700	-0.32312200
H	4.77542500	-3.42337400	-0.44651400
C	2.13472500	1.25276100	0.01836400
C	2.16497000	3.66307700	-0.28711300
H	2.71334900	4.59038700	-0.43362500
N	0.75776700	-1.36948600	0.24305900
C	-3.59025500	-3.60778800	-0.28415700
H	-4.11425800	-4.55311600	-0.40295800
H	-5.36957800	-2.42498100	-0.41067400
N	-1.57412400	0.01961100	0.28522200
C	0.01670900	4.91381500	-0.36321300
H	0.55884800	5.84471600	-0.50510000
N	0.79226200	1.35018800	0.24357200
C	4.29841400	2.38064900	-0.32236600
H	4.86026000	3.30237500	-0.44551200
C	2.79369000	-0.03508400	0.01414200
C	4.22398100	-0.05308500	-0.16130200
C	4.93514200	1.16893500	-0.28413200
C	4.90407700	-1.29261700	-0.28446300
H	5.98652800	-1.27216000	-0.38750400
H	6.01672100	1.12121300	-0.38723200
Fe	0.00429100	0.00037200	1.24571500
H	1.05376400	-0.01407000	2.71343000
H	1.62117900	-0.02855300	2.17602400

Fe-TS-1

C	-0.49011000	5.06462600	-0.65180400
C	-1.41598000	3.99538900	-0.48172500
C	-0.94558300	2.66546600	-0.24785400
C	0.48293500	2.44932900	-0.23170300
C	1.38406800	3.53411900	-0.49128100

C	-1.91971000	1.59875900	-0.19478300
C	1.81726200	-1.62641200	-0.30714500
H	-0.88652000	6.06494000	-0.80595700
C	-2.80973200	4.25042900	-0.61753200
C	-3.72284600	3.23557400	-0.61001900
C	-3.30626900	1.88268300	-0.43191800
H	-3.13167000	5.27738700	-0.76978100
H	-4.78087800	3.43521500	-0.75687500
C	-4.21112300	0.81331600	-0.45727800
C	-3.77070700	-0.51186100	-0.39611900
C	-2.37293500	-0.75119700	-0.17497300
H	-5.27174900	1.01747900	-0.58105100
C	-4.65929300	-1.62467100	-0.52375300
C	-1.85040900	-2.10248400	-0.26141100
C	-2.77705800	-3.16931600	-0.45924100
C	-0.43939700	-2.42537200	-0.31398600
C	-2.30544400	-4.50288500	-0.64761900
H	-3.04449600	-5.29267300	-0.75825400
C	3.23882200	1.94809500	-0.44464700
C	2.31019600	-2.94608200	-0.57608900
C	0.00165700	-3.76000500	-0.59294200
C	-0.97462200	-4.79606700	-0.72175300
H	-0.63474700	-5.81669900	-0.87518500
C	1.37937300	-3.98809000	-0.69054400
H	1.73739900	-4.99815000	-0.87450100
C	3.71796700	-3.14826700	-0.69637800
H	4.08873100	-4.15907300	-0.84328700
C	2.29338600	0.89377400	-0.21037700
C	2.75710900	3.25818200	-0.52798500
H	3.46027400	4.07593800	-0.66524100
N	0.48402800	-1.45462400	-0.10252400
C	-4.17516900	-2.89980000	-0.53312900
H	-4.85380800	-3.74153500	-0.64737800
H	-5.72276000	-1.42832300	-0.62936400
N	-1.55155400	0.31117100	0.08753600
C	0.85764300	4.84777100	-0.67270900
H	1.55199100	5.66604200	-0.84360500
N	0.99210100	1.21605300	0.04061100
C	4.62623200	1.62736900	-0.56562600
H	5.33837700	2.43913100	-0.68627200
C	2.71983100	-0.49225800	-0.27104700
C	4.10979300	-0.75214000	-0.45729600
C	5.03790000	0.32775800	-0.54820800
C	4.57580600	-2.08875700	-0.62576000
H	5.64661500	-2.24601100	-0.72835500
H	6.09265000	0.08685000	-0.65458000

Fe	0.01371000	-0.05277300	1.04433400
O	-0.48258800	0.06904500	4.03502300
C	0.14375900	-0.13328600	2.86173100
O	1.34536700	-0.41373500	2.78797200
H	-1.41341000	0.27081500	3.84168900
H	-0.75081800	-1.07203400	1.99939400

Fe-TS-1a

C	-4.74532400	0.83952100	-0.99491500
C	-3.94923200	-0.33304200	-0.83959200
C	-2.56495300	-0.22049200	-0.51420400
C	-2.00555800	1.10622100	-0.36859400
C	-2.80884400	2.25989400	-0.65284200
C	-1.79263500	-1.44149200	-0.45797600
C	2.26608900	1.39269200	-0.01811600
H	-5.80335900	0.71500100	-1.21007100
C	-4.52994200	-1.61420500	-1.06646200
C	-3.78705700	-2.76015300	-1.04190700
C	-2.38820000	-2.70661100	-0.76584800
H	-5.59419900	-1.65946300	-1.28254900
H	-4.24652000	-3.72775300	-1.22343900
C	-1.56338300	-3.84087700	-0.75435800
C	-0.18600700	-3.75352100	-0.51541200
C	0.36811300	-2.46157000	-0.23090900
H	-2.00282000	-4.81478100	-0.95503600
C	0.68229300	-4.88794000	-0.53078300
C	1.79893700	-2.28355200	-0.07097400
C	2.62003900	-3.45145100	-0.15519500
C	2.46198200	-0.99921100	0.03441700
C	4.03841700	-3.33080500	-0.12211600
H	4.62981600	-4.24201400	-0.16305300
C	-0.80397600	3.64600800	-0.48565200
C	3.68762600	1.52633400	-0.14139500
C	3.88961100	-0.90927100	-0.06059700
C	4.65655700	-2.11313000	-0.10032500
H	5.74007600	-2.03672500	-0.12419900
C	4.47106400	0.36503100	-0.09279800
H	5.55378700	0.45338300	-0.12800100
C	4.24704700	2.83216500	-0.27529600
H	5.32705300	2.92888900	-0.34460800
C	-0.03663900	2.47018400	-0.19157800
C	-2.19080300	3.51418600	-0.64257800
H	-2.79074300	4.40352900	-0.81751600
N	1.74217400	0.15293400	0.21605700
C	2.02619600	-4.73312900	-0.34720200
H	2.68288400	-5.59906400	-0.37337300

H	0.25023800	-5.87143100	-0.69346500
N	-0.47640900	-1.39968500	-0.12681400
C	-4.20175700	2.08819800	-0.92391000
H	-4.81141000	2.97374000	-1.08011400
N	-0.70302600	1.29215300	0.01333400
C	-0.13810000	4.90249700	-0.59609400
H	-0.73659700	5.78933600	-0.78519200
C	1.40446900	2.54404500	-0.11870000
C	2.02138000	3.82518700	-0.28694000
C	1.22117500	4.98385600	-0.48578000
C	3.44011600	3.93340500	-0.32758400
H	3.87403700	4.92359800	-0.44063500
H	1.72251500	5.94291300	-0.58708900
Fe	0.08721500	-0.04751700	1.01132400
O	-3.48304400	-0.11293000	3.18457800
C	-2.36572900	0.27798200	2.94236300
O	-1.41591400	-0.48148400	2.39484200
H	-2.03468600	1.31181200	3.17119800
H	-0.23300200	0.18025900	2.58843900

Fe-TS-2

C	3.42874000	-3.84006000	-0.36360000
C	3.53867900	-2.41590000	-0.26043000
C	2.38090000	-1.61322300	-0.10698100
C	1.08646100	-2.28022200	-0.10259800
C	1.01022000	-3.69226000	-0.34214500
C	2.56226500	-0.16808200	-0.12651500
C	-2.37248300	0.22739600	-0.30982600
H	4.34491100	-4.42009800	-0.43691600
C	4.83412000	-1.81411400	-0.37351500
C	4.99763500	-0.46360400	-0.42835600
C	3.86039000	0.40012900	-0.34734200
H	5.69567100	-2.47276500	-0.44627400
H	5.98469300	-0.02218500	-0.53670400
C	3.95597900	1.79201300	-0.44938300
C	2.81667900	2.60517700	-0.41305300
C	1.54827800	1.97530100	-0.19490100
H	4.93312300	2.25069100	-0.58185500
C	2.87482000	4.02543800	-0.56277200
C	0.32076800	2.75349300	-0.24241700
C	0.43948500	4.14899600	-0.45503600
C	-1.01598700	2.17263200	-0.25841100
C	-0.72595000	4.96304100	-0.63135600
H	-0.58912200	6.03453000	-0.74956700
C	-1.41211700	-3.49163500	-0.47030200
C	-3.53239600	1.00269000	-0.63560300

C	-2.14517600	3.00206900	-0.56677600
C	-1.96852300	4.41458000	-0.70671000
H	-2.84406100	5.03274700	-0.88564000
C	-3.39461500	2.39165100	-0.70291300
H	-4.27122500	3.00687900	-0.89126600
C	-4.78339500	0.34478900	-0.84867800
H	-5.66357300	0.94994700	-1.04776300
C	-1.28327300	-2.08790500	-0.21904500
C	-0.25286900	-4.27604500	-0.46810700
H	-0.33449400	-5.35150600	-0.60450400
N	-1.20860400	0.85215700	-0.01437400
C	1.72934600	4.76203000	-0.56581700
H	1.77168500	5.84088500	-0.68924900
H	3.84544800	4.50045900	-0.67806600
N	1.49876400	0.64632200	0.04503200
C	2.21758500	-4.45685000	-0.42311900
H	2.14291700	-5.53426200	-0.54309200
N	-0.06292300	-1.57939200	0.10422000
C	-2.71039600	-4.04677100	-0.69111500
H	-2.79881900	-5.12011200	-0.83609400
C	-2.44368300	-1.22372400	-0.31336700
C	-3.69619700	-1.82196600	-0.59783300
C	-3.80774400	-3.24148500	-0.73486000
C	-4.85806900	-1.01371200	-0.81442500
H	-5.80532200	-1.51684100	-0.98867300
H	-4.79280600	-3.66344900	-0.91475800
Fe	0.05385000	-0.03195600	1.12392100
O	-0.15952800	1.00336000	2.96876800
C	-1.12716400	0.08775400	2.58828500
O	-2.21468300	-0.05319300	3.08897700
H	0.76836400	0.19122700	2.77491300
H	1.18166900	-0.63995600	2.26160400

