

Supporting Information

Mechanism and Stereoselectivity of Benzylic C–H Hydroxylation by Ru-Porphyrin: A Computational Study

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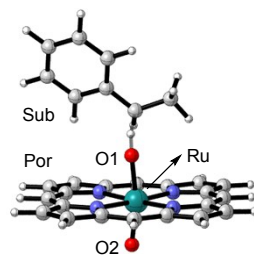
Table S1. The Calculated Free Energies of Benzylic C–H Hydroxylation by $^1\text{RuO}_2$ using Different Functionals^a

Functionals	$^1\text{TS1(OSS)}$	$^1\text{INT(OSS)}$	$^1\text{TS2(OSS)}$
UM06//UB3LYP	19.6	-0.3	0.2
UB97D// UB97D	15.2	8.4	9.4
UB3LYP-D3// UB3LYP-D3	15.6	0.9	3.0

^aIn method of DFT1//DFT2, the molecular geometries were optimized using the DFT2 functional and a mixed basis set of LANL2DZ for Ru and 6-31G(d) for other atoms in the gas-phase, single-point energies were computed at the DFT1/6-311+G(d,p)-SDD(SMD_{Dichloromethane}) level of the theory on the gas-phase optimized geometries. The energies are shown in kcal/mol.

OSS is open-shell singlet.

Table S2. The Spin Density (ζ) for the Reaction Species Calculated at the UM06/6-31G(d)-LANL2DZ Level of Theory



Structures	ζ_{Ru}	ζ_{O1}	ζ_{O2}	ζ_{Por}	ζ_{Sub}
$^1\text{RuO}_2(\text{OSS})$	0.0	0.6	-0.6	0.0	—
$^1\text{TS1(OSS)}$	-0.4	0.3	-0.6	0.0	0.7
$^1\text{TS1}\sigma'(\text{OSS})$	-0.3	0.5	-0.6	0.0	0.4
$^1\text{INT(OSS)}$	-0.5	0.1	-0.6	0.0	1.0
$^1\text{TS2(OSS)}$	-0.2	-0.2	-0.2	0.0	0.6
$^1\text{RuO(OSS)}$	0.0	—	0.0	0.0	—
$^3\text{RuO}_2$	0.3	1.1	0.6	0.0	—
$^3\text{TS1}$	0.4	0.4	0.6	0.0	0.6
^3INT	0.5	-0.1	0.6	0.0	1.0
$^3\text{TS2}$	0.5	-0.1	0.6	0.0	1.0
^3RuO	1.1	—	0.8	0.1	—
$^5\text{RuO}_2$	1.0	1.3	1.1	0.6	—
$^1\text{Ru}(\text{por}^*)\text{O}_2(\text{OSS})$	0.0	0.8	-0.8	0.0	—
S_ $^1\text{TS1(OSS)}$	-0.3	0.6	-0.7	0.0	0.4
R_ $^1\text{TS1(OSS)}$	-0.3	0.5	-0.7	0.0	0.5
S_ $^1\text{INT(OSS)}$	-0.4	0.1	-0.6	0.0	0.9

R_ ¹ INT(OSS)	-0.4	0.1	-0.6	0.0	0.9
S_ ¹ TS2(OSS)	0.4	0.1	0.4	0.0	-0.9
R_ ¹ TS2(OSS)	-0.4	0.0	-0.4	0.0	0.8
¹ Ru(por*)O(OSS)	0.0	—	0.0	0.0	—

OSS is open-shell singlet.

Table S3. The $\langle S^2 \rangle$ for the triplet and quintet Species Calculated at the UM06/6-31G(d)-LANL2DZ Level of Theory

Structures	$\langle S^2 \rangle$	Structures	$\langle S^2 \rangle$
³ RuO ₂	2.0003	³ TS2	2.0051
³ TS1	2.0005	³ RuO	2.0001
³ INT	2.0051	⁵ RuO ₂	6.0006

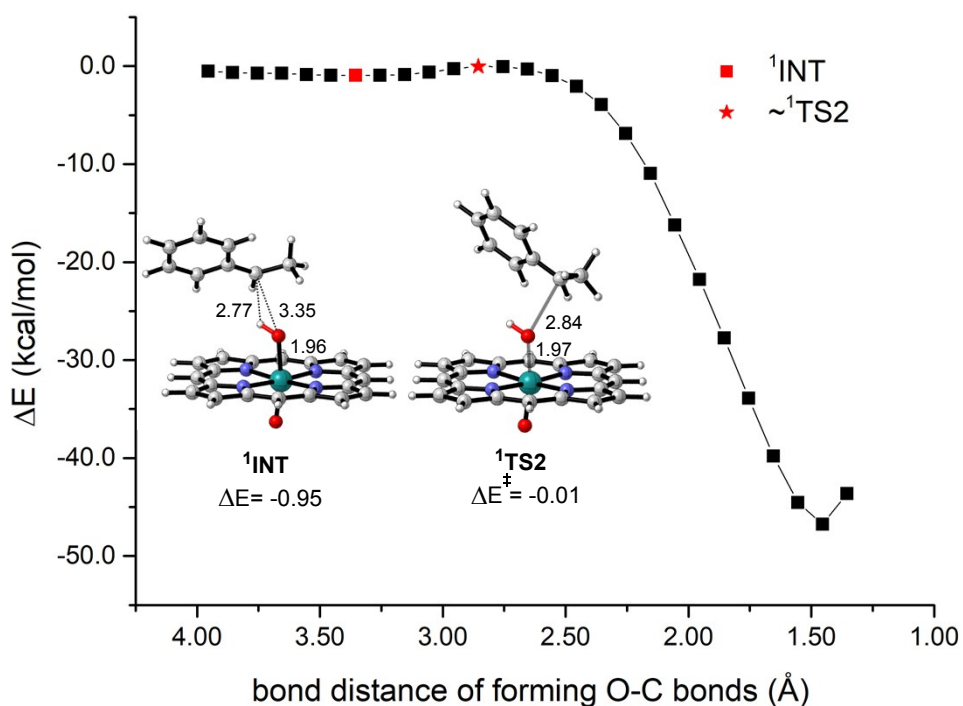


Figure S1. Geometry scans starting from ¹INT to form the 1-phenylethanol product. Calculations were done at the UB3LYP/6-31G(d)-LANL2DZ level of theory. The distances are shown in Å.

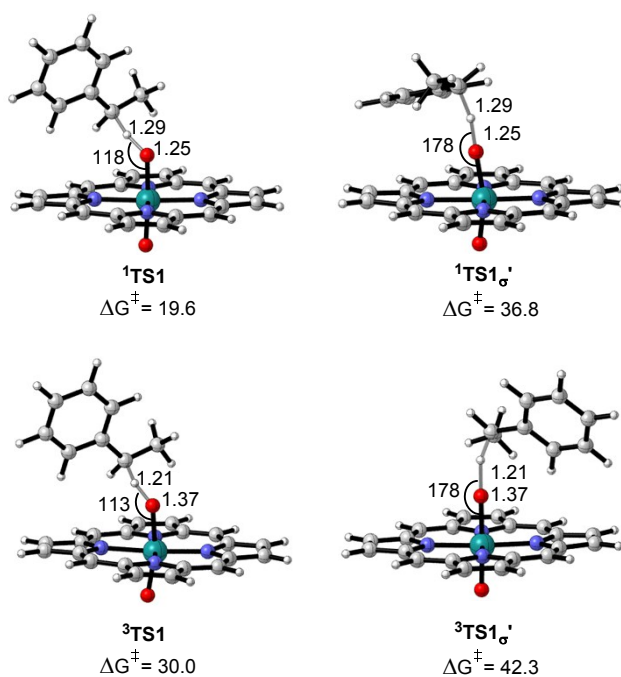


Figure S2. Optimized σ - and π -pathways transition structures. Calculations were done at the UM06/6-311+G(d,p)-SDD(SMD_{Dichloromethane})/UM06/6-31G(d)-LANL2DZ level of theory. The distances are shown in Å. The angles are shown in degrees, and energies are shown in kcal/mol.

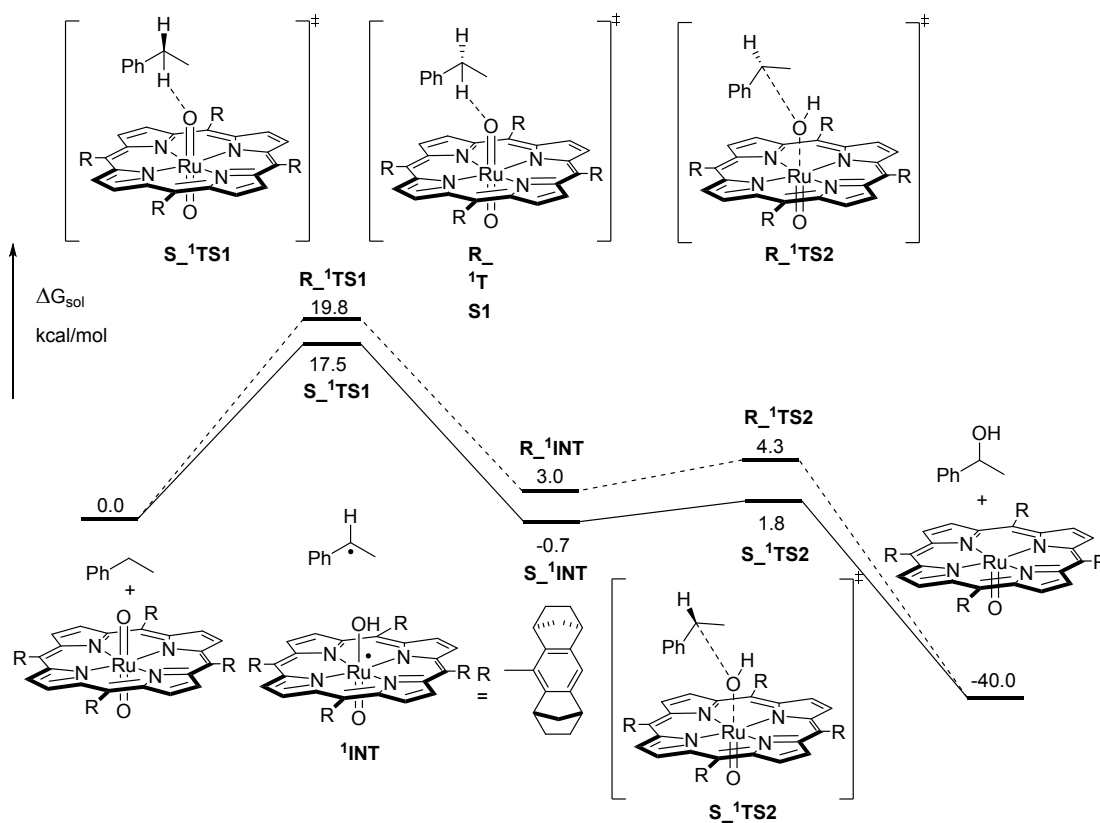


Figure S3. Gibbs free energy profiles for benzylic C–H hydroxylation with experimental chiral Ru-porphyrin ($\text{Ru}(\text{por}^*)\text{O}_2$) using ONIOM (UM06/6-311+G(d,p)-SDD:UFF

(SMD_{Dichloromethane})/UM06/6-31G(d)-LANL2DZ:UFF) level of theory.

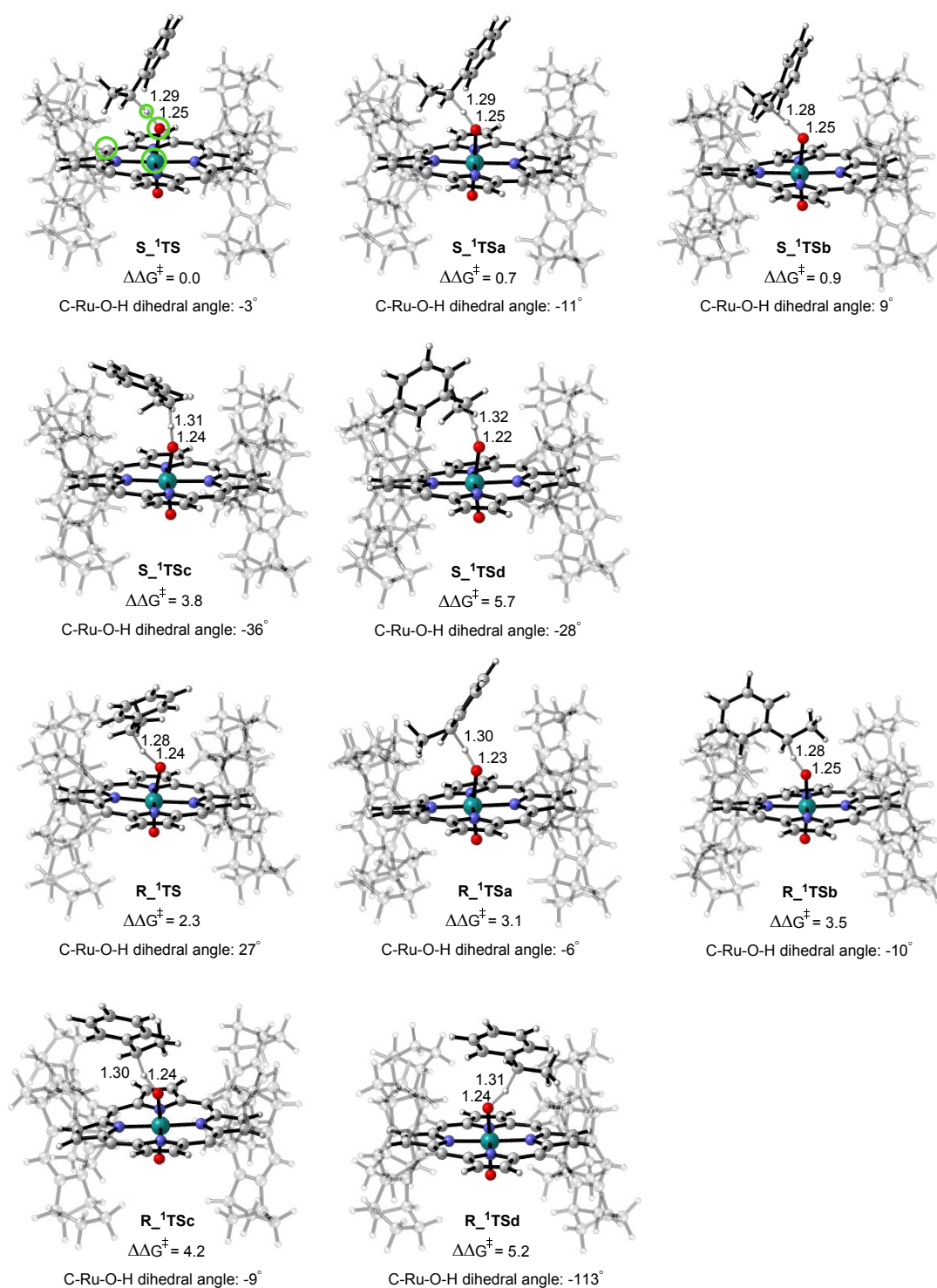


Figure S4. Different conformers for the hydrogen-atom abstraction transition structures. The distances are shown in Å. The energies are shown in kcal/mol. Calculations are based on ONIOM (UM06/6-311+G(d,p)-SDD:UFF(SMD_{Dichloromethane})/UM06/6-31G(d)-LANL2DZ:UFF) level of theory.

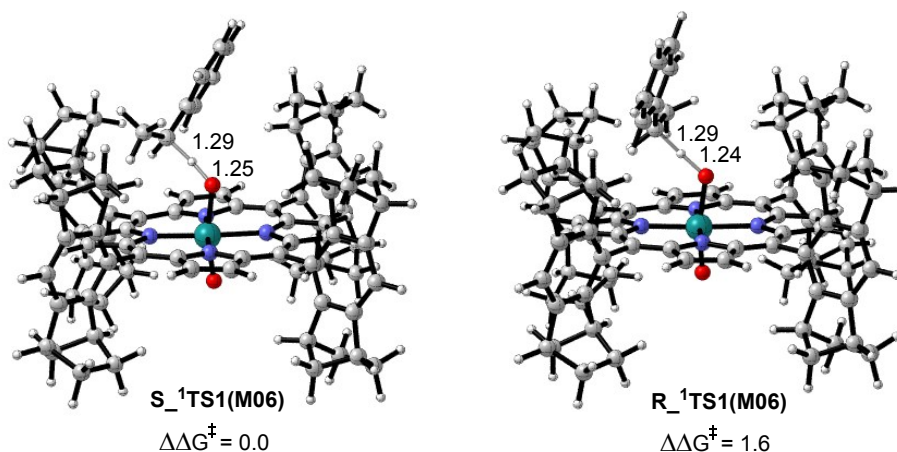


Figure S5. Optimized transition-state structures of $S_1TS1(M06)$ and $R_1TS1(M06)$. The distances are shown in Å. The energies are shown in kcal/mol. Calculations are based on UM06/6-31G(d)-LANL2DZ(SMD_{Dichloromethane})/UM06/6-31G(d)-LANL2DZ level of theory.

Table S4. Electronic Energies, Enthalpies, and Free Energies (in Hartree) of the Structures Calculated at the (U)M06/6-311+G(d,p)-SDD(SMD_{Dichloromethane})/ (U)M06/6-31G(d)-LANL2DZ Level of Theory

Structures	ZPVE	TCE	TCH	TCG	E_{sol}	$G_{sol}(E_{sol}+TCG)$	Imaginary Frequenc y	ΔG_{sol} (kcal/mol)
ethylbenzene	0.156401	0.163741	0.164685	0.124309	-310.709366384	-310.585057384	—	—
1-phenylethanol	0.161167	0.169484	0.170428	0.127913	-385.924638073	-385.796725073	—	—
$^1RuO_2(CSS)$	0.280728	0.300393	0.301337	0.234008	-1233.18694410	-1232.95293610	—	1.2
$^1RuO_2(OSS)$	0.279778	0.299731	0.300675	0.231775	-1233.18664727	-1232.95487227	—	—
3RuO_2	0.279070	0.299170	0.300114	0.230973	-1233.15144697	-1232.92047397	—	21.6
5RuO_2	0.276662	0.297187	0.298131	0.227316	-1233.13066350	-1232.90334750	—	32.3
$^1TS_1(OSS)$	0.430670	0.459152	0.460097	0.370774	-1543.87947235	-1543.50869835	2133.39i	19.6
$^1TS_1(CSS)^b$	0.432053	0.460306	0.461250	0.373039	-1543.87611667	-1543.50307767	297.27i	23.1
3TS_1	0.430831	0.459398	0.460343	0.370644	-1543.86282403	-1543.49218003	1194.94i	30.0
$^1TS_2(OSS)$	0.430953	0.457582	0.458526	0.375981	-1543.85733708	-1543.48135608	1800.39i	36.8
$^1INT(OSS)$	0.435443	0.464522	0.465466	0.377313	-1543.91483347	-1543.53752047	—	1.5
$^1INT(CSS)^b$	0.434611	0.463847	0.464792	0.374084	-1543.88379539	-1543.50971139	—	19.0
3INT	0.434179	0.463599	0.464544	0.373830	-1543.91437099	-1543.54054099	—	-0.4
$^1TS_2(OSS)$	0.434614	0.463373	0.464317	0.375973	-1543.91072724	-1543.53475424	129.36i	3.2
$^1TS_2(CSS)^b$	0.434965	0.463402	0.464346	0.377744	-1543.88920871	-1543.51146471	115.00i	17.9
3TS_2	0.434361	0.462988	0.463932	0.375576	-1543.91245695	-1543.53688095	84.12i	1.9

¹ RuO(OSS)	0.277519	0.295985	0.296929	0.23235	-1158.03885624	-1157.80650624	—	—
¹ RuO(CSS) ^b	0.277696	0.296077	0.297021	0.232666	-1158.02257457	-1157.78990857	—	—
³ RuO	0.277566	0.296008	0.296952	0.231398	-1158.05070567	-1157.81930767	—	—
¹ Ru(por ⁺)O ₂ (OSS) ^a	1.480529	1.542077	1.543021	1.371362	-1232.35938266	-1230.98802066	—	—
R_ ¹ TS1(OSS) ^a	1.632797	1.702365	1.703309	1.518113	-1543.05955472	-1541.54144172	2089.40 <i>i</i>	19.8
R_ ¹ INT(OSS) ^a	1.637290	1.707461	1.708405	1.523080	-1543.09145082	-1541.56837082	—	3.0
S_ ¹ TS1(OSS) ^a	1.633218	1.702559	1.703503	1.519424	-1543.06456462	-1541.54514062	2096.34 <i>i</i>	17.5
S_ ¹ INT(OSS) ^a	1.636774	1.707295	1.708239	1.520404	-1543.09456694	-1541.57416294	—	-0.7
R_ ¹ TS2(OSS) ^a	1.637061	1.706668	1.707612	1.524372	-1543.09061474	-1541.56624274	30.18 <i>i</i>	4.3
S_ ¹ TS2(OSS) ^a	1.636892	1.706549	1.707493	1.524317	-1543.09447297	-1541.57015597	43.56 <i>i</i>	1.8
¹ Ru(por ⁺)O(OSS) ^a	1.478216	1.538292	1.539236	1.371656	-1157.21178913	-1155.84013313	—	—

ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy. CSS is closed-shell singlet and OSS is open-shell singlet.

^aCalculated at the ONIOM (UM06/6-311+G(d,p)-SDD:UFF(SMD_{Dichloromethane})/UM06/6-31G(d)-LANL2DZ:UFF) Level of Theory.

^bThe wavefunction stability for the reaction species are instability.

