

Supporting Information

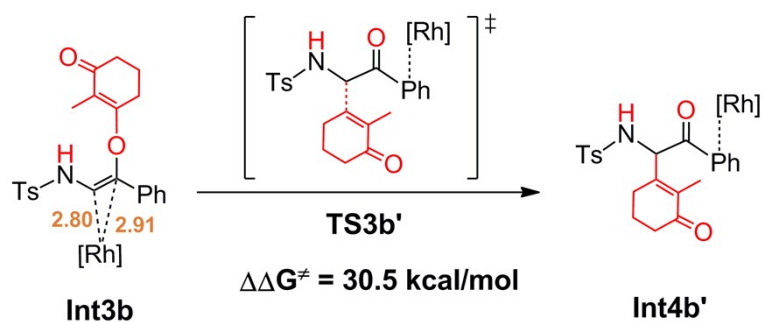
Computational Mechanistic Study of Substrate-Controlled Competitive O–H and C–H Insertion Reaction Catalyzed by dirhodium(II) carbenoid: Insight into the Origin of Chemoselectivity

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Scheme S1 Energies for [Rh]-catalyzed C-C bond formation process.

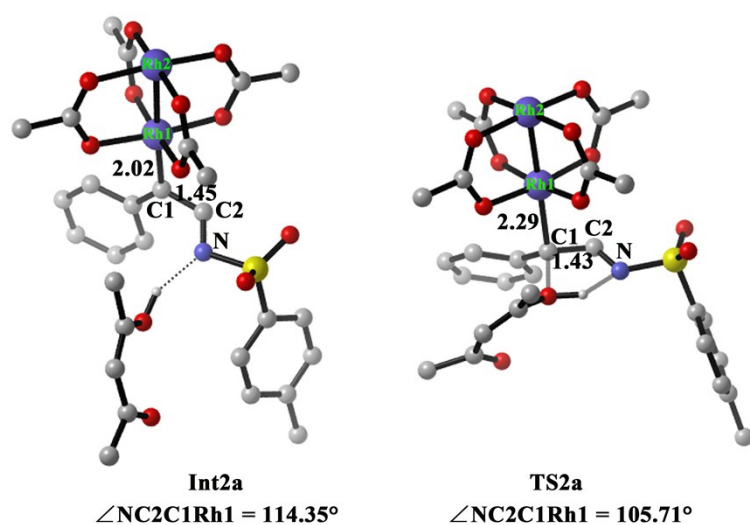


Fig. S1 Optimized structures of **Int2a** and **TS2a**, distances are given in Å.

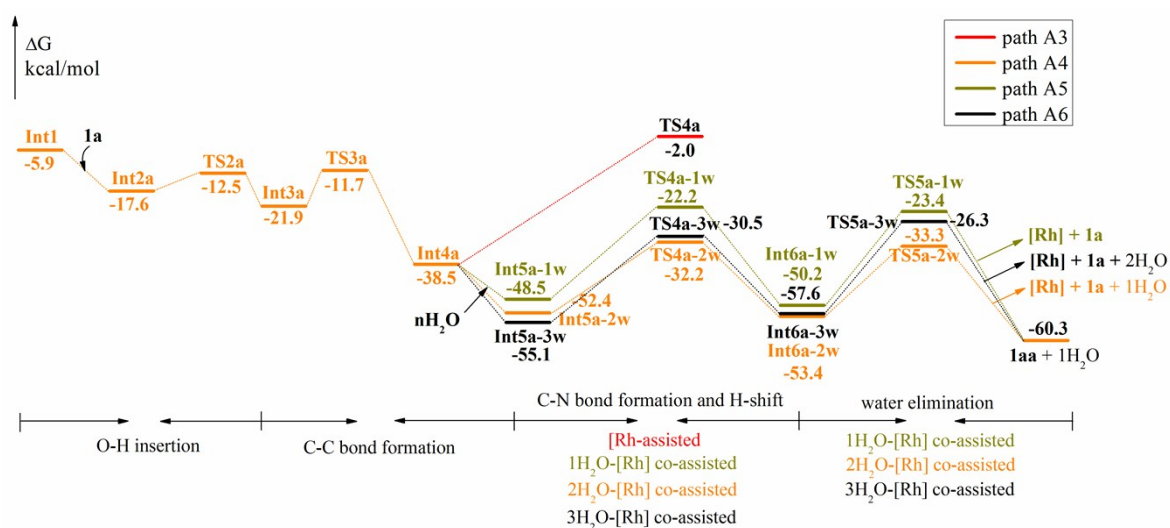


Fig. S2. DFT computed energy surfaces for [Rh]-assisted path A3, [Rh]-2H₂O co-assisted path A4, [Rh]-1H₂O co-assisted path A5, and [Rh]-3H₂O co-assisted path A6 in the solvent phase, and free energies are given in kcal/mol.

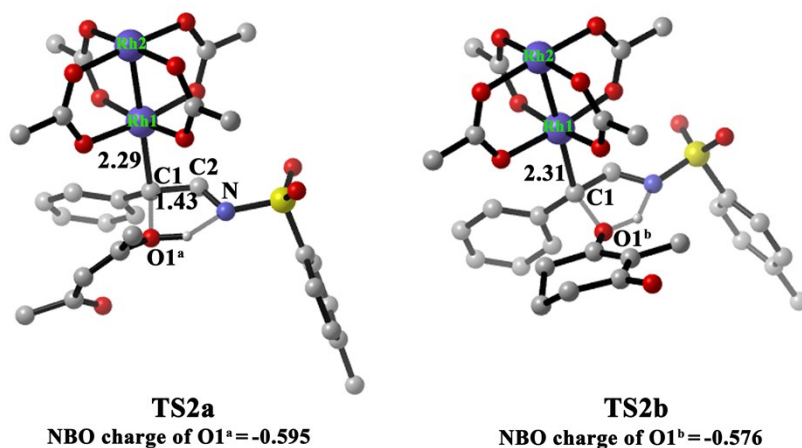


Fig. S3 Optimized structures of **TS2a** and **TS2b**, distances are given in Å.

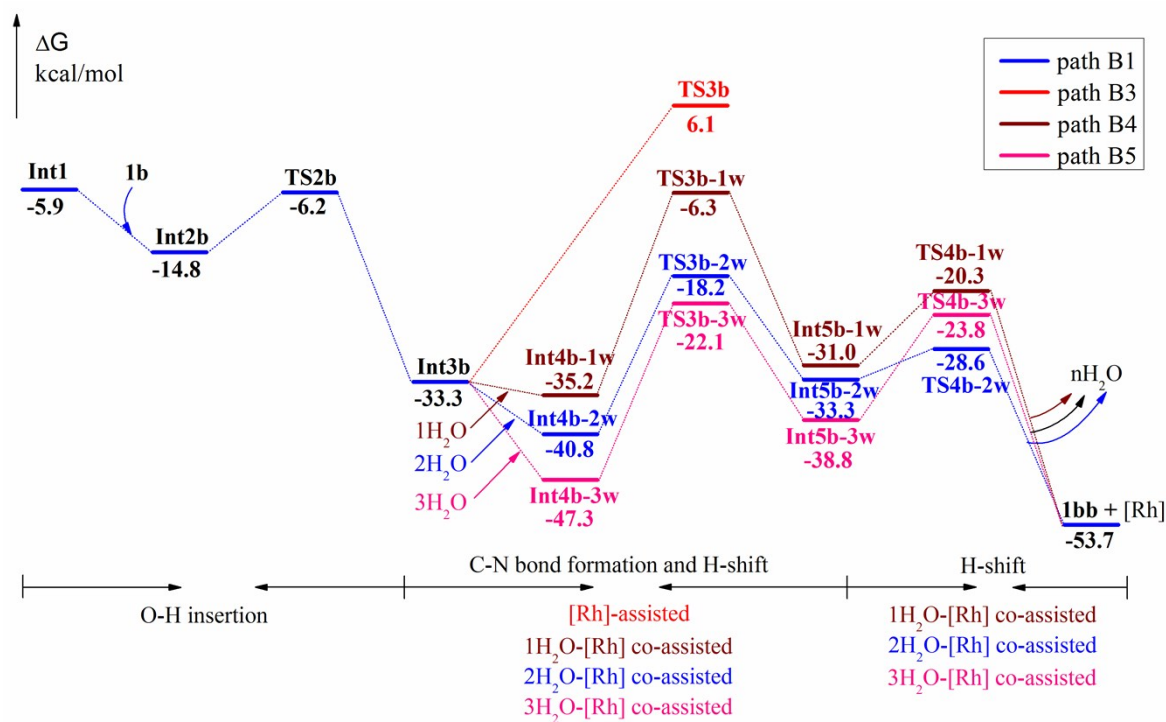


Fig. S4 DFT computed energy surfaces for paths B1, B2, B3, and B4 in the solvent phase, and free energies are given in kcal/mol.

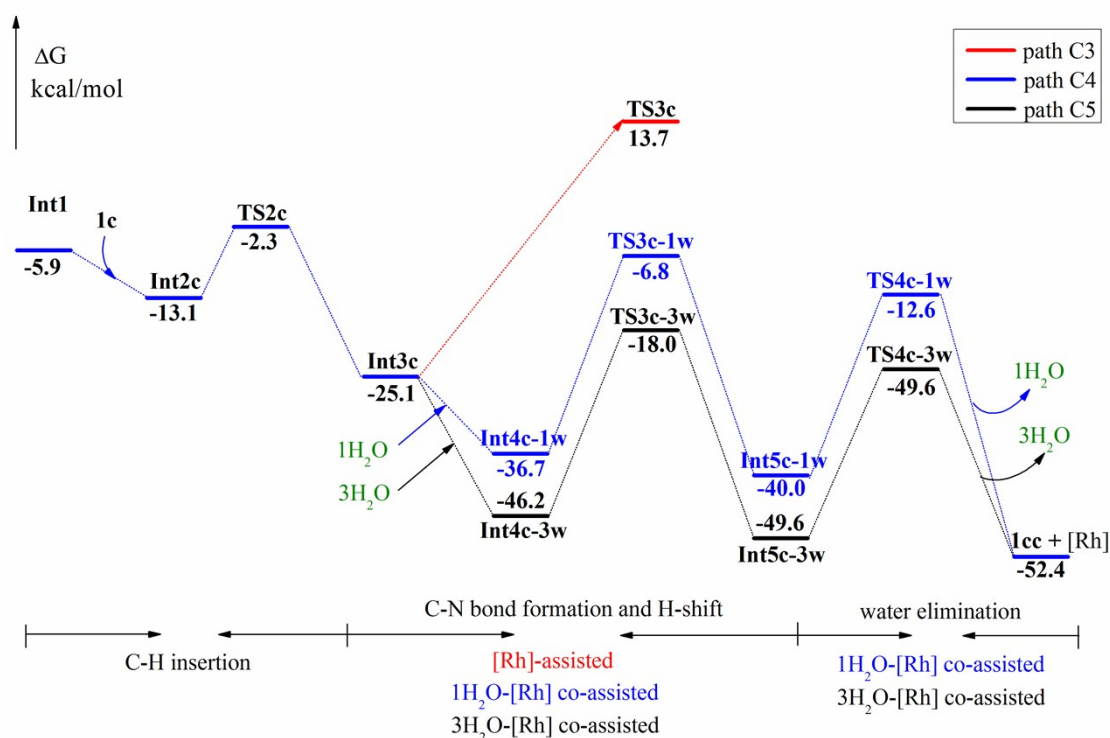


Fig. S5 DFT computed energy surfaces for paths C2, C3, and C4 in the solvent phase, and free energies are given in kcal/mol.

Distortion/interaction Analysis.

For the transition-metal catalysis reaction, it is important to figure out the factors governing the chemoselectivity within the established mechanism. To obtain deep insights into the origins of the difference of the reaction between three 1,3-diketones and the α -imino rhodium carbenoids, we then performed the distortion/interaction analysis of the rate-determining step transition states **TS4a-2w**, **TS3b-2w**, and **TS3c-2w**. The distortion/interaction model, or the activation strain model, has recently been used to elucidate the reactivities and selectivities organic synthesis in different systems. In bimolecular reaction, the transition state is divided into two fragments (the [Rh]-2H₂O catalyst and enol-tautomer substrate), followed by single point energy calculations on each distorted fragment. The energy differences between the distorted fragments and optimized ground-state geometries are the distortion energy of substrate ($\Delta E_{\text{sub}}^{\ddagger}$) and the catalyst ($\Delta E_{\text{cat}}^{\ddagger}$), respectively. The interaction energy ($\Delta E_{\text{int}}^{\ddagger}$) is the difference between the deformed fragments ($\Delta E_{\text{int}}^{\ddagger} = \Delta E^{\ddagger} - \Delta E_{\text{dist}}^{\ddagger}$).

The results in Figure 5 show that the distortion energy of **TS4a-2w** (28.6 kcal/mol) is larger than that of **TS3b-2w** (27.5 kcal/mol) and **TS3c-2w** (23.2 kcal/mol) by 1.1 and 5.4 kcal/mol.

However, the interaction energy (41.1 kcal/mol) is more favorable for **TS4a-2W** compared to that of the latter two ones (34.5 and 26.4 kcal/mol). Consequently, the interaction energy is the dominate factor determining the difference of the reaction between three 1,3-diketones and the α -imino rhodium carbenoids.

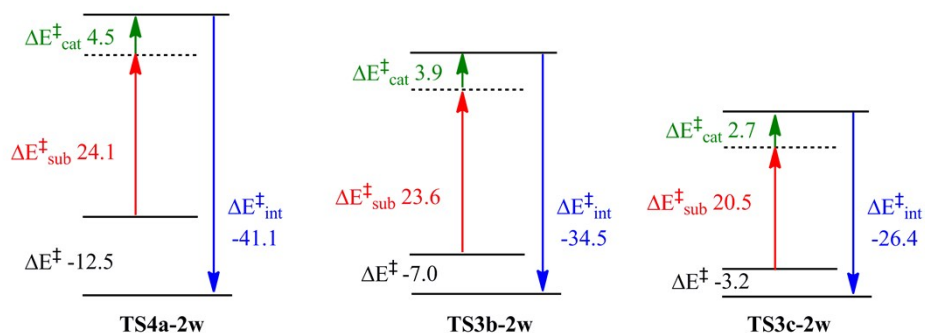


Fig. S6 Distortion, interaction and activation energies for the **TS4a-2w**, **TS3b-2w**, and **TS3c-2w** (green: distortion energy of catalyst; blue: distortion energy of substrate; red: interaction energy; black: activation energy, in kcal/mol).

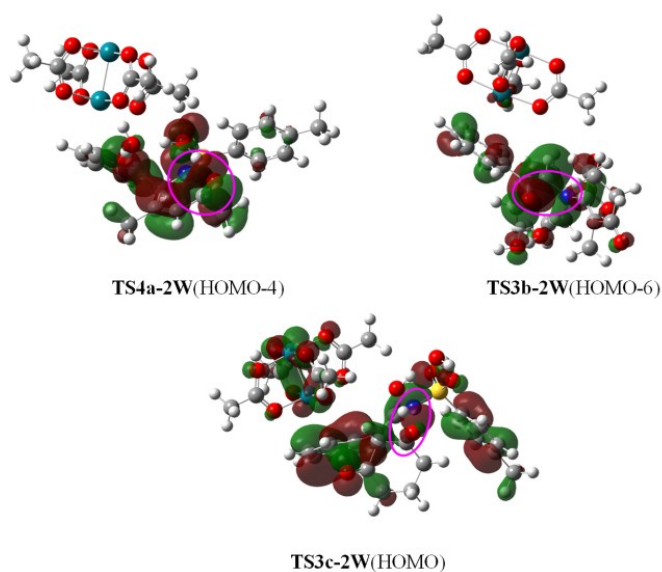


Fig. S7 Orbital interactions (pink ellipse) in HOMOs of the $2\text{H}_2\text{O}$ -[Rh] co-assisted transition states **TS4a-2w**, **TS3b-2w**, and **TS3c-2w**.

The higher activity of [Rh]- $2\text{H}_2\text{O}$ co-catalyzed C–N bond formation and H-shift process is also attributed to greater orbital overlap of the HOMO of **TS4a-2w**. As illustrated in Fig. S7, the electron delocalization of the reaction sites and the whole molecular fragments in HOMO-4 of **TS4a-2w** is larger than that in HOMO-6 of **TS3b-2w** and HOMO of **TS3c-2w**. In **TS4a-2w**, HOMO-4 shows a much stronger orbital interaction between N and carbonyl

oxygen O1 as well as the benzene rings. Consequently, the orbital interaction order of the TSs follows **TS4a-2w** > **TS3c-2w** > **TS3b-2w**, indicating that the substrate **1a** insertion path A1 is the most favored one.

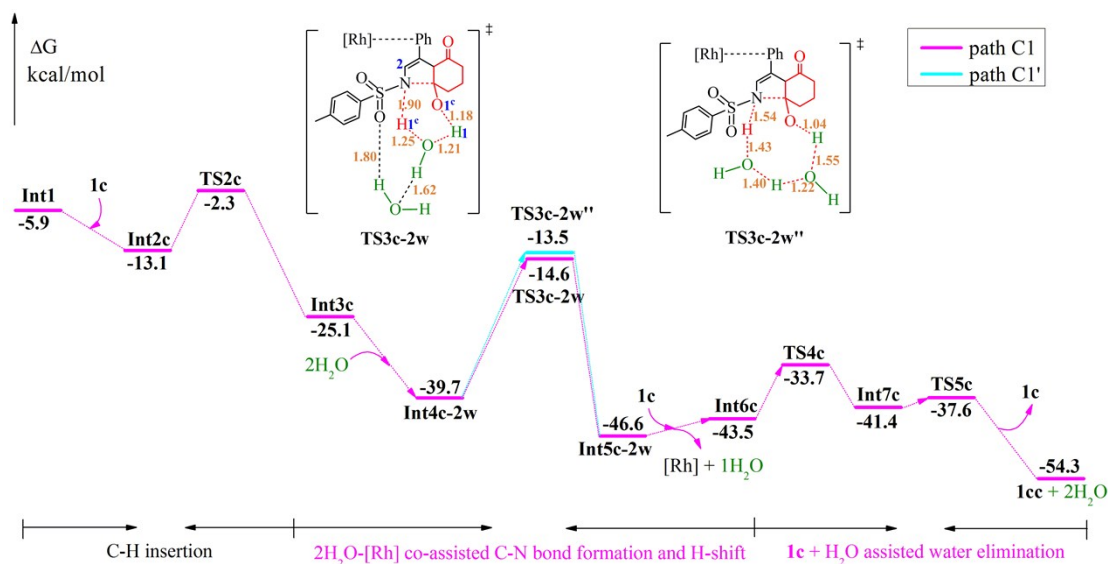


Fig. S8 DFT computed energy surfaces and the geometry structures of paths C1 and C1' in the solvent phase. The solvent-corrected free energies have been given in kcal/mol, and distances are in Å.

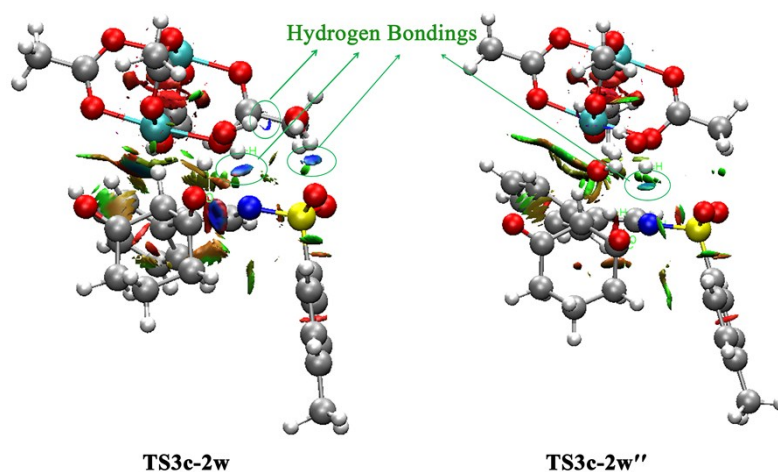


Fig. S9 Noncovalent interactions analysis (blue, strong interaction; green, weak interaction; and red, strong repulsion) for transition states **TS3c-2w** and **TS3c-2w''**.

Table S1. DFT calculated free energy profiles of enol-tautomer and keto-tautomer of **1a**, **1b**, and **1c**.

structures	enol-tautomer (kcal/mol)	keto-tautomer (kcal/mol)	$\Delta G^\ddagger$ (kcal/mol)
1a	-337206.5	-337221.2	14.7
1b	-265489.1	-265499.5	10.4
1c	-240830.3	-240839	8.7

Table S2. The comparison of free energy profiles in [Rh]-2H₂O co-assisted path A2 at M06-2X/6-311+G(d,p)(C, H, O, N, S), SDD (Rh) (olive line) and B3LYP-D3/6-311+G(d,p) (C, H, O, N, S), SDD (Rh) (red line). Activation free energies are given in kcal/mol.

Method TSs	B3LYP-D3/6- 311+G(d,p) (C, H, O, N, S), SDD (Rh) (red line)	M06-2X/6- 311+G(d,p)(C, H, O, N, S), SDD (Rh)	ΔG /kcal/mol
Com1	0	0	0
TS1	11.2	9.3	1.9
Int1	-3.4	-5.9	2.5
Int2a	-16.2	-17.6	1.4
TS2a	-3.1	-7.5	4.4
Int3a	-20.5	-21.9	1.4
TS3a	-7.2	-11.7	4.5
Int4a	-36.1	-38.5	1.6
Int5a-2w	-48.3	-52.4	4.1
TS4a-2w	-25.6	-32.2	6.6
Int6a-2w	-52.1	-53.4	1.3
Int7a	-53.5	-54.4	0.9
TS5a	-39.1	-43.8	4.7
Int8a	-54.3	-57.7	3.4
TS6a	-55.1	-57.3	2.2
1aa	-54.8	-58.9	4.1

Table S3. The comparison of free energy profiles in [Rh]-2H₂O co-assisted path B2 at M06-2X/6-311+G(d,p)(C, H, O, N, S), SDD (Rh) (olive line) and B3LYP-D3/6-311+G(d,p) (C, H, O, N, S), SDD (Rh) (red line). Activation free energies are given in kcal/mol.

TSs \ Method	B3LYP-D3/6-311+G(d,p) (C, H, O, N, S), SDD (Rh) (red line)	M06-2X/6-311+G(d,p)(C, H, O, N, S), SDD (Rh)	$\Delta G/\text{kcal/mol}$
Com1	0	0	0
TS1	11.2	9.3	1.9
Int1	-3.4	-5.9	2.5
Int2b	-10.4	-14.8	4.4
TS2b	-0.8	-1.2	0.4
Int3b	-28.5	-33.3	4.8
Int4b-2w	-24.5	-27.9	3.4
TS3b-2w	-13.1	-18.2	5.1
Int5b-2w	-28.3	-33.0	4.7
TS4b-2w	-24.8	-28.6	3.2
1bb	-30.1	-33.5	3.4

Table S4. The comparison of free energy profiles in [Rh]-2H₂O co-assisted path C2 at M06-2X/6-311+G(d,p)(C, H, O, N, S), SDD (Rh) (olive line) and B3LYP-D3/6-311+G(d,p) (C, H, O, N, S), SDD (Rh) (red line). Activation free energies are given in kcal/mol.