Fe-TS-2a

C	3.03142400	4.17881800	-0.45288300
C	1.62746900	3.94778500	-0.41006400
C	1.12199500	2.62365200	-0.21938600
C	2.07770800	1.54720100	-0.10479400
C	3.48118700	1.80493900	-0.23722500
C	-0.30920400	2.42913600	-0.28397400
C	0.51285300	-2.44232700	-0.25944400
H	3.37875300	5.20114000	-0.57781800
C	0.73149800	5.03312100	-0.62829700
C	-0.61540000	4.83658200	-0.73505600
C	-1.17354800	3.53016500	-0.59703200
H	1.15102300	6.02879100	-0.74644300

H	-1.28629100	5.66693600	-0.93768000
C	-2.54463100	3.27918000	-0.73536400
C	-3.05880200	1.97927100	-0.68800300
C	-2.15546100	0.90580400	-0.38773700
H	-3.21926900	4.11046900	-0.92435900
C	-4.43946300	1.68624400	-0.91235700
C	-2.60906400	-0.46843100	-0.47208400
C	-3.98392300	-0.70267600	-0.76685300
C	-1.72823900	-1.61767300	-0.42662800
C	-4.46110300	-2.03498100	-0.94930300
H	-5.52345000	-2.17413100	-1.13338500
C	3.89144300	-0.60134100	-0.14359500
C	0.06927400	-3.77812600	-0.53453100
C	-2.22317100	-2.93359000	-0.70883500
C	-3.62372300	-3.11258700	-0.93096800
H	-4.00236300	-4.11836400	-1.09059100
C	-1.30397600	-3.98788100	-0.72935200
H	-1.66159500	-4.99794000	-0.91436700
C	1.02842700	-4.83325900	-0.57398200
H	0.67870100	-5.84856300	-0.73954400
C	2.47616500	-0.80989600	-0.03653600
C	4.36255200	0.71475800	-0.18731600
H	5.43352800	0.89512100	-0.23488600
N	-0.41427600	-1.45649400	-0.13682600
C	-4.87866000	0.39437400	-0.93263500
H	-5.92718600	0.17648600	-1.11914500
H	-5.12384100	2.51283700	-1.08186800
N	-0.86666700	1.20508500	-0.05499400
C	3.92904600	3.15068700	-0.38550500
H	4.99742400	3.33805400	-0.45026400
N	1.65974600	0.27128900	0.13707600
C	4.75932200	-1.73654300	-0.18539800
H	5.83233100	-1.56775100	-0.21408500
C	1.92666500	-2.14776300	-0.12244300
C	2.84172600	-3.24139000	-0.21854800
C	4.24779300	-3.00117800	-0.20109800
C	2.35884900	-4.56736700	-0.40766100
H	3.08581600	-5.37443800	-0.44965000
H	4.91331600	-3.85951200	-0.24594700
Fe	0.02592100	-0.03798700	1.00053100
O	-2.23462700	0.24534900	4.31590300
C	-1.50586500	0.11372600	3.37693200
O	-1.46168000	-0.44854100	2.25080000
H	-0.15196800	0.80445100	3.22858300
H	0.50297200	0.84987700	2.59494600

Ru-1

C	4.74357200	1.81551600	-0.42195400
C	3.47114600	2.42444700	-0.27287400
C	2.30180600	1.60758600	-0.05885500
C	2.48892700	0.17435600	-0.03383500
C	3.77299000	-0.40722000	-0.30166000
C	1.02024800	2.27647900	-0.03675300
C	-1.09310000	-2.24272900	-0.03448700
H	5.60629200	2.46344900	-0.55702400
C	3.33696700	3.82837700	-0.42486900
C	2.11267400	4.44105500	-0.46031400
C	0.91577600	3.68190100	-0.30635500
H	4.24222400	4.41533800	-0.56010500
H	2.02936700	5.51316800	-0.61522200
C	-0.36697800	4.24665000	-0.37762900
C	-1.53383500	3.47029200	-0.30523700
C	-1.39561900	2.06770900	-0.03617800
H	-0.45959700	5.31677300	-0.54478700
C	-2.84329400	4.01303700	-0.45794300
C	-2.54342700	1.18899400	-0.05880600
C	-3.83554900	1.79308800	-0.27273900
C	-2.48188900	-0.25514800	-0.03402300
C	-4.98463900	0.97496200	-0.42228000
H	-5.94564300	1.46537500	-0.55758700
C	2.73134700	-2.63414100	-0.30261000
C	-2.23884400	-3.06372600	-0.30318100
C	-3.64718400	-1.04840700	-0.30176400
C	-4.90323800	-0.39165900	-0.45534200
H	-5.79017700	-1.00005200	-0.60874600
C	-3.49493100	-2.44165500	-0.37313500
H	-4.37554200	-3.05685500	-0.53962100
C	-2.05410400	-4.46874600	-0.45914400
H	-2.93046200	-5.09202200	-0.61377800
C	1.46166100	-2.02193600	-0.03426600
C	3.86206900	-1.80591200	-0.37299300
H	4.83509800	-2.26102000	-0.53966000
N	-1.31835800	-0.92116800	0.24654400
C	-3.94429700	3.19935400	-0.42334200
H	-4.93683400	3.62255100	-0.55795800
H	-2.94532700	5.08370100	-0.61176900
N	-0.13833800	1.60187500	0.24364800
C	4.89779700	0.45519800	-0.45508300
H	5.87596000	0.00788900	-0.60828100
N	1.45678100	-0.68132700	0.24673600
C	2.79052800	-4.05011200	-0.45775300
H	3.76088700	-4.51392600	-0.61161100

C	0.24177600	-2.79731200	-0.05948900
C	0.36455500	-4.21804500	-0.27587400
C	1.64762700	-4.80387100	-0.42598500
C	-0.79883300	-5.01527100	-0.42733000
H	-0.66885700	-6.08606000	-0.56466900
H	1.70351500	-5.88118700	-0.56241900
Ru	-0.00026600	0.00110300	1.36725600

Ru-2

C	-4.58729000	1.22667900	-1.32338700
C	-3.91977100	-0.00172000	-1.08847300
C	-2.52794800	-0.00113500	-0.68572500
C	-1.86657000	1.27805300	-0.56605900
C	-2.55009400	2.49238400	-0.92126000
C	-1.86554200	-1.27977800	-0.56588800
C	2.40206200	1.20356900	-0.05701600
H	-5.63729800	1.19162800	-1.60577300
C	-4.58629600	-1.23068000	-1.32327400
C	-3.93295400	-2.43374500	-1.25982900
C	-2.54808500	-2.49469400	-0.92098500
H	-5.63633000	-1.19650600	-1.60567000
H	-4.45279400	-3.36296100	-1.47694400
C	-1.82441300	-3.69374000	-0.87824000
C	-0.44419300	-3.72330400	-0.62105800
C	0.20544600	-2.49014300	-0.28006800
H	-2.33642100	-4.62564600	-1.10514400
C	0.32768400	-4.91945100	-0.66035800
C	1.63952800	-2.42973500	-0.13502900
C	2.37466500	-3.66468500	-0.25106100
C	2.40302900	-1.20180600	-0.05690200
C	3.79420900	-3.65062500	-0.25018100
H	4.31408400	-4.60367400	-0.31336000
C	-0.44718800	3.72272300	-0.62144700
C	3.83266400	1.22778400	-0.17520900
C	3.83365300	-1.22488700	-0.17509500
C	4.50536700	-2.48167700	-0.23438100
H	5.59113200	-2.48702100	-0.27603700
C	4.51134800	0.00172100	-0.18279900
H	5.59781400	0.00215800	-0.22728100
C	4.50336700	2.48511100	-0.23461500
H	5.58912700	2.49132500	-0.27627400
C	0.20344500	2.49012200	-0.28034500
C	-1.82738500	3.69201900	-0.87863500
H	-2.34014600	4.62348900	-1.10563100
N	1.79031300	0.00064300	0.14111700
C	1.68337000	-4.88347400	-0.46299200

H	2.26586500	-5.80020000	-0.51611400
H	-0.18133600	-5.85743800	-0.86522700
N	-0.58398200	-1.38319900	-0.10450800
C	-3.93492200	2.43028200	-1.26006700
H	-4.45551900	3.35905600	-1.47726400
N	-0.58508300	1.38254700	-0.10471800
C	0.32372500	4.91948900	-0.66084100
H	-0.18605000	5.85704800	-0.86579000
C	1.63757100	2.43087900	-0.13527300
C	2.37171600	3.66641000	-0.25140900
C	1.67943900	4.88462200	-0.46345800
C	3.79127100	3.65348600	-0.25052200
H	4.31038400	4.60694500	-0.31379000
H	2.26119600	5.80181200	-0.51665700
O	-3.57088100	0.00030600	3.67276200
C	-2.85517200	-0.00035000	2.54847100
O	-1.63819200	-0.00007800	2.59790700
H	-4.51965700	-0.00004800	3.45779300
H	-3.41414800	-0.00109600	1.60331200
Ru	0.06180800	0.00002600	1.16313000

Ru-2a

C	-0.00221400	5.05771900	-0.76759500
C	-1.04502200	4.13161000	-0.51459900
C	-0.73826700	2.73728900	-0.31431200
C	0.64454800	2.33844000	-0.41933300
C	1.65635600	3.28465700	-0.79309900
C	-1.85218000	1.81973300	-0.19308500
C	1.44016000	-1.89983300	-0.45030300
H	-0.26639800	6.10584100	-0.88569800
C	-2.39632000	4.56525400	-0.55248000
C	-3.44052200	3.68275100	-0.49729300
C	-3.20068800	2.28396100	-0.35703400
H	-2.58769300	5.62824900	-0.67801900
H	-4.46831200	4.02735800	-0.57079500
C	-4.22973700	1.33236100	-0.33517000
C	-3.97136200	-0.04349000	-0.26641200
C	-2.60871000	-0.46444000	-0.10288500
H	-5.26007100	1.67050200	-0.41452800
C	-5.00059200	-1.02973700	-0.31372600
C	-2.26377800	-1.87030400	-0.12946800
C	-3.34538700	-2.81737600	-0.23806600
C	-0.91765600	-2.38137200	-0.22535400
C	-3.06581000	-4.19755000	-0.39691900
H	-3.90480100	-4.88734800	-0.44826500
C	3.28328500	1.44844900	-0.92940400