Cartesian coordinates of the structures

ethylbenzene

C	1.62087300	-1.20284800	0.09527800
C	0.26004400	-1.19957700	-0.19177400
C	-0.43809500	-0.00002400	-0.34147800
C	0.26000900	1.19955400	-0.19180400
C	1.62083700	1.20287400	0.09524700
C	2.30598900	0.00002500	0.23924500
H	2.14991700	-2.14877900	0.20367300
H	-0.27626700	-2.14365200	-0.30561800
H	-0.27633200	2.14361000	-0.30567200
H	2.14985300	2.14882300	0.20361900
H	3.37211500	0.00004400	0.46060200
C	-1.92054000	-0.00004400	-0.59237700
C	-2.70982300	0.00003300	0.71386600
H	-2.19752500	-0.88143400	-1.18991900
H	-2.19753100	0.88127100	-1.19002700
H	-3.79212600	0.00001900	0.53323100

H	-2.46393200	-0.88472000	1.31649500
H	-2.46393700	0.88486000	1.31638900

1-phenylethanol

C	-1.79595000	1.23916000	0.32243900
C	-0.41887000	1.13136400	0.15336900
C	0.15073200	-0.08990300	-0.20178700
C	-0.67623200	-1.19830600	-0.38336800
C	-2.05133400	-1.09332700	-0.21005100
C	-2.61549500	0.12918100	0.14380500
H	-2.23218700	2.19958100	0.59404600
H	0.22787600	1.99673900	0.28178600
H	-0.23370600	-2.15488700	-0.66918200
H	-2.68543700	-1.96622400	-0.35859300
H	-3.69293300	0.21677900	0.27517500
C	1.64415600	-0.24778800	-0.32609600
C	2.23170000	-0.79413700	0.96843600
H	1.84760100	-0.97046700	-1.14101800
H	3.32023300	-0.93003100	0.88396200
H	2.02882400	-0.09196600	1.78800100
H	1.79101500	-1.76489400	1.22815300
O	2.20626200	1.01005900	-0.63876700
H	3.16637700	0.92744000	-0.57267400

¹RuO₂ (OSS)

C	-1.23929900	2.82041900	0.00048300
C	-2.51320900	3.49421400	0.00157200
C	-3.47383700	2.53012900	0.00143000
C	-2.79857500	1.25647100	0.00051000
N	-1.45808900	1.48176600	-0.00004500
C	0.01493700	3.43167500	-0.00002200
C	-3.41702100	0.00722400	0.00002300
C	-2.80393200	-1.24468300	-0.00049200
C	-3.48447500	-2.51557400	-0.00131600
C	-2.52779400	-3.48355900	-0.00145600

C	-1.25110600	-2.81492800	-0.00059500
N	-1.46446600	-1.47544900	-0.00002400
C	0.00061400	-3.43134200	-0.00013100
C	1.24631600	-2.81094700	0.00042100
C	2.51621400	-3.48520900	0.00145500
C	3.48492600	-2.52783700	0.00170900
C	2.82334500	-1.25170500	0.00053100
N	1.47581900	-1.46334800	-0.00009500
C	3.44808600	-0.00711300	0.00004200
C	2.82844900	1.23996400	-0.00048600
C	3.49532900	2.51328600	-0.00158400
C	2.53069400	3.47478000	-0.00141200
C	1.25796200	2.80599900	-0.00052500
N	1.48167200	1.45735500	0.00006500
H	-2.64246800	4.57156900	0.00220400
H	-4.55163600	2.65635800	0.00198300
H	-4.56278000	-2.63739500	-0.00177200
H	-2.66145000	-4.56037900	-0.00202000
H	2.63924700	-4.56334800	0.00198100
H	4.56155300	-2.66288700	0.00248900
H	4.57251900	2.64377800	-0.00225500
H	2.65833300	4.55238400	-0.00193500
Ru	0.03114400	0.00029800	-0.00001700
O	-0.15711900	-0.00146300	-1.74238100
O	-0.15713900	-0.00149400	1.74234800
H	0.02414200	4.52126700	-0.00001200
H	-4.50679600	0.00958900	0.00009400
H	4.53750000	-0.00930500	0.00010700
H	0.00526200	-4.52096700	-0.00012400

³RuO₂

C	2.03623200	2.31686300	-0.03130400
C	2.09142400	3.75364900	-0.06691100
C	0.80449100	4.19954900	-0.07372900
C	-0.04921600	3.04108300	-0.04353300
N	0.73742800	1.92672900	-0.01732500
C	3.12741600	1.44751300	-0.01644300
C	-1.44205500	3.06927200	-0.03322700

C	-2.31964300	1.98694900	-0.00647000
C	-3.75980300	2.06649400	-0.02771300
C	-4.22938800	0.78919700	-0.02231100
C	-3.07775000	-0.07881700	0.00227600
N	-1.95814900	0.67931800	0.02064000
C	-3.09244600	-1.47500300	-0.02171000
C	-1.99591600	-2.32707300	-0.04219300
C	-2.06569300	-3.76278900	-0.08356100
C	-0.78822300	-4.23150500	-0.08590700
C	0.08289900	-3.08856700	-0.04366900
N	-0.67514100	-1.95524600	-0.01930300
C	1.47398900	-3.12159600	-0.02930300
C	2.32882100	-2.02630600	-0.00511600
C	3.76248800	-2.08769900	-0.03107000
C	4.22469100	-0.80682200	-0.02726000
C	3.08261900	0.06130700	0.00028600
N	1.94421300	-0.71101600	0.02604600
H	3.00574000	4.33751400	-0.08397000
H	0.44964300	5.22482100	-0.09677500
H	4.11745200	1.90211300	-0.03371200
H	-1.89897700	4.05861600	-0.05678700
H	-4.32779000	2.99086800	-0.05055100
H	-5.26037400	0.45138600	-0.04045100
H	-4.07218900	-1.95196700	-0.04045500
H	-2.98946600	-4.33157700	-0.10813000
H	-0.45057600	-5.26232400	-0.11273100
H	1.94175400	-4.10520200	-0.05306700
H	4.33704700	-3.00785400	-0.05634800
H	5.25442600	-0.46534800	-0.04920700
Ru	0.03061800	-0.03377200	0.10272300
O	-0.16950500	0.26832700	-1.79163400
O	-0.20074100	0.19570200	1.83228100

¹TS1 (OSS)

C	1.41042200	1.25697400	-2.05978800
C	2.47471200	0.86204800	-2.94561900
C	2.38265600	-0.48818800	-3.10910500
C	1.26441400	-0.93228000	-2.31827400

N	0.71504700	0.14367200	-1.69579200
C	1.12787200	2.56401400	-1.66504800
C	0.82372700	-2.25018600	-2.18318400
C	-0.22812900	-2.70207600	-1.39199100
C	-0.62510900	-4.07450800	-1.23093100
C	-1.67945200	-4.09286700	-0.36848300
C	-1.94894500	-2.73077600	0.00562800
N	-1.04657800	-1.91942200	-0.62273200
C	-2.96816500	-2.30748900	0.85453600
C	-3.27777700	-0.99518900	1.20711300
C	-4.34592100	-0.58627000	2.08153600
C	-4.30024100	0.77164600	2.16221700
C	-3.20079600	1.21095800	1.34300800
N	-2.61556300	0.11415600	0.77943600
C	-2.79492400	2.53119100	1.17491800
C	-1.71071600	2.99236900	0.42742500
C	-1.28597700	4.36609500	0.30829300
C	-0.17901800	4.37167100	-0.48208700
C	0.08038500	3.00223100	-0.85639200
N	-0.86734200	2.21200100	-0.29068600
H	3.19233200	1.54406700	-3.39039700
H	3.00980700	-1.13608200	-3.71304300
H	1.79756800	3.33519200	-2.04556400
H	1.37083700	-3.00823500	-2.74332200
H	-0.14720100	-4.91517500	-1.72343900
H	-2.24046100	-4.95147900	-0.01389500
H	-3.60010900	-3.08695600	1.27942900
H	-5.03925400	-1.26484800	2.56775400
H	-4.94759000	1.43240500	2.72962400
H	-3.37853200	3.28631600	1.70117600
H	-1.77921200	5.20925500	0.78087200
H	0.42080500	5.22115700	-0.79230000
Ru	-0.98819900	0.12813600	-0.48655000
O	0.14681800	0.15569000	0.98245900
O	-1.94625100	0.44869000	-1.91982400
C	5.14170300	0.56213100	0.73330700
C	4.01125400	-0.18887200	0.45204400
C	3.24751300	-0.76353200	1.48362900

C	3.65726500	-0.54818700	2.80853300
C	4.79220900	0.20129000	3.08886400
C	5.53945800	0.76011000	2.05508800
H	5.72071500	0.99484100	-0.08145200
H	3.69870900	-0.34428600	-0.58307500
H	3.08181300	-0.97888500	3.62681100
H	5.09757500	0.35099500	4.12352000
H	6.42852800	1.34794100	2.27776800
C	2.03833500	-1.51743800	1.14453800
C	1.39211700	-2.41549100	2.16543000
H	2.07829000	-1.94902900	0.13533400
H	1.13579400	-0.61683700	0.97177300
H	0.49677400	-2.88960700	1.74296000
H	2.07485500	-3.21125300	2.50169400
H	1.07198500	-1.85166200	3.05208800

³TS1

C	1.23345700	1.70286700	-1.87349300
C	2.34979100	1.55007300	-2.77251500
C	2.43765400	0.22557100	-3.07994000
C	1.37945000	-0.44021000	-2.36235700
N	0.68725500	0.48002300	-1.64697100
C	0.77615500	2.91098600	-1.34570900
C	1.11657300	-1.81225400	-2.36304000
C	0.13445400	-2.47475100	-1.63554500
C	-0.06724400	-3.89744100	-1.61313800
C	-1.11272500	-4.14582500	-0.77630900
C	-1.57186600	-2.87710000	-0.28057900
N	-0.78966600	-1.88889100	-0.80684400
C	-2.64607600	-2.68105100	0.58376000
C	-3.13079800	-1.46336700	1.04997100
C	-4.23876200	-1.29190700	1.95088700
C	-4.37891500	0.04396000	2.16847200
C	-3.35557400	0.71056800	1.40949200
N	-2.62702600	-0.23385600	0.73335500
C	-3.13065200	2.08048500	1.39319900
C	-2.10945800	2.75433500	0.72078400
C	-1.85351200	4.17226500	0.76274300

C	-0.74991600	4.39723100	-0.00059100
C	-0.32327800	3.12044700	-0.51765200
N	-1.17753400	2.16343800	-0.06324500
H	2.97640100	2.36371900	-3.12353800
H	3.15051600	-0.26785100	-3.73282100
H	1.34334200	3.79983100	-1.62235700
H	1.76216800	-2.43402100	-2.98324500
H	0.52590300	-4.61134300	-2.17543300
H	-1.55034500	-5.10400300	-0.51560700
H	-3.16645800	-3.57548300	0.92504900
H	-4.82849500	-2.10455400	2.36248500
H	-5.10544600	0.54911900	2.79656800
H	-3.80749900	2.69017100	1.99125600
H	-2.44738700	4.89238600	1.31599700
H	-0.25446400	5.34123800	-0.20321000
Ru	-1.03800100	0.12206400	-0.49644500
O	0.18869300	0.27305700	0.98592800
O	-1.89564700	0.47278100	-1.99013700
C	5.14932300	0.66642200	0.71369200
C	4.00338200	-0.05967400	0.42822600
C	3.30325500	-0.73444700	1.44134200
C	3.78688200	-0.64734600	2.75281800
C	4.93883000	0.07571600	3.03875400
C	5.62412800	0.73580600	2.02278000
H	5.67795900	1.18140000	-0.08733600
H	3.62757900	-0.11182400	-0.59635100
H	3.25977600	-1.15858900	3.55719600
H	5.30471400	0.12459700	4.06341400
H	6.52516100	1.30365600	2.24948000
C	2.06913300	-1.46583500	1.08983200
C	1.44662900	-2.39447000	2.10181100
H	2.13853800	-1.91313900	0.08766500
H	1.23724600	-0.60612500	0.91614900
H	0.53283800	-2.84323600	1.69114500
H	2.13097900	-3.20825800	2.38493100
H	1.16153800	-1.85653200	3.01555900

¹TS1_σ' (OSS)

C	-1.72346900	2.96772200	-0.16031600
C	-2.81285800	3.72766000	-0.70528000
C	-3.79921900	2.84849500	-1.03954200
C	-3.33108700	1.53361500	-0.70637400
N	-2.07344800	1.64134400	-0.17789000
C	-0.52159800	3.49603200	0.29782500
C	-4.03047300	0.34541400	-0.89152500
C	-3.58732400	-0.93876800	-0.58671000
C	-4.31549900	-2.15616600	-0.80185600
C	-3.52211300	-3.18218600	-0.38190000
C	-2.29641900	-2.61042200	0.09951600
N	-2.37376100	-1.24881400	-0.03920800
C	-1.21656800	-3.32704100	0.60568400
C	-0.00652000	-2.81532600	1.07616100
C	1.12278900	-3.58168600	1.54415100
C	2.09748800	-2.68968900	1.86998600
C	1.57314600	-1.37198100	1.60561200
N	0.30487200	-1.49879500	1.14166000
C	2.26754900	-0.17496800	1.77522000
C	1.82500900	1.11549100	1.49598600
C	2.59770300	2.32206700	1.66795300
C	1.81931000	3.35904100	1.25706600
C	0.56351600	2.79435500	0.82624800
N	0.60693400	1.45264400	0.99863400
H	-2.81295800	4.80719700	-0.81588900
H	-4.76780700	3.06363700	-1.47879000
H	-0.41417500	4.57810100	0.22618900
H	-5.02594400	0.42788800	-1.32629300
H	-5.31217500	-2.21057000	-1.22729100
H	-3.74035200	-4.24512800	-0.39427200
H	-1.32708300	-4.41105200	0.62499600
H	1.15375400	-4.66462100	1.60581800
H	3.09422000	-2.89053000	2.25016600
H	3.28938000	-0.26106600	2.14391900
H	3.61452200	2.35057500	2.04656700
H	2.06257900	4.41631100	1.23510000
Ru	-0.92683300	0.09377000	0.49017400
O	0.09719500	-0.10445300	-0.96737700

O	-1.34394300	0.20690900	2.16584500
C	4.33939500	1.41829400	-1.09131500
C	3.25847400	1.08539800	-1.89384900
C	2.86935800	-0.25180500	-2.08306400
C	3.59353500	-1.23929300	-1.39947600
C	4.68061800	-0.90759600	-0.59555300
C	5.06532700	0.42029700	-0.44041900
H	4.61940700	2.46461700	-0.96970600
H	2.68859700	1.87071900	-2.39439100
H	3.30943400	-2.28593100	-1.50674900
H	5.23401000	-1.69887600	-0.08858900
H	5.92121500	0.67841900	0.18256900
C	1.66818100	-0.55133000	-2.89001500
C	1.41612000	-1.99070200	-3.27001100
H	1.55640700	0.14694800	-3.72984700
H	0.77788100	-0.24856100	-2.01183100
H	0.52300100	-2.07469400	-3.90085100
H	2.25690500	-2.44552700	-3.81838400
H	1.23543800	-2.60760300	-2.37541100

¹INT (OSS)

C	0.43311200	2.83187200	-0.71014600
C	1.65283700	3.47117700	-1.13021100
C	2.49879700	2.48831900	-1.54719900
C	1.80356900	1.23949300	-1.38468900
N	0.56930900	1.48532600	-0.87434400
C	-0.69845200	3.48369900	-0.22183100
C	2.30415700	-0.02711400	-1.68743800
C	1.65911400	-1.24389300	-1.51014900
C	2.22308600	-2.53210600	-1.79688400
C	1.28801500	-3.46808400	-1.46919900
C	0.13638200	-2.76577500	-0.97814000
N	0.39009100	-1.42208700	-1.01769000
C	-1.04154700	-3.35262800	-0.52568400
C	-2.16354300	-2.69225900	-0.03497300
C	-3.36201600	-3.31966700	0.45371500
C	-4.20507300	-2.32578400	0.84451200
C	-3.53455900	-1.07632100	0.60319700

N	-2.30273100	-1.33858600	0.06443300
C	-4.05853300	0.17987500	0.88037000
C	-3.43288300	1.41337400	0.69326000
C	-3.98061500	2.70316500	1.03317200
C	-3.03234500	3.62846700	0.72361800
C	-1.89955200	2.91090200	0.19201200
N	-2.19084800	1.58420400	0.18417100
H	1.82761500	4.54202000	-1.10540900
H	3.51149700	2.58497700	-1.92557000
H	-0.63326100	4.56953100	-0.15094600
H	3.31847800	-0.06899900	-2.08309500
H	3.22010200	-2.68929900	-2.19702000
H	1.36230800	-4.54791400	-1.54887100
H	-1.08602100	-4.44107000	-0.55113100
H	-3.52504100	-4.39189400	0.48970000
H	-5.20028100	-2.41693400	1.26739400
H	-5.06145300	0.20145100	1.30626100
H	-4.96455400	2.86488500	1.46118200
H	-3.07986300	4.70595700	0.84432000
Ru	-0.91757300	0.05877800	-0.49994400
O	-0.27587200	0.17454400	1.34799400
O	-1.56138500	0.43169900	-2.07461700
C	5.02467800	0.62266400	0.57352700
C	4.51341400	-0.65419600	0.71311800
C	3.36174400	-0.90680900	1.50401200
C	2.78454600	0.20147500	2.18099300
C	3.29329900	1.47996700	2.02115700
C	4.40918100	1.70504000	1.21048400
H	5.90779700	0.78674800	-0.04376600
H	4.98513400	-1.49413800	0.19935100
H	1.93924400	0.03377100	2.84851600
H	2.82166200	2.31463500	2.53906000
H	4.80243100	2.71267200	1.08677300
C	2.80933600	-2.20265900	1.57359300
C	1.55509600	-2.54202500	2.29642600
H	3.34637100	-2.99969100	1.05562400
H	0.63184300	0.52736800	1.33117600
H	1.23314900	-3.56540700	2.07222500

H	1.67484400	-2.46863900	3.39083600
H	0.73103900	-1.85921300	2.02417600

³INT

C	-3.20658200	-1.58985800	0.50932800
C	-4.50451700	-1.46245400	1.12198000
C	-4.73406200	-0.13147500	1.28719900
C	-3.57720100	0.56409800	0.78092200
N	-2.68779500	-0.35351000	0.31414000
H	-5.14694100	-2.29479600	1.39015000
H	-5.60440500	0.35190200	1.71920300
C	-3.39890300	1.94570400	0.79135400
C	-2.13686600	4.09688700	0.41181200
C	-0.90470100	4.38994300	-0.08876300
C	-0.29163700	3.13825000	-0.45239700
N	-1.15078500	2.12913900	-0.16450700
C	-2.28483300	2.66468500	0.36082800
H	-2.88905400	4.78269300	0.78824200
H	-0.44141500	5.36408100	-0.20726100
C	-2.56905700	-2.78724300	0.17965000
N	-0.46593000	-1.91166900	-0.74570000
C	0.67125700	-2.46366900	-1.26311400
C	0.54160500	-3.89448300	-1.24160200
C	-0.67784200	-4.18245700	-0.70602000
C	-1.31241500	-2.93263700	-0.39225400
H	1.29872500	-4.58625900	-1.59729700
H	-1.12160500	-5.15766300	-0.53344200
C	1.78027400	-1.75756200	-1.72151300
N	1.05199400	0.52450200	-1.22311800
C	1.58995400	1.77700200	-1.36440200
C	2.89137900	1.65456600	-1.96478700
C	3.11389700	0.33001300	-2.17779700
C	1.95365700	-0.37749100	-1.70649700
H	3.54775500	2.49051100	-2.18418600
H	3.99170400	-0.14443100	-2.60556600
C	0.97994700	2.97314700	-1.00643500
H	1.55555500	3.88131800	-1.18421200
H	2.60510700	-2.34969000	-2.11905300

H	-3.11159100	-3.70648400	0.39916100
H	-4.22275400	2.53304500	1.19711000
O	-0.26188100	0.09714500	1.34156400
H	0.42872500	0.77437100	1.44981800
C	2.55040600	-2.24754800	1.51012400
H	3.06858600	-2.97523000	0.88083300
C	3.11381600	-0.95793300	1.59850400
C	4.26684100	-0.62002500	0.84402800
C	4.80050100	0.65426100	0.87840100
C	4.20820900	1.64751400	1.66359000
C	3.08651700	1.33471000	2.43626600
C	2.54978200	0.05785600	2.41644100
H	4.71946300	-1.38858100	0.21419400
H	5.67915400	0.88838500	0.27793700
H	4.62552500	2.65285700	1.68447600
H	2.63519000	2.09780100	3.07005700
H	1.68792100	-0.17999300	3.03766900
C	1.30290400	-2.65773600	2.20023300
H	0.48768700	-1.94202500	1.98548800
H	0.98127400	-3.65709200	1.88549000
H	1.42245700	-2.67428500	3.29674400
O	-1.65324400	0.37752600	-2.05771200
Ru	-0.83914600	0.08469500	-0.54119400

¹TS2 (OSS)

C	-3.31425200	-0.66767500	1.03639200
C	-4.35839000	-0.13813800	1.87761700
C	-4.16659100	1.20672900	1.94660600
C	-3.00064800	1.50921900	1.15332600
N	-2.52875600	0.35352100	0.61464000
H	-5.13193500	-0.73303900	2.35215400
H	-4.75062000	1.94210300	2.49054700
C	-2.43762000	2.77353000	0.99533400
C	-0.71124900	4.42613300	0.19072300
C	0.42441500	4.31613500	-0.55185200
C	0.55888300	2.92750600	-0.90996200
N	-0.48151300	2.23442300	-0.37879600
C	-1.27767600	3.10558500	0.29719700