TSs \ Method	B3LYP-D3/6-311+G(d,p) (C, H, O, N, S), SDD (Rh) (red line)	M06-2X/6-311+G(d,p)(C, H, O, N, S), SDD (Rh)	$\Delta G/\text{kcal/mol}$
Com1	0	0	0
TS1	11.2	9.3	1.9
Int1	-3.4	-5.9	2.5
Int2c	-11.4	-13.1	2.3
TS2c	5.9	2.7	3.2
Int3c	-21.6	-25.1	3.5
Int4c-2w	-33.1	-39.7	6.1
TS3c-2w	-10.4	-14.6	4.2
Int5c-2w	-44.1	-46.6	2.5
Int6c	-41.5	-43.5	2.0
TS4c	-27.6	-33.7	6.1
Int7c	-37.2	-41.4	3.2
TS5c	-33.9	-37.6	3.7
1cc	-40.1	-42.7	1.6

S1. The B3LYP/6-31G(d) (C, H, O, N, S), SDD (Rh) optimized coordinates between α -Imino Rhodium carbenoids and 1,3-diketones in gas phase.

Com1

Rh	2.96552500	-1.66980200	-0.21013100
Rh	1.28814200	0.02491800	0.13567200
O	2.29242800	0.57627700	1.86143100
C	3.35340600	-0.06114900	2.18058700
O	3.86540200	-1.02304200	1.53070600
O	0.40320700	-0.64687500	-1.59966000
C	0.89815700	-1.64350500	-2.22532100
O	1.97316300	-2.24860800	-1.91473200
O	2.46622700	1.30615500	-0.98279500
C	3.56943200	0.87655500	-1.45452300
O	4.05065200	-0.28962800	-1.28763200
O	1.78223200	-2.97105400	0.86313500
C	0.67349400	-2.55294900	1.32479800
O	0.23301200	-1.35924200	1.23148100
C	4.06549200	0.39215800	3.43535200
H	4.82289700	-0.33608000	3.72931900
H	3.34361300	0.53687700	4.24410800
C	-0.22082600	-3.54411200	2.02999100
H	-0.49807800	-3.15770100	3.01566900
H	0.27604200	-4.51020400	2.13031100
C	4.36545900	1.83152700	-2.31528900
H	4.09478500	1.66905200	-3.36533700
H	5.43489800	1.63666500	-2.20756100
C	0.11740300	-2.14266700	-3.41582900
H	0.67901400	-2.90889200	-3.95243200
H	-0.12140800	-1.30747300	-4.08066600
C	-0.57765800	1.72675000	0.57283500
C	-0.03365500	3.07957100	0.24567700
C	-0.63362600	3.85117100	-0.76110300
C	1.06862300	3.59943600	0.94276400
C	-0.12550200	5.11157300	-1.07652800
H	-1.50279600	3.47853500	-1.29419000
C	1.55316700	4.86971600	0.63969400

H	1.56277800	2.99438600	1.69701100
C	0.96392500	5.62860400	-0.37453300
H	-0.59713100	5.69512900	-1.86228700
H	2.40571500	5.26072200	1.18833700
H	1.34997600	6.61542200	-0.61403600
C	-1.52817700	1.00995700	-0.26858200
N	-2.40365900	0.19866500	0.21593900
S	-3.28407100	-0.68712500	-0.95510700
O	-3.19415900	-0.05492700	-2.28298800
O	-2.90666800	-2.09656000	-0.78797000
C	-4.94703300	-0.46324900	-0.33697000
C	-5.82699200	0.37290500	-1.02276600
C	-5.34551500	-1.13781900	0.82025700
C	-7.12354700	0.53710700	-0.53493500
H	-5.49742400	0.87682300	-1.92496400
C	-6.64175900	-0.95796200	1.29388500
H	-4.65110900	-1.79487200	1.33301200
C	-7.55054500	-0.12149400	0.62560800
H	-7.81451200	1.18711500	-1.06602800
H	-6.95677700	-1.47703300	2.19592300
C	-8.96324300	0.03998400	1.13479200
H	-8.99354700	0.06892100	2.22944900
H	-9.42368500	0.95822000	0.75674400
H	-9.59451700	-0.79982900	0.81546800
N	-0.69261600	1.44793000	1.89022200
N	-0.74155100	1.17883600	2.98243200
H	4.55039800	1.35660500	3.24533500
H	-1.14181800	-3.65496100	1.44720000
H	4.13204600	2.86591400	-2.05522200
H	-0.83294700	-2.55492600	-3.05913500
H	-1.41835700	1.18474500	-1.34079600
TS1			
Rh	3.29001800	-1.32829900	-0.15865100
Rh	1.33131700	0.10884300	0.08733300
O	2.08119000	0.67764300	1.93149600
C	3.17217300	0.14906300	2.34853200
O	3.87762100	-0.69353400	1.72161200

O	0.75665200	-0.56733700	-1.78654300
C	1.48249000	-1.41200000	-2.41555900
O	2.58447300	-1.89074900	-2.01120100
O	2.45033200	1.60201300	-0.83344100
C	3.65414900	1.35791900	-1.18248400
O	4.27948600	0.26656900	-1.01359200
O	2.17247600	-2.85142700	0.68144900
C	0.98249800	-2.61578600	1.05246100
O	0.38855400	-1.48467600	0.98139600
C	3.63705400	0.57646400	3.72347000
H	3.67012200	1.66875900	3.78294400
H	4.62146900	0.15934700	3.94024700
C	0.17469500	-3.74709900	1.64386400
H	-0.82697300	-3.74543400	1.20403100
H	0.06505100	-3.58570100	2.72261400
C	4.38975300	2.47348700	-1.89381400
H	4.14001500	2.43739200	-2.96085600
H	5.46880600	2.34636300	-1.78685900
C	0.96924700	-1.85225800	-3.76759400
H	1.52758600	-2.71951600	-4.12365100
H	1.08688500	-1.02997700	-4.48274000
C	-0.49180300	1.30745400	0.25064900
C	-0.46584000	2.76948100	0.03150400
C	-1.48148600	3.40979900	-0.70552200
C	0.59533400	3.54050000	0.54435500
C	-1.42032200	4.77960200	-0.95054800
H	-2.31718300	2.83150600	-1.08891300
C	0.63206000	4.91451100	0.32835200
H	1.37983600	3.04746600	1.10752800
C	-0.36747000	5.53461600	-0.42804400
H	-2.20095200	5.25965600	-1.53375600
H	1.44945500	5.50273500	0.73581400
H	-0.32670300	6.60553100	-0.60789000
C	-1.52868700	0.48819700	-0.36338800
N	-2.43496800	-0.14694500	0.29275400
S	-3.32270800	-1.29621700	-0.63271100
O	-3.11315200	-1.08892500	-2.07645100
O	-3.05315600	-2.60440600	-0.02610200

C	-4.99695100	-0.81471900	-0.22989000
C	-5.77472200	-0.16440800	-1.18620400
C	-5.50981700	-1.11843000	1.03474500
C	-7.08485900	0.19248900	-0.86373300
H	-5.36126100	0.04161200	-2.16769400
C	-6.81654100	-0.75053000	1.33884500
H	-4.89601600	-1.64578200	1.75731300
C	-7.62344700	-0.08879700	0.39809800
H	-7.69946000	0.69263200	-1.60795500
H	-7.22219900	-0.98662600	2.31975300
C	-9.03743900	0.30928300	0.74939200
H	-9.04774100	1.10082100	1.50962800
H	-9.57895200	0.68120000	-0.12561500
H	-9.59921100	-0.53782500	1.16004700
N	-0.85665800	1.10881000	1.95752100
N	-0.59917700	1.02109300	3.03407400
H	2.91881000	0.22802400	4.47370300
H	0.67374300	-4.70258900	1.47385700
H	4.07550100	3.44605600	-1.50777400
H	-0.09766300	-2.08314800	-3.70015500
H	-1.40029700	0.36736200	-1.44527400
Int1			
Rh	3.51355900	-0.98422800	0.03390600
Rh	1.35290700	0.17285500	-0.17314400
O	1.82264800	1.14299200	1.59432300
C	2.91542000	0.85554300	2.20056800
O	3.79418600	0.03508300	1.80802500
O	1.09688100	-0.90003600	-1.92893100
C	1.99895100	-1.72269000	-2.32019700
O	3.10174200	-1.94711600	-1.74267300
O	2.37347200	1.64993000	-1.22085600
C	3.63306500	1.52870900	-1.41850100
O	4.36724300	0.58227600	-1.01146100
O	2.52569500	-2.48630900	1.05098500
C	1.27894500	-2.37834000	1.25317300
O	0.54142400	-1.40154600	0.87760000
C	3.14419200	1.55572500	3.52180100
H	2.85177900	2.60688800	3.45068800

H	4.18989300	1.46922100	3.82154500
C	0.58028100	-3.47062800	2.02828900
H	-0.48065800	-3.49970600	1.77077900
H	0.67039700	-3.25207700	3.09909600
C	4.28414800	2.62066600	-2.23986400
H	4.00348600	2.49082800	-3.29139900
H	5.37044400	2.56665200	-2.15174300
C	1.68615800	-2.49181100	-3.58372100
H	2.55840900	-3.06081200	-3.90887300
H	1.36762300	-1.80251300	-4.37137600
C	-0.44707800	1.05332100	-0.41995500
C	-0.78976800	2.44173600	-0.39541800
C	-2.07602100	2.89412100	-0.80563400
C	0.15827000	3.40681800	0.04106900
C	-2.39226700	4.24377200	-0.78233300
H	-2.81307800	2.17024900	-1.13373200
C	-0.17299700	4.75469400	0.07168900
H	1.13325100	3.06681000	0.36215500
C	-1.44189700	5.17471100	-0.34284600
H	-3.37492300	4.57832100	-1.10151100
H	0.55432200	5.48433200	0.41552800
H	-1.69326500	6.23201600	-0.32348500
C	-1.43660100	0.02237700	-0.68877600
N	-2.41340100	-0.18038900	0.13173100
S	-3.28542400	-1.64271600	-0.16166800
O	-2.99163600	-2.17370700	-1.50437500
O	-3.09796600	-2.48552900	1.02430100
C	-4.95680500	-1.00534200	-0.15603700
C	-5.65312500	-0.88929800	-1.35810600
C	-5.54292200	-0.63747700	1.05886200
C	-6.95689900	-0.39203900	-1.33884800
H	-5.18086200	-1.19456800	-2.28580400
C	-6.84205400	-0.13983200	1.05666200
H	-4.98889700	-0.74834600	1.98488700
C	-7.56940000	-0.01014200	-0.13833900
H	-7.50761800	-0.30406700	-2.27198200
H	-7.30366900	0.14931400	1.99781500
C	-8.98682700	0.51122100	-0.11752600

H	-9.06519100	1.43106300	0.47361500
H	-9.35157300	0.72446200	-1.12691200
H	-9.66893800	-0.22037400	0.33437500
N	-1.27868700	0.74066000	3.46395100
N	-0.53243000	-0.01779600	3.76101600
H	2.51378100	1.08590000	4.28537800
H	1.05965600	-4.43321000	1.83562100
H	3.92311300	3.60216000	-1.92048900
H	0.85365500	-3.17706200	-3.38951000
H	-1.23185300	-0.65075800	-1.53073400
Int2a			
Rh	-3.99617900	-0.07697900	-1.07998600
Rh	-1.93147000	-0.10109300	0.25770700
O	-2.11288000	1.95959500	0.38507200
C	-3.09134300	2.54287300	-0.20382900
O	-4.00726200	1.97705300	-0.86706000
O	-1.95576100	-2.15851700	0.01203400
C	-2.87969600	-2.71831000	-0.67879400
O	-3.85391600	-2.12922900	-1.22916200
O	-3.15824700	-0.28391800	1.92564300
C	-4.42921300	-0.34281200	1.77496200
O	-5.05677800	-0.27519600	0.67804600
O	-2.81021100	0.08856500	-2.76361000
C	-1.55079000	0.12442900	-2.63408600
O	-0.91093600	0.09335600	-1.52365000
C	-3.12565200	4.05144900	-0.09415400
H	-2.28373000	4.47333500	-0.65405300
H	-3.00965200	4.35451600	0.95073600
C	-0.70805700	0.24277900	-3.88276100
H	-1.19485800	-0.27775900	-4.71071500
H	0.29408700	-0.15421700	-3.70722500
C	-5.23858400	-0.53075800	3.03953500
H	-4.88611800	0.15203600	3.81785000
H	-5.09525900	-1.55288700	3.40784400
C	-2.76533700	-4.21643600	-0.84175300
H	-1.86246200	-4.44777800	-1.41723600
H	-3.64166800	-4.61089300	-1.35806700
C	-0.22136700	-0.23161500	1.33285000

C	0.11529300	0.33844200	2.59754500
C	1.33285500	0.00640600	3.25962800
C	-0.76237600	1.26944000	3.21936900
C	1.65424400	0.58310900	4.47818300
H	2.01638900	-0.69556100	2.79551900
C	-0.42731300	1.84440000	4.43711500
H	-1.68489200	1.52651400	2.71683200
C	0.77550300	1.50249500	5.06666600
H	2.58636200	0.32697600	4.97247200
H	-1.09796400	2.56077800	4.90229400
H	1.03190900	1.95522200	6.02087000
C	0.69758700	-1.07473800	0.59009200
N	1.79503500	-0.60058700	0.09936900
S	2.55988700	-1.62925400	-1.08547600
O	1.85026700	-2.91773100	-1.15378000
O	2.68187200	-0.78366200	-2.27823700
C	4.16952200	-1.90343000	-0.36164600
C	4.50348000	-3.19666300	0.04862500
C	5.07573400	-0.84388500	-0.24529200
C	5.77101800	-3.42623900	0.58100200
H	3.78528000	-4.00197900	-0.05980300
C	6.33264200	-1.09747100	0.29698100
H	4.82383800	0.16738700	-0.54228900
C	6.70304500	-2.38610700	0.71107500
H	6.04090400	-4.43090500	0.89727000
H	7.02587100	-0.26608200	0.39225700
C	8.08422600	-2.64808100	1.26260100
H	8.40962100	-1.83823700	1.92460300
H	8.12319700	-3.58712600	1.82394000
H	8.82195900	-2.71733800	0.45231000
H	-4.06109900	4.44120300	-0.49816000
H	-0.62290000	1.30219600	-4.15334300
H	-6.29874000	-0.36589500	2.84123300
H	-2.66028100	-4.69012200	0.13913700
H	0.34691500	-2.08088000	0.33008500
O	6.02382100	2.36056200	-0.35952000
C	4.18921600	3.45155300	-1.44138700
C	3.13707100	2.71147000	-0.99914300

C	1.74010300	2.87673900	-1.53015400
H	1.37828900	1.92082800	-1.92849600
H	1.05293200	3.16985500	-0.72525000
H	1.69767700	3.62823200	-2.32211800
O	3.29574200	1.79972300	-0.02783000
H	2.54948600	1.15753000	0.01309200
H	3.97086100	4.22756900	-2.16866900
C	5.59423000	3.27312000	-1.06342000
C	6.55755100	4.31096700	-1.63774600
H	7.57396700	4.08735300	-1.30701400
H	6.52309300	4.30604000	-2.73485900
H	6.28051400	5.32189500	-1.31240300

TS2a

Rh	-3.45339300	-1.44980900	-0.20738700
Rh	-1.37387200	-0.19455400	0.09649900
O	-2.08294300	1.12386000	-1.35335500
C	-3.22101400	0.90319800	-1.89450700
O	-3.99437400	-0.06654500	-1.64279700
O	-0.89551700	-1.61337600	1.53533600
C	-1.69353900	-2.57918200	1.78585900
O	-2.82208400	-2.77033400	1.23960000
O	-2.37572700	0.87252600	1.56847100
C	-3.59773200	0.60854200	1.82226300
O	-4.31568700	-0.26259800	1.24048600
O	-2.46474100	-2.60169900	-1.61094900
C	-1.24405600	-2.36366800	-1.85762900
O	-0.55264400	-1.40640200	-1.36310400
C	-3.66386800	1.88103200	-2.96315300
H	-3.24095500	1.57289800	-3.92696700
H	-3.30050500	2.88662200	-2.73806800
C	-0.51945000	-3.26738600	-2.82904800
H	-1.12025800	-4.15079000	-3.05136000
H	0.44853500	-3.55056500	-2.40521000
C	-4.23822400	1.39317000	2.94709200
H	-4.05116300	0.87093200	3.89296300
H	-5.31828800	1.45694400	2.79882300
C	-1.23857800	-3.55884100	2.84355900
H	-0.17853800	-3.78721500	2.70263000

H	-1.83863800	-4.46958100	2.80461900
C	0.55242300	1.01126800	0.39410900
C	0.40897800	2.23792300	1.20452700
C	1.30578700	2.52067300	2.24951700
C	-0.62209000	3.15369600	0.92914800
C	1.16692400	3.67862000	3.01180600
H	2.12430700	1.83646100	2.45459400
C	-0.74018900	4.32563800	1.67302000
H	-1.32830700	2.92787700	0.13878000
C	0.14823800	4.58774800	2.71942700
H	1.86455800	3.88060300	3.81984600
H	-1.53916600	5.02813900	1.44962000
H	0.04671000	5.49753000	3.30538600
C	1.35370600	-0.10795400	0.79183500
N	2.22569000	-0.58777700	-0.06032800
S	2.97061600	-2.08728200	0.24169600
O	2.64512000	-2.52054500	1.60778000
O	2.69201000	-2.95154400	-0.90860000
C	4.69694000	-1.61859600	0.18169200
C	5.35195200	-1.25060200	1.35870500
C	5.36463800	-1.62294600	-1.04372300
C	6.68985100	-0.86830400	1.29626100
H	4.82285000	-1.28123100	2.30543100
C	6.70292500	-1.23590700	-1.08602700
H	4.84584000	-1.94236300	-1.94133700
C	7.38308000	-0.84584000	0.07644200
H	7.20675000	-0.58645100	2.21027500
H	7.22956600	-1.24199200	-2.03708200
C	8.82267500	-0.39343000	0.01643500
H	8.88630600	0.70079400	-0.05131900
H	9.37609300	-0.69516700	0.91201000
H	9.33696100	-0.80550200	-0.85756300
H	-4.75209800	1.87794600	-3.05064900
H	-0.32672900	-2.72063400	-3.75966400
H	-3.79653600	2.38965900	3.01733700
H	-1.35256200	-3.09828400	3.83189200
H	1.15137400	-0.58752300	1.74818200
C	1.54342400	4.34620200	-1.39215000

O	2.39284200	4.08557700	-0.55747200
C	0.94288000	3.32559000	-2.30029400
C	0.93517300	1.98833500	-2.16348900
C	0.53609300	1.01018600	-3.22029200
H	1.40870700	0.41294800	-3.52152300
H	-0.21853000	0.31727800	-2.84546400
H	0.16150700	1.53344800	-4.10361500
O	1.41463800	1.42122600	-0.98216600
H	1.95942500	0.49049400	-1.04199200
H	0.50652700	3.70659600	-3.22038600
C	1.06591000	5.77194200	-1.62309100
H	1.23284200	6.07756500	-2.66388500
H	-0.01273700	5.84364800	-1.43408800
H	1.59906700	6.44840700	-0.95268200
Int3a			
Rh	3.37871400	-1.50189200	0.28893700
Rh	1.35553100	-0.20958100	-0.02216000
O	2.10953400	1.10892100	1.40740800
C	3.25627000	0.88470000	1.91822000
O	4.01284400	-0.10070800	1.65697200
O	0.79944500	-1.63630000	-1.40153500
C	1.53750100	-2.65569200	-1.60847800
O	2.67151800	-2.86862200	-1.07213700
O	2.32838900	0.81074000	-1.52173800
C	3.52979500	0.49390800	-1.80890100
O	4.22659700	-0.40125400	-1.23327400
O	2.40956700	-2.54274600	1.78685200
C	1.19913600	-2.26960300	2.04847800
O	0.50935900	-1.34033100	1.50313100
C	3.76641100	1.90168900	2.91737900
H	4.65713600	1.52697100	3.42404800
H	2.98662100	2.13249700	3.64923700
C	0.48966900	-3.11919600	3.07756300
H	1.19544100	-3.77856700	3.58484600
H	-0.27311400	-3.72089200	2.57044600
C	4.16960600	1.23612900	-2.96043400
H	3.92685200	0.71579900	-3.89459200
H	5.25559700	1.25030700	-2.84702700

C	0.99273600	-3.69186300	-2.56080500
H	0.07682000	-4.11096000	-2.13103700
H	1.72556100	-4.48186300	-2.73239600
C	-0.67035300	1.56610500	-0.00007000
C	-0.13137700	2.74540700	-0.71116100
C	-0.56888900	3.03838500	-2.01390600
C	0.80685000	3.59738800	-0.10523800
C	-0.05785300	4.13736900	-2.70217900
H	-1.33407100	2.42197300	-2.47390600
C	1.30439100	4.70315800	-0.79124900
H	1.17263000	3.36317500	0.88758300
C	0.87950200	4.97518300	-2.09408900
H	-0.40733700	4.34846300	-3.70921200
H	2.03386700	5.34982300	-0.31027200
H	1.26955100	5.83783400	-2.62778000
C	-1.06273500	0.41094900	-0.61255200
N	-1.82887500	-0.57074600	0.02703800
S	-2.52451400	-1.82958400	-0.87613300
O	-2.39239000	-1.46052100	-2.28744500
O	-2.02616300	-3.11707000	-0.37461400
C	-4.24663700	-1.70296000	-0.39526000
C	-4.89961200	-0.46687800	-0.44826400
C	-4.93058800	-2.86780600	-0.05048800
C	-6.25639900	-0.41456200	-0.14404400
H	-4.35746000	0.44002000	-0.69635400
C	-6.29190000	-2.79141900	0.24856200
H	-4.40133100	-3.81373800	-0.01509100
C	-6.97432500	-1.56984100	0.20712500
H	-6.76877700	0.54410200	-0.17778200
H	-6.82946500	-3.69720000	0.51781600
C	-8.44294100	-1.48402600	0.54985800
H	-8.59381000	-1.00877100	1.52799800
H	-8.98975200	-0.88398500	-0.18662100
H	-8.90498000	-2.47530100	0.58946300
H	4.01656200	2.83031300	2.39175300
H	-0.02053100	-2.48029900	3.80482000
H	3.77248900	2.25164900	-3.02358700
H	0.71807000	-3.21522700	-3.50660300

H	-0.95864600	0.30194100	-1.68412900
C	-3.21423600	3.46704500	0.43533400
O	-3.29179200	2.47703000	-0.28745400
C	-2.35295800	3.54809500	1.62373800
C	-1.38268800	2.69809200	2.04236700
C	-0.74717200	2.80092500	3.39915300
H	-0.87678500	1.85326700	3.93590000
H	0.33208000	2.96481600	3.30289700
H	-1.18926300	3.60543000	3.99060700
O	-0.85838500	1.63283400	1.37699400
H	-1.48550100	-0.88292100	0.93595900
H	-2.56287100	4.37169500	2.30044400
C	-4.06781800	4.69664900	0.15943200
H	-4.66755700	4.96531000	1.03793100
H	-3.42628700	5.55751400	-0.06844900
H	-4.72687100	4.50192700	-0.68884100