C	1.71850900	-3.28101000	-0.73103100
C	-0.67803000	-3.76864800	-0.50366200
C	-1.78534100	-4.66318000	-0.54333500
H	-1.59134100	-5.72014200	-0.70430600
C	0.64931700	-4.18618200	-0.69616700
H	0.84745000	-5.24075800	-0.87079400
C	3.06657600	-3.67246300	-0.98930800
H	3.27616400	-4.72665500	-1.14838400
C	2.24409900	0.53041800	-0.55390200
C	2.96502100	2.81252800	-0.98692000
H	3.74812700	3.52482500	-1.23448200
N	0.17469900	-1.57113600	-0.05441700
C	-4.68937800	-2.36173000	-0.28015600
H	-5.47916300	-3.10711400	-0.33518600
H	-6.03263200	-0.69838600	-0.38866100
N	-1.65741300	0.49672800	0.08199300
C	1.29922700	4.65749900	-0.92086600
H	2.08005300	5.37647300	-1.15334800
N	1.04247700	1.05152400	-0.16728400
C	4.59268800	0.93908300	-1.18117100
H	5.38536100	1.64530600	-1.41259800
C	2.48081700	-0.89880400	-0.56482400
C	3.81809500	-1.35478800	-0.88719700
C	4.84224600	-0.40825500	-1.14089900
C	4.07040600	-2.74097900	-1.04395000
H	5.08925600	-3.05291000	-1.26197600
H	5.84079700	-0.78198500	-1.35567900
O	1.52406700	0.85308200	4.05366400
C	2.27339800	0.16948000	3.41958700
O	1.83903000	-0.53960900	2.33581700
H	3.34455300	0.02155700	3.62928900
H	2.55996500	-0.89781700	1.77566400
Ru	-0.02924900	0.00588300	1.13004300

Ru-3

C	-1.26203900	4.96367300	-0.57923600
C	-2.02708800	3.76964700	-0.37907600
C	-1.38738900	2.51377200	-0.20725100
C	0.07401600	2.49126100	-0.28987400
C	0.79096600	3.68576200	-0.63345900
C	-2.24506700	1.33118100	-0.15652000
C	1.89440600	-1.37717600	-0.39411500
H	-1.79905000	5.90467700	-0.66417400
C	-3.45593400	3.86313400	-0.43829600
C	-4.24659600	2.75568800	-0.44567100
C	-3.66141900	1.45422100	-0.35271400

H	-3.89738900	4.85246800	-0.52492700
H	-5.32665600	2.83901400	-0.53342400
C	-4.41999500	0.28086500	-0.42990300
C	-3.81451500	-0.98176100	-0.40432000
C	-2.40047800	-1.04097400	-0.18374200
H	-5.49876700	0.35186600	-0.54737600
C	-4.55067000	-2.19743100	-0.55628000
C	-1.69058500	-2.31223700	-0.23874700
C	-2.46971800	-3.47434900	-0.47529300
C	-0.24058400	-2.45380900	-0.26142400
C	-1.84468900	-4.74385700	-0.68777900
H	-2.48175500	-5.61442400	-0.81872100
C	2.82371800	2.34943600	-0.81728300
C	2.51230000	-2.61535700	-0.77230500
C	0.34366800	-3.70624800	-0.63583500
C	-0.49348100	-4.85556900	-0.79293800
H	-0.02436100	-5.81102100	-1.01122400
C	1.72913500	-3.77121800	-0.80945800
H	2.19663000	-4.72719500	-1.03050000
C	3.90893300	-2.64222900	-1.07774000
H	4.37132400	-3.59962100	-1.30123200
C	2.05566000	1.19629700	-0.44598900
C	2.17144300	3.58558800	-0.84172900
H	2.74218000	4.48491400	-1.06129200
N	0.59918000	-1.41536900	0.04826800
C	-3.89613600	-3.39104200	-0.57761400
H	-4.44970600	-4.31681600	-0.71084000
H	-5.63094000	-2.14775900	-0.66367700
N	-1.71970600	0.10091500	0.05866700
C	0.09035000	4.92794000	-0.72799400
H	0.65593800	5.83301100	-0.93277800
N	0.77060300	1.35124200	-0.07000200
C	4.21351300	2.20319800	-1.11576900
H	4.79900400	3.08993600	-1.34271300
C	2.64694400	-0.13488700	-0.49795000
C	4.00572900	-0.21956200	-0.88981200
C	4.77444600	0.96382600	-1.13519900
C	4.62720100	-1.48849800	-1.11094700
H	5.68526800	-1.50517700	-1.35798000
H	5.82621400	0.84262100	-1.38047700
O	1.20504400	-0.13121900	3.98392500
C	1.51138100	-0.12995400	2.63473100
O	2.69382000	-0.08805200	2.33263400
H	0.26560800	-0.38444500	4.02516500
H	-0.74918100	-1.14052300	2.33627200
Ru	-0.04159900	-0.05115500	1.29759300

Ru-3a

C	4.64303500	-1.18258100	-1.26908500
C	3.95411700	0.04596700	-1.01978500
C	2.59413800	0.04645100	-0.62096900
C	1.91543200	-1.23998100	-0.52406800
C	2.59763400	-2.43523000	-0.92494700
C	1.93474600	1.34545500	-0.53882600
C	-2.36057300	-1.18190700	-0.08939000
H	5.69793800	-1.13713800	-1.52514500
C	4.65159300	1.27652400	-1.25518700
C	4.02088600	2.48165200	-1.21807300
C	2.62802900	2.54606600	-0.90256700
H	5.70640100	1.21884300	-1.50979200
H	4.55443500	3.40195800	-1.43911400
C	1.89931300	3.74023000	-0.90483100
C	0.52081200	3.75852800	-0.65828700
C	-0.11157800	2.51949500	-0.30673800
H	2.41000400	4.67384000	-1.12911000
C	-0.26081200	4.95294400	-0.71829500
C	-1.56384600	2.44082500	-0.14687200
C	-2.28686600	3.65502400	-0.29163900
C	-2.33469600	1.20441200	-0.04571300
C	-3.71804700	3.65852200	-0.29144400
H	-4.22752100	4.61584000	-0.36112400
C	0.50597600	-3.66773500	-0.74344700
C	-3.78099700	-1.19645900	-0.26289000
C	-3.76089700	1.23819100	-0.19489200
C	-4.43015600	2.49978200	-0.27049900
H	-5.51551000	2.50868700	-0.32271100
C	-4.45956800	0.02679500	-0.24171300
H	-5.54429700	0.03890700	-0.31017500
C	-4.45354900	-2.44955700	-0.41253000
H	-5.53806800	-2.45455500	-0.47866000
C	-0.14210400	-2.46000400	-0.32985600
C	1.88534400	-3.63819200	-0.96492100
H	2.40663500	-4.55785700	-1.21699900
N	-1.73605800	-0.00434700	0.19069700
C	-1.60683100	4.89477100	-0.52192700
H	-2.20797800	5.79807600	-0.58268300
H	0.23447900	5.89548700	-0.93506400
N	0.65054900	1.42052000	-0.14980200
C	3.98918400	-2.37470500	-1.25002600
H	4.50367600	-3.30037600	-1.49241300
N	0.62867500	-1.36428400	-0.06012800
C	-0.26668600	-4.86390700	-0.88185700

H	0.24786200	-5.78788700	-1.13044800
C	-1.59116700	-2.40780000	-0.22034200
C	-2.30944500	-3.61008100	-0.44821800
C	-1.61701600	-4.83279700	-0.71869300
C	-3.74000500	-3.60671400	-0.48348900
H	-4.24909600	-4.55812900	-0.61297000
H	-2.20585300	-5.73836600	-0.83790800
Ru	-0.01563000	-0.05181500	1.22693000
O	3.02624700	-0.26338700	4.06096600
C	2.05720600	-0.52675700	3.37390700
O	1.55388500	0.26981300	2.45019500
H	1.50913100	-1.48680700	3.47754500
H	-0.55334600	-1.20863700	2.25584700

Ru-4

C	-1.18264900	5.01045400	-0.51308600
C	-1.99418700	3.87053000	-0.28548500
C	-1.38836500	2.56943600	-0.14233400
C	0.04585900	2.48041900	-0.27667700
C	0.81715300	3.63902600	-0.62773300
C	-2.26895500	1.42877300	-0.04883600
C	1.73919000	-1.46707700	-0.48001800
H	-1.67059200	5.97903000	-0.59049400
C	-3.40664600	3.99952100	-0.30137200
C	-4.22967300	2.90642100	-0.27895700
C	-3.68795700	1.59072800	-0.19247000
H	-3.82818400	4.99828200	-0.38510700
H	-5.30883300	3.01799200	-0.33832400
C	-4.48634900	0.43865500	-0.20648300
C	-3.93400300	-0.84851500	-0.19553000
C	-2.51062700	-0.96991100	-0.04813000
H	-5.56620100	0.54775100	-0.26953100
C	-4.72555400	-2.03220900	-0.27645000
C	-1.87299200	-2.26642100	-0.12647100
C	-2.72436800	-3.42194000	-0.26961300
C	-0.44866200	-2.46445900	-0.25403400
C	-2.15093300	-4.70222900	-0.47458700
H	-2.81966200	-5.55703000	-0.54297000
C	2.79451500	2.20842100	-0.86905600
C	2.30579800	-2.74416900	-0.81473200
C	0.08347000	-3.75672000	-0.58276200
C	-0.80236600	-4.87241500	-0.63980400
H	-0.38256200	-5.85659300	-0.82890700
C	1.46376500	-3.86520600	-0.80167700
H	1.88711700	-4.84317600	-1.01671200
C	3.69733900	-2.82500900	-1.11488900

H	4.12746000	-3.80383300	-1.30862800
C	1.99026900	1.07463400	-0.50644100
C	2.19097400	3.47288400	-0.85793800
H	2.79585000	4.34722400	-1.08511900
N	0.43592700	-1.43853600	-0.06347500
C	-4.13401700	-3.26629000	-0.29195700
H	-4.74552500	-4.16202000	-0.37135000
H	-5.80555400	-1.92884400	-0.33401900
N	-1.78896000	0.16727800	0.17959200
C	0.16982400	4.90620400	-0.69909700
H	0.77210000	5.78297000	-0.92089700
N	0.71417800	1.30186400	-0.07082700
C	4.17163400	2.00894500	-1.18237700
H	4.78130700	2.87889600	-1.41037900
C	2.52951200	-0.26377400	-0.59129200
C	3.91781300	-0.40456200	-0.96379300
C	4.70651900	0.74905000	-1.20634400
C	4.46804700	-1.69449600	-1.17023800
H	5.52385400	-1.76636000	-1.42019400
H	5.75381100	0.60695500	-1.46197800
O	1.91800600	-0.11438900	2.53653800
C	3.08999800	-0.04617300	2.57547300
O	4.24729600	0.01994800	2.66579000
H	-0.73833200	-0.88817400	2.73140300
H	-0.94725800	-1.39063600	2.13238900
Ru	-0.09271600	-0.00173400	1.22218900