H	-1.13751300	5.31864700	0.63734300
H	1.11863900	5.09913500	-0.83906300
C	-3.12349300	-2.01174000	0.71745200
N	-1.12545500	-1.83913700	-0.70300800
C	-0.33205600	-2.72429900	-1.37617500
C	-0.84603100	-4.05187000	-1.17481200
C	-1.94253900	-3.94249100	-0.37405200
C	-2.11645000	-2.54684400	-0.07716800
H	-0.41073200	-4.95171100	-1.59727000
H	-2.58858600	-4.73445800	-0.00918000
C	0.80901600	-2.39952800	-2.10554000
N	0.88727000	0.01622300	-1.70215200
C	1.73538500	1.03759000	-2.03447300
C	2.81172300	0.50433300	-2.82505600
C	2.58896600	-0.83289500	-2.96015000
C	1.37615400	-1.13487600	-2.24739100
H	3.63060700	1.09245800	-3.22693600
H	3.18909600	-1.56322800	-3.49337400
C	1.58911700	2.37167700	-1.66888700
H	2.36092700	3.05688900	-2.01866200
H	1.32692700	-3.22476800	-2.59365500
H	-3.83671900	-2.71986000	1.13872400
H	-2.95200600	3.59562800	1.49298900
O	0.09289100	0.01235900	1.08141800
H	0.91014100	0.53975000	1.07303400
C	1.72756200	-2.03401000	1.53722400
H	1.58011600	-2.36241700	0.50710000
C	2.79124700	-1.13253900	1.77483100
C	3.55684000	-0.64275500	0.68594400
C	4.56241000	0.28633700	0.87716400
C	4.85514700	0.75459000	2.16157200
C	4.11830400	0.28133300	3.24984800
C	3.10152700	-0.64083500	3.06701100
H	3.32693400	-1.00476300	-0.31827200
H	5.12582900	0.65243300	0.01891300
H	5.64891800	1.48410700	2.31295400
H	4.34038900	0.64492700	4.25245600
H	2.52606800	-0.99143800	3.92310700

C	0.82949700	-2.57756300	2.58687800
H	0.31454800	-1.76440600	3.11987900
H	0.05852000	-3.22103000	2.14734800
H	1.37656900	-3.17107300	3.33796500
O	-1.86761100	0.63251000	-1.98000900
Ru	-0.86237200	0.19013900	-0.62344900

³TS2

C	-3.13386100	-1.33437000	0.62257300
C	-4.34464600	-1.11741300	1.37316400
C	-4.45466900	0.22453800	1.56695800
C	-3.30934200	0.83875200	0.94262500
N	-2.54852800	-0.13625500	0.37415400
H	-5.01482400	-1.90290900	1.70677200
H	-5.23381300	0.76589700	2.09384100
C	-3.02216100	2.20154500	0.95206600
C	-1.61973900	4.24952300	0.49532500
C	-0.41424900	4.44869800	-0.10498000
C	0.05193100	3.15912600	-0.54784000
N	-0.86804200	2.22127100	-0.20990100
C	-1.89748600	2.83688400	0.42752900
H	-2.27188800	4.98633500	0.95306800
H	0.12346900	5.38139600	-0.24092300
C	-2.62853200	-2.57131700	0.22267400
N	-0.57673300	-1.84429700	-0.92069900
C	0.44917900	-2.47315600	-1.57255700
C	0.20495400	-3.88828400	-1.55779400
C	-0.96273300	-4.09090600	-0.88412800
C	-1.45569700	-2.80276200	-0.48543700
H	0.85695800	-4.63027400	-2.00746000
H	-1.46067100	-5.03202400	-0.67387400
C	1.56591600	-1.85127900	-2.12264300
N	1.09330000	0.46683700	-1.49951900
C	1.73129600	1.66911600	-1.63854400
C	2.97668400	1.45297000	-2.32706300
C	3.06049900	0.12241300	-2.60029100
C	1.87027100	-0.49300500	-2.07422700
H	3.68835200	2.23522300	-2.57082600

H	3.85541400	-0.41032700	-3.11262200
C	1.25769700	2.90177700	-1.20218600
H	1.89805800	3.76171200	-1.39738500
H	2.29065000	-2.49860400	-2.61649200
H	-3.21201400	-3.45007900	0.49624400
H	-3.75101600	2.84304000	1.44742100
O	0.00869400	0.07885500	1.14366400
H	0.84233200	0.58049700	1.18621600
C	1.83634400	-2.31190400	1.54073100
H	2.03864200	-2.80351000	0.58702400
C	2.62568500	-1.18411700	1.86021100
C	3.56450400	-0.68106500	0.92356800
C	4.29000000	0.46877800	1.17892000
C	4.12563900	1.15364000	2.38618800
C	3.21983200	0.66647700	3.33322400
C	2.48144400	-0.47677200	3.08170400
H	3.68408000	-1.20492300	-0.02631700
H	4.98638900	0.84189600	0.42826600
H	4.69645700	2.05850700	2.58749900
H	3.08568600	1.19590100	4.27582100
H	1.75744900	-0.82758700	3.81591900
C	0.75059800	-2.85468000	2.39820100
H	-0.04330800	-2.10283300	2.53538800
H	0.29470100	-3.74139200	1.94172600
H	1.10937200	-3.14021300	3.40060800
O	-1.64900800	0.57395600	-2.09896500
Ru	-0.76623000	0.16681000	-0.64780800

¹RuO (OSS)

C	-2.86543100	-1.08979800	-0.12292300
C	-4.23605800	-0.66076600	-0.16705200
C	-4.22969300	0.70019400	-0.16734200
C	-2.85514000	1.11642500	-0.12292500
N	-2.04982900	0.00953500	-0.10225500
C	-2.43381400	-2.41122000	-0.11964100
C	-2.41125600	2.43376100	-0.11966900
C	-1.08978200	2.86527300	-0.12295200
C	-0.66077100	4.23594300	-0.16733500

C	0.70020600	4.22960800	-0.16725100
C	1.11643100	2.85500800	-0.12294200
N	0.00956500	2.04981200	-0.10193300
C	2.43382200	2.41120800	-0.11962500
C	2.86541400	1.08977900	-0.12289900
C	4.23604900	0.66076000	-0.16697200
C	4.22969800	-0.70019900	-0.16739800
C	2.85515100	-1.11643700	-0.12290700
N	2.04982300	-0.00956900	-0.10225100
C	2.41127000	-2.43378100	-0.11965400
C	1.08978600	-2.86528600	-0.12293100
C	0.66077200	-4.23594700	-0.16749500
C	-0.70020400	-4.22960500	-0.16706400
C	-1.11641600	-2.85499500	-0.12294600
N	-0.00953900	-2.04981000	-0.10193200
H	-5.09028300	-1.32931200	-0.19939100
H	-5.07764000	1.37667300	-0.19991400
H	-1.32943200	5.09007300	-0.19959700
H	1.37679100	5.07747700	-0.19944300
H	5.09026700	1.32931800	-0.19926300
H	5.07764400	-1.37667800	-0.20002500
H	1.32943600	-5.09007100	-0.19989100
H	-1.37680100	-5.07747000	-0.19911800
Ru	-0.00001300	0.00001700	0.15051200
O	0.00002800	-0.00000500	1.89714400
H	-3.20784700	-3.17822200	-0.13613300
H	-3.17813100	3.20791700	-0.13628700
H	3.17814100	-3.20793900	-0.13632600
H	3.20788100	3.17818300	-0.13614300

³RuO

C	1.09634200	2.86441700	-0.12157600
C	0.67053000	4.23687300	-0.16160700
C	-0.69044800	4.23368700	-0.16160400
C	-1.10983400	2.85925400	-0.12158000
N	-0.00483700	2.05266500	-0.10452400
C	2.41707300	2.42847600	-0.11791700
C	-2.42847900	2.41707100	-0.11793000

C	-2.86442500	1.09634200	-0.12147500
C	-4.23688500	0.67052900	-0.16131000
C	-4.23369700	-0.69045000	-0.16133200
C	-2.85926100	-1.10983500	-0.12145600
N	-2.05266900	-0.00483800	-0.10451200
C	-2.41707400	-2.42847900	-0.11789300
C	-1.09634300	-2.86442000	-0.12153700
C	-0.67053000	-4.23687700	-0.16152700
C	0.69044800	-4.23368900	-0.16154400
C	1.10983400	-2.85925600	-0.12152800
N	0.00483600	-2.05266700	-0.10449100
C	2.42847800	-2.41707300	-0.11787700
C	2.86442400	-1.09634300	-0.12144100
C	4.23688600	-0.67053100	-0.16125300
C	4.23369600	0.69044700	-0.16133400
C	2.85926100	1.10983300	-0.12145500
N	2.05266900	0.00483600	-0.10450200
H	1.34073900	5.08991200	-0.19120900
H	-1.36465800	5.08356600	-0.19120100
H	3.18584800	3.20090300	-0.13155400
H	-3.20090300	3.18584900	-0.13155900
H	-5.08992800	1.34073800	-0.19079800
H	-5.08357900	-1.36466000	-0.19083100
H	-3.18584900	-3.20090500	-0.13151500
H	-1.34073800	-5.08991700	-0.19110600
H	1.36465800	-5.08356800	-0.19113200
H	3.20090300	-3.18585000	-0.13148600
H	5.08992900	-1.34074000	-0.19070900
H	5.08357900	1.36465700	-0.19085200
Ru	-0.00000100	0.00000100	0.14224900
O	0.00000900	0.00001600	1.89153600

¹Ru (por*) O₂ (OSS)

C-C_R	0	2.55409300	1.72319900	-0.01429300	H
C-C_R	0	2.99239500	3.10188300	-0.03990700	H
C-C_R	0	1.88462100	3.87896900	-0.04450200	H
C-C_R	0	0.73918000	2.99617200	-0.01813500	H
N-N_R	0	1.19302300	1.71463500	-0.00429900	H

C-C_R	0	3.39624000	0.60197400	0.00086300	H
C-C_R	0	-0.60407400	3.40045600	-0.00404600	H
C-C_R	0	-1.71970400	2.55422600	0.01322600	H
C-C_R	0	-3.09615200	2.98866700	0.03984500	H
C-C_R	0	-3.87591500	1.88160100	0.04150100	H
C-C_R	0	-3.00035500	0.73531600	0.01826200	H
N-N_R	0	-1.71181700	1.18565900	0.00449400	H
C-C_R	0	-3.41026200	-0.60427500	0.00697300	H
C-C_R	0	-2.56306100	-1.71832200	-0.00769800	H
C-C_R	0	-2.99078100	-3.09465500	-0.03073200	H
C-C_R	0	-1.87953200	-3.86905200	-0.03635200	H
C-C_R	0	-0.73469400	-2.99272200	-0.01373800	H
N-N_R	0	-1.19419800	-1.70088000	-0.00019300	H
C-C_R	0	0.60241100	-3.40590200	-0.00375600	H
C-C_R	0	1.72316300	-2.56250400	0.00996600	H
C-C_R	0	3.10163300	-2.99449400	0.03474200	H
C-C_R	0	3.87310900	-1.88236900	0.03506200	H
C-C_R	0	2.98829100	-0.73903400	0.01250100	H
N-N_R	0	1.70501800	-1.20219800	0.00009500	H
H-H_	0	4.02433900	3.43776300	-0.05453500	H
H-H_	0	1.84791900	4.96345700	-0.06463100	H
H-H_	0	-3.43240800	4.02044300	0.05628300	H
H-H_	0	-4.96050600	1.84799500	0.05835100	H
H-H_	0	-4.02122400	-3.43496900	-0.04269100	H
H-H_	0	-1.84343700	-4.95354100	-0.05499400	H
H-H_	0	3.44167600	-4.02493100	0.05118100	H
H-H_	0	4.95758500	-1.84224000	0.05021800	H
Ru-Ru6+2	0	-0.02079900	-0.01146500	0.00005300	H
O-O_3	0	0.13229000	0.07635000	-1.74332300	H
O-O_3	0	0.13760300	0.07687500	1.74291700	H
C-C_3	0	0.98674400	-5.15652300	-2.63581500	L
C-C_3	0	1.39024700	-7.36759500	-2.63598300	L
C-C_R	0	1.29741200	-6.94874000	-1.19973800	L
C-C_3	0	0.36659300	-6.41168000	-3.24106200	L
H-H_	0	0.37280200	-6.41020100	-4.35608700	L
H-H_	0	-0.67169900	-6.60004700	-2.87770500	L
C-C_3	0	2.42077600	-5.24674800	-3.19757500	L
H-H_	0	2.45686900	-4.84182200	-4.23269500	L

H-H_	0	3.14670100	-4.69569000	-2.55989900	L
C-C_3	0	2.70036400	-6.77389600	-3.19671500	L
H-H_	0	2.87968100	-7.14011900	-4.23139400	L
H-H_	0	3.57343600	-7.03032700	-2.55661700	L
H-H_	0	0.44867300	-4.20526800	-2.83363900	L
H-H_	0	1.22461100	-8.44793000	-2.83306200	L
C-C_3	0	-0.19152000	-7.31006500	3.17637500	L
C-C_3	0	1.23939800	-7.40953300	2.60558100	L
C-C_3	0	0.85041100	-5.19596600	2.61800500	L
C-C_3	0	-0.45941700	-5.78086200	3.18575700	L
H-H_	0	-0.92557800	-7.85086900	2.53886700	L
H-H_	0	-0.22553800	-7.72027800	4.20953100	L
H-H_	0	-1.33561100	-5.51323400	2.55489300	L
H-H_	0	-0.62703700	-5.41824400	4.22361300	L
C-C_3	0	1.87173400	-6.16048600	3.21203800	L
H-H_	0	2.90837100	-5.97507700	2.84245900	L
H-H_	0	1.87292400	-6.16624200	4.32705800	L
C-C_R	0	1.17149700	-6.97809000	1.17165900	L
C-C_R	0	0.92941300	-5.61152900	1.17805400	L
H-H_	0	1.77095100	-8.36610800	2.79482400	L
H-H_	0	1.02607800	-4.11798700	2.81963300	L
C-C_R	0	0.85895500	-4.86458900	-0.00804000	L
C-C_R	0	1.36618100	-7.69530100	-0.01611700	L
H-H_	0	1.55880400	-8.75973700	-0.01908300	L
C-C_R	0	1.05013500	-5.58316200	-1.19832900	L
C-C_3	0	-5.21458400	-0.72704200	-2.61215300	L
C-C_3	0	-7.42658900	-1.12503700	-2.60633100	L
C-C_R	0	-6.97804600	-1.17651000	-1.17696200	L
C-C_3	0	-6.47952600	-0.04785000	-3.12651700	L
H-H_	0	-6.50079400	0.05678300	-4.23641400	L
H-H_	0	-6.65634700	0.94951600	-2.65790100	L
C-C_3	0	-5.32114000	-2.09850600	-3.31035600	L
H-H_	0	-4.93646300	-2.03347400	-4.35176800	L
H-H_	0	-4.76039800	-2.88423900	-2.75701900	L
C-C_3	0	-6.84915000	-2.37381700	-3.30677900	L
H-H_	0	-7.23640800	-2.44810300	-4.34666200	L
H-H_	0	-7.09634800	-3.30598000	-2.75210300	L
H-H_	0	-4.26569500	-0.17346800	-2.77570200	L

H-H_	0	-8.51009400	-0.93891400	-2.76345800	L
C-C_3	0	-7.24208000	-0.10982700	3.31961800	L
C-C_3	0	-7.36037500	-1.48389100	2.62565800	L
C-C_3	0	-5.14490900	-1.10518100	2.62874800	L
C-C_3	0	-5.71155500	0.15129400	3.32147700	L
H-H_	0	-7.79185100	0.67995600	2.76131000	L
H-H_	0	-7.63120300	-0.16677300	4.35989000	L
H-H_	0	-5.45185100	1.07841500	2.76383400	L
H-H_	0	-5.32729700	0.22577700	4.36240300	L
C-C_3	0	-6.10300100	-2.17194900	3.14851300	L
H-H_	0	-5.93005900	-3.17215500	2.68453200	L
H-H_	0	-6.08697500	-2.27239900	4.25889200	L
C-C_R	0	-6.95670300	-1.28949600	1.19523400	L
C-C_R	0	-5.58920600	-1.05372500	1.19632900	L
H-H_	0	-8.31577000	-2.02696100	2.78570300	L
H-H_	0	-4.06419500	-1.30217800	2.79255900	L
C-C_R	0	-4.86794300	-0.86360600	0.00791300	L
C-C_R	0	-7.70004500	-1.36100400	0.00963500	L
H-H_	0	-8.76568900	-1.54642100	0.01039500	L
C-C_R	0	-5.61198000	-0.93244100	-1.17972500	L
C-C_3	0	5.12171200	1.10114000	2.62957500	L
C-C_3	0	7.33650600	1.48359600	2.63478500	L
C-C_R	0	6.93886200	1.28579000	1.20320800	L
C-C_3	0	6.07589600	2.17047500	3.15130100	L
H-H_	0	6.05529000	2.27291800	4.26141800	L
H-H_	0	5.90321000	3.16954600	2.68477900	L
C-C_3	0	5.68796700	-0.15321100	3.32673000	L
H-H_	0	5.29972000	-0.22672800	4.36624700	L
H-H_	0	5.43240500	-1.08178000	2.76958700	L
C-C_3	0	7.21799200	0.11071600	3.33077000	L
H-H_	0	7.60274500	0.17047500	4.37251800	L
H-H_	0	7.77169300	-0.67903500	2.77630200	L
H-H_	0	4.04003100	1.29634500	2.78900900	L
H-H_	0	8.29034600	2.02864800	2.79748900	L
C-C_3	0	6.84938800	2.37667300	-3.29547300	L
C-C_3	0	7.42437600	1.12623500	-2.59614300	L
C-C_3	0	5.21252000	0.72731400	-2.61196000	L
C-C_3	0	5.32150400	2.10073200	-3.30609400	L

H-H_	0	7.09397700	3.30734200	-2.73711200	L
H-H_	0	7.24102600	2.45403500	-4.33348200	L
H-H_	0	4.75825600	2.88480000	-2.75298700	L
H-H_	0	4.94123000	2.03840700	-4.34927500	L
C-C_3	0	6.47995300	0.05007200	-3.12303100	L
H-H_	0	6.65549200	-0.94845600	-2.65640800	L
H-H_	0	6.50597500	-0.05152700	-4.23311600	L
C-C_R	0	6.96985100	1.17373900	-1.16864900	L
C-C_R	0	5.60382500	0.92906700	-1.17730700	L
H-H_	0	8.50864800	0.94097000	-2.74913000	L
H-H_	0	4.26460300	0.17372600	-2.78092500	L
C-C_R	0	4.85466400	0.85955200	0.00730800	L
C-C_R	0	7.68673000	1.35899800	0.02075100	L
H-H_	0	8.75196100	1.54692900	0.02580300	L
C-C_R	0	5.57158600	1.04825400	1.19886800	L
C-C_3	0	-0.98525800	5.15216300	-2.63495800	L
C-C_3	0	-1.38287700	7.36423200	-2.63415600	L
C-C_R	0	-1.29786700	6.94346900	-1.19803400	L
C-C_3	0	-0.35894400	6.40634700	-3.23571600	L
H-H_	0	-0.35998300	6.40630000	-4.35074700	L
H-H_	0	0.67815600	6.59141600	-2.86725700	L
C-C_3	0	-2.41651600	5.24686300	-3.20299000	L
H-H_	0	-2.44914100	4.84321900	-4.23872800	L
H-H_	0	-3.14670200	4.69704600	-2.56903000	L
C-C_3	0	-2.69195800	6.77476300	-3.20165300	L
H-H_	0	-2.86534100	7.14270500	-4.23672500	L
H-H_	0	-3.56731600	7.03287800	-2.56537500	L
H-H_	0	-0.44893100	4.19963700	-2.83167600	L
H-H_	0	-1.21346500	8.44434100	-2.82899700	L
C-C_3	0	0.19931800	7.30056500	3.17208000	L
C-C_3	0	-1.23388200	7.40303400	2.60754500	L
C-C_3	0	-0.84969900	5.18857600	2.61892300	L
C-C_3	0	0.46383600	5.77076000	3.18093600	L
H-H_	0	0.93175500	7.83940900	2.53104800	L
H-H_	0	0.23881400	7.71118900	4.20485900	L
H-H_	0	1.33678400	5.50094500	2.54654400	L
H-H_	0	0.63506000	5.40818400	4.21822700	L
C-C_3	0	-1.86626500	6.15549200	3.21713400	L

H-H_	0	-2.90491500	5.97222000	2.85217300	L
H-H_	0	-1.86256400	6.16163000	4.33214400	L
C-C_R	0	-1.17307900	6.97112100	1.17352200	L
C-C_R	0	-0.93414500	5.60420100	1.17926300	L
H-H_	0	-1.76259000	8.36076000	2.79867400	L
H-H_	0	-1.02689000	4.11099900	2.82157500	L
C-C_R	0	-0.86459800	4.85810000	-0.00726800	L
C-C_R	0	-1.36447400	7.68961500	-0.01400200	L
H-H_	0	-1.55153400	8.75494000	-0.01657500	L
C-C_R	0	-1.05410000	5.57736200	-1.19726700	L

R_1TS1 (OSS)