TS3a

Rh	3.61794300	-1.49974300	-0.75787600
Rh	2.55651700	0.42002200	0.22540100
O	4.01121200	0.38540200	1.69555500
C	4.91467400	-0.51344000	1.64419300
O	5.01344700	-1.42215300	0.75943400
O	1.16739300	0.32594700	-1.29151300
C	1.25322000	-0.60384100	-2.16165600
O	2.17017900	-1.48729200	-2.21337200
O	3.79385500	1.59327900	-0.95837800
C	4.61521700	1.02624000	-1.75014000
O	4.77493200	-0.22854300	-1.88752800
O	2.42528000	-2.70181500	0.40243400
C	1.57790000	-2.15430800	1.17907400
O	1.41084200	-0.89841900	1.32598200
C	5.98228200	-0.47245200	2.71442300
H	5.56951200	-0.08487900	3.64859000
H	6.78429200	0.20140200	2.39013900
C	0.67615700	-3.06303200	1.98042600
H	1.12479700	-4.05370900	2.07642000
H	-0.28710200	-3.16467300	1.46602100
C	5.45731200	1.92996400	-2.62319300

H	5.78232000	2.80608500	-2.05607500
H	4.84798700	2.28136400	-3.46405500
C	0.15707600	-0.67245900	-3.19635900
H	-0.05237300	0.32826400	-3.58476400
H	-0.75480700	-1.04260700	-2.71447900
C	-1.26629000	1.09279800	1.69028800
C	-0.29947000	2.08717700	1.15552000
C	-0.57554700	2.90792700	0.05809600
C	0.97561900	2.13644700	1.76037800
C	0.40071200	3.78876700	-0.42083700
H	-1.54174800	2.86510300	-0.43346500
C	1.95747900	2.99242500	1.25535600
H	1.16531000	1.51041900	2.62506300
C	1.66118800	3.82960700	0.16586100
H	0.17326400	4.42968700	-1.26807100
H	2.93621300	3.03011400	1.72331900
H	2.42524400	4.49594900	-0.22298500
C	-2.43241200	0.66126200	0.85455500
N	-2.93497000	-0.58252600	1.25130700
S	-3.26925500	-1.80921100	0.12930400
O	-2.57037500	-1.49865300	-1.12033100
O	-3.02666800	-3.05072900	0.87009400
C	-5.02205600	-1.66365000	-0.19010500
C	-5.46665000	-0.79805300	-1.19207200
C	-5.91847400	-2.42914300	0.55735700
C	-6.83534700	-0.70108000	-1.43599300
H	-4.75604700	-0.21493900	-1.76836400
C	-7.28229100	-2.31841400	0.29462500
H	-5.54790300	-3.10786000	1.31806700
C	-7.76192600	-1.45806900	-0.70401200
H	-7.18944200	-0.03187300	-2.21637000
H	-7.98542100	-2.91534200	0.87016200
C	-9.23904500	-1.37548500	-1.00785400
H	-9.51442300	-0.39015500	-1.39799400
H	-9.52564000	-2.11731200	-1.76503000
H	-9.84346500	-1.57104900	-0.11611600
H	6.40812500	-1.46647400	2.86493100
H	0.48753100	-2.62846000	2.96527000

H	6.31915000	1.38758300	-3.01593000
H	0.43878400	-1.34605600	-4.00755500
H	-2.43136300	0.85136000	-0.21009000
C	-4.41285400	2.95808000	-0.83661700
O	-3.56391800	2.32573400	-1.45900700
C	-4.55622100	2.93370200	0.63846700
C	-3.87842600	2.18351000	1.51167400
C	-4.05747100	2.08490900	2.97757200
H	-3.12967200	2.32577800	3.51032700
H	-4.85468800	2.74944300	3.33830000
H	-4.31382000	1.05410800	3.25581100
O	-1.12039400	0.56953100	2.79465100
H	-2.52752000	-0.93511600	2.11927200
H	-5.33647200	3.59085500	1.03684200
C	-5.41494600	3.83154600	-1.57435900
H	-6.43752400	3.47866000	-1.38778000
H	-5.36462600	4.86611000	-1.21220700
H	-5.20907200	3.80677700	-2.64599800

Int4a

Rh	3.56938200	-1.55814000	-0.70902400
Rh	2.54955100	0.43228600	0.17077600
O	4.02499800	0.46997100	1.62137900
C	4.91380400	-0.44502400	1.61255100
O	4.99537900	-1.39826700	0.77424400
O	1.13879300	0.26790300	-1.31549100
C	1.18228900	-0.72708500	-2.11274900
O	2.08714000	-1.62424500	-2.12950100
O	3.78342900	1.51684800	-1.10383200
C	4.57707200	0.88958600	-1.87833800
O	4.71721300	-0.37280700	-1.93993500
O	2.38923700	-2.67252400	0.54553000
C	1.56339000	-2.06712800	1.30329100
O	1.41347200	-0.80265000	1.37213600
C	5.94458100	-0.40710800	2.71844200
H	5.53204600	-0.90486300	3.60403400
H	6.17473200	0.62626500	2.98847100
C	0.67462500	-2.90972500	2.18564000

H	1.06410500	-3.92692000	2.25679400
H	-0.33540400	-2.94249000	1.76091300
C	5.40490100	1.72179300	-2.83255200
H	5.69021000	2.66679200	-2.36402800
H	4.80066100	1.95101400	-3.71833600
C	0.04597700	-0.85791300	-3.09663600
H	-0.16559900	0.11251700	-3.55454900
H	-0.84902000	-1.16927800	-2.54642600
C	-1.36341000	1.32497000	1.71484300
C	-0.36303300	2.17186100	1.02313800
C	-0.63913900	2.86439200	-0.15964400
C	0.93206000	2.24443700	1.58619000
C	0.35211300	3.64751100	-0.76340200
H	-1.61161800	2.78681500	-0.63379400
C	1.92412100	3.00630500	0.96715600
H	1.12676500	1.71397500	2.51128900
C	1.62397500	3.72015900	-0.20919900
H	0.12528300	4.18346400	-1.68058900
H	2.91072100	3.08093000	1.41359700
H	2.39823800	4.31098100	-0.68870300
C	-2.76806300	1.07587600	1.08785200
N	-3.27457000	-0.20514300	1.61697800
S	-3.23215900	-1.55892400	0.59122900
O	-2.32920800	-1.31576700	-0.54236000
O	-3.02422300	-2.69880800	1.49299700
C	-4.89696100	-1.64139700	-0.06144200
C	-5.19656500	-1.01492000	-1.27156100
C	-5.87295700	-2.33970400	0.65314000
C	-6.50054000	-1.08824000	-1.76258800
H	-4.42579200	-0.48061200	-1.81650400
C	-7.16702700	-2.40337600	0.14406700
H	-5.61261800	-2.83320400	1.58344500
C	-7.50163500	-1.78161600	-1.06930100
H	-6.74063000	-0.60377600	-2.70579500
H	-7.92985500	-2.94885400	0.69448600
C	-8.90272000	-1.88586100	-1.62384400
H	-9.65472400	-1.78850000	-0.83297300
H	-9.09611200	-1.11380300	-2.37517100

H	-9.06356900	-2.85988400	-2.10432800
H	6.84980200	-0.93609800	2.41421400
H	0.60053800	-2.45714700	3.17819300
H	6.29060000	1.16864600	-3.15087000
H	0.28374400	-1.59866700	-3.86207300
H	-2.69276900	1.01945600	0.00407400
C	-4.42401100	2.87128500	-0.87943600
O	-3.61958300	2.21661000	-1.53963200
C	-4.42707600	2.94682600	0.59951900
C	-3.74184100	2.18752400	1.48471000
C	-3.96943400	2.36642500	2.96315700
H	-3.03273400	2.58377700	3.48960400
H	-4.68012700	3.17223100	3.16487600
H	-4.36299300	1.43894400	3.39623100
O	-1.12700200	0.79908600	2.79506200
H	-2.76538500	-0.45432300	2.47124000
H	-5.12742200	3.67208500	1.01098100
C	-5.51317100	3.67330600	-1.57297100
H	-5.42556400	4.73749500	-1.31921300
H	-5.43087900	3.54776100	-2.65409700
H	-6.50521900	3.34572600	-1.23730500

TS4a

Rh	-3.47422400	-1.78199100	-0.40060700
Rh	-2.56599100	0.38971800	0.07711700
O	-3.86790100	1.17649500	-1.32719200
C	-4.65571900	0.38182400	-1.93951800
O	-4.73568100	-0.87465800	-1.76052900
O	-1.32348500	-0.51879400	1.43475000
C	-1.34847800	-1.78745100	1.55880300
O	-2.15251700	-2.57387400	0.95875900
O	-4.03042400	0.58831400	1.53926200
C	-4.84357300	-0.37420700	1.73079800
O	-4.86522300	-1.47206500	1.08969300
O	-2.05439700	-2.01762500	-1.85785600
C	-1.21292100	-1.07771500	-2.04511300
O	-1.19644400	0.03210300	-1.41807800
C	-5.55388700	0.98645300	-2.99551000

H	-6.44538000	0.37156400	-3.13416100
H	-5.00782200	1.02272200	-3.94567800
C	-0.13907000	-1.28359400	-3.08320800
H	-0.16311900	-0.45744400	-3.80119100
H	-0.28271500	-2.23386500	-3.60027800
C	-5.85473600	-0.20758800	2.84386400
H	-6.72226200	-0.84687000	2.66882900
H	-6.15939800	0.83823900	2.92869900
C	-0.33040900	-2.39255200	2.49414800
H	-0.48542500	-2.00009000	3.50505900
H	0.66998900	-2.08699600	2.16987300
C	1.56206700	2.18763900	-0.10874600
C	0.35509400	2.41064600	0.72824700
C	0.36757600	2.35980100	2.12793000
C	-0.86004100	2.69928500	0.06551800
C	-0.79529400	2.61995100	2.86039500
H	1.27033600	2.08888000	2.66237700
C	-2.02115600	2.95657800	0.79681200
H	-0.86290500	2.73910900	-1.01749200
C	-1.98148400	2.92468300	2.20417000
H	-0.76874600	2.56928300	3.94495400
H	-2.93786300	3.23084900	0.28389400
H	-2.88752900	3.11817300	2.76943700
C	2.98823600	2.16276000	0.52751800
N	3.86669800	1.10920900	0.02404600
S	3.30794200	-0.45187000	0.02496100
O	2.46014200	-0.58357000	1.22997100
O	2.76254600	-0.90516800	-1.26566500
C	4.83199400	-1.36904800	0.28078500
C	5.59847100	-1.14187100	1.42486300
C	5.20489800	-2.34298800	-0.64673000
C	6.75505800	-1.89153300	1.62988000
H	5.29539300	-0.38482400	2.14056800
C	6.36577500	-3.08356400	-0.42715500
H	4.58780500	-2.50638000	-1.52351200
C	7.15831600	-2.87066700	0.70990000
H	7.35565200	-1.71516500	2.51895600
H	6.65939700	-3.84054300	-1.15080300

C	8.41291200	-3.68198000	0.93435500
H	8.92623000	-3.38078300	1.85255200
H	8.18472500	-4.75203800	1.01378300
H	9.11741500	-3.56510800	0.10168000
H	-5.82889800	2.00798800	-2.72302400
H	0.83851100	-1.26107000	-2.58971400
H	-5.39088900	-0.50494700	3.79189700
H	-0.41591700	-3.48037000	2.50383400
H	2.93077500	2.11071600	1.61705000
C	4.62376800	1.90391300	-1.54958900
O	3.86639000	1.60564400	-2.61882900
C	4.46961700	3.28110300	-0.97324600
C	3.66577600	3.45075400	0.07898800
C	3.35559700	4.74703100	0.76601400
H	3.64934100	4.71111600	1.82355000
H	3.87998500	5.58303400	0.29403100
H	2.27961200	4.96393100	0.74482600
O	1.46724000	2.11078600	-1.33137000
H	2.93439500	1.85821400	-2.40038600
H	5.00067300	4.09735500	-1.45869200
C	6.02226500	1.36181700	-1.68902900
H	6.57265800	1.46560100	-0.75273800
H	5.99586400	0.31203500	-1.98890600
H	6.53999100	1.92783700	-2.47414000
Int5a-2w			
Rh	3.67669400	-1.57421400	-0.82181700
Rh	2.67223200	0.40089800	0.11043000
O	4.14108000	0.38052400	1.56709100
C	5.01889800	-0.54461000	1.53782100
O	5.09601200	-1.47290500	0.67140800
O	1.26734800	0.29471700	-1.38523300
C	1.30163400	-0.67866100	-2.20844000
O	2.19702300	-1.58450800	-2.24894500
O	3.92588400	1.50492400	-1.12781900
C	4.71906700	0.89210600	-1.91427600
O	4.84485500	-0.36936700	-2.01319900
O	2.47139500	-2.70810500	0.38791200
C	1.63720600	-2.11739600	1.14893800

O	1.51464300	-0.85448400	1.27312900
C	6.04043100	-0.55356500	2.65258700
H	5.61767300	-1.08241100	3.51505700
H	6.27376400	0.46749200	2.96338100
C	0.69157500	-2.98661900	1.94109100
H	1.13820200	-3.96732700	2.11813900
H	-0.22483600	-3.12237700	1.35410700
C	5.56549900	1.74307000	-2.83502800
H	5.85759800	2.66964700	-2.33496400
H	4.97269500	2.00669200	-3.71895500
C	0.16424100	-0.76862000	-3.19623000
H	-0.00467700	0.20746100	-3.66034700
H	-0.74542500	-1.03726700	-2.64761600
C	-1.33681000	1.42902500	1.49192800
C	-0.25097300	2.24126100	0.88295700
C	-0.42615000	3.00230300	-0.27780900
C	1.01512600	2.21747600	1.51103300
C	0.63626600	3.75286900	-0.79552000
H	-1.37606200	3.00673500	-0.80074600
C	2.07707600	2.95297800	0.98266700
H	1.13217800	1.63749600	2.41924400
C	1.87842100	3.73221100	-0.17328200
H	0.48768800	4.34061300	-1.69684800
H	3.03893500	2.95927900	1.48586100
H	2.70633700	4.30167100	-0.58369700
C	-2.73366500	1.38903500	0.81896800
N	-3.51398600	0.21810500	1.23008900
S	-3.21909000	-1.25222200	0.49767500
O	-2.12009500	-1.08193400	-0.46109000
O	-3.13051600	-2.27159800	1.56594700
C	-4.70519600	-1.62223300	-0.43302900
C	-4.96902100	-0.91397900	-1.60992200
C	-5.57249000	-2.61461800	0.02020800
C	-6.12308200	-1.21186100	-2.32853400
H	-4.28968600	-0.14116300	-1.95538300
C	-6.72296500	-2.89881700	-0.71683100
H	-5.34043800	-3.15853200	0.92909900
C	-7.01570800	-2.20752000	-1.89879700

H	-6.33390100	-0.66326700	-3.24345800
H	-7.40058600	-3.67377800	-0.36714300
C	-8.24627600	-2.53852800	-2.70946700
H	-8.98908700	-3.07488800	-2.11072000
H	-8.71876300	-1.63403300	-3.10828600
H	-7.99266000	-3.17551400	-3.56708100
H	6.94528400	-1.07610400	2.33624800
H	0.41558300	-2.51105300	2.88456300
H	6.44763700	1.18921600	-3.16187500
H	0.37375300	-1.52148500	-3.95797100
H	-2.60915200	1.34035400	-0.25978800
C	-4.27412900	3.16617400	-1.22322900
O	-3.59129300	2.35323800	-1.84378300
C	-4.20620300	3.37391000	0.24247800
C	-3.54818900	2.64044600	1.16804700
C	-3.62651700	3.00618200	2.62730600
H	-2.63460300	3.28005700	3.01046500
H	-4.29982000	3.85251200	2.78897800
H	-3.96649300	2.15997700	3.23718100
O	-1.14793800	0.80740200	2.52964000
H	-3.72451900	0.10948700	2.24052900
H	-4.79656300	4.21374400	0.60581900
O	-1.81009700	-1.51693400	4.01909000
H	-2.11680300	-1.99433900	3.22234500
H	-1.34673200	-0.74754500	3.63518200
O	-4.12531800	-0.09803900	4.00224700
H	-3.29916900	-0.61320200	4.20890900
H	-4.84349100	-0.74424700	4.08211100
C	-5.26628300	4.05232000	-1.95839800
H	-6.27985100	3.90181500	-1.56559900
H	-5.01988200	5.11110700	-1.80725300
H	-5.24703600	3.82167400	-3.02507100
TS4a-2w			
Rh	3.58804000	-1.61333400	0.82496200
Rh	2.68195200	0.33642700	-0.25168400
O	3.83913600	1.49164000	1.01913400
C	4.58738500	0.90433200	1.86908000
O	4.70710900	-0.35344200	2.01499100

O	1.58984400	-0.92700600	-1.44487500
C	1.64305200	-2.18340600	-1.23846200
O	2.40212600	-2.76595700	-0.39636500
O	4.26589100	0.23252300	-1.59040300
C	5.11085300	-0.71449100	-1.47053000
O	5.09473600	-1.61954200	-0.57712500
O	2.03918500	-1.55281800	2.17376000
C	1.15415800	-0.64805200	2.02651600
O	1.18330700	0.28502300	1.16173800
C	5.38029900	1.78572900	2.80808100
H	4.75466100	2.03422900	3.67367300
H	5.65883900	2.71823400	2.31191100
C	-0.05878900	-0.69995300	2.92403800
H	0.14890300	-1.28001400	3.82514100
H	-0.87512400	-1.17311300	2.36687200
C	6.21386200	-0.78469100	-2.50288500
H	5.84284300	-1.32515500	-3.38182300
H	7.07498300	-1.32426400	-2.10388700
C	0.70213600	-3.04013400	-2.04952700
H	0.77404700	-2.77366800	-3.10814500
H	-0.32099300	-2.82415700	-1.72256300
C	-1.29468100	2.29624500	-0.22734800
C	-0.20048700	2.18653500	-1.22490300
C	-0.39085800	1.72503000	-2.53402200
C	1.09475900	2.58939600	-0.82022100
C	0.68168300	1.68483400	-3.43297500
H	-1.35642500	1.35282300	-2.85783300
C	2.16084900	2.55301400	-1.72038200
H	1.23249300	2.96093000	0.18846200
C	1.94599200	2.10208900	-3.03775500
H	0.51916900	1.31438200	-4.44073700
H	3.13770100	2.92166300	-1.42367700
H	2.77829900	2.06979300	-3.73411400
C	-2.78012800	2.19873900	-0.66111200
N	-3.50522900	1.04080300	-0.06882100
S	-3.14956900	-0.42072100	-0.91608200
O	-3.27478000	-0.17030300	-2.36478800
O	-1.86646200	-0.92072700	-0.39091400

C	-4.43344000	-1.56688000	-0.43077900
C	-5.22190800	-2.12899200	-1.43575700
C	-4.56462900	-1.96608700	0.90216100
C	-6.16510800	-3.09685800	-1.09323200
H	-5.09046800	-1.81071800	-2.46393500
C	-5.51808500	-2.92810000	1.22185700
H	-3.94471800	-1.53029600	1.67706400
C	-6.33312700	-3.50584100	0.23622500
H	-6.77926600	-3.54059600	-1.87270900
H	-5.63150300	-3.23626200	2.25809800
C	-7.37932200	-4.52913300	0.60784900
H	-7.70647300	-5.10430200	-0.26394400
H	-7.00277100	-5.23222700	1.35892700
H	-8.26638700	-4.04360600	1.03537100
H	6.26778600	1.25950600	3.16509200
H	-0.38806200	0.31072700	3.17631400
H	6.50307600	0.22004400	-2.81994800
H	0.92379600	-4.09922600	-1.90850500
H	-2.84770700	2.14658300	-1.75235800
C	-5.23075500	1.63401600	0.26746100
O	-5.64127900	1.08379500	1.35265700
C	-4.76837700	3.07908900	0.30749700
C	-3.57080800	3.40779700	-0.17021700
C	-3.01396200	4.79470600	-0.31354200
H	-2.75917200	5.01120400	-1.36041400
H	-3.74192500	5.54115700	0.01689100
H	-2.09786400	4.92670100	0.27370700
O	-1.03637600	2.56396100	0.94443700
H	-3.25651900	0.86379500	1.24500600
H	-5.48238900	3.80769900	0.68424200
O	-2.07593400	2.72465000	3.48935400
H	-1.34414800	2.42867400	4.05209500
H	-1.67457300	2.86270100	2.60355800
O	-3.47559700	0.71852800	2.40337300
H	-3.02739800	1.44426300	2.92684400
H	-4.50564100	0.94923200	2.24399900
C	-6.06177800	1.33664700	-0.98330400
H	-6.39165500	0.29639600	-0.97606200

H	-6.95606800	1.97090300	-0.94098700
H	-5.52925600	1.55659500	-1.91278500
Int6a-2w			
Rh	3.55525400	-1.79390700	0.07740000
Rh	2.57552100	0.39824400	-0.01654000
O	3.84779100	0.96966800	1.51371100
C	4.66225400	0.10620000	1.98279800
O	4.77779900	-1.09833900	1.59198600
O	1.37320100	-0.29381700	-1.52756600
C	1.45290400	-1.51369200	-1.88879700
O	2.27259400	-2.37147400	-1.42023300
O	4.03111000	0.88771400	-1.41119200
C	4.87989900	0.00268500	-1.75972200
O	4.93981300	-1.18659900	-1.31408800
O	2.13371900	-2.34165100	1.44961400
C	1.26545900	-1.48012300	1.80111400
O	1.21160300	-0.27228500	1.39919400
C	5.54611000	0.55032400	3.12656700
H	4.98015900	0.47611200	4.06276300
H	5.84169200	1.59397600	2.99486800
C	0.22799000	-1.93369100	2.80468300
H	-0.08028200	-2.95662900	2.57421500
H	-0.64190900	-1.27422800	2.80957400
C	5.88611500	0.39880600	-2.81650900
H	6.23675100	1.41911700	-2.64057500
H	5.39861200	0.37604900	-3.79813600
C	0.49841400	-1.96001700	-2.96900100
H	0.79906200	-1.50920800	-3.92189500
H	-0.50706800	-1.59970600	-2.73263400
C	-1.48874400	2.07417300	0.24804200
C	-0.28544300	2.52172000	-0.49305900
C	-0.28098800	2.76388600	-1.87082700
C	0.91429100	2.68314900	0.23921900
C	0.89235900	3.17890400	-2.51165200
H	-1.17254000	2.59277200	-2.46311300
C	2.08067900	3.10382100	-0.40007400
H	0.89994800	2.51891700	1.31037600
C	2.06347400	3.35566500	-1.78508900