Ru-5

C	-1.67540800	4.88413200	-0.46215000
C	-2.37140400	3.66730100	-0.25052900
C	-1.63884700	2.43155800	-0.11917600
C	-0.20170500	2.49235200	-0.24326700
C	0.45489100	3.72356400	-0.57884600
C	-2.40488100	1.20774600	-0.03705300
C	1.87917700	-1.28057000	-0.47829900
H	-2.25688400	5.80053600	-0.52943200
C	-3.78989800	3.65355300	-0.26260600
C	-4.50281400	2.48483800	-0.24177300
C	-3.83421900	1.22779100	-0.16653800
H	-4.30896600	4.60606700	-0.33838100
H	-5.58811800	2.49151700	-0.29224600
C	-4.51166000	-0.00010400	-0.17536800
C	-3.83415900	-1.22796600	-0.16653400
C	-2.40482200	-1.20785100	-0.03705500
H	-5.59742900	-0.00013100	-0.23104500
C	-4.50269200	-2.48504700	-0.24176200

C	-1.63872800	-2.43162400	-0.11918700
C	-2.37122400	-3.66740400	-0.25053500
C	-0.20158400	-2.49234700	-0.24329200
C	-1.67516900	-4.88419900	-0.46216600
H	-2.25659900	-5.80063200	-0.52944400
C	2.56669300	2.49328300	-0.82555600
C	2.56681100	-2.49313600	-0.82559500
C	0.45507100	-3.72352400	-0.57888200
C	-0.31719800	-4.91961200	-0.63957400
H	0.19482500	-5.85635600	-0.84195700
C	1.83951700	-3.69217800	-0.80716900
H	2.35597200	-4.62271100	-1.02904800
C	3.95715600	-2.43070300	-1.13698800
H	4.48195600	-3.35847600	-1.34754000
C	1.87911700	1.28068000	-0.47827500
C	1.83934100	3.69229000	-0.80712000
H	2.35575100	4.62285100	-1.02898600
N	0.58537500	-1.38803800	-0.04785400
C	-3.78971900	-3.65372600	-0.26260000
H	-4.30874100	-4.60626600	-0.33836900
H	-5.58799700	-2.49177900	-0.29222800
N	-1.79996200	-0.00003700	0.17506500
C	-0.31743700	4.91961300	-0.63954400
H	0.19454200	5.85638200	-0.84192100
N	0.58531000	1.38808300	-0.04782100
C	3.95704200	2.43092200	-1.13694700
H	4.48179700	3.35872300	-1.34748400
C	2.54281900	0.00007200	-0.57803300
C	3.93813600	0.00010700	-0.95380400
C	4.61034900	1.22778600	-1.17992000
C	4.61040600	-1.22753600	-1.17994300
H	5.66656200	-1.19127300	-1.43629000
H	5.66650800	1.19157700	-1.43626600
O	1.85284100	0.00002000	2.57183400
C	3.02563800	0.00001100	2.64543600
O	4.18155200	-0.00005000	2.76897000
Ru	-0.09534000	-0.00000600	1.18414500

Ru-6

C	-4.91431900	1.21484400	-0.48246000
C	-4.21863700	-0.01180900	-0.32762500
C	-2.79580200	-0.00779100	-0.09513500
C	-2.12629600	1.27379000	-0.07307100
C	-2.84782300	2.48349800	-0.35108100
C	-2.11921300	-1.28559800	-0.07332500
C	2.18237000	1.21285000	-0.05777900

H	-5.99180300	1.17590300	-0.62409600
C	-4.90742200	-1.24233400	-0.48252800
C	-4.25036000	-2.44277300	-0.51028400
C	-2.83393400	-2.49944300	-0.35112000
H	-5.98512900	-1.20938400	-0.62403100
H	-4.79132000	-3.37274900	-0.66138100
C	-2.10377900	-3.69390000	-0.41499700
C	-0.70365200	-3.71879000	-0.32792400
C	-0.01982600	-2.48695200	-0.05534700
H	-2.63575300	-4.62668400	-0.58418800
C	0.06080500	-4.91296600	-0.47272900
C	1.42211400	-2.42478500	-0.07428500
C	2.13943700	-3.65745400	-0.28436300
C	2.18918500	-1.20058000	-0.05793700
C	3.54990400	-3.64119900	-0.43806100
H	4.05980000	-4.59204500	-0.57272200
C	-0.72455700	3.71481900	-0.32796800
C	3.59148500	1.23696700	-0.32906000
C	3.59839500	-1.21677700	-0.32918300
C	4.25847900	-2.47117400	-0.48159800
H	5.33245500	-2.47419300	-0.64590500
C	4.27035100	0.01199800	-0.39809700
H	5.34566400	0.01501000	-0.55772400
C	4.24444300	2.49508900	-0.48142800
H	5.31838400	2.50418100	-0.64572500
C	-0.03379500	2.48694500	-0.05500800
C	-2.12450900	3.68212000	-0.41501800
H	-2.66171900	4.61186600	-0.58433800
N	1.60471000	0.00446700	0.22478400
C	1.42868200	-4.87567300	-0.43271200
H	2.00252500	-5.79011600	-0.56187400
H	-0.46794900	-5.84971800	-0.62579500
N	-0.78692800	-1.38421900	0.21594100
C	-4.26390400	2.41887600	-0.51042200
H	-4.80999000	3.34578500	-0.66191100
N	-0.79460300	1.38007100	0.21683200
C	0.03315200	4.91324900	-0.47300700
H	-0.50093500	5.84692800	-0.62634600
C	1.40842300	2.43288700	-0.07400900
C	2.11879500	3.66956700	-0.28420300
C	1.40121500	4.88376600	-0.43274900
C	3.52931900	3.66112700	-0.43789000
H	4.03393500	4.61478700	-0.57260100
H	1.96992500	5.80139900	-0.56200400
Ru	-0.00493900	-0.00022200	1.40327100
H	-1.13509100	-0.00305200	2.87221500

H	-1.66031500	-0.00475500	2.24605400
---	-------------	-------------	------------

Ru-TS-1

C	2.23639400	-4.63636200	-0.61229200
C	2.73239300	-3.31222200	-0.46251700
C	1.82519300	-2.21698200	-0.26070200
C	0.41058500	-2.51417300	-0.25946000
C	-0.05424700	-3.84598600	-0.52240500
C	2.37564900	-0.88220900	-0.25013400
C	-2.27884200	0.84046600	-0.42854700
H	2.95694100	-5.44052200	-0.73789900
C	4.12454800	-3.07054500	-0.60963500
C	4.62778100	-1.80127300	-0.66104700
C	3.76855000	-0.67171500	-0.52270800
H	4.78335100	-3.92626300	-0.73343100
H	5.68740000	-1.62640800	-0.82583800
C	4.23902300	0.64515000	-0.61431500
C	3.36491700	1.73840300	-0.59914700
C	1.97619000	1.49171300	-0.33112100
H	5.30171000	0.81811600	-0.76328600
C	3.80613100	3.08086800	-0.80211200
C	1.01217000	2.56822300	-0.44253300
C	1.51082100	3.88808100	-0.70298300
C	-0.42132800	2.38233100	-0.46836100
C	0.60304300	4.96386700	-0.91042000
H	1.01776600	5.95706600	-1.06481000
C	-2.35049200	-3.00202000	-0.55567700
C	-3.19219000	1.90356300	-0.72823600
C	-1.30370300	3.46879500	-0.77857800
C	-0.74929400	4.77304100	-0.95438300
H	-1.42577300	5.60620000	-1.12401800
C	-2.67681600	3.20099000	-0.86398700
H	-3.36131000	4.02013600	-1.06915900
C	-4.58021700	1.59953500	-0.85896000
H	-5.27828500	2.41674800	-1.01852600
C	-1.84216200	-1.68302500	-0.30701400
C	-1.43628600	-4.06170600	-0.59648000
H	-1.80636700	-5.07441900	-0.73484300
N	-0.96957100	1.16171900	-0.20471100
C	2.90901200	4.11114100	-0.82654100
H	3.25191400	5.12912200	-0.99481600
H	4.86779600	3.25897700	-0.94862700
N	1.60448500	0.22029900	0.02679600
C	0.89694300	-4.89952300	-0.66217800
H	0.53113500	-5.90929500	-0.82644200

N	-0.51660600	-1.54592300	-0.00032000
C	-3.75618000	-3.18806600	-0.71741100
H	-4.13303500	-4.19758900	-0.85559200
C	-2.72344000	-0.53403100	-0.38959300
C	-4.11893000	-0.78148400	-0.60345900
C	-4.60132500	-2.11515800	-0.71284000
C	-5.01647200	0.30657800	-0.78800100
H	-6.07339300	0.08104700	-0.90644600
H	-5.67011800	-2.26204200	-0.84716800
O	0.47030700	0.65247300	4.18805200
C	-0.26912100	0.55736900	3.06403100
O	-1.49116300	0.39890600	3.09041000
H	1.40032300	0.78265000	3.93518500
H	0.27168400	1.47056300	2.12587300
Ru	-0.02892800	0.04114600	1.15564200

Ru- TS-Ia

C	2.79501100	4.40084600	-0.42157500
C	1.41359000	4.06815600	-0.38733900
C	1.00412000	2.70356800	-0.20261000
C	2.04543400	1.70831800	-0.07468300
C	3.42516800	2.06589800	-0.23046800
C	-0.40712200	2.41092500	-0.31504600
C	0.79049300	-2.41313100	-0.20692300
H	3.06483000	5.44701500	-0.54120500
C	0.44407700	5.07927700	-0.62778400
C	-0.88038900	4.78277600	-0.78346100
C	-1.34162100	3.43694700	-0.67621500
H	0.78979400	6.10480100	-0.72939200
H	-1.60540900	5.56109800	-1.00399300
C	-2.67787600	3.07533200	-0.89680300
C	-3.09241700	1.73707100	-0.89466900
C	-2.13949800	0.73279100	-0.52350500
H	-3.40149500	3.85131100	-1.13149600
C	-4.42230400	1.33704700	-1.22355700
C	-2.46942400	-0.67020100	-0.62534900
C	-3.80336700	-1.01038800	-1.01474700
C	-1.52194100	-1.75132200	-0.47921300
C	-4.16327500	-2.37188100	-1.21660100
H	-5.19493600	-2.59276300	-1.47786000
C	4.01588500	-0.30963900	-0.16259000
C	0.45027000	-3.77307700	-0.50687600
C	-1.88917800	-3.09907800	-0.79677100
C	-3.24808700	-3.38160900	-1.12761100
H	-3.53433600	-4.41403400	-1.30679900
C	-0.89503600	-4.08570100	-0.74501000