C-C_R	0	2.86447000	-0.82186300	-0.70090900	H
C-C_R	0	4.19330800	-0.26750300	-0.78223700	H
C-C_R	0	4.07223900	1.08109200	-0.78509800	H
C-C_R	0	2.66526900	1.39293100	-0.72709700	H
N-N_R	0	1.96946300	0.21294000	-0.70369100	H
C-C_R	0	2.55954600	-2.18205000	-0.57468600	H
C-C_R	0	2.12648400	2.68301200	-0.67859600	H
C-C_R	0	0.76127200	3.00455100	-0.67029900	H
C-C_R	0	0.21359500	4.34281800	-0.61820400	H
C-C_R	0	-1.13187500	4.22160800	-0.55921000	H
C-C_R	0	-1.43893700	2.80584900	-0.55455600	H
N-N_R	0	-0.26790200	2.11846000	-0.66593200	H
C-C_R	0	-2.71834100	2.25958400	-0.38343000	H
C-C_R	0	-3.03271300	0.89613700	-0.27603000	H
C-C_R	0	-4.36530400	0.35547600	-0.12168800	H
C-C_R	0	-4.25384000	-0.99361200	-0.08866900	H
C-C_R	0	-2.84801300	-1.30918000	-0.20516900	H
N-N_R	0	-2.15429800	-0.14444000	-0.30877100	H
C-C_R	0	-2.29748000	-2.60056500	-0.18156700	H
C-C_R	0	-0.93221400	-2.90516100	-0.22878500	H
C-C_R	0	-0.37536200	-4.23391400	-0.15907000	H
C-C_R	0	0.97076100	-4.11924700	-0.25624200	H
C-C_R	0	1.27737400	-2.71734900	-0.39716700	H
N-N_R	0	0.10492800	-2.01317000	-0.35508200	H
H-H_	0	5.11571000	-0.83845200	-0.81508500	H

H-H_	0	4.87826000	1.80663200	-0.82854100	H
H-H_	0	0.78840900	5.26325000	-0.62628300	H
H-H_	0	-1.85711700	5.02760600	-0.50789200	H
H-H_	0	-5.28099500	0.93475800	-0.05698700	H
H-H_	0	-5.05929100	-1.71392600	0.01407300	H
H-H_	0	-0.94411700	-5.15162400	-0.04769700	H
H-H_	0	1.69643900	-4.92623600	-0.24151000	H
Ru-Ru6+2	0	-0.07001000	0.03285200	-0.57331000	H
O-O_3	0	-0.41887500	-0.00518400	-2.28828400	H
O-O_3	0	-0.04064600	0.38683700	1.24286300	H
C-C_3	0	-3.67278700	-3.75922800	-2.79687500	L
C-C_3	0	-5.15093400	-5.45166400	-2.81146900	L
C-C_R	0	-4.73078900	-5.26163800	-1.38518900	L
C-C_3	0	-5.09793700	-4.00168000	-3.28256700	L
H-H_	0	-5.20918200	-3.89448200	-4.38684700	L
H-H_	0	-5.84619300	-3.35071500	-2.77070500	L
C-C_3	0	-2.91781400	-4.87094200	-3.55427700	L
H-H_	0	-2.68486000	-4.54343500	-4.59121400	L
H-H_	0	-1.97523600	-5.15259100	-3.03412100	L
C-C_3	0	-3.93897000	-6.04041800	-3.56518800	L
H-H_	0	-4.22226600	-6.30364300	-4.60794200	L
H-H_	0	-3.53563900	-6.94156000	-3.05234500	L
H-H_	0	-3.28197000	-2.72897600	-2.93603400	L
H-H_	0	-6.11713400	-5.97821500	-2.96166500	L
C-C_3	0	-5.51182200	-4.72113000	3.14164700	L
C-C_3	0	-4.76756300	-5.85358500	2.40122300	L
C-C_3	0	-3.26186400	-4.18713700	2.42644300	L
C-C_3	0	-4.46995400	-3.57027700	3.16013300	L
H-H_	0	-6.44119500	-4.42383400	2.60723800	L
H-H_	0	-5.76518700	-5.03692000	4.17745700	L
H-H_	0	-4.84814700	-2.66426100	2.63676600	L
H-H_	0	-4.19428400	-3.30589000	4.20457000	L
C-C_3	0	-3.34597600	-5.63230600	2.90563300	L
H-H_	0	-2.59980900	-6.29714800	2.40879100	L
H-H_	0	-3.25167100	-5.73370300	4.01205800	L
C-C_R	0	-4.59347000	-5.40983700	0.98031300	L
C-C_R	0	-3.66670700	-4.37625500	0.99449200	L
H-H_	0	-5.18015600	-6.87547900	2.53844600	L

H-H_	0	-2.28705300	-3.68793800	2.58851100	L
C-C_R	0	-3.25084900	-3.73567900	-0.18401500	L
C-C_R	0	-5.15730500	-5.89031500	-0.20853600	L
H-H_	0	-5.87941800	-6.69561200	-0.21711500	L
C-C_R	0	-3.81618000	-4.21810300	-1.37487700	L
C-C_3	0	-4.36445300	3.49925300	-2.81605700	L
C-C_3	0	-6.07644100	4.93647200	-2.57917600	L
C-C_R	0	-5.60254600	4.60267100	-1.19687100	L
C-C_3	0	-4.74268600	4.88877800	-3.31854600	L
H-H_	0	-4.85318000	4.93937000	-4.42693700	L
H-H_	0	-4.03075500	5.67955500	-2.98178300	L
C-C_3	0	-5.57565500	2.67829400	-3.30489700	L
H-H_	0	-5.44568900	2.39507000	-4.37243100	L
H-H_	0	-5.72165200	1.76015300	-2.69369100	L
C-C_3	0	-6.75856300	3.67064600	-3.14135000	L
H-H_	0	-7.22662400	3.88826800	-4.12643700	L
H-H_	0	-7.53040700	3.27680100	-2.44358700	L
H-H_	0	-3.36718600	3.12427300	-3.12972200	L
H-H_	0	-6.65328200	5.88067800	-2.67435200	L
C-C_3	0	-4.28396900	5.58270700	3.13757100	L
C-C_3	0	-5.50196000	4.77923800	2.63244900	L
C-C_3	0	-3.80369900	3.32509300	2.40547900	L
C-C_3	0	-3.11117700	4.57730900	2.98091500	L
H-H_	0	-4.11957300	6.50157700	2.53230500	L
H-H_	0	-4.42044000	5.86221800	4.20531200	L
H-H_	0	-2.32676400	4.96396700	2.29314700	L
H-H_	0	-2.65575600	4.34757600	3.96917500	L
C-C_3	0	-5.14349200	3.38259000	3.13149400	L
H-H_	0	-5.85841200	2.59960700	2.78305000	L
H-H_	0	-5.04408200	3.32448600	4.24056200	L
C-C_R	0	-5.31082500	4.57042700	1.16024600	L
C-C_R	0	-4.26101800	3.67446200	1.01950100	L
H-H_	0	-6.49744300	5.16552800	2.93760100	L
H-H_	0	-3.23972300	2.37375600	2.50209000	L
C-C_R	0	-3.84004300	3.21522800	-0.23769100	L
C-C_R	0	-6.02195600	5.06391600	0.05826400	L
H-H_	0	-6.84523100	5.75659700	0.16967000	L
C-C_R	0	-4.54661400	3.71391200	-1.34225300	L

C-C_3	0	4.29417200	-3.11811300	1.93141800	L
C-C_3	0	6.05974900	-4.50146200	1.79758400	L
C-C_R	0	5.49803600	-4.38836100	0.41273800	L
C-C_3	0	5.77320700	-3.08929400	2.29995800	L
H-H_	0	5.94950300	-2.96763900	3.39428000	L
H-H_	0	6.34229600	-2.30629600	1.74444800	L
C-C_3	0	3.82641200	-4.35679400	2.72444600	L
H-H_	0	3.62681000	-4.08819200	3.78434600	L
H-H_	0	2.91259100	-4.80778500	2.27809200	L
C-C_3	0	5.04521800	-5.31299800	2.63035400	L
H-H_	0	5.45646800	-5.52489900	3.64172600	L
H-H_	0	4.77743500	-6.27061800	2.13137000	L
H-H_	0	3.73073200	-2.17980300	2.11736500	L
H-H_	0	7.11659400	-4.83666100	1.86142600	L
C-C_3	0	5.89043200	-3.60328800	-4.11343100	L
C-C_3	0	5.39557400	-4.87378700	-3.38913600	L
C-C_3	0	3.62345900	-3.49642700	-3.26699100	L
C-C_3	0	4.66598500	-2.65234000	-4.02907500	L
H-H_	0	6.78308400	-3.16738900	-3.61252600	L
H-H_	0	6.13607600	-3.83290600	-5.17351100	L
H-H_	0	4.91107200	-1.71400500	-3.48396700	L
H-H_	0	4.29247500	-2.40220000	-5.04624900	L
C-C_3	0	3.93040400	-4.88656700	-3.81428100	L
H-H_	0	3.33950300	-5.68954100	-3.31266500	L
H-H_	0	3.79427300	-4.96331400	-4.91832400	L
C-C_R	0	5.22785100	-4.51750300	-1.94290200	L
C-C_R	0	4.13514600	-3.66610000	-1.86646900	L
H-H_	0	5.96995900	-5.80243300	-3.59163600	L
H-H_	0	2.56848300	-3.16122500	-3.35805000	L
C-C_R	0	3.69079600	-3.13540600	-0.64587800	L
C-C_R	0	5.95228000	-4.90427800	-0.80813700	L
H-H_	0	6.81506700	-5.55356900	-0.87169700	L
C-C_R	0	4.40658500	-3.53430800	0.49396000	L
C-C_3	0	3.51592000	4.35480300	-3.01954900	L
C-C_3	0	5.01009800	5.99781500	-2.67486300	L
C-C_R	0	4.56233300	5.53546500	-1.32105900	L
C-C_3	0	4.95240400	4.66980900	-3.42384300	L
H-H_	0	5.08372100	4.78116700	-4.52549000	L

H-H_	0	5.68482400	3.92118300	-3.03816000	L
C-C_3	0	2.78690600	5.60396600	-3.55618300	L
H-H_	0	2.57294800	5.49046100	-4.64158500	L
H-H_	0	1.83618300	5.79043000	-3.00965400	L
C-C_3	0	3.81828200	6.73947500	-3.31713500	L
H-H_	0	4.12389900	7.20081800	-4.28180900	L
H-H_	0	3.41318600	7.52585800	-2.64243900	L
H-H_	0	3.11756400	3.37707400	-3.36437900	L
H-H_	0	5.98378900	6.53123500	-2.70249900	L
C-C_3	0	5.37478600	4.00694500	2.95802500	L
C-C_3	0	4.62341500	5.27846500	2.50670100	L
C-C_3	0	3.11274200	3.64822400	2.17202600	L
C-C_3	0	4.32991000	2.88163700	2.72870000	L
H-H_	0	6.29550600	3.83975100	2.35637400	L
H-H_	0	5.64388200	4.07788300	4.03477100	L
H-H_	0	4.69843600	2.11814200	2.00865700	L
H-H_	0	4.06892200	2.38669700	3.68961000	L
C-C_3	0	3.20758100	4.94526200	2.96827200	L
H-H_	0	2.45594000	5.70552000	2.64813300	L
H-H_	0	3.12932000	4.79005300	4.06978100	L
C-C_R	0	4.42992000	5.17243200	1.02354300	L
C-C_R	0	3.50020300	4.16499200	0.81611500	L
H-H_	0	5.03996800	6.24205600	2.86897200	L
H-H_	0	2.13954300	3.11524000	2.22744200	L
C-C_R	0	3.07870500	3.79645100	-0.47059200	L
C-C_R	0	4.99852800	5.89065500	-0.03689000	L
H-H_	0	5.73701400	6.66425000	0.12493300	L
C-C_R	0	3.63741800	4.52192900	-1.53329500	L
C-C_R	0	2.75046400	-1.15099400	4.90037500	H
C-C_R	0	1.65163400	-1.58543100	4.17311800	H
C-C_R	0	0.54297700	-0.75153600	3.96403800	H
C-C_R	0	0.57794500	0.54458600	4.50418800	H
C-C_R	0	1.67810100	0.98101400	5.22794100	H
C-C_R	0	2.76861200	0.13697000	5.43053900	H
H-H_	0	3.59950300	-1.81585000	5.05233100	H
H-H_	0	1.63202700	-2.58923500	3.74784900	H
H-H_	0	-0.25578500	1.22274600	4.32734100	H
H-H_	0	1.69260900	1.99345900	5.62912500	H

H-H_	0	3.63265900	0.48538800	5.99408100	H
C-C_3	0	-0.55205100	-1.20142600	3.09944600	H
C-C_3	0	-1.96705900	-0.75494300	3.35930000	H
H-H_	0	-0.45069200	-2.25286500	2.80166800	H
H-H_	0	-0.27775900	-0.54599300	2.03017800	H
H-H_	0	-2.62890900	-1.07562900	2.54334900	H
H-H_	0	-2.35978300	-1.17012400	4.29993900	H
H-H_	0	-2.03716200	0.33872700	3.41852700	H

R_1INT (OSS)

C-C_R	0	-0.28562400	-2.99142000	-0.56517100	H
C-C_R	0	0.42321400	-4.23846900	-0.36982100	H
C-C_R	0	1.74394200	-3.95180000	-0.33494400	H
C-C_R	0	1.87346200	-2.51918000	-0.49185000	H
N-N_R	0	0.63463700	-1.98771700	-0.64040100	H
C-C_R	0	-1.67663400	-2.85690800	-0.66603200	H
C-C_R	0	3.08078000	-1.80300400	-0.46619900	H
C-C_R	0	3.20064000	-0.41024200	-0.47716500	H
C-C_R	0	4.44532600	0.31965500	-0.48598800	H
C-C_R	0	4.14705400	1.63797200	-0.41660700	H
C-C_R	0	2.71095400	1.75582600	-0.35439800	H
N-N_R	0	2.17310100	0.49914600	-0.42874200	H
C-C_R	0	1.99882600	2.94899500	-0.19194100	H
C-C_R	0	0.60300000	3.05978200	-0.14124700	H
C-C_R	0	-0.13117400	4.27510000	0.10285200	H
C-C_R	0	-1.45132100	3.97889700	0.02084000	H
C-C_R	0	-1.56499200	2.57323100	-0.27313600	H
N-N_R	0	-0.29594000	2.04524500	-0.33796500	H
C-C_R	0	-2.76514700	1.88997400	-0.50068100	H
C-C_R	0	-2.88344500	0.50717600	-0.70837500	H
C-C_R	0	-4.10470400	-0.20772400	-0.99509700	H
C-C_R	0	-3.79797900	-1.52630700	-1.02875300	H
C-C_R	0	-2.38226500	-1.64818500	-0.77196600	H
N-N_R	0	-1.86923800	-0.39602200	-0.60765700	H
H-H_	0	-0.03289000	-5.21710900	-0.26183000	H
H-H_	0	2.56114900	-4.65264900	-0.19823700	H
H-H_	0	5.43524300	-0.12192800	-0.54000500	H
H-H_	0	4.84939900	2.46523100	-0.40751700	H

H-H_	0	0.30635100	5.24573100	0.31393200	H
H-H_	0	-2.28170700	4.66602300	0.14856400	H
H-H_	0	-5.08117900	0.23912600	-1.15118000	H
H-H_	0	-4.47753800	-2.35028700	-1.22225000	H
Ru-Ru6+2	0	0.17965900	0.06260000	-0.59360900	H
O-O_3	0	0.07320000	-0.01212900	-2.33135900	H
O-O_3	0	0.06167800	-0.34444100	1.30786000	H
C-C_3	0	-3.57869300	3.71727600	-2.97166200	L
C-C_3	0	-5.53318900	4.81241000	-3.14737600	L
C-C_R	0	-5.53052800	4.15217200	-1.80175900	L
C-C_3	0	-4.04780700	5.13720900	-3.26934900	L
H-H_	0	-3.75753500	5.49100000	-4.28616300	L
H-H_	0	-3.70050500	5.87598900	-2.50832500	L
C-C_3	0	-4.31607100	2.93392900	-4.07739800	L
H-H_	0	-3.74862900	2.98537300	-5.03243500	L
H-H_	0	-4.46664700	1.86881700	-3.79257100	L
C-C_3	0	-5.66584700	3.69123600	-4.20031800	L
H-H_	0	-5.77979100	4.12679200	-5.21726600	L
H-H_	0	-6.53052700	3.02557300	-3.98363400	L
H-H_	0	-2.47864100	3.57214200	-2.92806900	L
H-H_	0	-6.22958300	5.67008600	-3.26024700	L
C-C_3	0	-6.35527400	3.66508900	2.75176000	L
C-C_3	0	-7.00626100	2.97987300	1.53302900	L
C-C_3	0	-5.05090600	1.89320600	1.73578100	L
C-C_3	0	-5.00237000	2.91836600	2.88916300	L
H-H_	0	-6.20742900	4.75423500	2.57964800	L
H-H_	0	-6.97993000	3.51507500	3.65960700	L
H-H_	0	-4.14046900	3.61386400	2.78262700	L
H-H_	0	-4.94044800	2.39786400	3.86974200	L
C-C_3	0	-6.53425800	1.54251000	1.73106800	L
H-H_	0	-6.81794500	0.87125600	0.88593100	L
H-H_	0	-6.88106400	1.09394300	2.69117100	L
C-C_R	0	-6.18492400	3.34682400	0.33375800	L
C-C_R	0	-4.97713600	2.67130800	0.45330400	L
H-H_	0	-8.10249600	3.12230800	1.42643100	L
H-H_	0	-4.35225700	1.03478300	1.82347900	L
C-C_R	0	-4.01045500	2.69313400	-0.56742400	L
C-C_R	0	-6.50984100	4.09867400	-0.80241400	L

H-H_	0	-7.46624600	4.59252000	-0.90959100	L
C-C_R	0	-4.32410400	3.47591400	-1.69065600	L
C-C_3	0	2.60659900	4.96364000	-2.58373600	L
C-C_3	0	3.76620800	6.87596900	-2.36161100	L
C-C_R	0	3.70169500	6.25290200	-0.99981600	L
C-C_3	0	3.83732000	5.61050700	-3.21097800	L
H-H_	0	3.72171700	5.80740000	-4.30241800	L
H-H_	0	4.77068800	5.02343400	-3.03861700	L
C-C_3	0	1.54391700	6.04775700	-2.86003200	L
H-H_	0	1.15067700	5.94834100	-3.89555100	L
H-H_	0	0.69953700	5.99107200	-2.13931000	L
C-C_3	0	2.34371000	7.36873000	-2.70273400	L
H-H_	0	2.35007900	7.93912100	-3.65742500	L
H-H_	0	1.92587500	8.00684500	-1.89281900	L
H-H_	0	2.35917300	3.94197900	-2.94229700	L
H-H_	0	4.58342500	7.61225500	-2.51458400	L
C-C_3	0	5.50071700	4.82144300	3.03944000	L
C-C_3	0	4.43496200	5.89829700	2.74535600	L
C-C_3	0	3.28653000	3.97906300	2.53624700	L
C-C_3	0	4.70641900	3.49574800	2.89772900	L
H-H_	0	6.34526800	4.87254000	2.31704600	L
H-H_	0	5.89121500	4.93562500	4.07446400	L
H-H_	0	5.13442300	2.84358000	2.10586700	L
H-H_	0	4.69196600	2.94194700	3.86206300	L
C-C_3	0	3.20139700	5.25270800	3.37005400	L
H-H_	0	2.26546900	5.83106600	3.18259800	L
H-H_	0	3.30847500	5.06852500	4.46453800	L
C-C_R	0	4.07031500	5.77236200	1.29675500	L
C-C_R	0	3.35937800	4.58753400	1.16592100	L
H-H_	0	4.67601300	6.92535700	3.09231700	L
H-H_	0	2.47521300	3.24010000	2.69239400	L
C-C_R	0	2.78414000	4.19796300	-0.05462700	L
C-C_R	0	4.26652600	6.64703300	0.22007200	L
H-H_	0	4.81875600	7.57120900	0.32476300	L
C-C_R	0	2.98453600	5.07256600	-1.13469600	L
C-C_3	0	-3.21420400	-3.76953400	1.96344800	L
C-C_3	0	-4.44505300	-5.64329900	2.12460600	L
C-C_R	0	-3.91940100	-5.59476200	0.72113000	L

C-C_3	0	-3.26771000	-5.00396900	2.85640800	L
H-H_	0	-3.49011900	-4.76413300	3.92253100	L
H-H_	0	-2.33731300	-5.61772100	2.80255900	L
C-C_3	0	-4.65093000	-3.23043100	2.13889900	L
H-H_	0	-4.73265400	-2.62851300	3.06813100	L
H-H_	0	-4.96938200	-2.60812400	1.27611300	L
C-C_3	0	-5.49969800	-4.52435600	2.25134200	L
H-H_	0	-6.00360700	-4.57765600	3.24136400	L
H-H_	0	-6.26223200	-4.58611700	1.44360200	L
H-H_	0	-2.39742600	-3.04823000	2.18012000	L
H-H_	0	-4.75640300	-6.64607300	2.48622900	L
C-C_3	0	-2.07224600	-7.29307100	-3.21736600	L
C-C_3	0	-3.47692500	-6.73274300	-2.91005100	L
C-C_3	0	-2.21833000	-4.87910800	-3.07889500	L
C-C_3	0	-1.20416700	-6.01246400	-3.33962500	L
H-H_	0	-1.70918200	-7.95829300	-2.40286800	L
H-H_	0	-2.08070100	-7.85402400	-4.17761200	L
H-H_	0	-0.37645500	-6.00591100	-2.59831600	L
H-H_	0	-0.78017300	-5.92289400	-4.36385200	L
C-C_3	0	-3.46195100	-5.45684500	-3.74653600	L
H-H_	0	-4.36930900	-4.82547900	-3.59255800	L
H-H_	0	-3.32635100	-5.64828100	-4.83663100	L
C-C_R	0	-3.42032100	-6.12743200	-1.53984000	L
C-C_R	0	-2.64184300	-4.98205900	-1.64176600	L
H-H_	0	-4.32494700	-7.42586900	-3.09404500	L
H-H_	0	-1.91019100	-3.86792500	-3.41968500	L
C-C_R	0	-2.48622500	-4.09413500	-0.56461800	L
C-C_R	0	-4.08933000	-6.47207500	-0.35760500	L
H-H_	0	-4.71302500	-7.35303500	-0.28727700	L
C-C_R	0	-3.15537400	-4.44157400	0.62088200	L
C-C_3	0	4.45829600	-3.43833900	-2.83593400	L
C-C_3	0	6.31672000	-4.67893700	-2.59779600	L
C-C_R	0	6.05446000	-4.04029900	-1.26728500	L
C-C_3	0	4.87878500	-4.88648300	-3.06334000	L
H-H_	0	4.80397400	-5.20257300	-4.12998900	L
H-H_	0	4.31448300	-5.60651600	-2.42401300	L
C-C_3	0	5.48371600	-2.69909500	-3.72011900	L
H-H_	0	5.14787800	-2.69342700	-4.78028500	L