H	0.88370600	3.35356600	-3.58351200
H	2.98459000	3.27762200	0.17521700
H	2.97370900	3.67544900	-2.28222600
C	-2.91165700	2.33621300	-0.29274400
N	-3.80223500	1.16891600	-0.12088900
S	-3.67681100	0.08031000	-1.41623000
O	-4.40268100	0.54848900	-2.60870500
O	-2.22296700	-0.13773100	-1.54547300
C	-4.47723900	-1.40118100	-0.82172500
C	-5.41112200	-2.01077000	-1.66035800
C	-4.11359500	-1.97718800	0.39949800
C	-5.99259300	-3.21519700	-1.26431900
H	-5.67500100	-1.54301700	-2.60241800
C	-4.70984600	-3.17650000	0.77516300
H	-3.40808200	-1.49164100	1.06364800
C	-5.65501900	-3.81421400	-0.04483900
H	-6.72174900	-3.69296600	-1.91369000
H	-4.44235800	-3.62120200	1.73043700
C	-6.30076900	-5.10653900	0.39446500
H	-6.95394600	-4.94463500	1.26135100
H	-6.90845900	-5.54367000	-0.40367300
H	-5.54875400	-5.84662300	0.69237000
H	6.42559100	-0.09194300	3.20051200
H	0.68138300	-1.95123900	3.80407200
H	6.72635100	-0.29759500	-2.82467900
H	0.51118600	-3.04690000	-3.06666000
H	-2.87347800	2.66583500	-1.33791400
C	-5.12024700	1.56016200	0.54006800
O	-5.45713000	0.68012800	1.56761800
C	-4.75646500	2.95169700	1.01107900
C	-3.58794000	3.40276300	0.55982800
C	-2.95220100	4.73903900	0.79634900
H	-2.73231800	5.25098300	-0.14987300
H	-3.61077200	5.38280900	1.38633900
H	-2.00151700	4.64405300	1.33706500
O	-1.37884900	1.59425800	1.37301800
H	-2.64590000	0.49798400	2.15298700
H	-5.44783700	3.50334500	1.64058000

O	-0.81384600	1.17741100	4.13086000
H	-0.14275100	0.50097400	4.30404300
H	-0.69186500	1.39218200	3.18749700
O	-3.10427500	0.02714900	2.87839600
H	-2.59636900	0.34283600	3.65390600
H	-4.69384900	0.56740800	2.18464700
C	-6.33140400	1.59894600	-0.40104600
H	-6.61219500	0.58826200	-0.70680300
H	-7.17565400	2.03011400	0.14617200
H	-6.12946300	2.20068300	-1.28941500
Int7a			
Rh	-4.35909800	-1.28924600	0.86124300
Rh	-3.21684700	0.57115700	-0.14287200
O	-4.71703200	0.63837600	-1.56499100
C	-5.65426300	-0.22439800	-1.50625000
O	-5.78074600	-1.12981100	-0.62115200
O	-1.79861500	0.39676100	1.33798900
C	-1.91104300	-0.53616400	2.19660400
O	-2.87095300	-1.36747700	2.28004100
O	-4.33857000	1.81819000	1.08540100
C	-5.18554600	1.29612900	1.88136900
O	-5.41232000	0.05203800	2.02152000
O	-3.26627400	-2.55542200	-0.32101800
C	-2.43709800	-2.04952200	-1.14903200
O	-2.22092800	-0.80370700	-1.30440900
C	-6.69142800	-0.18328700	-2.60567600
H	-6.31986200	-0.75622900	-3.46350600
H	-6.85772700	0.84564600	-2.93318800
C	-1.64225400	-2.99177000	-2.01703700
H	-1.99829800	-4.01625900	-1.89617100
H	-0.58385000	-2.93071800	-1.74460200
C	-6.01950000	2.24572700	2.71342600
H	-5.43870900	3.13365300	2.97419700
H	-6.38218500	1.74578700	3.61371100
C	-0.77870200	-0.68094000	3.18728200
H	-0.49386200	0.30065100	3.57676100
H	0.08182400	-1.09720300	2.65179700
C	0.87310500	0.96696300	-1.96960200

C	-0.03952100	1.92023200	-1.26167200
C	0.33883200	2.69471500	-0.15987800
C	-1.35444300	2.04638200	-1.76098600
C	-0.56765500	3.58036600	0.43647600
H	1.34089600	2.62320000	0.24949700
C	-2.26279600	2.92305600	-1.16282900
H	-1.62988700	1.45919200	-2.62925800
C	-1.86139200	3.69595700	-0.05656800
H	-0.25527200	4.17335800	1.29163500
H	-3.25567700	3.05000700	-1.58411700
H	-2.56921500	4.37387600	0.41044100
C	2.35955800	0.82308100	-1.52189600
N	2.87137600	-0.53047200	-1.77165500
S	2.29596700	-1.82054600	-0.90486200
O	1.16584600	-1.29914700	-0.11760000
O	2.13259100	-2.97865000	-1.78722200
C	3.54740500	-2.30737400	0.31105800
C	3.23453200	-2.19162400	1.66801700
C	4.75591100	-2.88665700	-0.08932000
C	4.14925800	-2.64315500	2.62726700
H	2.27075000	-1.78883500	1.96063800
C	5.65437700	-3.32478800	0.87952800
H	4.99458800	-2.96406000	-1.14349100
C	5.37128800	-3.21449100	2.25033600
H	3.89254500	-2.57365200	3.68200100
H	6.59658100	-3.76599900	0.56351800
C	6.35502400	-3.71423700	3.28142900
H	7.32933600	-3.22232600	3.17342000
H	5.99681100	-3.53477700	4.29993900
H	6.52629500	-4.79219600	3.17303000
H	-7.62540200	-0.63534700	-2.26620600
H	-1.72410900	-2.68178100	-3.06316800
H	-6.88559500	2.56795600	2.12317700
H	-1.06017800	-1.34960500	4.00247700
H	2.49272200	1.10197100	-0.47248600
C	3.82329800	-0.60470300	-2.94509100
O	5.04662200	-1.19358400	-2.59120000
C	3.96525800	0.87417800	-3.22805500

C	3.22814500	1.66409700	-2.44803100
C	3.18681000	3.16173700	-2.43587000
H	3.60492600	3.54888400	-1.49836000
H	3.78041800	3.56925400	-3.25999400
H	2.16390400	3.54572200	-2.53032000
O	0.49197800	0.35003000	-2.94782700
H	4.65018500	1.20790500	-4.00154200
H	5.50291500	-0.60217400	-1.93813600
C	5.41743000	3.51574700	1.23192900
O	5.52173200	2.96612500	0.13106900
C	4.98253100	2.84279200	2.45322600
C	4.58426900	1.54655600	2.55428900
C	4.15549200	0.92896100	3.85549800
H	3.11809400	0.57623000	3.78917900
H	4.78166300	0.05907700	4.09094700
H	4.22746400	1.64217900	4.67872600
O	4.54234300	0.75075000	1.47090700
H	4.29077900	-0.16382900	1.70613400
H	4.96923600	3.43104800	3.36465400
O	6.41190300	0.46710900	-0.85824300
H	6.93645600	1.04010800	-1.43773200
H	5.86879400	1.10442300	-0.34872500
C	3.26545500	-1.38762000	-4.13401300
H	3.92623000	-1.24055900	-4.99524600
H	3.22442400	-2.45252600	-3.89884600
H	2.26173400	-1.03216200	-4.37371600
C	5.75217700	4.99363200	1.37365800
H	4.88311900	5.55493900	1.73920400
H	6.55732100	5.13703200	2.10534500
H	6.06453900	5.39407800	0.40741700

TS5a

Rh	-4.56580500	-1.34368000	0.84682900
Rh	-3.22286200	0.25874400	-0.33913200
O	-3.14101100	-1.10663700	-1.89323600
C	-3.72872800	-2.23068200	-1.77145400
O	-4.41283000	-2.60752900	-0.76628000
O	-3.42501200	1.50521500	1.30846700
C	-4.08597500	1.09768400	2.31876800

O	-4.67062500	-0.02752400	2.42229800
O	-4.96919800	1.03743700	-1.13180800
C	-6.08211600	0.51276600	-0.79399200
O	-6.23342200	-0.46340400	0.00688500
O	-2.83670200	-2.14108000	1.61574900
C	-1.72060900	-1.61610400	1.29013200
O	-1.57010600	-0.61146300	0.52015700
C	-3.57543500	-3.20740600	-2.91456300
H	-3.65101600	-2.68307800	-3.87076200
H	-4.32768300	-3.99537400	-2.84899000
C	-0.46749700	-2.21470600	1.88202600
H	-0.15276200	-1.60460600	2.73710400
H	0.33898700	-2.19852000	1.14527200
C	-7.32864300	1.08768600	-1.42829000
H	-8.20845400	0.84333100	-0.83022900
H	-7.45235600	0.65188600	-2.42675900
C	-4.15424100	2.02369600	3.51234000
H	-5.02017500	1.78343400	4.13216000
H	-4.19365400	3.06486000	3.18332300
C	1.67531200	0.58602300	-2.29164400
C	0.43941300	1.29581600	-1.85233400
C	0.39821500	2.17074800	-0.74716700
C	-0.72299300	1.08232400	-2.60319500
C	-0.78334200	2.82047100	-0.41270800
H	1.27873700	2.35556600	-0.14346400
C	-1.91564600	1.73169000	-2.26589800
H	-0.68063100	0.40298400	-3.44706200
C	-1.94603100	2.60790400	-1.16805900
H	-0.80367100	3.48858200	0.44234900
H	-2.80037600	1.59169100	-2.87866800
H	-2.85885600	3.14161500	-0.92299300
C	3.00504600	0.86154000	-1.52360400
N	3.91119300	-0.30774700	-1.57276900
S	3.39336500	-1.88117000	-1.04728300
O	2.03211000	-1.64045800	-0.57488800
O	3.69139100	-2.82429800	-2.12305900
C	4.43357900	-2.28608300	0.34689000
C	4.24082700	-1.62331100	1.56331300

C	5.37539300	-3.30635200	0.20955600
C	5.03708800	-1.98580500	2.64548200
H	3.49968700	-0.83390900	1.66842900
C	6.15575000	-3.65385900	1.31195000
H	5.47844500	-3.82833900	-0.73541800
C	6.00449600	-2.99896900	2.54076200
H	4.90193200	-1.46943300	3.59271100
H	6.88892100	-4.45039900	1.21496700
C	6.85461100	-3.37012000	3.73204400
H	7.45485100	-2.51615200	4.06927100
H	6.23328800	-3.68075400	4.58074200
H	7.53913400	-4.19088800	3.49780300
H	-2.57867800	-3.66034600	-2.86121400
H	-0.66123000	-3.23116700	2.23030900
H	-7.23061300	2.16988300	-1.54389700
H	-3.24736800	1.89319700	4.11448900
H	2.83364600	1.15604500	-0.48258600
C	5.12120000	0.00342300	-2.14494100
O	6.25683900	0.24582600	-0.69059000
C	4.97842200	1.36940900	-2.66086400
C	3.80335900	1.90271400	-2.28459200
C	3.31424500	3.28837500	-2.54474800
H	3.31322700	3.84936000	-1.60029600
H	3.96961300	3.79863500	-3.25702500
H	2.29397400	3.29134300	-2.94371700
O	1.70138200	-0.13590300	-3.27053500
H	5.75731300	1.86006800	-3.23343000
H	7.07973700	0.66210200	-1.00158700
C	2.99930700	4.24910200	1.43266600
O	3.76773000	3.84257700	0.51289000
C	2.30022500	3.45697400	2.38018100
C	2.25989700	2.04978100	2.48280600
C	1.28268400	1.44382100	3.48356000
H	0.48306500	0.93506700	2.92996300
H	1.79684100	0.68420200	4.08331600
H	0.83068800	2.18428400	4.14968800
O	2.92702500	1.21324800	1.79328700
H	4.50629700	1.42692600	1.40098200

H	1.67352500	4.00006900	3.07994100
O	5.34098000	1.79014600	0.97690400
H	5.80083900	0.97176400	0.04124100
H	4.94452300	2.65497200	0.66760000
C	5.95384400	-1.02108200	-2.86934400
H	6.87871400	-0.55606300	-3.22237500
H	6.20278500	-1.87181100	-2.23668400
H	5.38555900	-1.38131900	-3.73215000
C	2.78161600	5.75950400	1.49143900
H	3.75235800	6.25705700	1.60044700
H	2.35541300	6.10198700	0.54055300
H	2.12520200	6.07525900	2.30717900

Int8a

Rh	-4.65792600	-1.27775900	0.92193200
Rh	-3.27507700	0.23035900	-0.33707000
O	-3.24479600	-1.19951500	-1.83415300
C	-3.86103500	-2.30147600	-1.65997300
O	-4.54591700	-2.61649300	-0.63455500
O	-3.42759100	1.55196800	1.25382300
C	-4.10508800	1.21432500	2.27898300
O	-4.71506100	0.10897300	2.43759600
O	-5.00349900	1.02803800	-1.15237700
C	-6.12905900	0.54735200	-0.79178800
O	-6.30342000	-0.39056800	0.04946800
O	-2.94983000	-2.08611100	1.72437000
C	-1.82078200	-1.60661400	1.37519400
O	-1.64328600	-0.65110700	0.55022600
C	-3.74291000	-3.33045800	-2.76061300
H	-3.78890600	-2.84403900	-3.73835200
H	-4.52902000	-4.08198300	-2.66870400
C	-0.58909400	-2.20118100	2.01416000
H	-0.35019300	-1.62829600	2.91842500
H	0.26162700	-2.13671700	1.33334000
C	-7.36250800	1.12553800	-1.44790900
H	-7.53697400	0.60391600	-2.39650800
H	-7.21586600	2.18577100	-1.66667800
C	-4.21337600	2.23163300	3.39229300
H	-4.96458500	2.98151100	3.11785100

H	-3.25895000	2.74704500	3.52587300
C	1.60786100	0.32837700	-2.28168900
C	0.41293600	1.11817800	-1.88807400
C	0.42337800	2.07249000	-0.85122900
C	-0.76871700	0.88791300	-2.60576500
C	-0.73268900	2.78043900	-0.54480200
H	1.32143400	2.27015200	-0.27874700
C	-1.93141500	1.60309500	-2.30103800
H	-0.76613100	0.14566200	-3.39590200
C	-1.91295200	2.55388100	-1.26644600
H	-0.71477200	3.50503600	0.26266800
H	-2.82840600	1.45540500	-2.89382100
H	-2.80619200	3.12828900	-1.04200800
C	2.98180700	0.64562400	-1.58253900
N	3.85364100	-0.53976200	-1.59955400
S	3.36923400	-2.06796500	-0.81521800
O	2.05373700	-1.74089700	-0.28275600
O	3.58019400	-3.12282800	-1.80014700
C	4.54675900	-2.25280300	0.50496700
C	4.47664400	-1.39454400	1.60784300
C	5.47478100	-3.29448500	0.43373200
C	5.38451400	-1.58747200	2.64454300
H	3.74463300	-0.58800700	1.65446100
C	6.36447600	-3.46759600	1.49214500
H	5.48765000	-3.96082200	-0.42158100
C	6.33902100	-2.61717500	2.60609600
H	5.34994800	-0.92053900	3.50220200
H	7.08771300	-4.27763500	1.45121600
C	7.31919600	-2.79199600	3.74039900
H	8.02786200	-1.95498900	3.77597100
H	6.80548100	-2.81912300	4.70823700
H	7.89662300	-3.71524500	3.63559400
H	-2.76788700	-3.82483500	-2.67928600
H	-0.77975300	-3.23619700	2.30637400
H	-8.23633400	0.98129600	-0.80954200
H	-4.52203900	1.74950000	4.32153100
H	2.86412700	0.99594200	-0.54045800
C	4.92905800	-0.32967700	-2.36443700

O	7.30905000	0.87955300	-0.87036200
C	4.88733900	1.00236000	-2.86828700
C	3.75852200	1.62267700	-2.42057000
C	3.32161500	3.01452200	-2.69726000
H	3.32784500	3.59375800	-1.75964100
H	3.98802700	3.49033500	-3.42180800
H	2.29676600	3.04014300	-3.08652600
O	1.59280400	-0.50553200	-3.16509800
H	5.67014500	1.43302700	-3.47743300
H	8.13498000	1.13927400	-0.43811800
C	2.76390900	4.32374700	1.17370100
O	3.50286700	3.96816900	0.21754100
C	2.17553100	3.46851600	2.14696700
C	2.28440500	2.06676200	2.23205600
C	1.52528000	1.36430000	3.35302800
H	0.78762700	0.68428800	2.90975000
H	2.22063700	0.74936500	3.93736600
H	1.01083100	2.05467200	4.02768100
O	2.93727800	1.30495100	1.44505500
H	4.67835800	1.65035000	1.06876300
H	1.57492200	3.95098900	2.91141000
O	5.46020400	2.10642300	0.68821000
H	6.60664700	1.31385900	-0.31851900
H	5.01833800	2.93466800	0.40359700
C	2.47057600	5.81986700	1.28591000
H	1.78745300	6.07267000	2.10214100
H	3.41391800	6.35929200	1.43361600
H	2.04660500	6.17749100	0.34012700
C	6.04141700	-1.28635100	-2.58426800
H	6.48844600	-1.10290600	-3.56489400
H	6.79968500	-1.03514100	-1.82663900
H	5.73132900	-2.32723900	-2.50815800
TS6a			
Rh	-4.77608000	-1.13851300	1.06784600
Rh	-3.37042100	0.20788000	-0.33974900
O	-3.48752700	-1.29922400	-1.75136100
C	-4.14690200	-2.35606900	-1.48028600
O	-4.79567600	-2.57143800	-0.40671400

O	-3.37143100	1.62975900	1.16579900
C	-4.01818200	1.39607100	2.23809800
O	-4.69288300	0.34634200	2.48979800
O	-5.08917700	1.05241600	-1.12681600
C	-6.22198600	0.65570600	-0.69469100
O	-6.40944000	-0.22057100	0.20812800
O	-3.08314500	-1.99854100	1.84706600
C	-1.94549600	-1.61722100	1.41647500
O	-1.74973000	-0.71662100	0.53423100
C	-4.11730600	-3.46284200	-2.50840800
H	-5.02770500	-4.06244100	-2.45094900
H	-3.26077000	-4.11390000	-2.29381000
C	-0.72399100	-2.26792000	2.01777200
H	-0.41825300	-1.69494500	2.90199300
H	0.10424500	-2.26641800	1.30778700
C	-7.45084700	1.25742000	-1.33801500
H	-8.29133600	1.23921900	-0.64134200
H	-7.72069300	0.66007100	-2.21722000
C	-3.96426400	2.44781900	3.32362000
H	-3.32554100	2.08554800	4.13700200
H	-4.96424700	2.60785100	3.73586100
C	1.36881900	-0.03512700	-2.00369800
C	0.24616200	0.94519400	-1.86975700
C	0.32384200	2.13743300	-1.13062500
C	-0.96470100	0.60972900	-2.49333100
C	-0.78840300	2.96813000	-1.00420800
H	1.24561800	2.42419900	-0.64036100
C	-2.07904900	1.44897400	-2.38455700
H	-1.02652400	-0.31937100	-3.04805400
C	-1.99045300	2.63148700	-1.63051300
H	-0.71570000	3.87498900	-0.41170300
H	-2.98848800	1.21440600	-2.92900900
H	-2.85733300	3.27858400	-1.53743800
C	2.79391600	0.35529300	-1.60117900
N	3.70550700	-0.77726800	-1.54383100
S	3.39592500	-2.20872100	-0.56045400
O	2.19331900	-1.87159700	0.19338100
O	3.47835300	-3.37186900	-1.43639900

C	4.78950500	-2.24979600	0.56311500
C	5.05951900	-1.15687500	1.39105800
C	5.52229100	-3.43455300	0.65665400
C	6.10312400	-1.25647800	2.30740000
H	4.47526000	-0.24411100	1.31635100
C	6.55191600	-3.51519700	1.59274600
H	5.28507900	-4.27311300	0.01111100
C	6.86355300	-2.43058600	2.42464700
H	6.32874600	-0.40401600	2.94272700
H	7.12201700	-4.43688800	1.67634500
C	8.00765700	-2.51002100	3.40612400
H	8.94127000	-2.15446900	2.94921600
H	7.82417900	-1.88915500	4.28906900
H	8.17689400	-3.53916000	3.73692400
H	-3.98181500	-3.05144700	-3.51077300
H	-0.96478800	-3.28315600	2.34046100
H	-7.24624600	2.27772100	-1.66977100
H	-3.55777600	3.38449700	2.93827000
H	2.87236700	0.91964600	-0.35693300
C	4.85042900	-0.51198100	-2.21783300
O	7.47889600	1.24241900	-1.40480100
C	4.74545500	0.77445800	-2.76772700
C	3.51644700	1.31522100	-2.43455100
C	3.07996500	2.69912300	-2.78833400
H	3.16589900	3.34264100	-1.90009800
H	3.72928300	3.10963300	-3.56681200
H	2.04372600	2.74115800	-3.13495800
O	1.16617800	-1.14975200	-2.45638300
H	5.54778800	1.26483000	-3.30153200
H	8.36492500	1.45756700	-1.07949900
C	3.01436300	4.43495300	1.23956800
O	3.71129900	4.34611400	0.21789600
C	2.33350600	3.33040700	1.89708100
C	2.41038600	1.99624400	1.57405400
C	1.52682300	0.98042800	2.25620600
H	0.84555300	0.52694600	1.52532300
H	2.13503500	0.16690000	2.66794200
H	0.92873300	1.42720100	3.05521700

O	3.25336500	1.51747600	0.67328100
H	4.99022100	2.11621800	0.52149500
H	1.67847400	3.59538300	2.72231400
O	5.86232100	2.54965300	0.40495900
H	6.87621900	1.72410200	-0.78522400
H	5.56924300	3.44701000	0.16812900
C	6.04827300	-1.39417800	-2.30062000
H	6.80383300	-1.01559500	-1.60128200
H	5.82287300	-2.44282300	-2.11096900
H	6.47677000	-1.29848600	-3.30295100
C	2.80876900	5.80667200	1.87754100
H	3.27367500	6.57464800	1.25589400
H	1.74220300	6.03098400	2.00335400
H	3.25968500	5.82841800	2.87813000

Int5a-2w'

C	2.12023600	-0.75947800	-0.07528400
C	3.28368900	0.02061000	-0.58652200
C	3.21053100	1.38942200	-0.89477300
C	4.49740300	-0.66377500	-0.77596900
C	4.33583000	2.05540400	-1.37989800
H	2.28075300	1.93728700	-0.78239800
C	5.61833700	0.00654100	-1.25204800
H	4.53497300	-1.72281100	-0.54323900
C	5.53883600	1.36958800	-1.55507500
H	4.26982800	3.11137700	-1.62648200
H	6.55291700	-0.52970500	-1.39141800
H	6.41304300	1.89417700	-1.93170300
C	0.86305200	0.00140900	0.41678000
N	-0.30308500	-0.86698800	0.58016500
S	-1.15823500	-1.32194900	-0.78194300
O	-0.44511900	-0.82799800	-1.96468400
O	-1.48004800	-2.75600100	-0.62592100
C	-2.71874200	-0.44286500	-0.68177100
C	-2.75837500	0.92154500	-0.98449900
C	-3.87460700	-1.13052800	-0.31582200
C	-3.97468600	1.59365000	-0.90676900
H	-1.85665200	1.45172000	-1.27259800
C	-5.08416700	-0.43900500	-0.24768900