H	-1.16774400	-5.11911200	-0.94183000
C	1.48953700	-4.75099000	-0.54055100
H	1.21775900	-5.78915200	-0.70926400
C	2.62681600	-0.63045200	-0.01112400
C	4.38290900	1.04277600	-0.20005200
H	5.43631900	1.30304400	-0.25973900
N	-0.24135600	-1.52190800	-0.05604200
C	-4.75818800	0.01442300	-1.26357900
H	-5.77081200	-0.28339100	-1.52268300
H	-5.15553800	2.10799400	-1.44220600
N	-0.90802400	1.15220600	-0.08701700
C	3.76859200	3.44312500	-0.37188000
H	4.81886800	3.70938900	-0.45013400
N	1.75087600	0.40093000	0.21292300
C	4.96545500	-1.37185800	-0.23289400
H	6.01974600	-1.12008500	-0.30458300
C	2.17285700	-2.00312500	-0.08407800
C	3.17542600	-3.02486300	-0.19847800
C	4.55274600	-2.67459500	-0.22369700
C	2.79481400	-4.38341800	-0.37782900
H	3.58196000	-5.13169200	-0.42373000
H	5.28219300	-3.47792500	-0.28852600
Ru	0.05944500	-0.01228600	1.15467100
O	-3.80446900	0.03236000	3.04322500
C	-2.62652500	0.26782900	2.90698600
O	-1.74644600	-0.60282900	2.41653300
H	-2.18098100	1.24355900	3.19839200
H	-0.48065900	-0.12494700	2.78191300

Ru-TS-2

C	2.95740900	-4.19704700	-0.56274000
C	3.24392400	-2.80524900	-0.38640200
C	2.19469700	-1.86784400	-0.21225200
C	0.82574500	-2.36693700	-0.25019400
C	0.57690100	-3.74205100	-0.57045700
C	2.56610400	-0.45568400	-0.19006300
C	-2.31535000	0.56426500	-0.41733100
H	3.79371900	-4.88546400	-0.65085000
C	4.60918400	-2.37330300	-0.45885500
C	4.94952500	-1.05533400	-0.47047900
C	3.93056800	-0.05533900	-0.38516200
H	5.37774800	-3.13712200	-0.54375000
H	5.98696100	-0.74423700	-0.55929100
C	4.19765800	1.31512300	-0.46967700
C	3.16522300	2.26260400	-0.45780700
C	1.82576400	1.79258000	-0.25807100

H	5.22588000	1.65158700	-0.58143100
C	3.40141800	3.66231000	-0.62090600
C	0.69719900	2.71473900	-0.32978200
C	0.99592500	4.08048400	-0.56900600
C	-0.70821800	2.31531000	-0.36035200
C	-0.04848300	5.03288200	-0.79972400
H	0.22935200	6.07396200	-0.93942000
C	-1.80128900	-3.24129000	-0.71014500
C	-3.35172100	1.47712900	-0.80033000
C	-1.70922800	3.27333900	-0.73293000
C	-1.34764800	4.64560200	-0.90713800
H	-2.12979500	5.36399100	-1.13703000
C	-3.02798700	2.83297100	-0.88582500
H	-3.80815900	3.55605400	-1.11082100
C	-4.67070200	0.98239200	-1.04734200
H	-5.46188800	1.69271900	-1.27060000
C	-1.51158300	-1.88005000	-0.37621300
C	-0.74619600	-4.16047500	-0.73691500
H	-0.95556700	-5.20932500	-0.93043400
N	-1.10274300	1.04895400	-0.05722300
C	2.35370300	4.53058600	-0.66000400
H	2.52772800	5.59378000	-0.80192400
H	4.42424400	4.01409600	-0.72703500
N	1.61724100	0.48248300	-0.01844900
C	1.67959700	-4.64829100	-0.67803200
H	1.47061800	-5.69917100	-0.85898400
N	-0.24333700	-1.55544600	0.01482300
C	-3.15368800	-3.62575600	-0.96978500
H	-3.36760800	-4.67346500	-1.16284500
C	-2.55650600	-0.87235400	-0.45321500
C	-3.86347100	-1.30397500	-0.79068700
C	-4.14447200	-2.69307700	-0.98667200
C	-4.91277400	-0.35557700	-1.01969800
H	-5.90962800	-0.73783400	-1.22179900
H	-5.17037300	-2.98368200	-1.19576300
O	-0.35440200	0.71826900	3.41099600
C	-1.35442700	0.02067700	2.76300000
O	-2.50056900	-0.10437600	3.11760400
H	0.55735400	-0.17759300	3.12569000
H	0.96870700	-0.92539100	2.54685200
Ru	-0.01132800	-0.05309400	1.29053900

Ru-TS-IIa

C	2.96945400	4.25407800	-0.49868200
---	------------	------------	-------------

C	1.57178200	3.98926600	-0.46047800
C	1.09369000	2.65359200	-0.25471100
C	2.08230400	1.60410500	-0.12444200
C	3.47766800	1.89349000	-0.28266000
C	-0.33128400	2.42954000	-0.35875700
C	0.61806500	-2.44049500	-0.29577500
H	3.29042400	5.28427000	-0.62954300
C	0.65723000	5.04778300	-0.71871600
C	-0.67940600	4.81575500	-0.87319000
C	-1.20944600	3.49802700	-0.73776700
H	1.05626500	6.05157500	-0.83922400
H	-1.36293200	5.62458100	-1.11592200
C	-2.56584900	3.20932400	-0.93810200
C	-3.04960100	1.89670100	-0.90901100
C	-2.14508700	0.84831900	-0.53257700
H	-3.24938800	4.02057400	-1.17438800
C	-4.40575500	1.56690100	-1.21227400
C	-2.55405100	-0.53933600	-0.62912900
C	-3.90769700	-0.80856600	-1.00478000
C	-1.65248000	-1.66867200	-0.53623900
C	-4.33918400	-2.14999200	-1.21029500
H	-5.38606400	-2.31602000	-1.45197400
C	3.94653400	-0.50408200	-0.19928400
C	0.21414000	-3.78103900	-0.60435900
C	-2.09431500	-2.99418000	-0.85721300
C	-3.47583500	-3.20664900	-1.14974400
H	-3.81988000	-4.22143600	-1.32899100
C	-1.14650000	-4.02539300	-0.84196500
H	-1.46981900	-5.04218300	-1.04995400
C	1.20332800	-4.80911700	-0.63507400
H	0.88348200	-5.83235500	-0.81162800
C	2.54014600	-0.74927600	-0.05840900
C	4.38365400	0.82508500	-0.24340300
H	5.44923600	1.03118100	-0.30277100
N	-0.35680800	-1.49396400	-0.15708900
C	-4.81347300	0.26425900	-1.23698800
H	-5.84359100	0.01952300	-1.48344200
H	-5.09655800	2.37491900	-1.43568300
N	-0.89504200	1.20586500	-0.10095800
C	3.89267800	3.24961800	-0.43536400
H	4.95565500	3.46144000	-0.51008200
N	1.71429800	0.31963700	0.15881400
C	4.84357600	-1.61385500	-0.25623900
H	5.91046200	-1.41548800	-0.30836100
C	2.01942600	-2.10188000	-0.14592500
C	2.96827300	-3.17014700	-0.25451100

C	4.36507500	-2.89219400	-0.25554700
C	2.52326200	-4.50742700	-0.45203000
H	3.27308800	-5.29340300	-0.49367700
H	5.05244100	-3.73258700	-0.31054600
O	-2.82124200	0.27340000	4.24364800
C	-1.98708800	0.08394400	3.41399300
O	-1.76433000	-0.46063500	2.31522000
H	-0.57413100	0.74345800	3.54672400
H	0.12893100	0.70298300	2.98230900
Ru	0.00387300	-0.02701900	1.12906200

Os-1

C	-0.11937600	5.07190500	-0.60295300
C	-1.11918600	4.07638500	-0.44204200
C	-0.74331100	2.70742000	-0.19607600
C	0.67555200	2.41564500	-0.14933900
C	1.65278000	3.42248500	-0.43707700
C	-1.81431200	1.73210100	-0.14947900
C	1.75436800	-1.79278400	-0.14965900
H	-0.44407100	6.09788100	-0.75825800
C	-2.48718100	4.42178100	-0.60271400
C	-3.47868600	3.47910100	-0.61894400
C	-3.16875000	2.09877300	-0.43680800
H	-2.73189000	5.46973000	-0.75794800
H	-4.51553900	3.76125300	-0.77849300
C	-4.13186400	1.07985900	-0.50912300
C	-3.79046700	-0.28002100	-0.43659700
C	-2.42975000	-0.62284800	-0.14931700
H	-5.16817300	1.35081200	-0.69294400
C	-4.73618900	-1.33222400	-0.61812200
C	-1.97280900	-1.99749100	-0.19559700
C	-2.97066000	-3.00758100	-0.44043500
C	-0.59257500	-2.43718100	-0.14991400
C	-2.58571500	-4.36497200	-0.60160000
H	-3.37094300	-5.10101900	-0.75597400
C	3.40215100	1.69482100	-0.43642200
C	2.13767800	-3.14235400	-0.43818100
C	-0.23308400	-3.79330000	-0.43829800
C	-1.27351100	-4.75195600	-0.61984000
H	-0.99928900	-5.79087300	-0.77975000
C	1.13081100	-4.11796100	-0.51138400
H	1.41439000	-5.15078800	-0.69573900
C	3.52177500	-3.43540700	-0.61929500
H	3.81654900	-4.46873000	-0.77889400
C	2.40731400	0.70534800	-0.14880300