H-H_	0	5.64147500	-1.65285300	-3.37564200	L
C-C_3	0	6.76758700	-3.55652400	-3.55672300	L
H-H_	0	7.07987800	-3.98497800	-4.53435300	L
H-H_	0	7.60526700	-2.96302600	-3.12803900	L
H-H_	0	3.39130800	-3.20628200	-3.03823900	L
H-H_	0	6.95832100	-5.58519500	-2.57759000	L
C-C_3	0	5.47866200	-4.18878800	3.29809600	L
C-C_3	0	6.53389900	-3.40848400	2.48459100	L
C-C_3	0	4.68459400	-2.15190700	2.25648300	L
C-C_3	0	4.20112000	-3.32074300	3.13926400	L
H-H_	0	5.32889500	-5.21558300	2.89690600	L
H-H_	0	5.78085900	-4.24932900	4.36666500	L
H-H_	0	3.37662300	-3.88722600	2.65186100	L
H-H_	0	3.85701700	-2.94314400	4.12714500	L
C-C_3	0	6.10703500	-1.97305600	2.77600700	L
H-H_	0	6.68877300	-1.21964000	2.19330600	L
H-H_	0	6.14872300	-1.71372500	3.85966200	L
C-C_R	0	6.13065400	-3.49701200	1.04347200	L
C-C_R	0	4.98876400	-2.72234400	0.90127200	L
H-H_	0	7.59447600	-3.65521000	2.70270000	L
H-H_	0	4.04747000	-1.24234700	2.26883900	L
C-C_R	0	4.32892700	-2.58994400	-0.33089100	L
C-C_R	0	6.70170900	-4.18767000	-0.03323800	L
H-H_	0	7.58202400	-4.80531400	0.08317000	L
C-C_R	0	4.90663100	-3.27301700	-1.41286900	L
C-C_R	0	-2.88957800	-1.61164300	5.05367800	H
C-C_R	0	-2.77546300	-0.38664500	4.42421200	H
C-C_R	0	-1.50505800	0.16455000	4.10934000	H
C-C_R	0	-0.35927800	-0.60044800	4.45571200	H
C-C_R	0	-0.48659200	-1.83352400	5.06887100	H
C-C_R	0	-1.74760400	-2.34974500	5.37639800	H
H-H_	0	-3.87536500	-2.00409700	5.29970500	H
H-H_	0	-3.67001700	0.18268700	4.17017400	H
H-H_	0	0.62910900	-0.21828100	4.20715000	H
H-H_	0	0.40766300	-2.40651400	5.31052900	H
H-H_	0	-1.84117800	-3.31986100	5.86148100	H
C-C_R	0	-1.40596100	1.42502700	3.47640800	H
C-C_3	0	-0.12925000	2.14590700	3.22364300	H

H-H_	0	-2.33987500	1.92897600	3.22593700	H
H-H_	0	-0.81795700	-0.12351800	1.66477900	H
H-H_	0	-0.30460600	3.08817200	2.69018700	H
H-H_	0	0.39722300	2.38460600	4.16296400	H
H-H_	0	0.56030900	1.54170500	2.61142500	H

S_1TS1 (OSS)

C-C_R	0	1.55853900	2.53910700	-0.66855300	H
C-C_R	0	1.47084300	3.97850300	-0.69394000	H
C-C_R	0	0.17893900	4.31536300	-0.46568300	H
C-C_R	0	-0.57242000	3.09195900	-0.32824800	H
N-N_R	0	0.29578400	2.04105600	-0.45799700	H
C-C_R	0	2.73678400	1.79144900	-0.78336200	H
C-C_R	0	-1.95513700	3.00972000	-0.11764400	H
C-C_R	0	-2.71720600	1.83379300	-0.12527100	H
C-C_R	0	-4.15221900	1.76061900	0.02372800	H
C-C_R	0	-4.50448400	0.45850200	-0.08702400	H
C-C_R	0	-3.29254200	-0.30510500	-0.27790300	H
N-N_R	0	-2.24112800	0.56891600	-0.30504200	H
C-C_R	0	-3.22176000	-1.69989200	-0.37428900	H
C-C_R	0	-2.04355100	-2.46040200	-0.42955600	H
C-C_R	0	-1.97230900	-3.90617800	-0.43479800	H
C-C_R	0	-0.66274500	-4.24255800	-0.39664900	H
C-C_R	0	0.09963500	-3.01080900	-0.38602500	H
N-N_R	0	-0.77688800	-1.97179500	-0.42120700	H
C-C_R	0	1.49921900	-2.91986100	-0.34822500	H
C-C_R	0	2.25758000	-1.74251400	-0.43238300	H
C-C_R	0	3.69936700	-1.67924000	-0.48807400	H
C-C_R	0	4.04441100	-0.37843400	-0.65091700	H
C-C_R	0	2.82208900	0.39151600	-0.67626700	H
N-N_R	0	1.77522700	-0.46780000	-0.53027200	H
H-H_	0	2.29842900	4.66091500	-0.85800500	H
H-H_	0	-0.23197500	5.31867300	-0.41521400	H
H-H_	0	-4.81532100	2.60455200	0.18431500	H
H-H_	0	-5.50748100	0.04788900	-0.02895900	H
H-H_	0	-2.82071800	-4.58279100	-0.45236300	H
H-H_	0	-0.24742000	-5.24530200	-0.38438400	H
H-H_	0	4.37355000	-2.52724500	-0.42172000	H

H-H_	0	5.04946900	0.02244000	-0.73687800	H
Ru-Ru6+2	0	-0.24425800	0.05723600	-0.47102800	H
O-O_3	0	-0.31008500	-0.11453400	-2.21449300	H
O-O_3	0	-0.17437900	-0.16330800	1.37242100	H
C-C_3	0	2.53044700	-4.67452600	-2.79821200	L
C-C_3	0	3.59018600	-6.64421400	-2.58268500	L
C-C_R	0	3.35755000	-6.12903800	-1.19433500	L
C-C_3	0	2.32991000	-6.11419900	-3.25974100	L
H-H_	0	2.34752500	-6.22587200	-4.36901900	L
H-H_	0	1.39495700	-6.57171100	-2.85702000	L
C-C_3	0	3.92926400	-4.38030900	-3.37848600	L
H-H_	0	3.85079700	-4.09367900	-4.45014600	L
H-H_	0	4.44526000	-3.57076800	-2.81706700	L
C-C_3	0	4.66247100	-5.74026000	-3.22766000	L
H-H_	0	4.95724000	-6.13909500	-4.22308100	L
H-H_	0	5.56453800	-5.65028100	-2.58275900	L
H-H_	0	1.72999200	-3.95827200	-3.08076800	L
H-H_	0	3.76524200	-7.73772700	-2.66615900	L
C-C_3	0	1.80238200	-6.58606600	3.13006300	L
C-C_3	0	3.23297900	-6.28215100	2.63545200	L
C-C_3	0	2.19235300	-4.30002600	2.43255600	L
C-C_3	0	1.08514300	-5.21610900	2.99237700	L
H-H_	0	1.31232700	-7.36918100	2.51017000	L
H-H_	0	1.82154200	-6.91317600	4.19281300	L
H-H_	0	0.21391200	-5.27555200	2.30371800	L
H-H_	0	0.74603200	-4.84873100	3.98583000	L
C-C_3	0	3.41328100	-4.86003100	3.15563500	L
H-H_	0	4.36931400	-4.39535800	2.81680600	L
H-H_	0	3.33888700	-4.78501200	4.26564400	L
C-C_R	0	3.13992400	-5.99466400	1.16722900	L
C-C_R	0	2.49482300	-4.77302100	1.04067100	L
H-H_	0	4.01455500	-7.01269700	2.93331900	L
H-H_	0	2.01678000	-3.20934200	2.54349000	L
C-C_R	0	2.24449700	-4.19211300	-0.21188700	L
C-C_R	0	3.58994000	-6.71871800	0.05548300	L
H-H_	0	4.07684100	-7.67943900	0.15525800	L
C-C_R	0	2.70508500	-4.91087100	-1.32618000	L
C-C_3	0	-4.99580900	-2.28545100	-2.95210900	L

C-C_3	0	-6.92119300	-3.44504200	-2.92491600	L
C-C_R	0	-6.42442500	-3.40532600	-1.51126300	L
C-C_3	0	-6.43959600	-2.07658600	-3.39721000	L
H-H_	0	-6.54253900	-1.93079000	-4.49787000	L
H-H_	0	-6.93903500	-1.23259700	-2.86446300	L
C-C_3	0	-4.63823500	-3.56807600	-3.73114500	L
H-H_	0	-4.34454200	-3.31821100	-4.77424000	L
H-H_	0	-3.81336500	-4.12934000	-3.23840900	L
C-C_3	0	-5.96817900	-4.36922600	-3.71316500	L
H-H_	0	-6.34658300	-4.52387900	-4.74744800	L
H-H_	0	-5.84601000	-5.35510500	-3.21232300	L
H-H_	0	-4.31258400	-1.42247000	-3.10052300	L
H-H_	0	-8.00592400	-3.64919200	-3.04742900	L
C-C_3	0	-6.80676100	-2.82484500	3.07429000	L
C-C_3	0	-6.47219200	-4.09303900	2.25993500	L
C-C_3	0	-4.53646900	-2.95145100	2.24042000	L
C-C_3	0	-5.46926000	-2.03655500	3.06040600	L
H-H_	0	-7.63070300	-2.24236700	2.60572500	L
H-H_	0	-7.09070300	-3.09663000	4.11465100	L
H-H_	0	-5.58542400	-1.03781700	2.58402100	L
H-H_	0	-5.07723900	-1.91033200	4.09343000	L
C-C_3	0	-5.02529200	-4.32617300	2.68421100	L
H-H_	0	-4.53739300	-5.16008100	2.12547900	L
H-H_	0	-4.91148100	-4.49950500	3.77978100	L
C-C_R	0	-6.24554200	-3.65818300	0.84341100	L
C-C_R	0	-5.05112100	-2.95175300	0.83050800	L
H-H_	0	-7.16405500	-4.95132700	2.39413200	L
H-H_	0	-3.44837700	-2.76225300	2.35823200	L
C-C_R	0	-4.50176700	-2.44397100	-0.35707400	L
C-C_R	0	-6.97219100	-3.91525800	-0.32672700	L
H-H_	0	-7.89666600	-4.47673600	-0.31684100	L
C-C_R	0	-5.23484100	-2.69100600	-1.52735600	L
C-C_3	0	4.25085100	3.51780500	1.44748400	L
C-C_3	0	6.24566800	4.50178600	1.13698800	L
C-C_R	0	5.87296200	3.86452900	-0.16757100	L
C-C_3	0	4.85818200	4.90546100	1.62089300	L
H-H_	0	4.84721300	5.25981100	2.67810000	L
H-H_	0	4.37653100	5.67287700	0.96928400	L

C-C_3	0	5.18982900	2.67907200	2.33770500	L
H-H_	0	4.87616300	2.74493500	3.40264200	L
H-H_	0	5.20760200	1.61310900	2.02169000	L
C-C_3	0	6.56887000	3.35940900	2.12456500	L
H-H_	0	6.95374700	3.77288000	3.08252800	L
H-H_	0	7.31437700	2.65052700	1.70102800	L
H-H_	0	3.16872500	3.44762200	1.67751700	L
H-H_	0	6.99681200	5.31749300	1.07612500	L
C-C_3	0	5.40442100	3.58056100	-4.78171900	L
C-C_3	0	6.33861400	2.81336200	-3.82216300	L
C-C_3	0	4.35912800	1.79392700	-3.52455000	L
C-C_3	0	4.03648000	2.87667200	-4.57491400	L
H-H_	0	5.35211100	4.66195500	-4.52567000	L
H-H_	0	5.74970000	3.46525100	-5.83260100	L
H-H_	0	3.26111600	3.58488900	-4.20706200	L
H-H_	0	3.68985800	2.40677400	-5.52140700	L
C-C_3	0	5.77176300	1.40254700	-3.94439900	L
H-H_	0	6.24819700	0.67994000	-3.23985400	L
H-H_	0	5.82441800	0.99647000	-4.98149300	L
C-C_R	0	5.89559800	3.13630800	-2.42704200	L
C-C_R	0	4.67214400	2.50727100	-2.24017300	L
H-H_	0	7.42663000	2.92017000	-4.01761200	L
H-H_	0	3.62784800	0.96143100	-3.45363900	L
C-C_R	0	4.00451900	2.53059700	-1.00372700	L
C-C_R	0	6.54504800	3.82547300	-1.39535200	L
H-H_	0	7.51156500	4.29052500	-1.53541600	L
C-C_R	0	4.64260900	3.25047400	0.02212800	L
C-C_3	0	-3.29087900	4.83079400	-2.36735800	L
C-C_3	0	-4.30333700	6.79554600	-1.96238500	L
C-C_R	0	-3.89519300	6.24172200	-0.63055700	L
C-C_3	0	-3.14446600	6.28236400	-2.81166900	L
H-H_	0	-3.30543000	6.42469000	-3.90579400	L
H-H_	0	-2.16274900	6.72702000	-2.52157800	L
C-C_3	0	-4.75480900	4.55499100	-2.76828300	L
H-H_	0	-4.81798600	4.29750200	-3.84831700	L
H-H_	0	-5.19740800	3.73139700	-2.16597100	L
C-C_3	0	-5.45501300	5.91161600	-2.48690900	L
H-H_	0	-5.87421800	6.33819500	-3.42452900	L

H-H_	0	-6.26632500	5.80561300	-1.73308300	L
H-H_	0	-2.53767900	4.12129500	-2.77093000	L
H-H_	0	-4.48200100	7.89124400	-1.99261100	L
C-C_3	0	-1.77238900	6.58730200	3.45018400	L
C-C_3	0	-3.25896900	6.29498400	3.15135400	L
C-C_3	0	-2.26291400	4.31853400	2.75973800	L
C-C_3	0	-1.08521800	5.22124700	3.18141100	L
H-H_	0	-1.37046100	7.38538000	2.78744500	L
H-H_	0	-1.64302400	6.88851500	4.51288000	L
H-H_	0	-0.31852800	5.29733300	2.37912000	L
H-H_	0	-0.61116900	4.83038200	4.10841500	L
C-C_3	0	-3.36978800	4.86032000	3.65820500	L
H-H_	0	-4.36406200	4.40012400	3.44577300	L
H-H_	0	-3.14134900	4.75959500	4.74496000	L
C-C_R	0	-3.37035500	6.04325700	1.67775500	L
C-C_R	0	-2.75284600	4.82530400	1.43469400	L
H-H_	0	-3.98948500	7.01815500	3.57166500	L
H-H_	0	-2.08232100	3.22447300	2.82061900	L
C-C_R	0	-2.67067400	4.27870100	0.14523100	L
C-C_R	0	-3.95787400	6.79827100	0.65418900	L
H-H_	0	-4.42021500	7.75792600	0.84211100	L
C-C_R	0	-3.27157600	5.02651700	-0.87933800	L
C-C_R	0	2.49753200	-1.12995400	5.70032600	H
C-C_R	0	1.86410600	-0.23554800	4.84833400	H
C-C_R	0	2.36336800	0.00357800	3.55839900	H
C-C_R	0	3.51231900	-0.69676600	3.15260600	H
C-C_R	0	4.15311300	-1.57737800	4.00973600	H
C-C_R	0	3.64684800	-1.80113100	5.28867800	H
H-H_	0	2.09460900	-1.30279600	6.69725300	H
H-H_	0	0.96889200	0.28694000	5.18331800	H
H-H_	0	3.89774900	-0.53211900	2.14470400	H
H-H_	0	5.05335200	-2.09430100	3.68070800	H
H-H_	0	4.14500700	-2.49764900	5.96109600	H
C-C_3	0	1.72299300	0.93000200	2.62402200	H
C-C_3	0	0.89767100	2.07962000	3.14041600	H
H-H_	0	0.84292100	0.25227700	1.97595500	H
H-H_	0	2.38688100	1.20099000	1.79421900	H
H-H_	0	1.49053500	2.74759200	3.78393900	H

H-H_	0	0.50625100	2.66885600	2.30098400	H
H-H_	0	0.03366700	1.73325600	3.72314700	H

S_1INT (OSS)

C-C_R	0	1.78322300	2.38118600	-0.67395500	H
C-C_R	0	1.82727200	3.82034200	-0.70503800	H
C-C_R	0	0.57062200	4.27635400	-0.48327600	H
C-C_R	0	-0.29178600	3.13112900	-0.34813400	H
N-N_R	0	0.47371400	2.00013300	-0.47609900	H
C-C_R	0	2.88822000	1.52981000	-0.77582800	H
C-C_R	0	-1.67468500	3.17941100	-0.13677000	H
C-C_R	0	-2.53931700	2.07850100	-0.14405000	H
C-C_R	0	-3.97225600	2.13523100	0.02848600	H
C-C_R	0	-4.44191200	0.87146600	-0.07907700	H
C-C_R	0	-3.30698800	0.00166500	-0.29240300	H
N-N_R	0	-2.17907700	0.77771400	-0.34043600	H
C-C_R	0	-3.36950400	-1.39189500	-0.39072200	H
C-C_R	0	-2.26867600	-2.26028900	-0.46185400	H
C-C_R	0	-2.33432800	-3.70644100	-0.46570000	H
C-C_R	0	-1.06173800	-4.16311900	-0.42846200	H
C-C_R	0	-0.18889300	-3.00661600	-0.41699800	H
N-N_R	0	-0.96482000	-1.89096300	-0.46058800	H
C-C_R	0	1.21204200	-3.04457300	-0.35521100	H
C-C_R	0	2.07691400	-1.94139500	-0.41715400	H
C-C_R	0	3.51815200	-2.01447000	-0.46427400	H
C-C_R	0	3.98542000	-0.75198600	-0.62370700	H
C-C_R	0	2.84173000	0.12899500	-0.65383600	H
N-N_R	0	1.71556600	-0.62480600	-0.50758200	H
H-H_	0	2.71479800	4.42358200	-0.86527200	H
H-H_	0	0.25520600	5.31372500	-0.43500300	H
H-H_	0	-4.55278600	3.03502000	0.20446600	H
H-H_	0	-5.47659200	0.55269100	-0.00323600	H
H-H_	0	-3.24238300	-4.30064400	-0.48017900	H
H-H_	0	-0.74134500	-5.20006300	-0.41394600	H
H-H_	0	4.10859900	-2.92264500	-0.39676700	H
H-H_	0	5.02398800	-0.44691000	-0.70406800	H
Ru-Ru6+2	0	-0.24776200	0.08885000	-0.52579800	H

O-O_3	0	-0.27592300	-0.14465800	-2.25348700	H
O-O_3	0	-0.25836900	-0.17987300	1.40170100	H
C-C_3	0	2.09478700	-4.88767700	-2.79647700	L
C-C_3	0	2.93620600	-6.95929400	-2.57491400	L
C-C_R	0	2.74670100	-6.42362400	-1.18781100	L
C-C_3	0	1.74619100	-6.29724700	-3.26264400	L
H-H_	0	1.76233900	-6.40908200	-4.37191200	L
H-H_	0	0.76399700	-6.65272100	-2.86947500	L
C-C_3	0	3.52262000	-4.74365200	-3.36259600	L
H-H_	0	3.48577700	-4.44884200	-4.43426700	L
H-H_	0	4.11641100	-3.99452600	-2.79407900	L
C-C_3	0	4.10499700	-6.17430200	-3.20786200	L
H-H_	0	4.36500700	-6.60120900	-4.20131200	L
H-H_	0	5.00531200	-6.18191500	-2.55432200	L
H-H_	0	1.37818300	-4.08978000	-3.08522100	L
H-H_	0	2.99444900	-8.06517100	-2.65888400	L
C-C_3	0	1.08670600	-6.72073700	3.10874600	L
C-C_3	0	2.55020000	-6.57544300	2.63875700	L
C-C_3	0	1.73914000	-4.48896700	2.43169700	L
C-C_3	0	0.52842700	-5.27878700	2.96932300	L
H-H_	0	0.52288200	-7.44129500	2.47582500	L
H-H_	0	1.05194300	-7.05343200	4.16937200	L
H-H_	0	-0.33356400	-5.23778000	2.26799300	L
H-H_	0	0.21712600	-4.88078100	3.96006500	L
C-C_3	0	2.87854800	-5.18484200	3.17028600	L
H-H_	0	3.88587500	-4.82982400	2.84869500	L
H-H_	0	2.79547700	-5.10677300	4.27948400	L
C-C_R	0	2.51442400	-6.27236400	1.17119300	L
C-C_R	0	2.00907500	-4.98679900	1.04155600	L
H-H_	0	3.24089300	-7.38956100	2.94450600	L
H-H_	0	1.68622000	-3.38562100	2.54715200	L
C-C_R	0	1.83354000	-4.38128300	-0.21241600	L
C-C_R	0	2.89650600	-7.03851700	0.06237600	L
H-H_	0	3.27245000	-8.04762500	0.16438600	L
C-C_R	0	2.22934400	-5.14249700	-1.32335300	L
C-C_3	0	-5.23686100	-1.83405900	-2.93061400	L
C-C_3	0	-7.25587200	-2.81951900	-2.85902400	L
C-C_R	0	-6.73388600	-2.80880300	-1.45400300	L