H	-3.82445100	-2.19216200	-0.10075100
C	-5.15540500	0.92797200	-0.54198300
H	-4.00873000	2.65535200	-1.13946300
H	-5.98750200	-0.97429300	0.03466600
C	-6.47268800	1.66527000	-0.49829700
H	-7.20658000	1.13990700	0.12093000
H	-6.35226200	2.67815900	-0.09869100
H	-6.90200000	1.76371800	-1.50408300
H	0.60776700	0.76305000	-0.31611000
C	0.25147100	2.98451200	1.06154000
O	0.10513000	2.80977800	-0.14685600
C	0.83880700	1.99060600	1.98988200
C	1.13272200	0.69220600	1.75805400
C	1.71304900	-0.16770600	2.84949500
H	2.71499300	-0.51955300	2.56901000
H	1.79829500	0.38496700	3.78915000
H	1.10829300	-1.06716500	3.01968900
O	2.16772600	-1.98059400	-0.00944300
H	-0.23835400	-1.64014000	1.26882300
H	1.01898700	2.36610500	2.99604800
O	0.66146000	-4.41560300	0.35499300
H	-0.09206600	-4.09306000	-0.17794500
H	1.36122100	-3.77314600	0.13293200
O	-0.13923600	-2.98403600	2.49430800
H	0.20129600	-3.64320300	1.82736200
H	-1.04807500	-3.26970400	2.67254400
C	-0.17109000	4.29681000	1.70036300
H	-0.91141800	4.11823100	2.49032400
H	0.68918400	4.78644800	2.17436400
H	-0.59463300	4.95703200	0.94152300
TS4a-2w'			
C	-2.35921800	0.42840000	-0.35847900
C	-3.31070100	-0.70802300	-0.24614000
C	-3.12083800	-1.78958100	0.63246100
C	-4.45825700	-0.68035000	-1.06111800
C	-4.06635100	-2.81219900	0.69400900
H	-2.22346500	-1.86914200	1.23609100
C	-5.40283300	-1.69666700	-0.98741100

H	-4.58919000	0.15369800	-1.74219100
C	-5.20832300	-2.76568000	-0.10657600
H	-3.90368800	-3.65101900	1.36444100
H	-6.28912700	-1.66094100	-1.61491700
H	-5.94434000	-3.56344700	-0.05009000
C	-1.26622900	0.65650800	0.71644900
N	0.08911500	0.43452800	0.18760300
S	0.51441300	-1.17805900	0.20186600
O	0.30724500	-1.75582100	1.55321200
O	-0.11668000	-1.87887900	-0.93451100
C	2.28123000	-1.11412400	-0.10315200
C	3.14658300	-1.61921200	0.86629800
C	2.77134900	-0.65402200	-1.32810800
C	4.51837700	-1.63932900	0.61302100
H	2.73982700	-1.99710500	1.79808200
C	4.14343200	-0.67378300	-1.56019200
H	2.09406900	-0.28754700	-2.09159100
C	5.03862200	-1.16182300	-0.59605000
H	5.19391900	-2.03703300	1.36663500
H	4.52661200	-0.30973300	-2.51049600
C	6.52644200	-1.15593500	-0.85548000
H	7.05543700	-1.82840700	-0.17288200
H	6.75549300	-1.46430300	-1.88162000
H	6.94606400	-0.15051600	-0.71916100
H	-1.46379000	-0.00232500	1.57242200
C	1.21411600	1.98409700	1.25429100
O	2.05203700	2.40594700	0.39399500
C	-0.10853800	2.66938600	1.43364100
C	-1.29328600	2.09017400	1.23163000
C	-2.61029600	2.74115300	1.55301600
H	-3.18590900	2.12468800	2.25696000
H	-2.46444100	3.72551000	2.00649200
H	-3.22922900	2.86398200	0.65732700
O	-2.46945200	1.22809400	-1.29090600
H	0.45734500	1.33927400	-1.19437700
H	-0.03977400	3.68677800	1.81815500
O	-1.26910900	3.54366800	-2.16789300
H	-1.48629700	3.53240000	-3.11311100

H	-1.80587500	2.81098000	-1.78375300
O	0.90976400	2.12624000	-1.68347200
H	0.16941300	2.76746600	-1.92034700
H	1.50087700	2.48548600	-0.74152100
C	1.77450800	1.29320200	2.47471100
H	2.71117600	0.79329900	2.22116200
H	1.98422900	2.06082400	3.23300300
H	1.06708300	0.57724800	2.89786900

Int6a-2w'

C	-2.00091800	0.22112000	-0.33396800
C	-3.20160300	-0.62984500	-0.54078700
C	-3.35578400	-1.88390600	0.07381900
C	-4.20687900	-0.15908400	-1.40404400
C	-4.49971300	-2.64328200	-0.16620100
H	-2.56190100	-2.29232000	0.68853200
C	-5.35522700	-0.91122000	-1.62540500
H	-4.07567600	0.80465200	-1.88536500
C	-5.50337700	-2.15569000	-1.00520400
H	-4.60326400	-3.62007000	0.29728800
H	-6.13339800	-0.53281600	-2.28224300
H	-6.39772000	-2.74709400	-1.18204900
C	-1.26012800	0.18434800	1.02051800
N	0.20784400	0.22481600	0.87499600
S	0.85756200	-1.30993800	0.55420500
O	1.04679500	-2.10834500	1.77621300
O	-0.04026300	-1.84869200	-0.48493600
C	2.46900900	-0.96080900	-0.13514000
C	3.55631500	-1.67890600	0.36200500
C	2.61610200	-0.06847300	-1.20062500
C	4.81168600	-1.49383900	-0.21658600
H	3.41463600	-2.36706000	1.18797700
C	3.87772100	0.10346000	-1.75917300
H	1.77572700	0.50575800	-1.57168700
C	4.99298400	-0.60227900	-1.28014500
H	5.66227200	-2.05090800	0.16797000
H	3.99999600	0.80633800	-2.57948000
C	6.35699200	-0.38284500	-1.88933800
H	6.75735500	0.60074900	-1.61187800

H	7.07331900	-1.13904800	-1.55393000
H	6.31529600	-0.41602100	-2.98407300
H	-1.59068200	-0.68840200	1.59783300
C	0.83752500	1.24036700	1.82748100
O	1.79605600	2.01768300	1.18405600
C	-0.40933300	2.00136800	2.22607300
C	-1.55077600	1.45163400	1.81634800
C	-2.95125400	1.91765300	2.07413600
H	-3.54930800	1.13741600	2.56304300
H	-2.95257700	2.80158500	2.71819500
H	-3.46960000	2.17891900	1.14250000
O	-1.66828300	1.04957200	-1.17900600
H	0.01717500	1.94108600	-1.06795100
H	-0.32021900	2.90274600	2.82478500
O	-1.61495600	3.60986700	-2.58402700
H	-1.28392800	3.42321600	-3.47608300
H	-1.89416600	2.73599500	-2.25503500
O	0.66706800	2.65807200	-1.20932900
H	0.09547800	3.36716400	-1.56723700
H	1.39442600	2.43415300	0.38034100
C	1.53097300	0.63105500	3.05192500
H	2.44128200	0.10638200	2.75299500
H	1.81616800	1.44656600	3.72397500
H	0.87618200	-0.06389700	3.58140500
Int7a'			
C	2.48323000	-1.31000300	-0.18575300
C	3.32239400	-0.34690900	-0.96983200
C	3.07821100	1.03407600	-1.03364900
C	4.42561300	-0.87353600	-1.66302200
C	3.92090000	1.86656100	-1.77119700
H	2.23872600	1.47496300	-0.50689600
C	5.25974800	-0.04415800	-2.40447300
H	4.60166000	-1.94235000	-1.60432700
C	5.00971700	1.33052300	-2.45953300
H	3.72441900	2.93477000	-1.80942700
H	6.10581500	-0.46556900	-2.94058200
H	5.66169200	1.98040900	-3.03747100
C	1.22519300	-0.80151300	0.57548400

N	0.14548900	-1.79464400	0.55093100
S	-0.59055600	-2.18842700	-0.88219400
O	0.29640700	-1.67849000	-1.93914000
O	-1.01288400	-3.58816400	-0.83610400
C	-2.11244300	-1.21678300	-1.03472500
C	-2.23173200	-0.33786600	-2.11361300
C	-3.18164900	-1.41148500	-0.15550700
C	-3.42928900	0.36465800	-2.29732700
H	-1.40367500	-0.23218700	-2.80692300
C	-4.36214700	-0.70025500	-0.35149600
H	-3.07268700	-2.09154700	0.68221300
C	-4.51092200	0.19525000	-1.42202800
H	-3.53011200	1.03207700	-3.15047800
H	-5.18750500	-0.84516100	0.34133100
C	-5.80931700	0.93884600	-1.62722100
H	-6.09250200	1.50281600	-0.73038600
H	-5.74368600	1.64223300	-2.46330800
H	-6.63108600	0.24447000	-1.84136400
H	0.88127600	0.15917500	0.17950600
C	-0.15292700	-2.39434800	1.90221400
O	-1.48360700	-2.16616300	2.29972600
C	0.82400500	-1.60099500	2.73991000
C	1.54276200	-0.70894100	2.06038000
C	2.54779100	0.26361800	2.59685800
H	2.19043600	1.29323400	2.47312400
H	2.71710300	0.09130200	3.66426200
H	3.51302500	0.17992200	2.08228800
O	2.80530200	-2.47948500	-0.08273500
H	0.86895000	-1.76816100	3.81183300
H	-1.61001000	-1.18781800	2.39134300
C	0.16667800	3.74505900	1.71967100
O	0.07202200	2.64079900	2.26343100
C	-0.40575700	4.07171500	0.41632900
C	-1.08579800	3.21860100	-0.39486300
C	-1.63678200	3.63382100	-1.72960300
H	-1.19060400	3.03272800	-2.53226600
H	-2.72140000	3.47110800	-1.76338700
H	-1.43649100	4.68740500	-1.93285700

O	-1.29140200	1.93877100	-0.03513400
H	-1.80110900	1.45332000	-0.71351700
H	-0.27128000	5.08615700	0.05609200
O	-1.85780300	0.57469300	2.63049600
H	-1.55432900	0.75179500	3.53354700
H	-1.29815000	1.17406600	2.09632700
C	0.09618000	-3.90032300	1.96857800
H	0.03416400	-4.22337300	3.01336100
H	-0.65496000	-4.43617300	1.38676200
H	1.08862500	-4.12698800	1.57314000
C	0.92414100	4.86867300	2.41193400
H	1.75968900	5.21409600	1.79034500
H	0.26724700	5.73230600	2.57489400
H	1.30616200	4.51691400	3.37198800
TS5a'			
C	1.56174300	-2.07266500	-0.13026000
C	2.74894600	-1.59672900	-0.89305300
C	3.12371600	-0.24606800	-0.98180900
C	3.52741700	-2.57130400	-1.54343500
C	4.25865500	0.11749300	-1.70672400
H	2.54770100	0.53327800	-0.49715100
C	4.65405900	-2.20325400	-2.26898700
H	3.22187900	-3.60945100	-1.46637200
C	5.02253400	-0.85585200	-2.35140100
H	4.53654900	1.16576900	-1.76619600
H	5.24681400	-2.96225800	-2.77218300
H	5.90353900	-0.56762500	-2.91908300
C	0.71480800	-1.03483700	0.66833100
N	-0.71696300	-1.40803600	0.68652200
S	-1.58664600	-1.70842400	-0.78897400
O	-0.58658900	-1.44069500	-1.81831000
O	-2.24156000	-3.00811500	-0.65226600
C	-2.86065200	-0.45697500	-0.86438000
C	-2.50958900	0.86597900	-1.14770400
C	-4.19199400	-0.84389400	-0.70812000
C	-3.52549200	1.81185100	-1.24507900
H	-1.47149800	1.16349800	-1.27692300
C	-5.19055900	0.12292700	-0.81691900

H	-4.43784400	-1.88441000	-0.52675200
C	-4.87518900	1.46190900	-1.07978000
H	-3.26139900	2.84495900	-1.45747500
H	-6.23078800	-0.17106400	-0.70240300
C	-5.95541000	2.51181300	-1.17910300
H	-6.95317100	2.06298900	-1.19310500
H	-5.91156500	3.20228200	-0.32716700
H	-5.84141300	3.11504400	-2.08707100
H	0.82922800	-0.01440400	0.28966200
C	-1.19217500	-1.55725700	1.96774800
O	-2.06477500	0.03491600	2.31065000
C	-0.01436300	-1.46963100	2.84110700
C	1.07860500	-1.13168800	2.13684000
C	2.45504700	-0.87945700	2.65375800
H	2.68304100	0.19056200	2.55781900
H	2.52862300	-1.16382200	3.70769500
H	3.20721900	-1.44008000	2.08739400
O	1.27058000	-3.25143000	-0.04349600
H	-0.07086800	-1.63009800	3.91191600
H	-2.27259300	0.08299100	3.25993000
C	2.54703700	3.00468800	1.28496800
O	1.94084100	2.14018800	1.98217300
C	2.20747600	3.44557400	-0.02047200
C	1.16926500	2.97894300	-0.85382900
C	1.08489900	3.54324700	-2.26678000
H	1.17798200	2.72197300	-2.98725800
H	0.09458400	3.98874100	-2.41995900
H	1.84943700	4.29496000	-2.48159200
O	0.29475300	2.10116600	-0.56194900
H	-0.50161100	2.09867100	0.86875900
H	2.85443700	4.20452100	-0.44803500
O	-0.68356300	2.00222100	1.85184100
H	-1.38146500	0.91372400	2.09816500
H	0.27237600	2.00575400	2.14655900
C	-2.33391000	-2.48454900	2.29139200
H	-2.55485500	-2.43366000	3.36142400
H	-3.23425500	-2.23866200	1.72996300
H	-2.03252300	-3.50557100	2.03934500

C	3.79991300	3.60395100	1.91909700
H	3.53952700	4.03245200	2.89374800
H	4.52713300	2.80476800	2.10810200
H	4.27462900	4.37391200	1.30459000
Int8a'			
C	1.57496700	-2.10463300	0.03305500
C	2.83335600	-1.66441400	-0.61726200
C	3.22018700	-0.31857100	-0.71774600
C	3.66311800	-2.66789600	-1.15225300
C	4.41964200	0.01411000	-1.34712900
H	2.60774000	0.47793200	-0.31259300
C	4.85571900	-2.32914700	-1.77874000
H	3.34591600	-3.70187400	-1.06751000
C	5.23551100	-0.98540400	-1.87779400
H	4.70242100	1.05955400	-1.42373200
H	5.49044400	-3.10734500	-2.19336200
H	6.16738100	-0.72084300	-2.37078800
C	0.65415900	-1.01997700	0.70270900
N	-0.75323900	-1.44672200	0.66642000
S	-1.58240400	-1.78484800	-0.88313300
O	-0.53859800	-1.50961200	-1.85932000
O	-2.20137700	-3.09769500	-0.73601100
C	-2.85735600	-0.54458500	-0.95760200
C	-2.50157500	0.79250300	-1.16092000
C	-4.19059800	-0.95356200	-0.87927100
C	-3.52310000	1.73199000	-1.26130800
H	-1.45673000	1.09865800	-1.22640300
C	-5.19061800	0.00957600	-0.99275700
H	-4.43525800	-2.00171600	-0.74814900
C	-4.87510400	1.36255900	-1.17782600
H	-3.26132000	2.77669800	-1.40891300
H	-6.23191400	-0.29685500	-0.93950100
C	-5.96015700	2.40690900	-1.27444500
H	-5.98574800	3.02758000	-0.36970900
H	-5.78877700	3.08057400	-2.12144300
H	-6.94797800	1.95225000	-1.39453600
H	0.74098000	-0.02631200	0.22817300
C	-1.21592400	-1.66191100	1.89982600

O	-2.35266500	0.78359000	3.36599900
C	-0.18987200	-1.36007500	2.84208300
C	0.93206100	-0.96293100	2.17828200
C	2.23642600	-0.55677000	2.76019600
H	2.43856500	0.49837200	2.51816900
H	2.23156300	-0.68711400	3.84565000
H	3.05793900	-1.14703000	2.33607300
O	1.24697300	-3.27126600	0.12652400
H	-0.33406700	-1.40625000	3.91272100
H	-2.86347000	1.48878800	3.78819500
C	2.68464000	3.09456500	0.80920700
O	2.16915800	2.32039600	1.65842300
C	2.25148800	3.27729300	-0.53342200
C	1.17627100	2.63394000	-1.17670000
C	0.90081300	2.99441600	-2.63261500
H	0.91701800	2.08140500	-3.23914900
H	-0.10846100	3.41647900	-2.71862600
H	1.61549500	3.71220600	-3.04501500
O	0.40422500	1.75590000	-0.66898100
H	-0.45063900	2.06969300	0.90391900
H	2.80408300	4.00001200	-1.12531700
O	-0.56649600	2.19079600	1.87125200
H	-1.68697500	1.27411000	2.81708400
H	0.37614000	2.30390500	2.11607900
C	3.89642500	3.90257200	1.27289500
H	4.32870200	4.53271700	0.49012500
H	3.60175000	4.53743900	2.11701000
H	4.66637300	3.21720800	1.64655000
C	-2.60118600	-2.05915000	2.25204800
H	-2.58427000	-2.65983700	3.16539300
H	-3.12725500	-1.12188200	2.48801500
H	-3.10401700	-2.60923000	1.45864200
TS6a'			
C	1.63320100	-2.05014300	0.25329100
C	3.03894300	-1.72502100	-0.14073200
C	3.52802800	-0.42088500	-0.30413300
C	3.89451300	-2.81257900	-0.39169300
C	4.84629000	-0.20972800	-0.71007600

H	2.89427700	0.43750800	-0.12136300
C	5.20967800	-2.59932600	-0.78851100
H	3.49861800	-3.81539100	-0.27301000
C	5.68903700	-1.29511200	-0.94988000
H	5.20822600	0.80594200	-0.84113400
H	5.86253300	-3.44721400	-0.97680200
H	6.71600200	-1.12773600	-1.26389900
C	0.69929600	-0.95394400	0.77281900
N	-0.69284000	-1.36703200	0.83499400
S	-1.55737000	-2.00894600	-0.56692700
O	-0.61756800	-1.84624600	-1.66960200
O	-2.11356600	-3.30244900	-0.18591400
C	-2.91201900	-0.85474700	-0.77333400
C	-2.65484900	0.50848600	-0.94632500
C	-4.20722900	-1.36738600	-0.84534700
C	-3.72762500	1.36532600	-1.17017000
H	-1.64013300	0.89308500	-0.89196600
C	-5.26442800	-0.49004500	-1.08496700
H	-4.37978000	-2.43008000	-0.71449500
C	-5.04495900	0.88393500	-1.24499400
H	-3.53677900	2.42904600	-1.28727700
H	-6.27630500	-0.88213400	-1.14508900
C	-6.19345900	1.83479500	-1.48030200
H	-6.33742400	2.49781900	-0.61793700
H	-6.00683200	2.47528800	-2.34998700
H	-7.13178000	1.29832400	-1.64918900
H	0.68120300	0.16150200	-0.02100600
C	-1.23487900	-1.06141600	2.03750500
O	-2.28716900	1.79810400	3.22918200
C	-0.23812700	-0.46994000	2.82819400
C	0.94059200	-0.40864200	2.10740400
C	2.20544500	0.20914600	2.60601400
H	2.35084200	1.18571000	2.12181100
H	2.14276900	0.37185300	3.68566100
H	3.08606800	-0.40295900	2.39202500
O	1.22128100	-3.19659100	0.18590300
H	-0.41646300	-0.07076700	3.81709800
H	-2.89879500	2.50938300	3.46813100

C	2.43996500	3.56995500	-0.26404300
O	2.14212500	3.26244500	0.89944700
C	2.04363500	2.84112700	-1.45854900
C	1.19826300	1.75976200	-1.52757600
C	0.97505000	1.02807800	-2.82850600
H	1.21660400	-0.03434500	-2.70729500
H	-0.08497700	1.07135300	-3.10634200
H	1.57550500	1.43930700	-3.64407800
O	0.51327400	1.30995800	-0.48828500
H	-0.30502200	2.42834800	0.72156500
H	2.47656600	3.18291500	-2.39454400
O	-0.62906600	3.05105100	1.40663500
H	-1.65707800	2.23435500	2.60421800
H	0.21803700	3.42126600	1.70869600
C	-2.66044700	-1.24868900	2.42941700
H	-3.18705900	-0.29542000	2.30364300
H	-3.15293000	-2.04365700	1.86996500
H	-2.69698400	-1.48621500	3.49635800
C	3.31667500	4.79678700	-0.50334700
H	3.63782900	5.20962700	0.45513000
H	4.19632200	4.54487600	-1.10835400
H	2.75672900	5.56182300	-1.05653700
1aa + 2H₂O			
C	2.26032500	-0.90023100	-0.32749800
C	3.55643100	-0.15746900	-0.44922400
C	3.65246300	1.23520000	-0.31999200
C	4.70064700	-0.89762200	-0.78641000
C	4.87870300	1.87346300	-0.50975100
H	2.76363400	1.82711500	-0.12763900
C	5.92750500	-0.26082900	-0.95185400
H	4.60620400	-1.97115100	-0.91579300
C	6.01888900	1.12723700	-0.81248100
H	4.94065700	2.95527400	-0.42850000
H	6.81124600	-0.84322300	-1.19801700
H	6.97461700	1.62603100	-0.95038900
C	1.28157700	-0.51347100	0.72137400
N	-0.06062500	-0.96610700	0.65160700
S	-0.90913600	-1.17543300	-0.88482000

O	-0.22089800	-0.25812300	-1.79983800
O	-1.04187600	-2.60058200	-1.15643200
C	-2.54453800	-0.51089200	-0.59379800
C	-2.71196800	0.84961000	-0.32425700
C	-3.64127600	-1.35780500	-0.75592800
C	-3.99880900	1.35824800	-0.19125900
H	-1.86762600	1.51810200	-0.21111000
C	-4.92418900	-0.82635500	-0.62610300
H	-3.48806100	-2.40748600	-0.98102100
C	-5.12435400	0.53149000	-0.34241300
H	-4.10701700	2.41960400	0.01405600
H	-5.78362600	-1.47966700	-0.75291100
C	-6.51524700	1.10504400	-0.22141100
H	-6.62687000	1.68556800	0.70154800
H	-6.73117100	1.78497800	-1.05503900
H	-7.27728700	0.31996300	-0.22469100
C	-0.61472200	-0.97809300	1.92569600
O	-1.88359000	3.99996100	0.09357500
C	0.35508000	-0.51674400	2.78958300
C	1.53923000	-0.22486500	2.06460500
C	2.83327100	0.19221700	2.70992600
H	3.08248500	1.23763100	2.49719600
H	2.75714900	0.08175300	3.79606400
H	3.67937100	-0.40944300	2.36534400
O	2.04342600	-1.87341400	-1.04047100
H	0.23488200	-0.43781200	3.86297300
H	-1.65135800	4.30187600	0.98398500
H	0.60427600	1.78352800	0.22959800
O	0.38326000	2.35860700	-0.52336800
H	-1.06346800	3.56931400	-0.22397000
H	0.24900400	1.71321000	-1.24427000
C	-1.98827000	-1.45479700	2.28270100
H	-2.76837400	-0.71749600	2.06798100
H	-2.24719700	-2.37900200	1.75687800
H	-2.00796600	-1.66061200	3.35682400
Int2b			
Rh	-3.92987600	-0.67933400	-0.60462100
Rh	-1.68699600	-0.37711200	0.34789900