C	3.00124400	3.03835600	-0.50929000
H	3.75386400	3.80048600	-0.69327200
N	0.43221500	-1.57365900	0.17400700
C	-4.33276500	-2.63948700	-0.60111800
H	-5.05888100	-3.43377700	-0.75612500
H	-5.77847600	-1.07090700	-0.77763100
N	-1.57869300	0.41272700	0.17360100
C	1.21445400	4.76757500	-0.61925500
H	1.96196300	5.53950300	-0.77885300
N	1.14683100	1.16116700	0.17450600
C	4.75252900	1.27301000	-0.61839600
H	5.51514100	2.02995500	-0.77827000
C	2.71647200	-0.70988700	-0.19522100
C	4.09018700	-1.06894000	-0.44023700
C	5.07331600	-0.05694400	-0.60121700
C	4.45235700	-2.43260300	-0.60121500
H	5.50331400	-2.66449100	-0.75576500
H	6.10320800	-0.36909500	-0.75631000
Os	-0.00026800	-0.00007000	1.22820000

Os-2

C	4.00780200	-2.84487100	-1.17510900
C	3.79068400	-1.44847700	-0.99106300
C	2.49358400	-0.96437400	-0.64305900
C	1.42226600	-1.93045500	-0.53356800
C	1.65110200	-3.30883100	-0.84276700
C	2.30687600	0.46807300	-0.57447100
C	-2.59522600	-0.35309300	-0.26306000
H	5.01775800	-3.17913500	-1.39891400
C	4.86053100	-0.53407400	-1.21088400
C	4.66698300	0.81574700	-1.19146400
C	3.37300800	1.35843300	-0.91946200
H	5.84345400	-0.94203800	-1.43271200
H	5.48522800	1.50267400	-1.38830700
C	3.10892800	2.73289000	-0.94726000
C	1.80889400	3.22902900	-0.78651100
C	0.75703200	2.31530900	-0.45446500
H	3.91871600	3.42609200	-1.15831000
C	1.50289500	4.61734800	-0.92742000
C	-0.61776500	2.76371100	-0.40967500
C	-0.86782400	4.15312800	-0.63744600
C	-1.77083800	1.88673300	-0.31643100
C	-2.20350300	4.64028300	-0.73992100
H	-2.34612300	5.70835200	-0.88302400
C	-0.74918800	-3.71208100	-0.65402000
C	-3.93362300	0.10647100	-0.49349600

C	-3.09069500	2.39533500	-0.55034100
C	-3.27749600	3.80059600	-0.72275400
H	-4.28765800	4.17896600	-0.85218800
C	-4.15469900	1.48649600	-0.56496700
H	-5.16981100	1.85739400	-0.68107000
C	-4.99014800	-0.84759700	-0.60642400
H	-6.00686200	-0.48544800	-0.73083400
C	-0.94953900	-2.32481500	-0.35960600
C	0.55808900	-4.18190100	-0.83121900
H	0.72067800	-5.24047200	-1.01553700
N	-1.61759700	0.56577100	-0.00492000
C	0.21494600	5.05560200	-0.84103700
H	-0.01486000	6.11039300	-0.96792900
H	2.31864300	5.30912700	-1.11822600
N	1.10155700	1.00459600	-0.17350900
C	2.98452700	-3.74427900	-1.11920600
H	3.15867800	-4.80321600	-1.28814900
N	0.16577100	-1.54192200	-0.13175400
C	-1.88462100	-4.57414900	-0.74299000
H	-1.71620100	-5.63539600	-0.90358400
C	-2.28685100	-1.77159700	-0.30676500
C	-3.38188700	-2.67406300	-0.48110900
C	-3.14698900	-4.06970100	-0.64343500
C	-4.71680400	-2.18279900	-0.57546700
H	-5.52014600	-2.90834800	-0.67458400
H	-4.00848300	-4.72689000	-0.72970800
O	2.47629000	0.32292100	2.97594400
C	1.39593300	-0.47848700	2.62275600
O	0.11759900	-0.01124100	3.03239200
H	2.41863600	1.14876500	2.47009000
H	1.59780700	-1.48876100	2.98291500
Os	0.03385500	-0.02370900	1.13788700

Os-2a

C	2.57419500	4.49090900	-0.62329300
C	1.20776600	4.09846300	-0.60194000
C	0.85331100	2.72378100	-0.38319800
C	1.93720900	1.77628300	-0.22160200
C	3.29978400	2.18997000	-0.37605100
C	-0.54606900	2.37470400	-0.50004200
C	0.85750700	-2.39868000	-0.33854000
H	2.79972900	5.54532400	-0.76156100
C	0.20141700	5.06171000	-0.88408100
C	-1.10772000	4.70784300	-1.04919400
C	-1.51559200	3.34820000	-0.90534000
H	0.50718400	6.09718600	-1.01060900

H	-1.86044500	5.44952400	-1.30109100
C	-2.83541500	2.92783400	-1.12273900
C	-3.19864800	1.57628700	-1.07230000
C	-2.21040200	0.62191600	-0.66377900
H	-3.58631000	3.66661400	-1.38981900
C	-4.51378500	1.11487100	-1.38358800
C	-2.48101800	-0.80008500	-0.72904500
C	-3.80067700	-1.20163400	-1.12099500
C	-1.48559200	-1.84247800	-0.58507300
C	-4.10201800	-2.57945700	-1.30677400
H	-5.12422200	-2.84647800	-1.56361200
C	3.98981100	-0.15449300	-0.28986700
C	0.57815600	-3.76811700	-0.65227500
C	-1.79351800	-3.20449200	-0.90550500
C	-3.14389700	-3.54879900	-1.21847500
H	-3.38577000	-4.59347100	-1.39239500
C	-0.75535900	-4.14365700	-0.87344600
H	-0.98133500	-5.18722500	-1.07621700
C	1.65944100	-4.69680900	-0.70600100
H	1.43381800	-5.74397200	-0.88717600
C	2.61670700	-0.53424500	-0.14009700
C	4.30122200	1.21057900	-0.33156500
H	5.34261300	1.51483700	-0.39459700
N	-0.21565800	-1.55705800	-0.14967300
C	-4.79545200	-0.22171200	-1.38932200
H	-5.79467600	-0.56629200	-1.64405400
H	-5.27700000	1.84968400	-1.62344600
N	-1.00041200	1.10393700	-0.22293900
C	3.58690500	3.57845200	-0.53684300
H	4.62630500	3.88840800	-0.59843700
N	1.69223700	0.45906200	0.09420400
C	4.98579300	-1.17498800	-0.35863400
H	6.02890600	-0.87698600	-0.41613000
C	2.22093200	-1.92602700	-0.22085400
C	3.26712100	-2.90203000	-0.34565400
C	4.62938600	-2.49315200	-0.36199900
C	2.94809700	-4.27304400	-0.54043900
H	3.76797800	-4.98459600	-0.59798700
H	5.39234700	-3.26473800	-0.42822200
O	-3.12401700	0.33115600	3.91005000
C	-2.22140300	0.06401300	3.19362500
O	-1.77455000	-0.49179900	2.19853100
H	-0.60187800	0.90256000	3.50348100
H	0.02425300	0.66659900	2.97435900
Os	0.01703600	-0.00374900	1.03891100

Os-3

C	-0.99197700	5.01588500	-0.73918900
C	-1.81608000	3.86754500	-0.52505900
C	-1.23902800	2.57890900	-0.33781600
C	0.21855300	2.48825300	-0.41213900
C	0.99496500	3.63669600	-0.77719600
C	-2.15367300	1.44504200	-0.27987300
C	1.84669500	-1.46884300	-0.50546000
H	-1.48060700	5.98183000	-0.83629400
C	-3.23541300	4.02826400	-0.58891600
C	-4.07799200	2.95912400	-0.59026400
C	-3.55950200	1.63075600	-0.48715400
H	-3.62950200	5.03666900	-0.68453700
H	-5.15256000	3.09295000	-0.68087300
C	-4.37875400	0.49853500	-0.56908800
C	-3.83787000	-0.79355200	-0.54940500
C	-2.43455000	-0.93295600	-0.31409000
H	-5.45085900	0.62603500	-0.69480300
C	-4.63203600	-1.96964200	-0.71953200
C	-1.79020200	-2.23329100	-0.38054500
C	-2.62526800	-3.35723600	-0.63014500
C	-0.35220500	-2.44863500	-0.38765000
C	-2.05850700	-4.65321700	-0.83323700
H	-2.73517700	-5.49226500	-0.97256200
C	2.95713600	2.19898400	-0.94945800
C	2.39991500	-2.74105900	-0.86276400
C	0.17932000	-3.72682300	-0.74677900
C	-0.71262800	-4.83376400	-0.91210300
H	-0.28745700	-5.81291800	-1.11375200
C	1.56183700	-3.85914600	-0.90005900
H	1.98567900	-4.83680400	-1.11235200
C	3.79528600	-2.83975100	-1.15612300
H	4.21005000	-3.82218600	-1.36326100
C	2.13995100	1.08892500	-0.55890600
C	2.36862300	3.46655100	-0.98372500
H	2.98302400	4.33361100	-1.21326600
N	0.53729000	-1.44298300	-0.06556700
C	-4.04084000	-3.19687200	-0.74542600
H	-4.64255700	-4.09050800	-0.89005100
H	-5.70733700	-1.86263000	-0.83297800
N	-1.69549200	0.17827400	-0.03160100
C	0.35696500	4.91054400	-0.88888800
H	0.96789500	5.78246400	-1.10570000
N	0.86491600	1.31631700	-0.15671900
C	4.33655200	1.98091700	-1.25070500
H	4.96179700	2.83631900	-1.49078500

C	2.65890900	-0.26916900	-0.61060000
C	4.01725700	-0.42496500	-0.99508100
C	4.83977600	0.71643300	-1.25262100
C	4.57237000	-1.72428700	-1.19947700
H	5.62932600	-1.79850100	-1.44064800
H	5.88451300	0.54314900	-1.49681100
O	1.03437000	-0.07958300	3.96483700
C	1.37680100	-0.12011400	2.63291700
O	2.56863700	-0.16067200	2.35796900
H	0.07845200	-0.26079400	3.99457700
H	-0.87086500	-1.10005800	2.15864600
Os	-0.04764700	-0.04084000	1.14486300