C-C_3	0	-6.66399200	-1.50373500	-3.35517500	L
H-H_	0	-6.77222200	-1.36092500	-4.45571000	L
H-H_	0	-7.07832400	-0.61353800	-2.82464300	L
C-C_3	0	-5.00632600	-3.15118600	-3.69988400	L
H-H_	0	-4.70951400	-2.93898500	-4.75040500	L
H-H_	0	-4.22559000	-3.77755200	-3.21376700	L
C-C_3	0	-6.40089600	-3.83216400	-3.65113500	L
H-H_	0	-6.80874000	-3.96401000	-4.67733700	L
H-H_	0	-6.35709000	-4.81956200	-3.14039000	L
H-H_	0	-4.48312300	-1.03602300	-3.09975600	L
H-H_	0	-8.35622100	-2.92870700	-2.96189900	L
C-C_3	0	-6.97178900	-2.17556100	3.13739400	L
C-C_3	0	-6.76778000	-3.47055200	2.32201500	L
C-C_3	0	-4.73962000	-2.50479000	2.25744800	L
C-C_3	0	-5.57037700	-1.50886000	3.09256200	L
H-H_	0	-7.75052600	-1.52362400	2.68325000	L
H-H_	0	-7.25692600	-2.41838000	4.18457700	L
H-H_	0	-5.60758400	-0.50489900	2.61448200	L
H-H_	0	-5.14720400	-1.41539500	4.11674500	L
C-C_3	0	-5.33859000	-3.82969200	2.71743200	L
H-H_	0	-4.93807700	-4.70497300	2.15255700	L
H-H_	0	-5.21765500	-4.00946800	3.81120400	L
C-C_R	0	-6.53333900	-3.06128400	0.89908300	L
C-C_R	0	-5.28177700	-2.46321000	0.85840800	L
H-H_	0	-7.52985400	-4.26385700	2.47444700	L
H-H_	0	-3.63681700	-2.41230500	2.35206900	L
C-C_R	0	-4.71228300	-2.01428000	-0.34340300	L
C-C_R	0	-7.30141900	-3.26173800	-0.25564200	L
H-H_	0	-8.27005600	-3.74212400	-0.22467100	L
C-C_R	0	-5.48666500	-2.20217800	-1.49768900	L
C-C_3	0	4.57606700	3.16834300	1.40718300	L
C-C_3	0	6.64797900	3.96026000	1.05706800	L
C-C_R	0	6.20912600	3.32082200	-0.22553900	L
C-C_3	0	5.30623100	4.50059300	1.53568700	L
H-H_	0	5.33530000	4.88543400	2.58184500	L
H-H_	0	4.89001400	5.28854300	0.86386200	L
C-C_3	0	5.44387000	2.27573900	2.31749700	L
H-H_	0	5.14612500	2.40097200	3.38167800	L

H-H_	0	5.36416700	1.20348200	2.03393600	L
C-C_3	0	6.87616600	2.82330200	2.07662600	L
H-H_	0	7.30410200	3.22870900	3.01966500	L
H-H_	0	7.55202100	2.03842800	1.67057100	L
H-H_	0	3.49411100	3.20427300	1.64521000	L
H-H_	0	7.46855600	4.70321400	0.96765500	L
C-C_3	0	5.66366600	3.00448900	-4.82291000	L
C-C_3	0	6.53628000	2.16753200	-3.86378100	L
C-C_3	0	4.47610500	1.33708900	-3.52858500	L
C-C_3	0	4.24000700	2.43132700	-4.59011400	L
H-H_	0	5.71364700	4.08935000	-4.58136300	L
H-H_	0	5.98335900	2.84466300	-5.87604000	L
H-H_	0	3.53748900	3.21219900	-4.22295600	L
H-H_	0	3.83959000	1.98313000	-5.52581900	L
C-C_3	0	5.84163200	0.81299100	-3.95948500	L
H-H_	0	6.25932300	0.05906800	-3.25048700	L
H-H_	0	5.84363100	0.39049400	-4.99133600	L
C-C_R	0	6.14239100	2.54764200	-2.46849300	L
C-C_R	0	4.86935200	2.03541000	-2.25797700	L
H-H_	0	7.62694600	2.17204400	-4.07316300	L
H-H_	0	3.67301300	0.57580700	-3.43774600	L
C-C_R	0	4.21804100	2.14460100	-1.01714700	L
C-C_R	0	6.86127300	3.19770100	-1.45821100	L
H-H_	0	7.86213700	3.57555500	-1.61811100	L
C-C_R	0	4.93016400	2.82435400	-0.01172400	L
C-C_3	0	-2.85617200	5.12630400	-2.36676700	L
C-C_3	0	-3.68072000	7.17361300	-1.94491000	L
C-C_R	0	-3.31335300	6.57851900	-0.61906800	L
C-C_3	0	-2.58124100	6.56041900	-2.80674600	L
H-H_	0	-2.73802300	6.72202500	-3.89879300	L
H-H_	0	-1.56039200	6.91190500	-2.52391300	L
C-C_3	0	-4.34267200	4.98751900	-2.75505500	L
H-H_	0	-4.43879100	4.74169000	-3.83537100	L
H-H_	0	-4.85333900	4.20521700	-2.15149000	L
C-C_3	0	-4.91309100	6.40131300	-2.46222300	L
H-H_	0	-5.29957900	6.86880200	-3.39436700	L
H-H_	0	-5.72405100	6.36665500	-1.70140400	L
H-H_	0	-2.17467300	4.35269000	-2.77987200	L

H-H_	0	-3.75844600	8.28120100	-1.96923300	L
C-C_3	0	-1.13438600	6.71081100	3.44496400	L
C-C_3	0	-2.64342400	6.55502000	3.15717300	L
C-C_3	0	-1.83274800	4.49881700	2.74856000	L
C-C_3	0	-0.57538400	5.28975500	3.16493200	L
H-H_	0	-0.66727000	7.47263900	2.78230900	L
H-H_	0	-0.97016500	6.99399600	4.50781700	L
H-H_	0	0.18942100	5.30010200	2.35737000	L
H-H_	0	-0.13225700	4.85377200	4.08700900	L
C-C_3	0	-2.87922800	5.13348200	3.65855100	L
H-H_	0	-3.91257300	4.76589500	3.45227400	L
H-H_	0	-2.65235900	5.00699000	4.74293900	L
C-C_R	0	-2.78837200	6.32206600	1.68344000	L
C-C_R	0	-2.28573900	5.05445800	1.42978600	L
H-H_	0	-3.30249500	7.33888700	3.58667200	L
H-H_	0	-1.75009100	3.39264800	2.80317700	L
C-C_R	0	-2.26709200	4.50798200	0.13759500	L
C-C_R	0	-3.31395100	7.13220600	0.66839300	L
H-H_	0	-3.68565400	8.12890100	0.86446700	L
C-C_R	0	-2.80599400	5.31245900	-0.87831900	L
C-C_R	0	2.52623300	-1.30674500	5.75566100	H
C-C_R	0	2.04868200	-0.28658800	4.95218600	H
C-C_R	0	2.55151100	-0.09966700	3.63899800	H
C-C_R	0	3.55046800	-1.00090100	3.18477000	H
C-C_R	0	4.03253400	-2.00393600	4.00240700	H
C-C_R	0	3.52323600	-2.16948600	5.29382100	H
H-H_	0	2.12304600	-1.43430300	6.75950500	H
H-H_	0	1.27605900	0.38415400	5.32636500	H
H-H_	0	3.93491900	-0.88215800	2.16984900	H
H-H_	0	4.81358700	-2.66882500	3.63636600	H
H-H_	0	3.89906900	-2.96619600	5.93338100	H
C-C_R	0	2.10517100	0.93824800	2.79252800	H
C-C_3	0	1.11158900	1.98029600	3.16590400	H
H-H_	0	0.63627400	-0.35477000	1.75055900	H
H-H_	0	2.57355700	0.99937300	1.80839300	H
H-H_	0	1.49521100	2.64790800	3.95546300	H
H-H_	0	0.85286400	2.59926700	2.29850200	H
H-H_	0	0.17413700	1.54106600	3.53813900	H

R_1TS2 (OSS)

C-C_R	0	-1.29649600	2.88337600	-0.16730200	H
C-C_R	0	-0.95770700	4.28863800	-0.14407900	H
C-C_R	0	0.39194400	4.37389900	-0.14982400	H
C-C_R	0	0.91075400	3.02323600	-0.19367700	H
N-N_R	0	-0.14611400	2.16215700	-0.21071500	H
H-H_	0	-1.66488600	5.11128500	-0.11949000	H
H-H_	0	0.98721800	5.28119500	-0.12797900	H
C-C_R	0	2.26965900	2.68262500	-0.22144100	H
C-C_R	0	4.20492100	1.06068000	-0.37069800	H
C-C_R	0	4.30511800	-0.28694800	-0.43785600	H
C-C_R	0	2.96292300	-0.82058800	-0.36923200	H
N-N_R	0	2.09307700	0.21996900	-0.26854200	H
C-C_R	0	2.79902500	1.38507000	-0.27414200	H
H-H_	0	5.02106500	1.77584100	-0.39390800	H
H-H_	0	5.21769500	-0.86754500	-0.52409500	H
C-C_R	0	-2.59600100	2.35785400	-0.12628700	H
N-N_R	0	-2.04347700	-0.05728000	-0.16957100	H
C-C_R	0	-2.76625600	-1.22237400	-0.16322600	H
C-C_R	0	-4.16455900	-0.88505400	-0.06790300	H
C-C_R	0	-4.25811100	0.46585400	-0.02694000	H
C-C_R	0	-2.92173300	0.99845100	-0.10491600	H
H-H_	0	-4.98512800	-1.59438700	-0.02966500	H
H-H_	0	-5.16836100	1.05187700	0.05070800	H
C-C_R	0	-2.25308500	-2.52563500	-0.22222300	H
N-N_R	0	0.15538100	-1.98070700	-0.23220100	H
C-C_R	0	1.32339600	-2.70011100	-0.30569200	H
C-C_R	0	0.98882400	-4.10352900	-0.31106100	H
C-C_R	0	-0.36179900	-4.20250000	-0.27137400	H
C-C_R	0	-0.89259300	-2.86145600	-0.23485400	H
H-H_	0	1.70182400	-4.92124000	-0.34399400	H
H-H_	0	-0.94993900	-5.11460100	-0.26706300	H
C-C_R	0	2.62137500	-2.18291100	-0.39114000	H
O-O_3	0	0.18843700	0.26175800	1.62957600	H
H-H_	0	0.81802600	-0.39243800	1.98007100	H
C-C_3	0	-1.63697600	-1.08451700	3.20246000	H
H-H_	0	-1.91847600	-1.58703100	2.27764100	H

C-C_R	0	-0.53221300	-1.60795600	3.90920200	H
C-C_R	0	0.17682700	-2.72308600	3.39161900	H
C-C_R	0	1.26176200	-3.25519800	4.06105200	H
C-C_R	0	1.70283100	-2.68956000	5.26066300	H
C-C_R	0	1.03446900	-1.57711100	5.77748500	H
C-C_R	0	-0.06116100	-1.04276100	5.12080700	H
H-H_	0	-0.14523800	-3.15688500	2.44314600	H
H-H_	0	1.76390600	-4.12760600	3.64942100	H
H-H_	0	2.56007800	-3.10931400	5.78410200	H
H-H_	0	1.37723300	-1.12362600	6.70689300	H
H-H_	0	-0.56972100	-0.17296100	5.53510200	H
C-C_3	0	-2.39758200	0.12763300	3.59363300	H
H-H_	0	-1.76572600	1.02531200	3.49212800	H
H-H_	0	-3.27400900	0.26457400	2.94865200	H
H-H_	0	-2.74849900	0.09123000	4.63688200	H
O-O_3	0	0.15099300	0.19908100	-2.03704800	H
Ru-Ru6+2	0	-0.00623100	0.08221700	-0.30358300	H
C-C_3	0	-4.08829800	3.32044400	-2.76475500	L
C-C_3	0	-5.82578800	4.74594800	-2.78857400	L
C-C_R	0	-5.43500400	4.56996100	-1.35223000	L
C-C_3	0	-4.44814100	4.64195900	-3.43592600	L
H-H_	0	-4.48980600	4.57233600	-4.54802200	L
H-H_	0	-3.76660500	5.47594500	-3.14348400	L
C-C_3	0	-5.25824600	2.43271000	-3.23768700	L
H-H_	0	-5.05874200	2.04234800	-4.25973300	L
H-H_	0	-5.43385300	1.58028200	-2.54556000	L
C-C_3	0	-6.45906900	3.41646000	-3.25187700	L
H-H_	0	-6.86841500	3.52041200	-4.28068400	L
H-H_	0	-7.26781500	3.08583200	-2.56314500	L
H-H_	0	-3.06971400	2.93075300	-2.97510900	L
H-H_	0	-6.40484800	5.66498800	-3.01963400	L
C-C_3	0	-4.43993000	6.01471400	2.95244900	L
C-C_3	0	-5.59821100	5.13596400	2.43445800	L
C-C_3	0	-3.86066300	3.71294800	2.47203300	L
C-C_3	0	-3.24004400	5.03064000	2.98027300	L
H-H_	0	-4.24672100	6.87780800	2.27757000	L
H-H_	0	-4.66470500	6.38779500	3.97573400	L
H-H_	0	-2.41099800	5.37498100	2.32427300	L

H-H_	0	-2.86056400	4.90386400	4.01793500	L
C-C_3	0	-5.25315000	3.80057400	3.08694500	L
H-H_	0	-5.92376400	2.97047400	2.76009900	L
H-H_	0	-5.23869600	3.84663500	4.20092600	L
C-C_R	0	-5.28927500	4.79808200	1.00706600	L
C-C_R	0	-4.21588000	3.91797800	1.02870200	L
H-H_	0	-6.62176700	5.52200000	2.62596500	L
H-H_	0	-3.28620200	2.79312700	2.69895600	L
C-C_R	0	-3.71874700	3.32492500	-0.14300700	L
C-C_R	0	-5.93929000	5.15244600	-0.18237600	L
H-H_	0	-6.78233700	5.83002300	-0.19595900	L
C-C_R	0	-4.36345800	3.68873500	-1.33571900	L
C-C_3	0	3.50739900	3.89346700	2.44685000	L
C-C_3	0	5.01450600	5.56022500	2.49983400	L
C-C_R	0	4.70585700	5.30715600	1.05496600	L
C-C_3	0	3.64489000	5.26336900	3.10313700	L
H-H_	0	3.65659300	5.21693200	4.21714800	L
H-H_	0	2.85890600	5.98305600	2.77172100	L
C-C_3	0	4.77752600	3.19469000	2.97442500	L
H-H_	0	4.60159800	2.79242700	3.99618500	L
H-H_	0	5.10024700	2.36875600	2.30274200	L
C-C_3	0	5.81922700	4.34543800	3.01026700	L
H-H_	0	6.17094800	4.52339500	4.05019200	L
H-H_	0	6.69246900	4.12816700	2.35607800	L
H-H_	0	2.55019300	3.36079900	2.63065000	L
H-H_	0	5.44358400	6.55793000	2.73177700	L
C-C_3	0	3.65444200	6.50996400	-3.30555800	L
C-C_3	0	4.91827700	5.83000300	-2.73670300	L
C-C_3	0	3.42432400	4.15225500	-2.80106200	L
C-C_3	0	2.62307200	5.35042900	-3.35080500	L
H-H_	0	3.30766900	7.34172600	-2.65314800	L
H-H_	0	3.85153100	6.89931800	-4.32849000	L
H-H_	0	1.73066600	5.56937700	-2.72385900	L
H-H_	0	2.30040900	5.15284600	-4.39655500	L
C-C_3	0	4.80610600	4.44858500	-3.37462600	L
H-H_	0	5.58671400	3.73791900	-3.01238200	L
H-H_	0	4.82155200	4.47719600	-4.48917700	L
C-C_R	0	4.61943800	5.46757300	-1.31323600	L

C-C_R	0	3.69521300	4.43286400	-1.35186800	L
H-H_	0	5.87497700	6.36841300	-2.90461200	L
H-H_	0	3.00925600	3.14756400	-3.02899300	L
C-C_R	0	3.24228600	3.79899300	-0.18462800	L
C-C_R	0	5.16162800	5.93844300	-0.10991000	L
H-H_	0	5.89105200	6.73668400	-0.08234800	L
C-C_R	0	3.77723300	4.27689900	1.02120800	L
C-C_3	0	4.67253500	-3.18446700	1.84528400	L
C-C_3	0	6.51411200	-4.39164100	1.40166700	L
C-C_R	0	5.73269300	-4.31505900	0.12425700	L
C-C_3	0	6.18183400	-3.02089500	1.98348200	L
H-H_	0	6.51425500	-2.89998900	3.04089100	L
H-H_	0	6.58493300	-2.17980000	1.37093500	L
C-C_3	0	4.44852100	-4.47826600	2.65719800	L
H-H_	0	4.37466400	-4.24800800	3.74271800	L
H-H_	0	3.53355900	-5.01557000	2.32362100	L
C-C_3	0	5.72509900	-5.30711800	2.35846600	L
H-H_	0	6.30482500	-5.48437500	3.29090300	L
H-H_	0	5.47988900	-6.28288800	1.88358300	L
H-H_	0	4.05831300	-2.31152600	2.15274900	L
H-H_	0	7.59436200	-4.62457500	1.29101400	L
C-C_3	0	5.60335700	-3.14160800	-4.25963100	L
C-C_3	0	5.23960700	-4.52141700	-3.66970200	L
C-C_3	0	3.40736300	-3.29051000	-3.24901600	L
C-C_3	0	4.33715600	-2.29144000	-3.96863300	L
H-H_	0	6.50618600	-2.71216700	-3.77153500	L
H-H_	0	5.77791300	-3.22265600	-5.35497200	L
H-H_	0	4.57027200	-1.41316800	-3.32675600	L
H-H_	0	3.87154700	-1.94329500	-4.91662600	L
C-C_3	0	3.74957100	-4.57858700	-3.98940300	L
H-H_	0	3.24614800	-5.47463600	-3.55449700	L
H-H_	0	3.53246600	-4.52772900	-5.08195600	L
C-C_R	0	5.16555700	-4.35700700	-2.18157700	L
C-C_R	0	4.03472600	-3.59691800	-1.91989300	L
H-H_	0	5.84607500	-5.37981400	-4.02831300	L
H-H_	0	2.33033400	-3.02052700	-3.22364100	L
C-C_R	0	3.72671400	-3.14288300	-0.62749300	L
C-C_R	0	6.06830000	-4.71868700	-1.17436000	L

H-H_	0	6.98522800	-5.25023700	-1.39064100	L
C-C_R	0	4.59704000	-3.56066600	0.39386100	L
C-C_3	0	-3.35128700	-4.32974700	2.18794600	L
C-C_3	0	-4.99649300	-5.84243900	1.97122700	L
C-C_R	0	-4.71122200	-5.31701600	0.59703600	L
C-C_3	0	-3.58888000	-5.79111800	2.55211400	L
H-H_	0	-3.55970900	-5.97989700	3.65071500	L
H-H_	0	-2.88121800	-6.48532800	2.03942900	L
C-C_3	0	-4.53243600	-3.65670600	2.91495000	L
H-H_	0	-4.28549300	-3.49674200	3.98745900	L
H-H_	0	-4.79935200	-2.68265800	2.44853200	L
C-C_3	0	-5.67195400	-4.70040500	2.76242800	L
H-H_	0	-6.00573200	-5.06434300	3.75887400	L
H-H_	0	-6.54183200	-4.27914400	2.21148200	L
H-H_	0	-2.34460500	-3.94336000	2.43223400	L
H-H_	0	-5.50467700	-6.82901200	2.01260600	L
C-C_3	0	-4.13553800	-5.40646300	-4.02983500	L
C-C_3	0	-5.27825800	-4.83933800	-3.16077400	L
C-C_3	0	-3.66733100	-3.28788900	-2.95497100	L
C-C_3	0	-3.02219200	-4.33419100	-3.88673000	L
H-H_	0	-3.79670900	-6.40083200	-3.66362000	L
H-H_	0	-4.46184300	-5.49365900	-5.08944500	L
H-H_	0	-2.09500200	-4.76037700	-3.44296800	L
H-H_	0	-2.78546700	-3.87989600	-4.87382400	L
C-C_3	0	-5.11741800	-3.34528400	-3.42246800	L
H-H_	0	-5.79823300	-2.71855300	-2.79846200	L
H-H_	0	-5.24329800	-3.07144200	-4.49595600	L
C-C_R	0	-4.81380400	-4.89084400	-1.73635500	L
C-C_R	0	-3.81650800	-3.93381000	-1.60739600	L
H-H_	0	-6.28726100	-5.26181300	-3.35270100	L
H-H_	0	-3.19636800	-2.28215600	-2.96208600	L
C-C_R	0	-3.23420200	-3.62833100	-0.36622500	L
C-C_R	0	-5.31071200	-5.60084000	-0.63628100	L
H-H_	0	-6.12190100	-6.31023100	-0.73002700	L
C-C_R	0	-3.69931900	-4.37571000	0.72892700	L

S_1TS2 (OSS)