O	-1.85158200	1.61506100	-0.15820800
C	-2.88832500	2.02957200	-0.79431400
O	-3.89050700	1.32176500	-1.10646200
O	-1.73020700	-2.41013900	0.77058800
C	-2.76215100	-3.10743000	0.46634600
O	-3.82067000	-2.67288900	-0.07240000
O	-2.63874700	0.02013200	2.15067500
C	-3.91843800	0.00050400	2.21275700
O	-4.71071700	-0.23010500	1.25363100
O	-3.02462600	-1.12512600	-2.40283600
C	-1.76088700	-1.09099800	-2.48694300
O	-0.95546800	-0.80924000	-1.53092500
C	-2.88551900	3.48776900	-1.18358600
H	-2.91479400	4.10335800	-0.27703400
H	-3.75596500	3.71426100	-1.80141800
C	-1.12806800	-1.37458500	-3.82879800
H	-0.08359800	-1.66830100	-3.70808900
H	-1.16743200	-0.46123000	-4.43420400
C	-4.52101600	0.25509500	3.57725800
H	-4.40099200	-0.64393000	4.19276200
H	-5.58417100	0.48370900	3.48645900
C	-2.67619500	-4.58441900	0.77812000
H	-3.64366900	-5.06352200	0.62081600
H	-2.34385300	-4.73015500	1.81022200
C	0.15871900	-0.21487200	1.15251600
C	0.63549100	0.67891300	2.16004000
C	1.90861000	0.49418700	2.77177200
C	-0.15571600	1.78892500	2.56581100
C	2.35928100	1.37126400	3.74595400
H	2.52980600	-0.33975300	2.46538800
C	0.31248200	2.66954900	3.53151100
H	-1.11575000	1.94171600	2.09230100
C	1.56253600	2.45987300	4.12551600
H	3.32953300	1.21860500	4.20896700
H	-0.29327300	3.52077900	3.82808900
H	1.91975800	3.14798800	4.88734400
C	1.00499700	-1.22229600	0.54300100
N	2.03720800	-0.88690500	-0.16338700

S	2.71903200	-2.17201700	-1.10783200
O	2.07895100	-3.45300100	-0.76953200
O	2.72794000	-1.67915700	-2.48832300
C	4.39303500	-2.19347500	-0.47882600
C	4.82459200	-3.29477300	0.26139100
C	5.24895800	-1.12161900	-0.75077200
C	6.13642900	-3.31918900	0.73343300
H	4.14271000	-4.11645800	0.45176700
C	6.55219900	-1.16347200	-0.26384000
H	4.90158300	-0.26742900	-1.32132200
C	7.01853200	-2.26024100	0.47848900
H	6.48023100	-4.17641900	1.30682100
H	7.22112800	-0.33071800	-0.46596600
C	8.44676700	-2.30573400	0.96666500
H	8.79552000	-1.31523300	1.27810900
H	8.56080500	-2.99025400	1.81310500
H	9.12095100	-2.65125500	0.17185700
H	-1.96045100	3.73450100	-1.71591000
H	-1.69453000	-2.14922000	-4.35149600
H	-3.99516900	1.07228400	4.07829400
H	-1.92944500	-5.04620000	0.12266000
H	0.65096600	-2.25944600	0.57844800
C	1.22320000	4.40390500	-1.66587300
C	1.86300300	5.57792300	-0.92448900
C	3.55957600	4.02381700	0.07134400
C	2.83597500	2.89593900	-0.61584100
H	1.67534800	6.48240700	-1.51151800
H	4.62207100	3.75816400	0.13300600
H	3.20234400	4.08832700	1.11121200
H	1.32233600	5.70258200	0.02692500
C	1.80477700	3.06653100	-1.49063500
C	3.35154600	5.35688300	-0.65045900
H	3.76651400	6.18038400	-0.05753400
H	3.89828900	5.34028900	-1.60229900
O	0.22005800	4.59143600	-2.35573000
O	3.34202200	1.69723800	-0.25151600
H	2.75033600	0.94198500	-0.47339000
C	1.16847200	1.92975700	-2.25048100

H	0.76995700	2.31312600	-3.19414100
H	1.88086400	1.12908400	-2.47545000
H	0.32755100	1.48501200	-1.70736700
TS2b			
Rh	-3.37725700	-1.32369600	-0.83210400
Rh	-1.36359700	-0.36290300	0.17510200
O	-2.58614200	1.23752400	0.75525800
C	-3.83704700	1.21223600	0.48557600
O	-4.44863600	0.29133600	-0.12874900
O	-0.37724700	-2.03790700	-0.54483600
C	-1.00148500	-2.91902600	-1.22909400
O	-2.23989000	-2.89863700	-1.50428600
O	-1.84592000	-1.41399000	1.89448300
C	-2.87990100	-2.16555800	1.90178100
O	-3.70287700	-2.31644500	0.94899800
O	-2.91753400	-0.28483800	-2.55454800
C	-1.84297200	0.38782800	-2.60698600
O	-1.01655100	0.56296600	-1.64711000
C	-4.64821300	2.41505500	0.92056900
H	-4.31585100	2.76873200	1.90020100
H	-5.71074000	2.16686600	0.94589500
C	-1.48572300	1.01645200	-3.93633500
H	-0.82167300	0.33238600	-4.47843500
H	-0.95263100	1.95985900	-3.79782400
C	-3.11990200	-2.96765000	3.16234800
H	-4.16918000	-3.26058500	3.23271900
H	-2.81951300	-2.39423900	4.04272500
C	-0.16978100	-4.06721000	-1.74876600
H	-0.79838000	-4.79213300	-2.26821300
H	0.35690200	-4.54381600	-0.91641900
C	0.50371300	0.51091000	1.20978400
C	0.46980800	0.98244100	2.63669900
C	1.68367500	1.15944800	3.32858400
C	-0.73178300	1.24425200	3.30929800
C	1.69688100	1.59105700	4.65288000
H	2.62325800	0.96476300	2.81704200
C	-0.71732900	1.66793600	4.63999700
H	-1.66851200	1.11649800	2.78381600

C	0.49169300	1.84452400	5.31373200
H	2.64340100	1.72225600	5.17040800
H	-1.65707300	1.86138700	5.15065500
H	0.49706700	2.17560300	6.34889200
C	1.35580600	-0.61187900	0.91647900
N	2.24807300	-0.47846400	-0.02829400
S	3.08652300	-1.85067400	-0.59866300
O	2.81022000	-2.98546500	0.29202300
O	2.83774200	-1.93779100	-2.03968700
C	4.78438700	-1.33815500	-0.35457600
C	5.43974700	-1.67899000	0.82972300
C	5.43122400	-0.60677000	-1.35302900
C	6.75839900	-1.26773400	1.01491600
H	4.92663300	-2.26786300	1.58279600
C	6.74893400	-0.20321900	-1.14825900
H	4.91231400	-0.37430300	-2.27700200
C	7.43233300	-0.52547700	0.03419300
H	7.27492900	-1.53270900	1.93407500
H	7.25775100	0.36623500	-1.92212400
C	8.87128900	-0.11113200	0.23021200
H	9.55435400	-0.83922200	-0.22696800
H	9.07585100	0.85996000	-0.23284100
H	9.12865600	-0.04425500	1.29209000
H	-4.49750700	3.22802900	0.20025200
H	-2.38505500	1.16863700	-4.53634400
H	-2.50620100	-3.87561200	3.12629600
H	0.59754600	-3.67562700	-2.42443400
H	1.19997400	-1.54499700	1.45475900
C	0.47893400	4.19988800	-2.23454500
C	-0.56401500	5.00148900	-1.46589800
C	-0.20292200	3.55638400	0.57196200
C	0.70796800	2.74552800	-0.29516500
H	-0.58278600	6.01338600	-1.88143700
H	0.18248400	3.55311500	1.59675300
H	-1.18656700	3.06903400	0.61005200
H	-1.54315100	4.54841900	-1.68571700
C	1.10060500	3.03133000	-1.55249400
C	-0.31318700	4.99297000	0.04305700

H	-1.11593600	5.51973000	0.57026700
H	0.61894600	5.53092400	0.25981100
O	0.74887000	4.46807500	-3.39797000
O	1.26846800	1.62675100	0.34049300
H	1.89981600	0.95214000	-0.23182700
C	2.06348600	2.18662400	-2.34787600
H	2.20343700	2.64780200	-3.32755500
H	3.04478000	2.11216800	-1.86197400
H	1.67847500	1.17046300	-2.49375100

Int3b

Rh	-3.66808800	-0.96460100	-0.66433200
Rh	-1.46531800	-0.37538600	0.11484700
O	-2.24353100	1.47897300	0.62987900
C	-3.47854200	1.71681900	0.41640400
O	-4.31173800	0.91250900	-0.10720700
O	-0.89482600	-2.27709000	-0.42553700
C	-1.73535500	-3.08194300	-0.94363300
O	-2.95832000	-2.81569200	-1.18596000
O	-2.02430600	-1.09942300	1.97076400
C	-3.19085400	-1.59692400	2.12054100
O	-4.08840800	-1.66969500	1.22362700
O	-3.12489200	-0.24615800	-2.51829000
C	-1.94564000	0.19232900	-2.69515800
O	-1.04214700	0.29117000	-1.79732100
C	-3.98432900	3.08741500	0.80818100
H	-3.63767900	3.33860500	1.81460600
H	-5.07386900	3.12219400	0.76204700
C	-1.56875300	0.60510900	-4.09963200
H	-1.18129500	-0.27248100	-4.63074200
H	-0.78606500	1.36670100	-4.08284000
C	-3.51621100	-2.17046500	3.48049300
H	-4.59211100	-2.31831900	3.58671200
H	-3.14128100	-1.51088800	4.26769500
C	-1.23691700	-4.46727200	-1.27318800
H	-1.92387900	-4.96721500	-1.95841800
H	-1.17214900	-5.04746000	-0.34526700
C	1.26963400	0.97991700	0.89673400
C	1.01262900	1.74936700	2.13064100

C	1.80492100	2.87723400	2.42009300
C	0.05170600	1.34010300	3.07326500
C	1.64155900	3.57082400	3.61805900
H	2.56294700	3.20193300	1.71550300
C	-0.09566200	2.03283100	4.27349000
H	-0.59616900	0.49701800	2.86019500
C	0.69265400	3.15181200	4.55225300
H	2.26664200	4.43567000	3.82355100
H	-0.84349400	1.70200300	4.98940900
H	0.56660600	3.69306300	5.48585400
C	1.23895200	-0.38447200	0.81819800
N	1.73679900	-1.06998700	-0.28322200
S	2.32056100	-2.64811700	-0.22651000
O	1.80023100	-3.23314800	1.00836000
O	2.07304900	-3.21855500	-1.55178800
C	4.09686700	-2.47747500	-0.05177400
C	4.65458500	-2.35233600	1.22317200
C	4.90056900	-2.44971100	-1.19348100
C	6.03251600	-2.18914400	1.34576300
H	4.01996000	-2.39940700	2.10180800
C	6.27703500	-2.28582100	-1.04961800
H	4.45282200	-2.57156000	-2.17409600
C	6.86455900	-2.15275300	0.21656000
H	6.47080300	-2.09352100	2.33613200
H	6.90593500	-2.26627700	-1.93617500
C	8.36050800	-2.00781300	0.36429700
H	8.83782900	-2.98729200	0.50107200
H	8.80854000	-1.54790200	-0.52235400
H	8.61996200	-1.39580800	1.23443600
H	-3.57147300	3.83448700	0.12071400
H	-2.44758300	0.96729100	-4.63728900
H	-3.01050800	-3.13699800	3.58788100
H	-0.23048800	-4.40707400	-1.69393200
H	0.98404400	-0.99764700	1.67313000
C	2.30449300	4.73925400	-2.05271600
C	0.85518800	5.21018200	-2.11881800
C	0.15254600	3.29356100	-0.63658000
C	1.58011600	2.82905800	-0.69351200

H	0.86096400	6.29260300	-2.27866000
H	-0.30301500	3.02592400	0.31865400
H	-0.41584100	2.73661200	-1.39487300
H	0.40351100	4.75840700	-3.01614800
C	2.59046900	3.48504200	-1.31735200
C	0.05727800	4.80375300	-0.87840500
H	-0.99395000	5.09620500	-0.98306300
H	0.44991800	5.33337900	-0.00045900
O	3.19406200	5.36379400	-2.61918300
O	1.90279000	1.59011900	-0.17344500
H	1.89441500	-0.56170700	-1.14609200
C	4.00682900	2.96980600	-1.34883500
H	4.68717800	3.79852000	-1.55665100
H	4.28519600	2.48907500	-0.40643800
H	4.14445000	2.22689500	-2.14618200
TS3b			
Rh	3.83852900	-1.05433000	0.05214700
Rh	1.61921200	-0.07560100	-0.14913600
O	2.51771400	1.54452400	-1.05312900
C	3.78487300	1.55236300	-1.20546600
O	4.58869600	0.63646800	-0.84649100
O	0.90922800	-1.77744800	0.80707600
C	1.71611600	-2.71943000	1.14447100
O	2.96293600	-2.70605700	0.94928200
O	1.49948400	-0.97477000	-2.00799100
C	2.46575400	-1.70004400	-2.41775000
O	3.55231400	-1.92006700	-1.79645300
O	3.99524700	-0.13371900	1.89283900
C	3.02813800	0.57173900	2.31838500
O	1.91730700	0.76689500	1.71986900
C	4.37980800	2.75616500	-1.90230000
H	4.57728900	2.49958800	-2.94980000
H	5.33337200	3.02226100	-1.43944300
C	3.21622400	1.27464400	3.64487000
H	3.92196500	0.72412000	4.27037200
H	2.25757100	1.39264500	4.15487500
C	2.28249300	-2.36474700	-3.76392900
H	1.99357600	-1.61805800	-4.50991600

H	1.46719000	-3.09300100	-3.69548700
C	1.11227800	-3.90924500	1.85216200
H	1.10038800	-3.71174000	2.93100800
H	1.71987700	-4.79902700	1.67575400
C	-0.70044000	1.72554600	0.25911000
C	-0.32294300	3.04785300	-0.25868800
C	-0.42038200	4.16455700	0.58991900
C	0.08158100	3.23081800	-1.59193500
C	-0.12254800	5.43770300	0.11210400
H	-0.74041400	4.01801100	1.61551900
C	0.37055100	4.50755500	-2.06675900
H	0.18262100	2.37750900	-2.25328400
C	0.27103200	5.61319600	-1.21751600
H	-0.20299500	6.29470800	0.77490100
H	0.67626500	4.63985000	-3.10092300
H	0.49802400	6.60804700	-1.59130400
C	-0.64742300	0.49880300	-0.43448600
N	-1.41996900	-0.46471100	0.36655200
S	-2.32802000	-1.84721300	-0.54001100
O	-1.45664400	-2.12822000	-1.67614600
O	-2.51524300	-2.79215800	0.56073900
C	-3.89802900	-1.30574400	-1.15522300
C	-3.97568100	-0.85592800	-2.47685300
C	-5.03184900	-1.41375100	-0.34445400
C	-5.22188500	-0.49333200	-2.98210600
H	-3.08701000	-0.81453200	-3.09647300
C	-6.26171200	-1.03706700	-0.86976300
H	-4.95332800	-1.77985200	0.67041500
C	-6.37634700	-0.56724900	-2.18876200
H	-5.29794800	-0.14717500	-4.00917300
H	-7.14226100	-1.09512600	-0.23708200
C	-7.71956400	-0.14471700	-2.72980700
H	-8.07792700	0.75537500	-2.21501400
H	-7.67288500	0.07535200	-3.80034700
H	-8.47289000	-0.92547300	-2.57368300
H	3.68767400	3.59951900	-1.86917900
H	3.62741000	2.27403500	3.45918700
H	3.20003900	-2.86836300	-4.07194100

H	0.08369600	-4.07088100	1.52163500
H	-0.72230900	0.39608000	-1.50984800
C	-4.56070800	0.51130000	2.36752300
C	-4.17386600	-0.14523200	3.69802600
C	-1.83213500	-0.39434100	2.88423700
C	-2.21994900	0.32182500	1.60797600
H	-4.84806700	0.25524200	4.46175600
H	-0.76823800	-0.21648400	3.07449100
H	-1.96699500	-1.47527200	2.74104800
H	-4.38664800	-1.22357100	3.62933000
C	-3.52120000	0.76757000	1.38688400
C	-2.70356900	0.07065600	4.05238000
H	-2.42857200	-0.48111200	4.95946200
H	-2.51573400	1.13354800	4.24833800
O	-5.75190500	0.77926800	2.16012600
O	-1.15648300	1.63657100	1.47136500
H	-0.74746300	-1.09491800	0.84909300
C	-3.87607800	1.64693300	0.21066500
H	-3.46370100	2.65807400	0.33380700
H	-3.51459800	1.27411200	-0.75433900
H	-4.96365500	1.73112300	0.15889200

Int4b-2w

Rh	-4.28036800	-0.40079600	-1.08612200
Rh	-2.53519200	0.02463000	0.51119000
O	-4.00619700	0.03258800	1.97302900
C	-5.22075400	-0.16299700	1.63804700
O	-5.64340500	-0.35994600	0.45454500
O	-1.20766800	-0.02507500	-1.07690900
C	-1.64563200	-0.23978100	-2.25836100
O	-2.86508800	-0.42863800	-2.56787300
O	-2.33484600	-2.02339600	0.73140400
C	-3.08512000	-2.79230000	0.04105500
O	-3.98461800	-2.41667900	-0.77470300
O	-4.48356700	1.63115600	-1.31826400
C	-3.73814700	2.40481200	-0.63387400
O	-2.84035900	2.03881300	0.19347100
C	-6.24301000	-0.19323000	2.75164900

H	-5.95972900	0.50046400	3.54664200
H	-6.27479600	-1.20325000	3.17728900
C	-3.96059900	3.89132200	-0.79379400
H	-4.30518200	4.11606200	-1.80551500
H	-3.04501900	4.44111700	-0.56646300
C	-2.86126100	-4.28042900	0.18358800
H	-2.10085800	-4.59380000	-0.54176700
H	-3.78297200	-4.82475900	-0.03177000
C	-0.62618900	-0.27658500	-3.37088600
H	-1.11909700	-0.41835700	-4.33379500
H	0.08547700	-1.08964500	-3.19188800
C	1.97043200	0.70334200	0.61706600
C	0.89095100	0.99152400	1.57576700
C	0.79539100	2.24213400	2.20119700
C	-0.05722200	-0.00090100	1.92458900
C	-0.22800900	2.51409700	3.11749500
H	1.52078300	3.01663600	1.97604400
C	-1.06916700	0.27042400	2.85067400
H	0.03933700	-1.00694700	1.53174600
C	-1.16391200	1.54065700	3.44362900
H	-0.27878600	3.49656700	3.57893600
H	-1.74053700	-0.52381900	3.15952500
H	-1.95329500	1.74649700	4.15982900
S	3.18168400	-2.04996600	-1.88403200
O	1.86861400	-2.60341900	-2.22519800
O	4.24088300	-1.86193400	-2.88166600
C	3.85185200	-3.04910700	-0.55279800
C	2.99103800	-3.76489100	0.28018800
C	5.23303600	-3.05615100	-0.32997400
C	3.52242400	-4.48407500	1.35133800
H	1.92481000	-3.77272100	0.08037100
C	5.74561500	-3.78013400	0.74514200
H	5.89353400	-2.52290400	-1.00571100
C	4.90065400	-4.50370000	1.60345100
H	2.85276900	-5.04392800	1.99918100
H	6.81998200	-3.79703500	0.91224700
C	5.47150100	-5.31181700	2.74376800
H	5.82564200	-6.28912700	2.39034600

H	6.32577700	-4.80597400	3.20608300
H	4.72233000	-5.49585200	3.51995600
H	-7.23455400	0.04949600	2.36463300
H	-4.73823400	4.21043400	-0.08968300
H	-2.49887200	-4.51890700	1.18608000
H	-0.05815000	0.65932300	-3.37790300
C	4.51681000	4.82186000	-0.00134400
C	3.89984500	5.05034000	-1.37574400
C	2.52181500	2.95425800	-1.13027600
C	3.29144300	2.70450600	0.13606100
H	3.90778700	6.12594000	-1.57504800
H	1.50262000	2.56329500	-1.03074500
H	2.99911200	2.38218000	-1.93964800
H	4.56242300	4.57733300	-2.11666700
C	4.18082700	3.55730600	0.69884600
C	2.49696000	4.44733100	-1.47907300
H	2.09019600	4.58360700	-2.48722400
H	1.82188200	4.96959800	-0.78830400
O	5.28703900	5.63788400	0.48961700
O	3.14330100	1.46749400	0.75260600
C	4.89489400	3.26649200	1.99500600
H	5.28997600	4.20054800	2.40006900
H	4.22609300	2.80315300	2.72739800
H	5.74363000	2.58609000	1.84682800
C	1.93660900	-0.27721800	-0.30777500
H	1.04798100	-0.88580900	-0.41539100
N	2.93776900	-0.52188700	-1.23988300
H	3.77922500	0.08496000	-1.32394600
O	5.76420300	0.07868200	0.86235900
H	5.62125000	-0.86173500	1.05610900
H	4.91024500	0.51058400	1.05775500
O	5.33697300	0.79023400	-1.76488600
H	5.77164200	0.53122700	-0.91933600
H	5.55390200	0.09498200	-2.40887000
TS3b-2w			
Rh	4.14641300	-0.19536700	-1.37706600
Rh	2.59589600	-0.08504700	0.46030500

O	4.21865600	0.37919300	1.67177900
C	5.38094900	0.45999700	1.15492000
O	5.66469400	0.27538400	-0.07083200
O	1.10091800	-0.54740900	-0.89717200
C	1.40932300	-0.75702400	-2.11808500
O	2.57959400	-0.66967500	-2.61181900
O	2.34645700	1.92897500	0.04011900
C	2.99796000	2.43457200	-0.93304700
O	3.80291700	1.81416100	-1.69644100
O	4.41221800	-2.19030700	-0.96710400
C	3.75675400	-2.70826300	-0.00479700
O	2.94410000	-2.09568000	0.76080200
C	6.51547100	0.82848400	2.08484700
H	6.42216500	1.88437500	2.36319600
H	7.47837800	0.67102700	1.59633000
C	3.94184400	-4.19019200	0.23105000
H	4.96117900	-4.48732600	-0.02593400
H	3.25270600	-4.74270900	-0.41820100
C	2.80461200	3.90975000	-1.20931700
H	2.47697800	4.04818000	-2.24453300
H	3.76252800	4.42832300	-1.09821700
C	0.29765500	-1.17173100	-3.05166200
H	0.61368700	-1.05719800	-4.09010900
H	-0.60695400	-0.59119500	-2.85839100
C	-2.08731800	-0.89308800	1.59414900
C	-0.74146700	-0.81713700	2.25646600
C	-0.35420100	-1.86253500	3.10234300
C	0.11677700	0.29036600	2.12219900
C	0.86810200	-1.82562100	3.78168400
H	-1.03390200	-2.70025200	3.22011200
C	1.33550200	0.33960600	2.81253000
H	-0.18604100	1.13812300	1.51607500
C	1.71351700	-0.72929500	3.64496000
H	1.15205600	-2.65502000	4.42432400
H	1.94188400	1.23949500	2.77723100
H	2.66035600	-0.68858300	4.17486500
N	-3.64751300	-0.17767900	-0.14784200
S	-3.71425200	0.99199300	-1.53436600