Os-3a

C	1.30523100	-4.84852600	-0.97248400
C	2.02407500	-3.62087100	-0.86058300
C	1.34184000	-2.40468000	-0.56963900
C	-0.10793000	-2.45280000	-0.46043400
C	-0.80299800	-3.67906500	-0.71263000
C	2.14107000	-1.18625200	-0.59431400
C	-2.21060400	1.27506100	-0.37536700
H	1.87018300	-5.76015300	-1.14752000
C	3.42944000	-3.62765300	-1.12489800
C	4.15038700	-2.47662400	-1.22060500
C	3.51423700	-1.21616400	-1.00326100
H	3.90655300	-4.58820900	-1.30051800
H	5.20690100	-2.49376700	-1.47297800
C	4.18485500	0.00435600	-1.13911800
C	3.51183600	1.22353500	-1.00285600
C	2.13872500	1.19075500	-0.59392800
H	5.24240900	0.00542000	-1.39097500
C	4.14555400	2.48527600	-1.21978600
C	1.33711300	2.40763700	-0.56900400
C	2.01700900	3.62524800	-0.85950000
C	-0.11271700	2.45289700	-0.45986700
C	1.29576200	4.85152800	-0.97099400
H	1.85894600	5.76431800	-1.14568300
C	-2.92425800	-2.48626100	-0.64772300
C	-2.92910300	2.48089700	-0.64717800
C	-0.81019300	3.67785700	-0.71166400
C	-0.06346700	4.87914300	-0.91907700
H	-0.61029400	5.80898300	-1.04858100
C	-2.20988600	3.67514200	-0.73724600
H	-2.74108000	4.61129400	-0.88542300
C	-4.35235600	2.42506300	-0.78250900
H	-4.89610800	3.35546200	-0.91972900

C	-2.20807400	-1.27911800	-0.37555400
C	-2.20268500	-3.67907200	-0.73819900
H	-2.73205900	-4.61619800	-0.88674700
N	-0.86543300	1.34501500	-0.09798600
C	3.42235900	3.63486900	-1.12375100
H	3.89759700	4.59640900	-1.29907800
H	5.20203500	2.50452000	-1.47213700
N	1.58353800	0.00162400	-0.25314800
C	-0.05393700	-4.87881700	-0.92052300
H	-0.59895800	-5.80966300	-1.05040800
N	-0.86277900	-1.34656600	-0.09834100
C	-4.34762100	-2.43324800	-0.78305300
H	-4.88947900	-3.36471600	-0.92051900
C	-2.88920800	-0.00269900	-0.39241200
C	-4.29459200	-0.00408100	-0.60954700
C	-4.99946700	-1.23800700	-0.74927700
C	-5.00184000	1.22853100	-0.74902000
H	-6.08167300	1.18759300	-0.86673500
H	-6.07937600	-1.19911500	-0.86696000
O	1.36724100	-0.00454500	4.94298700
C	0.60358500	-0.00046000	4.00997300
O	1.01059100	0.00094200	2.72455600
H	-0.49611400	0.00261200	4.11194300
H	-1.38051000	-0.00086300	2.05934200
Os	-0.03870700	0.00005300	1.07664300

Os-4a

C	-1.53522400	4.85293400	-0.90829300
C	-2.22511100	3.62981600	-0.63737700
C	-1.50623900	2.42925400	-0.38486700
C	-0.05445200	2.50084900	-0.47101000
C	0.59460800	3.71072100	-0.87353000
C	-2.27533600	1.20215000	-0.25140800
C	2.00234700	-1.29926300	-0.59067400
H	-2.13093800	5.75122400	-1.04884200
C	-3.65348600	3.62649500	-0.69572500
C	-4.36071000	2.46690800	-0.63625700
C	-3.68912100	1.21466900	-0.46935900
H	-4.16256800	4.57587800	-0.84010800
H	-5.44312800	2.46334700	-0.73094000
C	-4.38099000	0.00023300	-0.49195300
C	-3.68926600	-1.21427400	-0.46944600
C	-2.27547200	-1.20191200	-0.25147900
H	-5.46246100	0.00030600	-0.59645200
C	-4.36097600	-2.46644300	-0.63640800
C	-1.50650500	-2.42910000	-0.38495100

C	-2.22549500	-3.62957400	-0.63750800
C	-0.05472500	-2.50081500	-0.47106500
C	-1.53572000	-4.85275400	-0.90842300
H	-2.13151300	-5.75098700	-1.04900700
C	2.70184500	2.49098000	-0.97473700
C	2.70158100	-2.49120700	-0.97473400
C	0.59423500	-3.71075300	-0.87357200
C	-0.18185100	-4.89905200	-1.04115700
H	0.32828000	-5.82723600	-1.28408700
C	1.98271600	-3.68792700	-1.05130600
H	2.50485900	-4.60913200	-1.29747000
C	4.10478200	-2.42650900	-1.24362700
H	4.63635300	-3.34823000	-1.46437800
C	2.00249800	1.29910700	-0.59065200
C	1.98309300	3.68775900	-1.05129700
H	2.50530700	4.60892100	-1.29747600
N	0.70419100	-1.40701800	-0.17904800
C	-3.65386900	-3.62609900	-0.69589700
H	-4.16304800	-4.57542500	-0.84031300
H	-5.44339200	-2.46277100	-0.73110700
N	-1.67993300	0.00005600	0.08844900
C	-0.18135500	4.89910000	-1.04108100
H	0.32886200	5.82723500	-1.28401800
N	0.70438200	1.40698900	-0.17900600
C	4.10503900	2.42612400	-1.24364600
H	4.63671700	3.34777800	-1.46442000
C	2.66880500	-0.00012100	-0.65971200
C	4.04590400	-0.00019500	-1.01524400
C	4.74696700	1.22704100	-1.23854100
C	4.74684400	-1.22749600	-1.23853600
H	5.80983300	-1.17322600	-1.45919000
H	5.80995000	1.17265900	-1.45919700
O	1.91006100	0.00028400	2.46003100
C	1.55969900	-0.00020600	3.59015600
O	1.31996800	-0.00070400	4.72583300
H	-0.59376500	1.10801700	2.27694900
H	-0.59376000	-1.10822200	2.27672700
Os	-0.04666700	0.00000500	1.12859900

Os-5a

C	-4.88611200	1.23269200	-0.75321600
C	-4.18911000	-0.00000500	-0.57720400
C	-2.79668000	-0.00000300	-0.27687900
C	-2.12586900	1.28249700	-0.21118000
C	-2.82671500	2.48932400	-0.52179700
C	-2.12586600	-1.28250200	-0.21118100

C	2.22492800	1.18983200	-0.18940000
H	-5.95737400	1.19130600	-0.93382200
C	-4.88610900	-1.23270400	-0.75321700
C	-4.23924200	-2.43185400	-0.74026100
C	-2.82670800	-2.48933100	-0.52179800
H	-5.95737100	-1.19132000	-0.93382300
H	-4.77724700	-3.36192100	-0.90068800
C	-2.10169100	-3.68435700	-0.56777500
C	-0.70493700	-3.69166100	-0.46174200
C	-0.02149400	-2.46649700	-0.17378600
H	-2.62469100	-4.61968400	-0.74746200
C	0.05540700	-4.88992100	-0.62793700
C	1.42923800	-2.41032100	-0.20916200
C	2.12799200	-3.62905300	-0.46156700
C	2.22493100	-1.18982600	-0.18940000
C	3.54310400	-3.63267400	-0.65474400
H	4.03098100	-4.59180400	-0.80815700
C	-0.70494600	3.69165900	-0.46174200
C	3.61803700	1.21967600	-0.52671300
C	3.61804000	-1.21966700	-0.52671300
C	4.26507900	-2.47900200	-0.71359200
H	5.33301400	-2.49351300	-0.91289600
C	4.29760800	0.00000500	-0.62190100
H	5.36718600	0.00000600	-0.81640500
C	4.26507300	2.47901200	-0.71359300
H	5.33300800	2.49352600	-0.91289700
C	-0.02150000	2.46649700	-0.17378600
C	-2.10170000	3.68435200	-0.56777400
H	-2.62470200	4.61967800	-0.74746000
N	1.65287900	0.00000200	0.13661200
C	1.41644600	-4.85608300	-0.60911500
H	1.99102300	-5.76715500	-0.75415100
H	-0.47962100	-5.82252100	-0.78451900
N	-0.79822600	-1.36294100	0.14254900
C	-4.23924800	2.43184400	-0.74026000
H	-4.77725500	3.36190900	-0.90068700
N	-0.79823000	1.36293900	0.14255000
C	0.05539500	4.88992100	-0.62793700
H	-0.47963500	5.82251900	-0.78452000
C	1.42923200	2.41032400	-0.20916200
C	2.12798300	3.62905800	-0.46156800
C	1.41643400	4.85608600	-0.60911600
C	3.54309500	3.63268300	-0.65474500
H	4.03097000	4.59181400	-0.80815900
H	1.99100900	5.76716000	-0.75415300
Os	-0.06401500	0.00000000	1.34605500

H	-1.48697500	-0.00000300	2.19153700
H	0.39727100	0.00000600	2.97585000

Os-TS-1

C	2.34167300	-4.56162900	-0.78205400
C	2.82022800	-3.23428800	-0.62253400
C	1.89614400	-2.15497400	-0.40095700
C	0.48933700	-2.47370500	-0.38805800
C	0.03839300	-3.80544100	-0.66361500
C	2.43151900	-0.81521300	-0.36080100
C	-2.26750100	0.84935600	-0.53656800
H	3.07138700	-5.35561800	-0.91942500
C	4.20756800	-2.96597800	-0.76625500
C	4.69512700	-1.68940300	-0.78561200
C	3.81984700	-0.57518600	-0.62036700
H	4.87904400	-3.80928300	-0.90718400
H	5.75359100	-1.49714200	-0.93719300
C	4.26873300	0.75143000	-0.66424000
C	3.37693500	1.83069900	-0.61143100
C	1.99168000	1.55667700	-0.36615900
H	5.32861900	0.94729500	-0.80350200
C	3.79981600	3.18562300	-0.76280000
C	1.00910700	2.61994500	-0.44714400
C	1.49153400	3.95508300	-0.66832600
C	-0.42361800	2.42328500	-0.48860600
C	0.57259700	5.02217700	-0.86964100
H	0.97644900	6.02396300	-0.99412300
C	-2.27044800	-2.99427800	-0.71482000
C	-3.17717000	1.90133900	-0.87587500
C	-1.31303300	3.49698000	-0.81607500
C	-0.77428400	4.81241300	-0.95648700
H	-1.45880600	5.63643700	-1.13707400
C	-2.67691900	3.20973500	-0.95881500
H	-3.36511300	4.02229100	-1.17667600
C	-4.55077600	1.57905900	-1.08342900
H	-5.25099700	2.38740600	-1.27413600
C	-1.79552400	-1.67042600	-0.44481100
C	-1.34074600	-4.04060100	-0.74978800
H	-1.69368700	-5.05576600	-0.91037700
N	-0.97829100	1.19637400	-0.22165200
C	2.88697000	4.20218200	-0.76721700
H	3.21569400	5.22996300	-0.90031700
H	4.86036400	3.38479700	-0.88832500
N	1.63210800	0.26224500	-0.05210700
C	1.00486000	-4.84283700	-0.81894000
H	0.65118000	-5.85714900	-0.98099400