C-C_R	0	-1.29649600	2.88337600	-0.16730200	H
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C-C_R	0	-0.95770700	4.28863800	-0.14407900	H
C-C_R	0	0.39194400	4.37389900	-0.14982400	H
C-C_R	0	0.91075400	3.02323600	-0.19367700	H
N-N_R	0	-0.14611400	2.16215700	-0.21071500	H
H-H_	0	-1.66488600	5.11128500	-0.11949000	H
H-H_	0	0.98721800	5.28119500	-0.12797900	H
C-C_R	0	2.26965900	2.68262500	-0.22144100	H
C-C_R	0	4.20492100	1.06068000	-0.37069800	H
C-C_R	0	4.30511800	-0.28694800	-0.43785600	H
C-C_R	0	2.96292300	-0.82058800	-0.36923200	H
N-N_R	0	2.09307700	0.21996900	-0.26854200	H
C-C_R	0	2.79902500	1.38507000	-0.27414200	H
H-H_	0	5.02106500	1.77584100	-0.39390800	H
H-H_	0	5.21769500	-0.86754500	-0.52409500	H
C-C_R	0	-2.59600100	2.35785400	-0.12628700	H
N-N_R	0	-2.04347700	-0.05728000	-0.16957100	H
C-C_R	0	-2.76625600	-1.22237400	-0.16322600	H
C-C_R	0	-4.16455900	-0.88505400	-0.06790300	H
C-C_R	0	-4.25811100	0.46585400	-0.02694000	H
C-C_R	0	-2.92173300	0.99845100	-0.10491600	H
H-H_	0	-4.98512800	-1.59438700	-0.02966500	H
H-H_	0	-5.16836100	1.05187700	0.05070800	H
C-C_R	0	-2.25308500	-2.52563500	-0.22222300	H
N-N_R	0	0.15538100	-1.98070700	-0.23220100	H
C-C_R	0	1.32339600	-2.70011100	-0.30569200	H
C-C_R	0	0.98882400	-4.10352900	-0.31106100	H
C-C_R	0	-0.36179900	-4.20250000	-0.27137400	H
C-C_R	0	-0.89259300	-2.86145600	-0.23485400	H
H-H_	0	1.70182400	-4.92124000	-0.34399400	H
H-H_	0	-0.94993900	-5.11460100	-0.26706300	H
C-C_R	0	2.62137500	-2.18291100	-0.39114000	H
O-O_3	0	0.18843700	0.26175800	1.62957600	H
H-H_	0	0.81802600	-0.39243800	1.98007100	H
C-C_3	0	-1.63697600	-1.08451700	3.20246000	H
H-H_	0	-1.91847600	-1.58703100	2.27764100	H
C-C_R	0	-0.53221300	-1.60795600	3.90920200	H
C-C_R	0	0.17682700	-2.72308600	3.39161900	H
C-C_R	0	1.26176200	-3.25519800	4.06105200	H

C-C_R	0	1.70283100	-2.68956000	5.26066300	H
C-C_R	0	1.03446900	-1.57711100	5.77748500	H
C-C_R	0	-0.06116100	-1.04276100	5.12080700	H
H-H_	0	-0.14523800	-3.15688500	2.44314600	H
H-H_	0	1.76390600	-4.12760600	3.64942100	H
H-H_	0	2.56007800	-3.10931400	5.78410200	H
H-H_	0	1.37723300	-1.12362600	6.70689300	H
H-H_	0	-0.56972100	-0.17296100	5.53510200	H
C-C_3	0	-2.39758200	0.12763300	3.59363300	H
H-H_	0	-1.76572600	1.02531200	3.49212800	H
H-H_	0	-3.27400900	0.26457400	2.94865200	H
H-H_	0	-2.74849900	0.09123000	4.63688200	H
O-O_3	0	0.15099300	0.19908100	-2.03704800	H
Ru-Ru6+2	0	-0.00623100	0.08221700	-0.30358300	H
C-C_3	0	-4.08829800	3.32044400	-2.76475500	L
C-C_3	0	-5.82578800	4.74594800	-2.78857400	L
C-C_R	0	-5.43500400	4.56996100	-1.35223000	L
C-C_3	0	-4.44814100	4.64195900	-3.43592600	L
H-H_	0	-4.48980600	4.57233600	-4.54802200	L
H-H_	0	-3.76660500	5.47594500	-3.14348400	L
C-C_3	0	-5.25824600	2.43271000	-3.23768700	L
H-H_	0	-5.05874200	2.04234800	-4.25973300	L
H-H_	0	-5.43385300	1.58028200	-2.54556000	L
C-C_3	0	-6.45906900	3.41646000	-3.25187700	L
H-H_	0	-6.86841500	3.52041200	-4.28068400	L
H-H_	0	-7.26781500	3.08583200	-2.56314500	L
H-H_	0	-3.06971400	2.93075300	-2.97510900	L
H-H_	0	-6.40484800	5.66498800	-3.01963400	L
C-C_3	0	-4.43993000	6.01471400	2.95244900	L
C-C_3	0	-5.59821100	5.13596400	2.43445800	L
C-C_3	0	-3.86066300	3.71294800	2.47203300	L
C-C_3	0	-3.24004400	5.03064000	2.98027300	L
H-H_	0	-4.24672100	6.87780800	2.27757000	L
H-H_	0	-4.66470500	6.38779500	3.97573400	L
H-H_	0	-2.41099800	5.37498100	2.32427300	L
H-H_	0	-2.86056400	4.90386400	4.01793500	L
C-C_3	0	-5.25315000	3.80057400	3.08694500	L
H-H_	0	-5.92376400	2.97047400	2.76009900	L

H-H_	0	-5.23869600	3.84663500	4.20092600	L
C-C_R	0	-5.28927500	4.79808200	1.00706600	L
C-C_R	0	-4.21588000	3.91797800	1.02870200	L
H-H_	0	-6.62176700	5.52200000	2.62596500	L
H-H_	0	-3.28620200	2.79312700	2.69895600	L
C-C_R	0	-3.71874700	3.32492500	-0.14300700	L
C-C_R	0	-5.93929000	5.15244600	-0.18237600	L
H-H_	0	-6.78233700	5.83002300	-0.19595900	L
C-C_R	0	-4.36345800	3.68873500	-1.33571900	L
C-C_3	0	3.50739900	3.89346700	2.44685000	L
C-C_3	0	5.01450600	5.56022500	2.49983400	L
C-C_R	0	4.70585700	5.30715600	1.05496600	L
C-C_3	0	3.64489000	5.26336900	3.10313700	L
H-H_	0	3.65659300	5.21693200	4.21714800	L
H-H_	0	2.85890600	5.98305600	2.77172100	L
C-C_3	0	4.77752600	3.19469000	2.97442500	L
H-H_	0	4.60159800	2.79242700	3.99618500	L
H-H_	0	5.10024700	2.36875600	2.30274200	L
C-C_3	0	5.81922700	4.34543800	3.01026700	L
H-H_	0	6.17094800	4.52339500	4.05019200	L
H-H_	0	6.69246900	4.12816700	2.35607800	L
H-H_	0	2.55019300	3.36079900	2.63065000	L
H-H_	0	5.44358400	6.55793000	2.73177700	L
C-C_3	0	3.65444200	6.50996400	-3.30555800	L
C-C_3	0	4.91827700	5.83000300	-2.73670300	L
C-C_3	0	3.42432400	4.15225500	-2.80106200	L
C-C_3	0	2.62307200	5.35042900	-3.35080500	L
H-H_	0	3.30766900	7.34172600	-2.65314800	L
H-H_	0	3.85153100	6.89931800	-4.32849000	L
H-H_	0	1.73066600	5.56937700	-2.72385900	L
H-H_	0	2.30040900	5.15284600	-4.39655500	L
C-C_3	0	4.80610600	4.44858500	-3.37462600	L
H-H_	0	5.58671400	3.73791900	-3.01238200	L
H-H_	0	4.82155200	4.47719600	-4.48917700	L
C-C_R	0	4.61943800	5.46757300	-1.31323600	L
C-C_R	0	3.69521300	4.43286400	-1.35186800	L
H-H_	0	5.87497700	6.36841300	-2.90461200	L
H-H_	0	3.00925600	3.14756400	-3.02899300	L

C-C_R	0	3.24228600	3.79899300	-0.18462800	L
C-C_R	0	5.16162800	5.93844300	-0.10991000	L
H-H_	0	5.89105200	6.73668400	-0.08234800	L
C-C_R	0	3.77723300	4.27689900	1.02120800	L
C-C_3	0	4.67253500	-3.18446700	1.84528400	L
C-C_3	0	6.51411200	-4.39164100	1.40166700	L
C-C_R	0	5.73269300	-4.31505900	0.12425700	L
C-C_3	0	6.18183400	-3.02089500	1.98348200	L
H-H_	0	6.51425500	-2.89998900	3.04089100	L
H-H_	0	6.58493300	-2.17980000	1.37093500	L
C-C_3	0	4.44852100	-4.47826600	2.65719800	L
H-H_	0	4.37466400	-4.24800800	3.74271800	L
H-H_	0	3.53355900	-5.01557000	2.32362100	L
C-C_3	0	5.72509900	-5.30711800	2.35846600	L
H-H_	0	6.30482500	-5.48437500	3.29090300	L
H-H_	0	5.47988900	-6.28288800	1.88358300	L
H-H_	0	4.05831300	-2.31152600	2.15274900	L
H-H_	0	7.59436200	-4.62457500	1.29101400	L
C-C_3	0	5.60335700	-3.14160800	-4.25963100	L
C-C_3	0	5.23960700	-4.52141700	-3.66970200	L
C-C_3	0	3.40736300	-3.29051000	-3.24901600	L
C-C_3	0	4.33715600	-2.29144000	-3.96863300	L
H-H_	0	6.50618600	-2.71216700	-3.77153500	L
H-H_	0	5.77791300	-3.22265600	-5.35497200	L
H-H_	0	4.57027200	-1.41316800	-3.32675600	L
H-H_	0	3.87154700	-1.94329500	-4.91662600	L
C-C_3	0	3.74957100	-4.57858700	-3.98940300	L
H-H_	0	3.24614800	-5.47463600	-3.55449700	L
H-H_	0	3.53246600	-4.52772900	-5.08195600	L
C-C_R	0	5.16555700	-4.35700700	-2.18157700	L
C-C_R	0	4.03472600	-3.59691800	-1.91989300	L
H-H_	0	5.84607500	-5.37981400	-4.02831300	L
H-H_	0	2.33033400	-3.02052700	-3.22364100	L
C-C_R	0	3.72671400	-3.14288300	-0.62749300	L
C-C_R	0	6.06830000	-4.71868700	-1.17436000	L
H-H_	0	6.98522800	-5.25023700	-1.39064100	L
C-C_R	0	4.59704000	-3.56066600	0.39386100	L
C-C_3	0	-3.35128700	-4.32974700	2.18794600	L

C-C_3	0	-4.99649300	-5.84243900	1.97122700	L
C-C_R	0	-4.71122200	-5.31701600	0.59703600	L
C-C_3	0	-3.58888000	-5.79111800	2.55211400	L
H-H_	0	-3.55970900	-5.97989700	3.65071500	L
H-H_	0	-2.88121800	-6.48532800	2.03942900	L
C-C_3	0	-4.53243600	-3.65670600	2.91495000	L
H-H_	0	-4.28549300	-3.49674200	3.98745900	L
H-H_	0	-4.79935200	-2.68265800	2.44853200	L
C-C_3	0	-5.67195400	-4.70040500	2.76242800	L
H-H_	0	-6.00573200	-5.06434300	3.75887400	L
H-H_	0	-6.54183200	-4.27914400	2.21148200	L
H-H_	0	-2.34460500	-3.94336000	2.43223400	L
H-H_	0	-5.50467700	-6.82901200	2.01260600	L
C-C_3	0	-4.13553800	-5.40646300	-4.02983500	L
C-C_3	0	-5.27825800	-4.83933800	-3.16077400	L
C-C_3	0	-3.66733100	-3.28788900	-2.95497100	L
C-C_3	0	-3.02219200	-4.33419100	-3.88673000	L
H-H_	0	-3.79670900	-6.40083200	-3.66362000	L
H-H_	0	-4.46184300	-5.49365900	-5.08944500	L
H-H_	0	-2.09500200	-4.76037700	-3.44296800	L
H-H_	0	-2.78546700	-3.87989600	-4.87382400	L
C-C_3	0	-5.11741800	-3.34528400	-3.42246800	L
H-H_	0	-5.79823300	-2.71855300	-2.79846200	L
H-H_	0	-5.24329800	-3.07144200	-4.49595600	L
C-C_R	0	-4.81380400	-4.89084400	-1.73635500	L
C-C_R	0	-3.81650800	-3.93381000	-1.60739600	L
H-H_	0	-6.28726100	-5.26181300	-3.35270100	L
H-H_	0	-3.19636800	-2.28215600	-2.96208600	L
C-C_R	0	-3.23420200	-3.62833100	-0.36622500	L
C-C_R	0	-5.31071200	-5.60084000	-0.63628100	L
H-H_	0	-6.12190100	-6.31023100	-0.73002700	L
C-C_R	0	-3.69931900	-4.37571000	0.72892700	L

¹Ru (por*) O (OSS)

C-C_R	0	3.03849100	-0.45317100	0.04364900	H
C-C_R	0	4.01996100	-1.50708500	0.11015700	H
C-C_R	0	3.35115400	-2.68335700	0.11470000	H
C-C_R	0	1.94339300	-2.37956800	0.04751800	H

N-N_R	0	1.78746600	-1.01641100	0.01757900	H
C-C_R	0	3.32712300	0.91479500	0.01901100	H
C-C_R	0	0.91553500	-3.32737200	0.02379100	H
C-C_R	0	-0.45284600	-3.03983600	0.00827300	H
C-C_R	0	-1.50767900	-4.02250400	0.01658100	H
C-C_R	0	-2.68407800	-3.35390500	0.01503800	H
C-C_R	0	-2.37926900	-1.94485000	0.00298200	H
N-N_R	0	-1.01592700	-1.78856700	0.00147400	H
C-C_R	0	-3.32625900	-0.91596700	0.01095300	H
C-C_R	0	-3.03703700	0.45204800	0.03310600	H
C-C_R	0	-4.01850800	1.50618400	0.09438000	H
C-C_R	0	-3.34967500	2.68242000	0.09988900	H
C-C_R	0	-1.94171800	2.37865900	0.03899400	H
N-N_R	0	-1.78578600	1.01534100	0.01002400	H
C-C_R	0	-0.91396800	3.32687400	0.02167500	H
C-C_R	0	0.45443100	3.03922400	0.01205700	H
C-C_R	0	1.50950300	4.02160800	0.02469800	H
C-C_R	0	2.68571500	3.35274000	0.02461500	H
C-C_R	0	2.38044100	1.94377900	0.01009700	H
N-N_R	0	1.01719600	1.78779900	0.00571700	H
H-H_	0	5.09558500	-1.36863400	0.15450200	H
H-H_	0	3.78257200	-3.67808800	0.16431100	H
H-H_	0	-1.36999200	-5.09906500	0.02631600	H
H-H_	0	-3.67948900	-3.78643600	0.02476700	H
H-H_	0	-5.09430500	1.36789800	0.13409600	H
H-H_	0	-3.78121300	3.67722800	0.14619500	H
H-H_	0	1.37220700	5.09818700	0.03577500	H
H-H_	0	3.68124300	3.78497100	0.03774000	H
Ru-Ru6+2	0	0.00131000	-0.00049200	-0.23792900	H
O-O_3	0	0.00608500	-0.00078800	-1.98401200	H
C-C_3	0	-1.33076500	5.04555200	2.66940400	L
C-C_3	0	-1.93099900	7.21120300	2.69017800	L
C-C_R	0	-1.81823600	6.81144700	1.24989500	L
C-C_3	0	-2.44180400	5.89755600	3.27424500	L
H-H_	0	-2.44652100	5.88527700	4.38920500	L
H-H_	0	-3.45476700	5.61916600	2.89742500	L
C-C_3	0	-0.08493600	5.74448100	3.25201900	L
H-H_	0	0.11371300	5.38312800	4.28484100	L

H-H_	0	0.81487300	5.57245400	2.62120600	L
C-C_3	0	-0.49866000	7.24074000	3.26529300	L
H-H_	0	-0.50698800	7.63582200	4.30485000	L
H-H_	0	0.18167200	7.85963700	2.63933200	L
H-H_	0	-1.40239800	3.95261400	2.85353900	L
H-H_	0	-2.55259400	8.10904800	2.89226700	L
C-C_3	0	-3.34024500	6.52246100	-3.11197600	L
C-C_3	0	-2.08910800	7.23200000	-2.55117600	L
C-C_3	0	-1.47485300	5.07013700	-2.58432100	L
C-C_3	0	-2.91527400	5.02935100	-3.13548200	L
H-H_	0	-4.22915600	6.68542100	-2.46311000	L
H-H_	0	-3.56151000	6.88330600	-4.14039900	L
H-H_	0	-3.57979400	4.40286100	-2.50034600	L
H-H_	0	-2.92048400	4.63625100	-4.17575600	L
C-C_3	0	-0.98291600	6.38710000	-3.17589500	L
H-H_	0	0.03516900	6.66970900	-2.81645000	L
H-H_	0	-0.99739100	6.39984900	-4.29076400	L
C-C_R	0	-1.94577900	6.80493100	-1.12160000	L
C-C_R	0	-1.56820300	5.46966700	-1.14079100	L
H-H_	0	-2.02947900	8.32579500	-2.73401400	L
H-H_	0	-0.84929800	4.17776500	-2.79866300	L
C-C_R	0	-1.30733500	4.75520400	0.03844200	L
C-C_R	0	-2.08467700	7.52358900	0.07307600	L
H-H_	0	-2.38220200	8.56347300	0.08621800	L
C-C_R	0	-1.44570400	5.47465200	1.23572400	L
C-C_3	0	-4.98831700	-1.57417700	2.64556200	L
C-C_3	0	-7.15636600	-2.16611700	2.65876300	L
C-C_R	0	-6.78587500	-1.92738200	1.22606400	L
C-C_3	0	-5.83372700	-2.73118100	3.16772000	L
H-H_	0	-5.79840900	-2.83439900	4.27739800	L
H-H_	0	-5.56854100	-3.70784300	2.69717000	L
C-C_3	0	-5.66826500	-0.38167100	3.34941000	L
H-H_	0	-5.28411200	-0.27479600	4.38755800	L
H-H_	0	-5.50469800	0.56878000	2.79468500	L
C-C_3	0	-7.16611100	-0.79014900	3.35875600	L
H-H_	0	-7.53881500	-0.88920900	4.40189100	L
H-H_	0	-7.79482600	-0.05509700	2.80910600	L
H-H_	0	-3.89228900	-1.66588000	2.79993100	L

H-H_	0	-8.05318200	-2.80000800	2.82386800	L
C-C_3	0	-6.60120700	-3.02766400	-3.26383300	L
C-C_3	0	-7.29273000	-1.83273600	-2.57293400	L
C-C_3	0	-5.12930700	-1.22352600	-2.59625200	L
C-C_3	0	-5.10682900	-2.60649400	-3.27955500	L
H-H_	0	-6.75462800	-3.97314600	-2.69790900	L
H-H_	0	-6.98486500	-3.15035400	-4.30045300	L
H-H_	0	-4.47024800	-3.32847900	-2.72140500	L
H-H_	0	-4.73551800	-2.51621500	-4.32391900	L
C-C_3	0	-6.45653500	-0.67511100	-3.10998900	L
H-H_	0	-6.72646000	0.30561300	-2.65073600	L
H-H_	0	-6.49352500	-0.58518200	-4.22076700	L
C-C_R	0	-6.83392500	-1.82526200	-1.14604400	L
C-C_R	0	-5.49768500	-1.45072300	-1.15943900	L
H-H_	0	-8.38997000	-1.75349400	-2.72513700	L
H-H_	0	-4.23908600	-0.58282000	-2.77111200	L
C-C_R	0	-4.75506700	-1.30791100	0.02246300	L
C-C_R	0	-7.52620700	-2.07625500	0.04592500	L
H-H_	0	-8.56755900	-2.36883200	0.05444500	L
C-C_R	0	-5.44757800	-1.56022100	1.21686100	L
C-C_3	0	5.11894000	1.22027600	-2.59530800	L
C-C_3	0	7.28156000	1.83264600	-2.58158700	L
C-C_R	0	6.82889200	1.82524700	-1.15268100	L
C-C_3	0	6.44474700	0.67352000	-3.11443800	L
H-H_	0	6.47705000	0.58303300	-4.22531500	L
H-H_	0	6.71812800	-0.30654600	-2.65582600	L
C-C_3	0	5.09144700	2.60286200	-3.27915300	L
H-H_	0	4.71554900	2.51153600	-4.32178400	L
H-H_	0	4.45637500	3.32423000	-2.71847300	L
C-C_3	0	6.58528700	3.02613100	-3.27027000	L
H-H_	0	6.96415500	3.14858900	-4.30868200	L
H-H_	0	6.73991300	3.97223400	-2.70573000	L
H-H_	0	4.22891300	0.57814600	-2.76592400	L
H-H_	0	8.37822000	1.75490900	-2.73852700	L
C-C_3	0	7.17864600	0.79779500	3.35361100	L
C-C_3	0	7.16534400	2.17219700	2.65054100	L
C-C_3	0	4.99778100	1.57837600	2.64624000	L
C-C_3	0	5.68113600	0.38805300	3.35041000	L