O	-2.59728500	0.68626900	-2.43302000
O	-5.09604600	0.95772600	-2.00750400
C	-3.39768800	2.57066000	-0.75388600
C	-2.09324000	3.07576600	-0.72207400
C	-4.47338600	3.31010900	-0.25770900
C	-1.87111900	4.32830300	-0.15819500
H	-1.27463200	2.50321000	-1.14325200
C	-4.22651700	4.56252000	0.30531400
H	-5.48208100	2.91752600	-0.31886000
C	-2.92891500	5.08882100	0.36768100
H	-0.85939200	4.72508200	-0.13060200
H	-5.05959600	5.14372600	0.69131700
C	-2.66551600	6.44604500	0.97424300
H	-1.97202600	6.37410800	1.82083900
H	-2.20922500	7.12297300	0.24190500
H	-3.58820900	6.91153800	1.33233800
H	6.45396300	0.23729800	3.00286300
H	3.71694200	-4.44337000	1.26896300
H	2.07315000	4.34133900	-0.52375000
H	0.06338400	-2.22753600	-2.86974300
C	-5.89344500	-3.20086600	-0.88836500
C	-4.88069300	-4.14153000	-1.52473100
C	-3.11064900	-2.39791200	-1.24624900
C	-4.13792300	-1.50385700	-0.59565300
H	-5.21387300	-5.16619400	-1.33309100
H	-2.12485300	-2.17063800	-0.83395900
H	-3.06268300	-2.16566200	-2.32151500
H	-4.93786700	-3.98834600	-2.61417100
C	-5.43617000	-1.84562200	-0.42711900
C	-3.45655300	-3.87332900	-1.04045700
H	-2.74014000	-4.50843200	-1.57402500
H	-3.37129100	-4.10667600	0.02799800
O	-7.06457500	-3.53275400	-0.77213100
O	-2.96981800	-1.68484200	2.12034200
C	-6.50548500	-1.01248800	0.23161900
H	-7.48091000	-1.35500700	-0.11889600
H	-6.48755500	-1.15650500	1.31984300
H	-6.40618200	0.05049400	0.01317500

C	-2.30083400	-0.15479000	0.45408400
H	-4.36381100	0.39821600	0.88240800
H	-1.49435400	0.23695000	-0.14738600
O	-4.74635100	0.99502600	1.80749100
H	-3.99097400	1.57286300	2.01811800
H	-4.83862800	0.27102900	2.64286400
O	-4.80150400	-0.76450100	3.50796800
H	-4.00284400	-1.26123300	3.03001400
H	-4.50049400	-0.52436200	4.39857000

Int5b-2w

Rh	4.31282600	-0.31084600	-1.32749600
Rh	2.71027100	0.23283700	0.37672000
O	4.27671900	1.07070100	1.45028400
C	5.45287000	1.04628300	0.95788900
O	5.77874300	0.54162800	-0.16256000
O	1.27264000	-0.63573800	-0.83265800
C	1.61430700	-1.12706000	-1.96134600
O	2.79740300	-1.14150800	-2.42987200
O	2.40271900	2.03806100	-0.58428000
C	3.05677500	2.28466200	-1.65280400
O	3.92219600	1.52141100	-2.18678700
O	4.61899700	-2.11180400	-0.38368800
C	3.95489300	-2.37269200	0.67149000
O	3.10492000	-1.60335500	1.22825300
C	6.54815300	1.68917400	1.77835800
H	6.38991100	2.77308200	1.80492700
H	7.52675900	1.47780800	1.34483400
C	4.17093800	-3.72868900	1.30321100
H	5.17122900	-4.10055500	1.07232000
H	3.43797700	-4.43203800	0.89044700
C	2.75109200	3.58511700	-2.35933400
H	1.88416900	3.43524100	-3.01379200
H	3.59899600	3.89277000	-2.97425100
C	0.52404400	-1.74716100	-2.80039300
H	0.92017800	-2.05719700	-3.76854700
H	-0.29553500	-1.03410000	-2.93319000
C	-1.90340500	-0.32048200	1.58585700

C	-0.64191300	0.01926000	2.28907800
C	-0.29858900	-0.63766200	3.47976800
C	0.21087800	1.03412500	1.80881400
C	0.87385600	-0.30901100	4.16833400
H	-0.94764500	-1.41961300	3.86293100
C	1.37595500	1.37354500	2.50651600
H	-0.05854100	1.58508900	0.91368900
C	1.71153500	0.69347000	3.68914100
H	1.12514300	-0.84103300	5.08165300
H	1.98208700	2.20889400	2.17147000
H	2.61968900	0.95744200	4.22211000
N	-3.19724600	-0.69547300	-0.43682100
S	-3.46641300	0.18885900	-1.89372100
O	-2.15665300	0.48475700	-2.49251800
O	-4.49602300	-0.52317400	-2.64845100
C	-4.13780100	1.75024600	-1.32327800
C	-3.28332200	2.72026100	-0.79201800
C	-5.51044200	1.98399000	-1.42810300
C	-3.82557300	3.92063200	-0.32815100
H	-2.21321400	2.54754100	-0.76206000
C	-6.03144600	3.19252100	-0.97072800
H	-6.15287500	1.22985900	-1.86820700
C	-5.20487200	4.17383800	-0.40326000
H	-3.16377700	4.68060400	0.08015200
H	-7.09937800	3.37632000	-1.05544100
C	-5.78924600	5.46391200	0.12011100
H	-5.02022900	6.23227400	0.24565400
H	-6.55658600	5.85647600	-0.55579600
H	-6.26676200	5.30920900	1.09632400
H	6.50375700	1.32373900	2.80849200
H	4.01879800	-3.67370300	2.38333500
H	2.49894400	4.36276600	-1.63450800
H	0.11976900	-2.61998600	-2.27574900
C	-5.54521800	-3.67407300	-0.13933800
C	-4.57104100	-4.79530000	-0.46978400
C	-2.69299300	-3.13580500	-0.54113100
C	-3.71474600	-2.03683600	-0.34213000
H	-4.97106800	-5.72337900	-0.05047100

H	-1.74396600	-2.83456000	-0.08504200
H	-2.49955700	-3.22955900	-1.62263100
H	-4.56155900	-4.91417800	-1.56458200
C	-5.02997200	-2.27272600	-0.11779000
C	-3.15970000	-4.47739300	0.02638200
H	-2.45980800	-5.27133300	-0.25843800
H	-3.15887700	-4.42525200	1.12305700
O	-6.72683900	-3.90738300	0.07881600
C	-6.06824000	-1.21761000	0.13214000
H	-6.66117100	-1.03845300	-0.77314300
H	-6.76478200	-1.56301100	0.90077200
H	-5.62321300	-0.27114000	0.44376300
C	-1.98255700	-0.35665700	0.23807400
H	-4.40381800	0.78527800	2.00563500
H	-1.09495800	-0.19531000	-0.36133300
O	-4.67945300	1.67325200	2.30538100
H	-4.36801800	2.27210800	1.60725100
H	-3.74688200	1.48002600	3.86951600
O	-3.14511200	0.96539000	4.46083500
H	-2.33580800	1.49445500	4.53346600
O	-2.97508700	-0.67004000	2.35192200
H	-2.91211700	-0.22843300	3.24675500

TS4b-2w

Rh	4.22880800	-0.05197200	-1.39279200
Rh	2.65175200	0.13713000	0.41119800
O	4.24517700	0.71392500	1.61786100
C	5.41522500	0.77115100	1.11524500
O	5.71912700	0.51552500	-0.09258900
O	1.19244000	-0.44327900	-0.93132800
C	1.51431600	-0.70012200	-2.14075000
O	2.68922900	-0.61279000	-2.62396500
O	2.36213800	2.11105700	-0.13975300
C	3.01280600	2.57051800	-1.13738400
O	3.85975600	1.92724100	-1.83323700
O	4.51403800	-2.01795000	-0.86499000
C	3.86672200	-2.48572500	0.12710100
O	3.03112900	-1.84336400	0.84350800

C	6.54451400	1.14771200	2.04791500
H	6.20848400	1.89889700	2.76695200
H	7.40108900	1.51627400	1.48057600
C	4.13536200	-3.92309100	0.51029000
H	4.49280500	-4.48657500	-0.35381000
H	3.23306000	-4.38024700	0.92264900
C	2.72758800	3.99754800	-1.54722000
H	1.90999000	3.99796900	-2.27798600
H	3.60718100	4.43852300	-2.02079500
C	0.41372200	-1.16133800	-3.06331000
H	0.77252900	-1.19465300	-4.09333800
H	-0.45517900	-0.50264800	-2.97852600
C	-1.91547200	-0.85096700	1.55163800
C	-0.60236500	-0.57642300	2.24105800
C	-0.19581300	-1.46711500	3.24253500
C	0.19670500	0.55675200	1.98547500
C	0.98365600	-1.25270000	3.96503200
H	-0.81943500	-2.33332300	3.43991500
C	1.36375900	0.78731000	2.72486200
H	-0.10872000	1.28527400	1.24156800
C	1.76192000	-0.12738200	3.71573200
H	1.28637200	-1.96799500	4.72513700
H	1.92454300	1.70482500	2.57803000
H	2.67449200	0.05122000	4.27595000
N	-3.36745400	-0.52330000	-0.41708300
S	-3.64690300	0.50346100	-1.75584400
O	-2.37344800	0.75437500	-2.45168700
O	-4.79283600	-0.03906200	-2.48438500
C	-4.11716100	2.06551000	-1.00475500
C	-3.14048200	3.03001300	-0.75028300
C	-5.45687500	2.30187900	-0.68903000
C	-3.51180700	4.22963900	-0.13728000
H	-2.11219600	2.84708500	-1.04326600
C	-5.81152600	3.50702700	-0.08809500
H	-6.20587500	1.55145100	-0.91505300
C	-4.84890900	4.48746300	0.20217300
H	-2.75520700	4.98709900	0.05493400
H	-6.85427800	3.69280000	0.15713200

C	-5.25421200	5.80350500	0.82315500
H	-4.39669900	6.32431000	1.26093900
H	-5.69332200	6.47073300	0.07019700
H	-6.00694400	5.66374700	1.60683400
H	6.85349000	0.25794700	2.60915400
H	4.91215200	-3.94508800	1.28386900
H	2.41825900	4.59030800	-0.68350900
H	0.09666700	-2.16620900	-2.76093300
C	-5.54330200	-3.63236400	-0.48801200
C	-4.53746100	-4.64015000	-1.02820200
C	-2.75164100	-2.88371700	-0.98025300
C	-3.80308900	-1.89304800	-0.53689000
H	-4.86456600	-5.63775400	-0.71919700
H	-1.78118200	-2.59604800	-0.56305900
H	-2.64894500	-2.81156100	-2.07586200
H	-4.59572800	-4.60963700	-2.12765500
C	-5.08827800	-2.22917800	-0.27471200
C	-3.11164200	-4.31505900	-0.57799300
H	-2.39670100	-5.02413300	-1.01149900
H	-3.03940400	-4.40345500	0.51345600
O	-6.69940500	-3.96042900	-0.25144400
C	-6.12874200	-1.27208900	0.23226200
H	-6.79409300	-1.78916700	0.92860100
H	-5.66396200	-0.41735900	0.72963100
H	-6.75217200	-0.90330600	-0.59201700
H	-2.90888400	0.92978600	1.35021600
O	-3.58035600	1.44135000	2.04662700
H	-3.37722300	2.39272200	2.05497900
H	-3.50963400	0.91426900	3.03884700
O	-3.42846600	0.02755800	4.03197700
H	-2.62274000	0.16162800	4.55902100
O	-2.76957200	-1.57309000	2.17247000
H	-3.21546200	-0.79229200	3.43382200
C	-2.17364800	-0.19674100	0.33538000
H	-1.32996600	0.15873700	-0.24773700
Int4b-2w'			
C	0.83292600	1.08362900	-0.29384300
C	1.65120400	2.24035300	0.10505400

C	2.30715400	2.25996100	1.34900300
C	1.79090900	3.35642800	-0.74197600
C	3.05767700	3.36719300	1.73946700
H	2.21630300	1.40852200	2.01438700
C	2.53010800	4.46652000	-0.34110100
H	1.33805600	3.34277200	-1.72907400
C	3.16859700	4.47783600	0.90108900
H	3.55456600	3.36208200	2.70591100
H	2.62438400	5.31707000	-1.01085000
H	3.75587100	5.33905800	1.20715900
S	-2.51474000	0.06269700	-2.02494000
O	-2.78714300	1.35551100	-2.65325400
O	-2.75657100	-1.21693300	-2.70120800
C	-3.41312700	0.02522900	-0.46981900
C	-3.64569700	1.21285700	0.22567000
C	-3.83263900	-1.20160600	0.05294800
C	-4.28950500	1.16386200	1.46145300
H	-3.34095900	2.16182300	-0.20263200
C	-4.47633900	-1.23153400	1.28987800
H	-3.67550800	-2.11154900	-0.51666500
C	-4.71284900	-0.05246400	2.01473000
H	-4.47049100	2.08889600	2.00303300
H	-4.81370100	-2.18394300	1.69191200
C	-5.44029900	-0.09190600	3.33684300
H	-6.52640200	-0.03444900	3.18670200
H	-5.23640600	-1.02031800	3.88010300
H	-5.15485900	0.74875500	3.97699300
C	3.96308100	-2.48597300	0.73291800
C	4.46104800	-2.53581000	-0.70612800
C	2.83775800	-0.71997600	-1.34626500
C	2.29902000	-0.82169600	0.05332900
H	5.50099100	-2.87487100	-0.69107600
H	2.75180200	0.31041100	-1.70716600
H	2.19741500	-1.33366000	-1.99833100
H	3.87647500	-3.30862900	-1.22856600
C	2.80708300	-1.60250700	1.03474900
C	4.29343500	-1.19256600	-1.41889100
H	4.60639400	-1.26852100	-2.46604300

H	4.93951500	-0.44272400	-0.94421100
O	4.47697100	-3.17785500	1.60283900
O	1.11365300	-0.14494800	0.32699200
C	2.23094700	-1.68126800	2.42553900
H	3.00323100	-2.03337500	3.11269000
H	1.85205400	-0.71294500	2.76685900
H	1.39751900	-2.39366000	2.47253000
C	-0.21434800	1.14012400	-1.14226000
H	-0.56342000	2.09582000	-1.51676600
N	-0.88743400	0.02809100	-1.63234900
H	-0.50910600	-0.93461500	-1.52391200
O	-0.86412200	-2.22733800	1.10602200
H	-1.74852900	-1.86772400	1.28298400
H	-0.28268100	-1.44536100	1.04898700
O	-0.24675600	-2.68790200	-1.53987200
H	-0.54080800	-2.80749300	-0.60716400
H	-1.02896200	-2.86557100	-2.08880600
TS3b-2w'			
C	0.46086200	1.79602200	0.25424600
C	-0.05084600	3.18006700	-0.02421100
C	0.72282100	4.27045500	0.40000600
C	-1.27329600	3.43363400	-0.66649400
C	0.29900600	5.57823100	0.16818200
H	1.65977500	4.06525800	0.90755200
C	-1.69780400	4.74101800	-0.89935800
H	-1.90558100	2.60144000	-0.96387000
C	-0.91154300	5.81917900	-0.48515800
H	0.91490500	6.41182100	0.49664500
H	-2.64883300	4.91977400	-1.39512600
H	-1.24414100	6.83835800	-0.66432800
N	0.52242000	-0.59583700	-0.19004600
S	-0.37426400	-1.85238200	-1.14624600
O	-0.33841000	-1.45354500	-2.55575900
O	0.16982700	-3.13468200	-0.70302300
C	-2.06307900	-1.70658300	-0.56569000
C	-2.96572900	-0.90221700	-1.26767900
C	-2.47588000	-2.47048400	0.52851600
C	-4.28983300	-0.84469400	-0.84275900

H	-2.63613800	-0.35052700	-2.14058900
C	-3.80631100	-2.39551300	0.93919700
H	-1.77090000	-3.11482500	1.04162900
C	-4.73123200	-1.58573500	0.26485400
H	-4.99519200	-0.21961600	-1.38443500
H	-4.13252500	-2.98680800	1.79080500
C	-6.17742000	-1.53672900	0.69400400
H	-6.58255400	-0.52176600	0.62160800
H	-6.79542500	-2.17834400	0.05259700
H	-6.30350300	-1.88323200	1.72411800
C	4.16677500	-1.70533600	0.26137800
C	4.78123800	-1.13214700	-1.00608500
C	2.55431700	-0.19000400	-1.65000600
C	1.97788900	-0.79692100	-0.39341900
H	5.84285900	-0.95391700	-0.80981000
H	1.99932500	0.71927100	-1.89342900
H	2.39682000	-0.88290100	-2.49072500
H	4.72699200	-1.91733200	-1.77667800
C	2.69974200	-1.49889900	0.50908000
C	4.04429300	0.11583800	-1.48912800
H	4.46121700	0.46919000	-2.43900600
H	4.16371600	0.92544100	-0.75823300
O	4.84773500	-2.34617100	1.04923100
O	1.34788600	1.65150400	1.18801700
C	2.18192800	-2.08652700	1.79604900
H	2.90663600	-2.81390900	2.16577300
H	2.08361300	-1.30560300	2.56060700
H	1.21762000	-2.58157300	1.67298100
C	0.01134800	0.74739600	-0.51594000
H	0.05689500	-0.69832500	1.12656500
H	-0.47247300	0.87060600	-1.47354700
O	-0.54802700	-0.66179500	2.11495500
H	-1.39223300	-0.26060400	1.84295500
H	-0.06384300	0.04978400	2.80480000
O	0.64582200	1.00798100	3.46730400
H	1.00648200	1.45468200	2.58799800
H	0.09562100	1.66599100	3.92011300

Int5b-2w'

C	1.72904600	-0.57584400	0.08466100
C	3.19140600	-0.49613400	-0.15561500
C	4.08434800	-1.15461500	0.70787400
C	3.71707200	0.23757300	-1.23343300
C	5.46057800	-1.08906400	0.49189600
H	3.69595700	-1.73511600	1.53916400
C	5.09175700	0.29584300	-1.45026500
H	3.04339000	0.77539700	-1.89411700
C	5.96975300	-0.36612800	-0.58799800
H	6.13447600	-1.61085900	1.16589300
H	5.47937300	0.86923000	-2.28797700
H	7.04202500	-0.31542700	-0.75541200
N	-0.57254500	-0.69090600	-0.69271800
S	-1.53126300	0.30009800	-1.73746200
O	-0.80106100	0.45326000	-3.00159500
O	-2.89295400	-0.23120900	-1.70263000
C	-1.52256600	1.90467900	-0.93398900
C	-0.41677800	2.74531700	-1.07906300
C	-2.63212300	2.30370800	-0.18614300
C	-0.41633500	3.98399100	-0.43428700
H	0.41834300	2.44361100	-1.70148300
C	-2.61798500	3.54653200	0.44203500
H	-3.49237800	1.64856400	-0.10929500
C	-1.51059400	4.40194700	0.33952300
H	0.43932700	4.64462300	-0.55123200
H	-3.48285000	3.85844500	1.02192900
C	-1.49975400	5.73428300	1.04943000
H	-0.69340800	6.37795500	0.68506400
H	-2.44771700	6.26580100	0.91140300
H	-1.35822600	5.60176600	2.12960700
C	-2.67344100	-3.31439200	1.08747000
C	-2.32013400	-4.53215000	0.24735000
C	-0.64444600	-3.16404900	-1.02120200
C	-1.12562200	-1.94935600	-0.25748600
H	-2.52216400	-5.42506200	0.84650700
H	0.41768300	-3.04450900	-1.25931400
H	-1.17434900	-3.19036000	-1.98751000
H	-3.01212200	-4.55500000	-0.60897200

C	-2.03583000	-2.00865700	0.74392700
C	-0.87800700	-4.46820400	-0.25678800
H	-0.65288400	-5.32682400	-0.89954100
H	-0.18877700	-4.51627400	0.59667400
O	-3.48143000	-3.39097100	2.00360200
C	-2.51148300	-0.83822800	1.55431800
H	-3.51524400	-0.53176500	1.23518000
H	-2.59435000	-1.12855500	2.60524300
H	-1.84491400	0.02074100	1.46627700
C	0.83329500	-0.59116400	-0.92719000
H	0.16797100	0.91888600	1.90411600
H	1.16824400	-0.57307900	-1.95673400
O	0.23994600	1.81219000	2.29286600
H	0.12498600	2.41229400	1.53815900
H	1.90819600	1.44641100	2.95169500
O	2.68176200	0.83995100	3.05244200
H	3.41372100	1.27485200	2.58901500
O	1.30746400	-0.71939800	1.37068500
H	1.97096400	-0.31689100	2.00095900

TS4b-2w'

C	1.54517900	0.99154800	0.20405300
C	2.20134500	2.31654300	-0.10675600
C	3.36179500	2.64709000	0.61184400
C	1.71145500	3.24012600	-1.04616600
C	4.01975500	3.85754700	0.39267700
H	3.74237600	1.92767500	1.32998100
C	2.36580500	4.45170100	-1.26138700
H	0.80677500	3.02159300	-1.60571200
C	3.52362300	4.76532800	-0.54418900
H	4.92347000	4.08900400	0.95056700
H	1.96959100	5.15469300	-1.98952100
H	4.03354600	5.70937700	-0.71618200
N	0.05794200	-0.83991800	-0.50577100
S	-1.30379000	-1.19500400	-1.48598100
O	-1.10397500	-0.62902700	-2.82881300
O	-1.59165200	-2.61900800	-1.31362400
C	-2.62548200	-0.24369500	-0.72603000
C	-2.95617400	1.00971900	-1.24227000