N	-0.46675400	-1.52151900	-0.10193200
C	-3.66915900	-3.19844700	-0.91786400
H	-4.02813900	-4.21405800	-1.05824900
C	-2.68536200	-0.53456500	-0.54580700
C	-4.06820300	-0.79746100	-0.82193600
C	-4.52732300	-2.13724300	-0.95004700
C	-4.97007500	0.27869100	-1.04064800
H	-6.01656800	0.03875700	-1.21184300
H	-5.58864100	-2.29897000	-1.12155900
O	-0.07864700	-0.01169900	4.17686300
C	-0.52191600	0.35858100	2.93669100
O	-1.71110400	0.06919600	2.56237000
H	0.84951200	0.26230200	4.26824600
H	-0.09718800	1.43951700	2.62061200
Os	-0.02287100	0.01902700	1.03992500

Os-TS-1a

C	-4.75842900	-0.21591400	-1.36953300
C	-3.76126600	-1.19463600	-1.10207700
C	-2.44623200	-0.79338800	-0.70145000
C	-2.18574300	0.62735200	-0.61617600
C	-3.17510800	1.58347500	-1.01305800
C	-1.45692400	-1.83770300	-0.53882000
C	1.96603300	1.79400200	-0.17671600
H	-5.75434600	-0.56273700	-1.63262300
C	-4.06175300	-2.57146000	-1.29712700
C	-3.10498900	-3.54054400	-1.20184400
C	-1.76055400	-3.19773000	-0.86708800
H	-5.08149600	-2.83670100	-1.56407400
H	-3.34403500	-4.58441600	-1.38362100
C	-0.72299000	-4.13880900	-0.82966200
C	0.61049500	-3.76546700	-0.61047600
C	0.89097600	-2.39792100	-0.29119200
H	-0.95003800	-5.18142800	-1.03530500
C	1.69337800	-4.69259900	-0.67845900
C	2.25553600	-1.91932300	-0.19426400
C	3.30247000	-2.89461300	-0.33506400
C	2.65468600	-0.53164700	-0.10880600
C	4.66198600	-2.48249300	-0.36283000
H	5.42575100	-3.25193100	-0.44286200
C	-1.49827900	3.36281300	-0.82576900
C	3.32846300	2.20591100	-0.32867700
C	4.02375400	-0.14391900	-0.26161500
C	5.01827800	-1.16313400	-0.34848400
H	6.06095000	-0.86517800	-0.41240300

C	4.33041800	1.22478100	-0.29384600
H	5.37081700	1.53085100	-0.36082900
C	3.61016900	3.59608600	-0.48323600
H	4.64821200	3.91011000	-0.54579600
C	-0.52418800	2.38764100	-0.43607800
C	-2.81695300	2.93821100	-1.04328500
H	-3.57139200	3.67644400	-1.30132000
N	1.73211400	0.46818600	0.13564200
C	2.98232400	-4.26582400	-0.52900100
H	3.80288800	-4.97557100	-0.59759600
H	1.46747300	-5.73944000	-0.86017100
N	-0.18650500	-1.56154700	-0.08852700
C	-4.48394400	1.12090100	-1.34458500
H	-5.24970400	1.85495600	-1.57801300
N	-0.97636400	1.11273000	-0.16819600
C	-1.09297700	4.72442700	-0.95986400
H	-1.84854600	5.46836000	-1.19560900
C	0.87837100	2.73472300	-0.33133200
C	1.22883700	4.11399700	-0.53910400
C	0.21791200	5.07690300	-0.80416600
C	2.59419400	4.50671100	-0.56281400
H	2.81820700	5.56227400	-0.69480400
H	0.52114800	6.11407600	-0.92287300
O	-3.88222900	0.09004300	2.77050800
C	-2.69202800	0.27353800	2.76707000
O	-1.79912000	-0.64565000	2.35602900
H	-2.22375200	1.21516300	3.11869400
H	-0.67949800	-0.26736300	2.69708500
Os	0.07655100	0.00125900	1.05610500

Os-TS-2

C	3.03083100	-4.06088300	-0.90402400
C	3.28772700	-2.67576000	-0.70166400
C	2.20498700	-1.77221400	-0.45303700
C	0.86419200	-2.31901300	-0.46465400
C	0.63639500	-3.69481200	-0.78999700
C	2.51900600	-0.36465300	-0.35668900
C	-2.40033900	0.52460200	-0.46660000
H	3.88230500	-4.72113500	-1.04872600
C	4.61776600	-2.18188200	-0.80893600
C	4.89569000	-0.84571500	-0.77703900
C	3.84808900	0.10880800	-0.59892600
H	5.41833600	-2.90174600	-0.95977400
H	5.91242300	-0.48207400	-0.89523500
C	4.06647100	1.49153000	-0.62414100
C	3.00401700	2.40544600	-0.56346100

C	1.68242500	1.90990300	-0.32735400
H	5.07766400	1.86609100	-0.75726300
C	3.19598800	3.81102800	-0.71519100
C	0.53940100	2.79091300	-0.38828800
C	0.79388400	4.18716400	-0.61095800
C	-0.84543100	2.36197900	-0.40287000
C	-0.28424800	5.09194800	-0.81200200
H	-0.04770900	6.14383200	-0.94986800
C	-1.77251700	-3.25978300	-0.81266900
C	-3.47378300	1.41662800	-0.78825400
C	-1.89328100	3.28171800	-0.73105000
C	-1.57794500	4.66308000	-0.89423500
H	-2.38715700	5.35905800	-1.09598600
C	-3.19973100	2.78713000	-0.84742100
H	-4.01305200	3.48264500	-1.03651500
C	-4.77924200	0.87884300	-1.00357400
H	-5.59926200	1.56640600	-1.18975200
C	-1.51805800	-1.88620400	-0.49926400
C	-0.68594600	-4.14071700	-0.89830300
H	-0.87447300	-5.19167900	-1.10024100
N	-1.19346700	1.06694000	-0.10785100
C	2.12890700	4.66266900	-0.71964800
H	2.28194000	5.73039000	-0.85359100
H	4.20871300	4.18325400	-0.84155000
N	1.55000100	0.56257200	-0.03540400
C	1.76138100	-4.55885200	-0.95965400
H	1.58050500	-5.61541200	-1.13526200
N	-0.22504800	-1.53366000	-0.17547800
C	-3.12080300	-3.68446900	-1.00997400
H	-3.31066900	-4.74032700	-1.18054100
C	-2.58655200	-0.91074800	-0.52985600
C	-3.90593900	-1.38841000	-0.81004800
C	-4.14187800	-2.77938700	-0.99316100
C	-4.98036400	-0.46990200	-0.98772200
H	-5.97314800	-0.87611500	-1.16323200
H	-5.16482000	-3.10630900	-1.16076800
O	0.15036000	-0.45690800	3.95206100
C	-0.63300200	-0.17951600	2.98786600
O	-1.84227800	-0.30697200	2.76496200
H	1.02632800	-0.76975500	2.96427900
H	1.29550200	-0.97150200	2.03897500
Os	0.02148600	-0.00945200	1.05837900

Os-TS-2a

C	-1.24140600	4.96245000	-0.76870900
C	-2.02465300	3.80474200	-0.52920900

C	-1.38764000	2.52576600	-0.34273400
C	0.05356300	2.48576800	-0.44703300
C	0.79992300	3.65182800	-0.81719500
C	-2.24997700	1.36545200	-0.22892200
C	1.85027200	-1.45035800	-0.61491900
H	-1.75614600	5.91448200	-0.87324700
C	-3.44172100	3.89845300	-0.56669800
C	-4.24006700	2.78947200	-0.52767000
C	-3.66740700	1.48863300	-0.40221800
H	-3.88439000	4.88510700	-0.67999600
H	-5.32065400	2.87465500	-0.60147700
C	-4.43706000	0.31736700	-0.40897700
C	-3.85130600	-0.95543800	-0.37771600
C	-2.43110600	-1.04219700	-0.20418400
H	-5.51769600	0.39784700	-0.49546500
C	-4.61239300	-2.15823600	-0.47759700
C	-1.75225600	-2.32060400	-0.29087300
C	-2.57393600	-3.49352200	-0.45213500
C	-0.32145000	-2.49869000	-0.39079100
C	-1.97312100	-4.76015600	-0.66427200
H	-2.62448400	-5.62647200	-0.75059100
C	2.81829800	2.26816200	-1.01641500
C	2.44447600	-2.71076100	-0.95720500
C	0.24179100	-3.77134700	-0.73298900
C	-0.61967800	-4.90221900	-0.81856300
H	-0.17956900	-5.87510500	-1.01946100
C	1.62842000	-3.84967600	-0.94661700
H	2.07166300	-4.81690500	-1.16915000
C	3.84139100	-2.75398200	-1.25170400
H	4.29842100	-3.72036600	-1.44572000
C	2.04327700	1.11923200	-0.64597400
C	2.18174100	3.51642800	-1.03259600
H	2.76432200	4.40114200	-1.27635600
N	0.55457100	-1.46141700	-0.15917000
C	-3.98904800	-3.37478300	-0.49148800
H	-4.57449500	-4.28625700	-0.58494200
H	-5.69359800	-2.08214200	-0.55214800
N	-1.74295500	0.11932800	0.05341700
C	0.11730200	4.89712600	-0.92667700
H	0.69735200	5.78878800	-1.14805600
N	0.76499100	1.33440300	-0.19358000
C	4.20553400	2.09541900	-1.30930000
H	4.80161200	2.97773000	-1.52528800
C	2.60740700	-0.21634400	-0.72280500
C	4.00546500	-0.32566900	-1.08372900
C	4.76843300	0.84726900	-1.32002100

C	4.58448900	-1.60455700	-1.29074800
H	5.64362400	-1.65057300	-1.53357700
H	5.82215600	0.72896100	-1.56190000
O	1.51102700	0.25616600	4.29696400
C	2.31715300	0.04262100	3.44351200
O	1.96376900	-0.14048300	2.13111300
H	3.40661400	-0.03764400	3.58796700
H	2.72712200	-0.25539100	1.52551500
Os	-0.02216800	0.00242900	1.03244300