H-H_	0	7.80608100	0.06202200	2.80347100	L
H-H_	0	7.55483500	0.89949800	4.39523800	L
H-H_	0	5.51646000	-0.56381100	2.79845800	L
H-H_	0	5.30062400	0.28326000	4.39010700	L
C-C_3	0	5.84400100	2.73728900	3.16281600	L
H-H_	0	5.57640700	3.71267100	2.69097300	L
H-H_	0	5.81242700	2.84297500	4.27237400	L
C-C_R	0	6.79007300	1.93001000	1.21961700	L
C-C_R	0	5.45220300	1.56151700	1.21603600	L
H-H_	0	8.06217600	2.80715600	2.81120700	L
H-H_	0	3.90220600	1.66953000	2.80414700	L
C-C_R	0	4.75547300	1.30697400	0.02466400	L
C-C_R	0	7.52551700	2.07869800	0.03631400	L
H-H_	0	8.56628100	2.37322400	0.04035200	L
C-C_R	0	5.49324300	1.44881600	-1.16026600	L
C-C_3	0	1.33015600	-5.04873300	2.66971800	L
C-C_3	0	1.92734200	-7.21526100	2.68849900	L
C-C_R	0	1.81704200	-6.81349200	1.24855700	L
C-C_3	0	2.43919800	-5.90307900	3.27492800	L
H-H_	0	2.44244200	-5.89222100	4.38990800	L
H-H_	0	3.45306200	-5.62566400	2.89981800	L
C-C_3	0	0.08255000	-5.74662000	3.24971800	L
H-H_	0	-0.11706300	-5.38621100	4.28268300	L
H-H_	0	-0.81610300	-5.57257100	2.61778100	L
C-C_3	0	0.49419700	-7.24346700	3.26174000	L
H-H_	0	0.50063300	-7.63975500	4.30085200	L
H-H_	0	-0.18618100	-7.86069600	2.63419300	L
H-H_	0	1.40313300	-3.95613000	2.85530800	L
H-H_	0	2.54739600	-8.11421800	2.89029800	L
C-C_3	0	3.33930700	-6.52141300	-3.11354100	L
C-C_3	0	2.08765000	-7.23031000	-2.55304600	L
C-C_3	0	1.47555800	-5.06780400	-2.58380200	L
C-C_3	0	2.91589000	-5.02782400	-3.13518000	L
H-H_	0	4.22832000	-6.68606800	-2.46524900	L
H-H_	0	3.55975400	-6.88129200	-4.14248000	L
H-H_	0	3.58112000	-4.40278500	-2.49929000	L
H-H_	0	2.92130300	-4.63344100	-4.17496700	L
C-C_3	0	0.98211500	-6.38365900	-3.17656100	L

H-H_	0	-0.03613600	-6.66562600	-2.81706800	L
H-H_	0	0.99622000	-6.39524600	-4.29144400	L
C-C_R	0	1.94518800	-6.80457500	-1.12296000	L
C-C_R	0	1.56898900	-5.46894100	-1.14076000	L
H-H_	0	2.02688200	-8.32384000	-2.73702700	L
H-H_	0	0.85083200	-4.17457600	-2.79702200	L
C-C_R	0	1.30870300	-4.75554000	0.03914700	L
C-C_R	0	2.08273700	-7.52476600	0.07100500	L
H-H_	0	2.37844100	-8.56514900	0.08308000	L
C-C_R	0	1.44634400	-5.47624000	1.23568900	L

S_1TS1 (M06)

C		1.09840800	2.75833300	-0.58495700	
C		0.76688300	4.15770600	-0.60514100	
C		-0.57658900	4.26286200	-0.41357100	
C		-1.09951800	2.92792300	-0.30531600	
N		-0.06027700	2.04218900	-0.40989600	
C		2.39377100	2.23724600	-0.69044500	
C		-2.45179200	2.60878100	-0.13462300	
C		-2.98864100	1.31409500	-0.11492100	
C		-4.38487200	0.99979200	0.03825200	
C		-4.49947100	-0.35527500	-0.01249600	
C		-3.17434400	-0.89187500	-0.18528000	
N		-2.29120100	0.15154300	-0.25106900	
C		-2.86431700	-2.25574800	-0.24312600	
C		-1.56952700	-2.79560800	-0.32785700	
C		-1.25148200	-4.20300900	-0.34168400	
C		0.10445000	-4.30366900	-0.37021900	
C		0.62988300	-2.95890500	-0.38994500	
N		-0.41353100	-2.08842300	-0.37127300	
C		1.99341200	-2.62630400	-0.41302400	
C		2.53302600	-1.33124500	-0.46293400	
C		3.93870800	-1.02822200	-0.53831200	
C		4.05557400	0.32579300	-0.64044500	
C		2.72137400	0.86879400	-0.62397200	
N		1.83708600	-0.15734100	-0.50034200	
H		1.48469900	4.95884300	-0.74514800	
H		-1.17716000	5.16558800	-0.36996300	

H	-5.17212300	1.73467600	0.17070100
H	-5.40113500	-0.95382300	0.06467300
H	-1.98337200	-5.00370100	-0.32015200
H	0.70880500	-5.20469100	-0.38111300
H	4.73219100	-1.76829200	-0.51555700
H	4.96359800	0.91488100	-0.71867600
Ru	-0.24547900	0.00282800	-0.42914700
O	-0.26203000	-0.19749400	-2.17029000
O	-0.10140300	-0.21214300	1.41218800
C	2.79202200	-4.33471800	-2.97574400
C	4.24141900	-6.06485300	-2.95077800
C	4.13381400	-5.58252200	-1.52548800
C	2.80729400	-5.80015400	-3.44301900
H	2.69750400	-5.90693700	-4.53204600
H	2.05532000	-6.41901900	-2.93541200
C	4.01809500	-3.77688700	-3.74220600
H	3.73451300	-3.50663900	-4.76824900
H	4.41652900	-2.87357000	-3.26244600
C	5.01331200	-4.96645600	-3.72812100
H	5.23684800	-5.30875700	-4.74784400
H	5.96746300	-4.72218900	-3.24500900
H	1.86709600	-3.76699800	-3.12590100
H	4.64002100	-7.07727300	-3.08296100
C	3.72819200	-5.92023400	3.00037100
C	4.95484800	-5.37866600	2.21987100
C	3.51015600	-3.64287000	2.18415600
C	2.73817300	-4.72668600	2.97658600
H	3.31996600	-6.82625100	2.53556200
H	4.01624700	-6.17744400	4.02893900
H	1.77858800	-4.96962300	2.50231100
H	2.52217700	-4.36471000	3.99132000
C	4.94516200	-3.90733200	2.67136500
H	5.69281700	-3.29217800	2.15098300
H	5.05858400	-3.78472200	3.75902500
C	4.51678000	-5.22228500	0.78492700
C	3.61909200	-4.14448300	0.76652800
H	5.87824000	-5.94810400	2.37672300
H	3.11664300	-2.62690400	2.30984600

C	2.95634700	-3.76136100	-0.39855000
C	4.79165700	-5.96091500	-0.36029200
H	5.49152500	-6.79815400	-0.34576000
C	3.23405100	-4.50716400	-1.54396000
C	-4.74942300	-2.94401500	-2.70202500
C	-6.45636000	-4.41866600	-2.62841600
C	-5.88381200	-4.36410400	-1.23393600
C	-6.24120600	-2.96182600	-3.07546000
H	-6.41888900	-2.80893600	-4.14986200
H	-6.83526800	-2.24067600	-2.49816100
C	-4.22472800	-4.13034000	-3.55009600
H	-4.01877900	-3.80291000	-4.57789700
H	-3.29027000	-4.53462200	-3.13954900
C	-5.40011200	-5.14137200	-3.50539800
H	-5.80346300	-5.32533000	-4.51061600
H	-5.11550600	-6.11191500	-3.08068100
H	-4.20357900	-2.00571900	-2.84933300
H	-7.47004700	-4.82683000	-2.71279600
C	-5.92210100	-4.16820200	3.30735200
C	-5.41609100	-5.35430400	2.44522100
C	-3.70210800	-3.88797900	2.36153300
C	-4.74539000	-3.15971400	3.24644000
H	-6.86135000	-3.75573400	2.91865100
H	-6.10768700	-4.49974300	4.33817700
H	-5.02945100	-2.18908700	2.82004100
H	-4.33045500	-2.97103200	4.24573300
C	-3.92008400	-5.34436000	2.80643400
H	-3.32991700	-6.06350500	2.22278200
H	-3.73345800	-5.50020800	3.87896300
C	-5.35673500	-4.85271900	1.02391200
C	-4.29123800	-3.94218200	0.97371800
H	-5.96465900	-6.29083600	2.59783700
H	-2.68604600	-3.48525200	2.43520900
C	-3.99812400	-3.21711500	-0.18183500
C	-6.17145400	-5.08266500	-0.07905400
H	-6.99716700	-5.79513100	-0.04024800
C	-4.82313200	-3.44799000	-1.28258100
C	3.45297100	4.24624200	1.57472000

C	5.19290700	5.65363600	1.29940900
C	4.99500400	4.95853200	-0.02470800
C	3.73654600	5.74333700	1.78433700
H	3.64848400	6.05416700	2.83548700
H	3.11041500	6.39126100	1.15635900
C	4.55479400	3.61604100	2.46272700
H	4.22442100	3.56737700	3.51010500
H	4.78848700	2.58945300	2.14973100
C	5.74911300	4.58909500	2.28110700
H	6.02555500	5.06000800	3.23428600
H	6.64493800	4.09697100	1.88310200
H	2.43621900	3.90206700	1.79516100
H	5.77102000	6.58418000	1.26651000
C	4.61242200	4.64875200	-4.52364900
C	5.74242700	4.01802900	-3.66799600
C	4.02239800	2.58450900	-3.38708800
C	3.42806100	3.66775200	-4.32298800
H	4.38202200	5.67175100	-4.20160900
H	4.91583800	4.69400300	-5.57853000
H	2.54397700	4.14235700	-3.87727200
H	3.11591200	3.21856800	-5.27519600
C	5.46951600	2.52231200	-3.90346400
H	6.11189000	1.86556600	-3.30149000
H	5.53719800	2.23227200	-4.96194400
C	5.30744300	4.15363000	-2.23033300
C	4.23967700	3.26178000	-2.05606300
H	6.74699900	4.38991500	-3.89989600
H	3.45578800	1.64767200	-3.36385700
C	3.51657400	3.19802200	-0.86256800
C	5.70996200	5.01377100	-1.21524300
H	6.54482600	5.70380300	-1.34809200
C	3.91526300	4.07888900	0.14661700
C	-3.76552000	4.30895300	-2.50036700
C	-5.18640700	6.03391400	-2.18262700
C	-4.78877400	5.55522900	-0.80837900
C	-3.88077300	5.77412400	-2.95545900
H	-3.99445400	5.88011800	-4.04413700
H	-3.04416900	6.39667800	-2.61097200

C	-5.11864500	3.74605900	-3.00403600
H	-5.04751000	3.47884400	-4.06692100
H	-5.40814400	2.84012400	-2.45603600
C	-6.09533300	4.93100300	-2.78619300
H	-6.52442800	5.27162200	-3.73837600
H	-6.92921700	4.68217700	-2.11830300
H	-2.88678700	3.74507000	-2.83285000
H	-5.60775500	7.04446000	-2.23243000
C	-3.42286100	5.92768700	3.51060900
C	-4.79255500	5.38052900	3.02818400
C	-3.39362700	3.64056800	2.69598700
C	-2.46140100	4.73197700	3.28063300
H	-3.12752500	6.82762600	2.95727200
H	-3.47453700	6.19547600	4.57479300
H	-1.63531500	4.96722800	2.59559800
H	-2.01872900	4.38984800	4.22649900
C	-4.68458100	3.91501900	3.48624300
H	-5.52845000	3.29578500	3.15463900
H	-4.55578700	3.81077200	4.57345400
C	-4.67993100	5.20838200	1.53347500
C	-3.80719500	4.13017800	1.33109000
H	-5.65741300	5.95479200	3.37951400
H	-2.98400500	2.62417600	2.73374700
C	-3.39696100	3.74273900	0.05614500
C	-5.18873900	5.94072900	0.46630400
H	-5.86852400	6.78011800	0.62174500
C	-3.90907200	4.48108100	-1.00924700
C	2.79503000	-0.90697400	5.54184800
C	1.96323200	-0.10979800	4.76680900
C	2.39451600	0.38675800	3.52628000
C	3.68302900	0.03602800	3.08597700
C	4.51998700	-0.74570500	3.86841700
C	4.07978200	-1.22158900	5.10243400
H	2.44192500	-1.28095400	6.50194000
H	0.96303700	0.13278300	5.12397700
H	4.01627700	0.38708300	2.10692800
H	5.52047300	-0.99073300	3.51338200
H	4.73505900	-1.83593600	5.71880700

C	1.54570400	1.22143100	2.67282700
C	0.50100000	2.11771600	3.28622100
H	0.81522400	0.40823600	1.98734900
H	2.11775700	1.70567600	1.87090500
H	0.95221100	2.86504700	3.95915100
H	-0.04871500	2.65343900	2.49859300
H	-0.23948300	1.54924200	3.86554300

R_1TS1 (M06)

C	2.65819700	1.45142500	-0.35518700
C	3.26427400	2.75589200	-0.36444700
C	2.25580600	3.67009400	-0.36045300
C	1.01473100	2.94202600	-0.35368600
N	1.30064100	1.60155800	-0.35227100
C	3.35918400	0.23807400	-0.35508200
C	-0.25612200	3.52725000	-0.33891100
C	-1.47719400	2.83190300	-0.30822400
C	-2.78307000	3.44201800	-0.24038800
C	-3.69071600	2.43134700	-0.17983400
C	-2.95165900	1.19165000	-0.22380500
N	-1.62567000	1.48433400	-0.30977000
C	-3.52410700	-0.08858400	-0.17248500
C	-2.82995000	-1.30941400	-0.20507200
C	-3.44974900	-2.61052500	-0.23613900
C	-2.45082700	-3.53111900	-0.33335000
C	-1.20784000	-2.80316700	-0.34805200
N	-1.47874100	-1.47480800	-0.25785700
C	0.07190400	-3.38107000	-0.41563700
C	1.28051300	-2.67673400	-0.37519500
C	2.58518800	-3.28159000	-0.40019800
C	3.50181900	-2.27570800	-0.36335500
C	2.77500100	-1.03533800	-0.33035300
N	1.43513300	-1.31316200	-0.31391500
H	4.33393400	2.93862200	-0.36416800
H	2.33450800	4.75224800	-0.36209900
H	-2.96756000	4.51112300	-0.22820600
H	-4.77109600	2.50514900	-0.11203500
H	-4.51962300	-2.78725800	-0.19884700

H	-2.53764300	-4.61105000	-0.39319400
H	2.76748900	-4.35043600	-0.44119600
H	4.58389600	-2.35587500	-0.37686100
Ru	-0.07123300	0.07995200	-0.35369300
O	-0.32139700	0.03381500	-2.08750300
O	-0.28252200	0.18142800	1.48896800
C	-0.38568000	-4.76852500	-3.19750700
C	-0.27336600	-6.99277000	-3.56613100
C	-0.04121500	-6.79574500	-2.08885600
C	-1.26598900	-5.85030800	-3.84612800
H	-1.43777900	-5.68050200	-4.91888600
H	-2.22954700	-5.97993300	-3.33539800
C	0.91595800	-4.92289800	-4.02460600
H	0.83661600	-4.36222300	-4.96549800
H	1.78708200	-4.53336300	-3.48214700
C	0.99078300	-6.45015700	-4.28297100
H	0.94275500	-6.67391500	-5.35745200
H	1.90759800	-6.90744500	-3.89082700
H	-0.78195800	-3.74757600	-3.16496600
H	-0.56850100	-8.00304600	-3.87197100
C	-0.47832700	-7.63043300	2.35760500
C	0.81815700	-7.77437200	1.51967500
C	0.69287900	-5.55294100	1.89116100
C	-0.56650200	-6.10294700	2.60888900
H	-1.35154900	-8.02825600	1.82622900
H	-0.38497500	-8.18316300	3.30238300
H	-1.48716500	-5.65269400	2.21463100
H	-0.52221900	-5.87507700	3.68322400
C	1.69377400	-6.68771200	2.16813100
H	2.65523100	-6.54583900	1.65680300
H	1.86910800	-6.85583100	3.24065600
C	0.53493500	-7.13533900	0.18328200
C	0.46112000	-5.75265800	0.41320100
H	1.22330500	-8.79209900	1.48412000
H	0.98360700	-4.54171700	2.20027200
C	0.13999400	-4.85655600	-0.60717600
C	0.28624700	-7.68256800	-1.06982400
H	0.34660800	-8.75802400	-1.24480300

C	-0.11253900	-5.41417600	-1.86169300
C	-5.52653300	0.37416200	-2.61364800
C	-7.77451600	0.25162700	-2.45068000
C	-7.23598100	0.01677300	-1.06135300
C	-6.73412600	1.25073000	-2.98741700
H	-6.82134600	1.42580600	-4.06956800
H	-6.74568000	2.21273500	-2.45768100
C	-5.86487400	-0.92485200	-3.38802700
H	-5.54277300	-0.83835900	-4.43439500
H	-5.35361500	-1.79571400	-2.95796400
C	-7.40972800	-1.00780600	-3.27954900
H	-7.88037800	-0.95926400	-4.27103900
H	-7.75699400	-1.92796400	-2.79361800
H	-4.52861200	0.77673500	-2.81868800
H	-8.82955700	0.54256200	-2.51026600
C	-6.98140200	0.45627100	3.45213100
C	-7.33571200	-0.84173700	2.67966900
C	-5.08845000	-0.73275200	2.50471600
C	-5.43738000	0.53363900	3.32651900
H	-7.49041800	1.33146700	3.02998400
H	-7.28998400	0.36878500	4.50290500
H	-5.08883400	1.44599000	2.82554200
H	-4.95471300	0.49451200	4.31233500
C	-6.13018200	-1.72456400	3.04926300
H	-6.12159300	-2.68727000	2.52074500
H	-6.03768600	-1.89761800	4.13141800
C	-7.03726100	-0.56633900	1.22668500
C	-5.64092000	-0.49804200	1.12131400
H	-8.33450700	-1.23809400	2.89543300
H	-4.03421800	-1.02906400	2.55183300
C	-5.00697400	-0.16345000	-0.07527500
C	-7.86142200	-0.31201500	0.13613500
H	-8.94834800	-0.36748600	0.21602900
C	-5.83919300	0.09316000	-1.16488400
C	5.32159800	0.63068000	2.12789600
C	7.57034700	0.71710400	1.97488900
C	7.05381100	0.58292800	0.56341000
C	6.44846800	1.56269400	2.60359800

H	6.51924300	1.62887400	3.69991600
H	6.37725600	2.57231900	2.17798400
C	5.76711200	-0.71019200	2.76685200
H	5.43664200	-0.76827600	3.81338800
H	5.33229300	-1.57068400	2.24089800
C	7.31356600	-0.64836800	2.66518900
H	7.77646400	-0.66369800	3.66132100
H	7.73872800	-1.48011300	2.09018900
H	4.29194400	0.93320700	2.35529800
H	8.59645400	1.08874100	2.07520100
C	6.74401900	1.43540000	-3.89493800
C	7.21643000	0.10919000	-3.24303400
C	4.96859500	-0.00219600	-3.07137100
C	5.19961300	1.35952000	-3.77435400
H	7.17130900	2.31058800	-3.39010400
H	7.05849200	1.47397700	-4.94682100
H	4.76917600	2.18874800	-3.19814400
H	4.72189200	1.36287300	-4.76322400
C	6.09494100	-0.84138900	-3.69861500
H	6.17497500	-1.84514400	-3.26049200
H	6.01473000	-0.92211200	-4.79239100
C	6.89847900	0.21998500	-1.77255100
C	5.50135100	0.15355200	-1.66928000
H	8.24654300	-0.17359100	-3.48834800
H	3.94639100	-0.38789000	-3.15396200
C	4.84452800	0.30598500	-0.44806900
C	7.70150100	0.43374000	-0.65776700
H	8.78881500	0.48050200	-0.73748000
C	5.65619300	0.52534200	0.66326800
C	0.09693100	5.34947000	-2.92216800
C	-0.01554200	7.60357700	-2.91556700
C	-0.18533900	7.16719300	-1.48160400
C	0.95613000	6.52304700	-3.42242700
H	1.08037300	6.53186100	-4.51506500
H	1.94172700	6.56780700	-2.93987800
C	-1.23770700	5.63625600	-3.65577300
H	-1.20351400	5.23821200	-4.67876700
H	-2.08662800	5.16230200	-3.14621400

C	-1.31293800	7.18541900	-3.65639700
H	-1.30976800	7.58226400	-4.68084200
H	-2.20890300	7.57166900	-3.15502400
H	0.48862100	4.33752200	-3.07326300
H	0.27325000	8.65027200	-3.06494200
C	0.45521000	7.23752700	3.01819900
C	-0.87438000	7.53644700	2.27710700
C	-0.77024700	5.28153600	2.26131600
C	0.52778300	5.68839200	3.00394100
H	1.31134500	7.71195100	2.52277600
H	0.41201700	7.62341900	4.04591700
H	1.42107600	5.30206500	2.49659700
H	0.52638200	5.27919200	4.02304900
C	-1.73917400	6.36258900	2.77014100
H	-2.72361700	6.31790100	2.28528400
H	-1.86608200	6.34830900	3.86241500
C	-0.66063600	7.13257800	0.83945600
C	-0.59598600	5.73164400	0.83219100
H	-1.26266100	8.54917400	2.43518000
H	-1.06279600	4.23520600	2.40174900
C	-0.32188200	5.01408400	-0.33227400
C	-0.45804100	7.87665600	-0.31747400
H	-0.51098100	8.96665300	-0.31206400
C	-0.11584100	5.76641700	-1.48844200
C	2.84494300	0.27623200	4.76437200
C	2.19588100	-0.45385300	3.78101200
C	0.96980900	-1.08956700	4.04298200
C	0.41837300	-0.96168900	5.32563800
C	1.07527400	-0.23843700	6.31388400
C	2.28831700	0.38523300	6.03883700
H	3.79060300	0.77177200	4.54007400
H	2.61888500	-0.53455200	2.77490900
H	-0.53059200	-1.44465300	5.55491800
H	0.63557300	-0.16015400	7.30728400
H	2.79882200	0.95709200	6.81202900
C	0.29302000	-1.79948500	2.95240800
C	-0.98300500	-2.54601500	3.22160500
H	0.99450700	-2.32143400	2.28437500

H	-0.04233000	-0.83109600	2.16573100
H	-1.40104400	-2.95400800	2.29122800
H	-0.82815300	-3.39009000	3.91439100
H	-1.74281900	-1.88896400	3.66688000