C	-3.31186000	-0.77035800	0.36978600
C	-3.96441500	1.75589700	-0.62643200
H	-2.43868600	1.38300600	-2.11953400
C	-4.32034000	-0.01849200	0.96625000
H	-3.05539900	-1.75445100	0.74585300
C	-4.66133800	1.25534900	0.48386600
H	-4.23141800	2.72953900	-1.03134900
H	-4.85554200	-0.42721600	1.81973700
C	-5.78200100	2.04436400	1.11851900
H	-6.75727700	1.70188000	0.74899300
H	-5.79075000	1.92592300	2.20737400
H	-5.70402800	3.11214300	0.89023100
C	1.70021500	-3.96183000	0.89114400
C	2.77194700	-4.18656400	-0.16649000
C	2.10932900	-2.04828500	-1.29648200
C	0.98226800	-1.93099500	-0.29732100
H	3.56803700	-4.78678600	0.28454000
H	2.44140900	-1.04692300	-1.59034900
H	1.71327500	-2.51749700	-2.21206300
H	2.32367100	-4.79587300	-0.96694200
C	0.79912500	-2.78363200	0.73716000
C	3.28046800	-2.86559000	-0.74758600
H	4.01983700	-3.04803600	-1.53601700
H	3.78104900	-2.28719700	0.03979600
O	1.56476000	-4.73933100	1.82725500
C	-0.28183000	-2.63720600	1.76915500
H	0.08510100	-2.98761400	2.73715500
H	-0.60239100	-1.59598600	1.84690900
H	-1.15064000	-3.25681100	1.51226400
H	-0.47921600	1.25655500	0.42483000
O	-1.04295800	1.51862700	1.31725200
H	-1.76482700	2.12674300	1.08285000
H	-0.32136100	1.87765200	2.10165800
O	0.70935800	2.03792100	2.93312200
H	1.14523000	2.89455800	2.78934800
O	1.83222500	0.43262000	1.31635100
H	1.32720400	1.35425100	2.46160000
C	0.57041800	0.50213400	-0.68357400

H	0.54822300	0.88065800	-1.70090300
1bb + 2H₂O			
C	0.57719300	1.59391300	0.30348700
C	0.71296900	3.03908700	-0.04816700
C	1.34025300	3.88598000	0.88156300
C	0.22655900	3.57740600	-1.24990100
C	1.49060900	5.24281500	0.60956200
H	1.71866700	3.45712300	1.80445000
C	0.36648600	4.93922700	-1.51285900
H	-0.29661900	2.94776500	-1.96087700
C	1.00227200	5.77139000	-0.58908100
H	1.99004000	5.88808900	1.32697300
H	-0.02632600	5.35180400	-2.43764900
H	1.11596200	6.83098400	-0.80159700
N	0.57158100	-0.78328100	-0.42631100
S	-0.39196200	-1.92824400	-1.28466100
O	-0.46256300	-1.55805800	-2.70637100
O	0.10572200	-3.24557700	-0.88590600
C	-2.02198500	-1.66760600	-0.58257800
C	-3.04793600	-1.20199300	-1.40293500
C	-2.25893000	-1.98274500	0.75877600
C	-4.32670700	-1.03888300	-0.86449000
H	-2.84290600	-0.97338200	-2.44304000
C	-3.53709600	-1.81082300	1.27866900
H	-1.45382900	-2.35340400	1.38296500
C	-4.59171600	-1.33794100	0.47868200
H	-5.13003900	-0.67820700	-1.50190400
H	-3.72314100	-2.04842700	2.32307200
C	-5.97806700	-1.17977500	1.05509800
H	-6.63344500	-0.62310700	0.37873500
H	-6.44063500	-2.15844600	1.23598700
H	-5.95293300	-0.65308100	2.01571700
C	3.66850000	-2.33096700	1.13480600
C	4.60054900	-2.32375800	-0.06613600
C	2.89685800	-1.02984100	-1.38159100
C	1.94217100	-1.20161500	-0.21825800
H	5.62889600	-2.38939400	0.30130800
H	2.70543000	-0.08297400	-1.89865800

H	2.67739200	-1.81755900	-2.11985500
H	4.40190900	-3.24186000	-0.64063700
C	2.28494100	-1.78550300	0.95382800
C	4.36536500	-1.10106200	-0.95441700
H	5.01304400	-1.13405500	-1.83776400
H	4.62765100	-0.19031000	-0.39939800
O	4.02035200	-2.80116300	2.20704000
C	1.34887000	-1.97880200	2.11230900
H	1.90903800	-1.92739000	3.04905400
H	0.56434000	-1.22231400	2.10270900
H	0.89266200	-2.97665200	2.06642200
O	-2.52614000	1.98983800	-0.13863900
H	-3.15277500	1.25203400	-0.09112500
H	-2.34571000	2.21396800	0.80158200
O	-1.68006400	2.58320400	2.50255200
H	-1.40426700	3.51052700	2.43801400
O	0.63968400	1.22676900	1.47117000
H	-0.84052900	2.08725800	2.43931900
C	0.32950700	0.60212400	-0.83086800
H	-0.73723300	0.72957700	-1.05723500
H	0.88576200	0.89244300	-1.72959100

Int2c

Rh	-3.75636100	0.46022100	-0.93776400
Rh	-1.78864500	-0.53953900	0.15530800
O	-1.77479900	1.11507400	1.39927200
C	-2.61528500	2.05991100	1.20137500
O	-3.54747400	2.06952700	0.34639200
O	-1.98710700	-2.10098100	-1.18969200
C	-2.93368100	-2.08716400	-2.05344200
O	-3.82141100	-1.19344800	-2.17220200
O	-3.12040900	-1.47648800	1.44792700
C	-4.37798600	-1.27432800	1.31227500
O	-4.92967600	-0.52934000	0.45134600
O	-2.47146300	1.37022600	-2.26871200
C	-1.22270300	1.18191600	-2.14426300
O	-0.66032800	0.47542900	-1.23715800
C	-2.43690900	3.28849700	2.06703000
H	-2.26923000	2.99964100	3.10836400

H	-3.30671500	3.94305200	1.98883200
C	-0.29459000	1.86235100	-3.12124500
H	0.62279400	1.28142200	-3.23897400
H	-0.02536100	2.84159500	-2.70971800
C	-5.27610600	-2.02494100	2.27252500
H	-5.27665900	-3.08785200	2.00572800
H	-6.29612900	-1.64110500	2.21924500
C	-2.96323100	-3.25174300	-3.01742600
H	-3.88067800	-3.23401200	-3.60768400
H	-2.88294400	-4.19424100	-2.46788300
C	-0.14393300	-1.37523600	0.97194800
C	0.16743500	-1.62670200	2.34559400
C	1.33627100	-2.34950100	2.71811100
C	-0.69339800	-1.15800600	3.37503500
C	1.62516900	-2.58899000	4.05298000
H	2.00795700	-2.70651000	1.94606900
C	-0.39009700	-1.39605700	4.70879900
H	-1.57994900	-0.60504100	3.09728700
C	0.76333100	-2.11188800	5.04894800
H	2.51887800	-3.14255400	4.32537900
H	-1.04967500	-1.02770400	5.48918400
H	0.99321800	-2.29950300	6.09466600
C	0.78686600	-1.70440400	-0.09726000
N	1.91281700	-1.08080300	-0.18666700
S	2.73398300	-1.31464800	-1.69053800
O	2.20739300	-2.49506500	-2.39995300
O	2.74629100	-0.00616200	-2.35641000
C	4.37477100	-1.68828000	-1.09305100
C	4.89832700	-2.96498700	-1.29821400
C	5.11015700	-0.68928400	-0.44733400
C	6.18776600	-3.24468000	-0.84610500
H	4.30460500	-3.71603200	-1.80823900
C	6.39298800	-0.99521200	-0.00031300
H	4.70101300	0.30505400	-0.29024500
C	6.95289900	-2.26824700	-0.19381000
H	6.60577500	-4.23575500	-1.00541400
H	6.96866200	-0.22388200	0.50539500
C	8.35914600	-2.56715200	0.26986400

H	8.55845800	-2.12693800	1.25330300
H	8.54106200	-3.64468700	0.33515400
H	9.09926000	-2.14977000	-0.42566400
H	-1.54292700	3.82176900	1.72414700
H	-0.79908300	2.00861700	-4.07913400
H	-4.89091900	-1.94205500	3.29285700
H	-2.09775600	-3.18557300	-3.68609200
H	0.42498600	-2.38068300	-0.88227200
C	3.91579900	3.38578100	0.35005700
C	4.40818400	4.80648200	0.63124200
C	2.06386900	5.68875200	0.31328400
C	1.66654500	4.28238100	-0.05555600
H	5.27397400	4.73892200	1.29656400
H	1.22349700	6.18340400	0.82246100
H	2.24773000	6.26079700	-0.60990200
H	4.77047400	5.22198500	-0.32171200
C	2.51023000	3.22634500	-0.02254000
C	3.31025700	5.70522800	1.20857400
H	3.67084500	6.73306900	1.32699800
H	3.03316600	5.34469100	2.20730200
O	4.69743100	2.43990700	0.40477400
O	0.38139000	4.09717300	-0.46652100
H	-0.09480900	4.94252200	-0.45171100
H	2.16703400	2.23478700	-0.30349100
TS2c			
Rh	-3.38127800	-1.58910400	-0.33457600
Rh	-1.42211500	-0.20338800	0.14910700
O	-0.70249100	-0.78978500	-1.68877200
C	-1.41508900	-1.52060400	-2.45666700
O	-2.55368200	-2.00415000	-2.17618500
O	-2.29732500	0.21610300	1.98621300
C	-3.41896800	-0.32202200	2.27948600
O	-4.10354800	-1.08669600	1.53518400
O	-2.50123400	1.37680100	-0.65593800
C	-3.65211200	1.16704500	-1.17298900
O	-4.28045600	0.06712800	-1.16849100
O	-2.38244500	-3.20111100	0.47121400
C	-1.21069500	-3.02965500	0.92444500

O	-0.58233300	-1.91615800	0.96591400
C	-0.83101800	-1.81432300	-3.81829900
H	-0.67706500	-0.86647700	-4.34456200
H	-1.49880600	-2.45842200	-4.39240800
C	-0.46567000	-4.23013700	1.45830200
H	-1.10379000	-5.11507300	1.44338500
H	-0.12084300	-4.02830600	2.47715500
C	-4.29340800	2.34980400	-1.86188700
H	-4.35357200	3.19794700	-1.17182900
H	-5.29065200	2.09236800	-2.22179400
C	-3.95856600	-0.03297000	3.66414600
H	-3.46202400	-0.69513100	4.38323000
H	-5.03329200	-0.22047800	3.70100900
C	0.31806200	1.02692800	0.58524200
C	0.26567000	2.20469900	1.44859000
C	1.38180600	2.57976500	2.23701600
C	-0.91244300	2.97995300	1.54851100
C	1.31423000	3.66509400	3.10601600
H	2.30235100	2.00697200	2.16264100
C	-0.96895800	4.07297900	2.40926100
H	-1.77137400	2.69790400	0.95224900
C	0.13704600	4.41479500	3.19358600
H	2.17606200	3.92725600	3.71339400
H	-1.88387300	4.65488600	2.47986300
H	0.08265000	5.26244700	3.87147900
C	1.31470100	0.01935800	0.83945700
N	2.24963900	-0.43177100	0.05419800
S	3.01965700	-1.88108200	0.58427600
O	2.85287100	-2.04206000	2.03718800
O	2.61654800	-2.94942600	-0.33593900
C	4.72992300	-1.47514800	0.24765900
C	5.54668500	-1.01216600	1.27989300
C	5.22769700	-1.64394800	-1.04685500
C	6.87853000	-0.70747300	1.00266600
H	5.14407200	-0.90841500	2.28199300
C	6.55989600	-1.33016700	-1.30470900
H	4.58291900	-2.02936300	-1.82982000
C	7.40530700	-0.86061900	-0.28779000

H	7.52122000	-0.34986600	1.80330000
H	6.95260700	-1.45926000	-2.31025200
C	8.85798600	-0.56129600	-0.57195400
H	8.99519500	-0.16462900	-1.58342100
H	9.26475600	0.16549300	0.13836100
H	9.46730000	-1.47154000	-0.49449500
H	0.14495200	-2.29662600	-3.70218900
H	0.42539900	-4.39450700	0.84333100
H	-3.65435000	2.64631600	-2.70041100
H	-3.73768600	0.99808300	3.95163700
H	1.15091400	-0.47400000	1.80673400
C	-0.15450400	2.54837800	-2.20382300
C	-0.21171500	4.03693700	-1.88911500
C	2.17849100	3.92952300	-1.06718100
C	2.09852200	2.43742200	-1.19482000
H	-0.91294300	4.50682600	-2.58395300
H	3.21428800	4.23924000	-1.24153600
H	1.95873000	4.15952900	-0.01086900
H	-0.60237400	4.16482800	-0.86968400
C	0.92390000	1.76526200	-1.53641100
C	1.18922600	4.66270500	-1.98280500
H	1.15469300	5.72396500	-1.71392600
H	1.54399900	4.60917100	-3.02007500
O	-0.89934600	2.03415900	-3.02395600
O	3.22207400	1.81843000	-0.89465300
H	3.02429400	0.83535200	-0.76627800
H	0.97070400	0.71874500	-1.82202000

Int3c

Rh	-3.36380200	-1.55204000	-0.36834400
Rh	-1.39313800	-0.23613500	0.08063500
O	-0.66404500	-0.86426600	-1.75228800
C	-1.34670000	-1.69327700	-2.44489300
O	-2.48848700	-2.15481100	-2.13510000
O	-2.24599700	0.30340700	1.87838900
C	-3.41261100	-0.12843300	2.15789000
O	-4.12928400	-0.88014600	1.42224700
O	-2.36395000	1.33550400	-0.84819300
C	-3.51317500	1.15355900	-1.36982900

O	-4.17712700	0.06926200	-1.33924300
O	-2.48384600	-3.14063100	0.59064000
C	-1.30294000	-2.99246100	1.04341900
O	-0.61767900	-1.91908300	0.98368400
C	-0.71935100	-2.18308900	-3.72956800
H	-0.23442000	-1.35429600	-4.25236500
H	-1.47053400	-2.65014600	-4.36864600
C	-0.63829500	-4.18071300	1.69418000
H	-1.33739300	-5.01405700	1.77986000
H	-0.25904200	-3.89516300	2.67973100
C	-4.13941900	2.34405900	-2.05831500
H	-4.62801300	2.97502000	-1.30585500
H	-4.89423900	2.01546300	-2.77548800
C	-3.98208300	0.26698200	3.50170100
H	-3.67468500	-0.47536000	4.24786600
H	-5.07335700	0.28103300	3.46250100
C	0.73689500	1.55678500	0.19511700
C	0.32816200	2.57197400	1.21598200
C	1.15523000	2.81047500	2.32942100
C	-0.85653500	3.32207000	1.09812300
C	0.80819300	3.75331100	3.29887000
H	2.08596000	2.25812400	2.42919500
C	-1.19532000	4.27128400	2.06140600
H	-1.52424700	3.13091300	0.26600500
C	-0.36832300	4.49082600	3.16643600
H	1.46454100	3.91648600	4.14964800
H	-2.11890100	4.83441700	1.95390100
H	-0.63836000	5.23096600	3.91489600
C	1.21832300	0.35690500	0.66829500
N	1.90287400	-0.60163100	-0.04335800
S	2.61231700	-1.97127100	0.66348300
O	2.31313100	-1.90565200	2.09371400
O	2.26115000	-3.12310600	-0.16800100
C	4.36492100	-1.67117900	0.44052700
C	5.09131600	-1.06795200	1.46807700
C	4.98179000	-2.04099900	-0.75751500
C	6.45227100	-0.82744400	1.28353800
H	4.59967300	-0.81021200	2.40014600

C	6.34076000	-1.78862800	-0.92362800
H	4.40824700	-2.52944400	-1.53805900
C	7.09707700	-1.17997100	0.08999700
H	7.02379700	-0.36305800	2.08329200
H	6.82421100	-2.07339600	-1.85485600
C	8.57632800	-0.93895500	-0.09575200
H	8.79520400	-0.54900500	-1.09603800
H	8.96247500	-0.22627700	0.63952500
H	9.14415300	-1.87157600	0.01858300
H	0.05174700	-2.92299600	-3.48526900
H	0.22626500	-4.47244800	1.08895700
H	-3.36369000	2.93556100	-2.55000300
H	-3.59271200	1.24023500	3.80818200
H	1.12368800	0.12240100	1.72319300
C	0.33113600	3.28561100	-1.76059100
C	1.08909100	4.55881500	-1.40634100
C	3.22607000	3.19933300	-1.21806100
C	2.45268300	1.95003300	-1.59167300
H	0.58837500	5.39408200	-1.90333000
H	4.26149100	3.07544000	-1.54643200
H	3.22100200	3.28977000	-0.12173700
H	1.03342300	4.72027000	-0.32331200
C	0.93691500	1.94198100	-1.29362600
C	2.56692100	4.45099700	-1.82697400
H	3.10881300	5.34644300	-1.50457600
H	2.64212500	4.41023800	-2.92117300
O	-0.64443000	3.30237900	-2.48383100
O	2.98744600	0.98047100	-2.10603400
H	2.05024700	-0.49585800	-1.04616800
H	0.48825500	1.16804900	-1.92262800
TS3c			
Rh	-0.94404700	-3.09614000	-0.54309400
Rh	-0.69030900	-0.75900400	0.00584100
O	1.09602300	-0.81986900	-1.03123500
C	1.45496100	-1.89435700	-1.61750900
O	0.83578500	-3.00416200	-1.56988200
O	-2.48101600	-0.90694200	1.01870200
C	-3.10193800	-2.01877400	1.04620700

O	-2.72363600	-3.09660100	0.48416100
O	-1.69289000	-0.33895900	-1.75112000
C	-2.07824900	-1.29680000	-2.50209200
O	-1.92179800	-2.53506100	-2.26274500
O	0.04010000	-3.54909500	1.20931200
C	0.41435200	-2.60554800	1.97295500
O	0.28498300	-1.35733500	1.73976900
C	2.72087200	-1.82573000	-2.43773700
H	2.93600200	-2.79347000	-2.89354000
H	3.55472100	-1.51708900	-1.79991600
C	1.04189800	-3.00101800	3.29131000
H	1.65235200	-3.89842200	3.16442700
H	0.24273100	-3.23880700	4.00329800
C	-2.76760100	-0.91083000	-3.79009300
H	-3.58950900	-0.22006400	-3.57864800
H	-3.14377400	-1.79614300	-4.30472300
C	-4.38632100	-2.06499400	1.84120100
H	-5.05123200	-2.83404300	1.44233400
H	-4.87140400	-1.08672500	1.83194400
C	-1.05191800	2.08916600	0.24295600
C	-2.37171400	2.08800700	0.90421800
C	-2.45635800	2.17343800	2.30711700
C	-3.56474200	2.04619400	0.16127400
C	-3.69329300	2.19816900	2.94561800
H	-1.54780400	2.24336800	2.89799200
C	-4.80130000	2.07550600	0.80383000
H	-3.52360500	1.98948300	-0.91998900
C	-4.87217700	2.14868700	2.19676500
H	-3.73660300	2.27206900	4.02893800
H	-5.71208200	2.04614000	0.21181000
H	-5.83764600	2.18210900	2.69471800
C	0.09884500	1.62339100	0.81172300
N	1.29593300	1.94752700	0.12225400
S	2.66691900	2.27953800	1.13911800
O	3.25066400	3.53489600	0.65372200
O	2.24417600	2.14618000	2.53893300
C	3.82054000	0.96373700	0.76276200
C	4.90521800	1.23077800	-0.07233400

C	3.64961700	-0.29162600	1.35115400
C	5.83260900	0.21833500	-0.31856600
H	5.02360300	2.21714200	-0.50684900
C	4.58663900	-1.28879800	1.09247100
H	2.79454400	-0.48332800	1.98990200
C	5.69366900	-1.05049100	0.26120100
H	6.68219800	0.42146500	-0.96552500
H	4.46127500	-2.26842600	1.54733700
C	6.72472300	-2.12846900	0.02482700
H	6.26477200	-3.12141900	-0.01813800
H	7.27105500	-1.96386600	-0.90920000
H	7.46290300	-2.14737100	0.83748800
H	2.60227900	-1.06285600	-3.21411900
H	1.63665900	-2.18334800	3.70334200
H	-2.05521200	-0.38540100	-4.43539200
H	-4.15020200	-2.32024800	2.88120100
H	0.16425100	1.20767100	1.81044100
C	-1.57890000	4.08100600	-1.29300400
C	-0.96279000	5.29986700	-0.62252800
C	1.18721900	4.28827300	-1.55021400
C	0.66754000	2.87272900	-1.46374800
H	-1.27680700	6.17013500	-1.20785400
H	0.92298400	4.63576700	-2.56362300
H	2.27653800	4.26693300	-1.49330700
H	-1.43321200	5.40421000	0.36541500
C	-0.84692100	2.73657100	-1.12327500
C	0.57404500	5.21053500	-0.48814900
H	0.86031500	4.83851600	0.50004600
H	1.00978400	6.21092900	-0.57382700
O	-2.58109900	4.15800300	-1.97678000
O	1.23022500	1.93568900	-2.16955900
H	1.48224700	1.40064600	-1.04483400
H	-1.25163700	2.05497600	-1.88268600
Int4c-2w			
Rh	3.26070300	-1.83949000	0.35496200
Rh	1.38765100	-0.36560700	-0.06417000
O	0.56445900	-1.12139800	1.71472900
C	1.20774800	-2.00822300	2.38388100

O	2.33287500	-2.49215700	2.06589400
O	2.35000800	0.21046600	-1.78524200
C	3.48545700	-0.29309500	-2.07409000
O	4.12720000	-1.13503700	-1.37024600
O	2.41001800	1.06983100	1.03688000
C	3.53817500	0.78000500	1.55982000
O	4.14594500	-0.32948500	1.44676600
O	2.28776400	-3.29167000	-0.72209100
C	1.15021200	-3.02289500	-1.22808200
O	0.54748700	-1.90215600	-1.13775400
C	0.57525900	-2.49541300	3.66773000
H	1.12074500	-3.35798900	4.05247600
H	-0.47447600	-2.75499500	3.50327900
C	0.43684400	-4.11274900	-1.98763100
H	1.08744600	-4.97862500	-2.11985200
H	0.10440100	-3.72911800	-2.95658600
C	4.21077300	1.86988000	2.36390500
H	4.68648800	2.58105500	1.67786200
H	4.97851400	1.44640100	3.01381800
C	4.10358900	0.13718400	-3.38436900
H	3.69915100	-0.48927400	-4.18820100
H	5.18713900	0.00617000	-3.35523500
C	-0.48299500	1.63770300	-0.45921300
C	0.18187000	2.50210200	-1.48929000
C	-0.49039000	2.78499900	-2.69410700
C	1.46614800	3.04935600	-1.31599300
C	0.09339200	3.57658800	-3.68531200
H	-1.48991800	2.38829200	-2.85243800
C	2.04483800	3.85093900	-2.29982800
H	2.02800500	2.80681900	-0.42099500
C	1.36312600	4.11922100	-3.48980200
H	-0.45245500	3.77508700	-4.60384100
H	3.04115900	4.25619300	-2.14092800
H	1.81768300	4.74324400	-4.25450500
C	-1.13404500	0.51548000	-0.93683000
N	-2.08839800	-0.23874800	-0.30631800
S	-2.72841100	-1.64616700	-1.05020000
O	-2.47463700	-1.50706300	-2.48741200

O	-2.29123300	-2.83041600	-0.30870900
C	-4.47477900	-1.43083800	-0.73310200
C	-5.32133100	-1.08859200	-1.78611600
C	-4.96612400	-1.64491400	0.55922900
C	-6.68782600	-0.95778300	-1.53613300
H	-4.91505500	-0.93936300	-2.78072500
C	-6.33129300	-1.49967500	0.78594600
H	-4.28957400	-1.90281100	1.36792200
C	-7.21290500	-1.16050700	-0.25356600
H	-7.35593800	-0.69656100	-2.35297200
H	-6.72155400	-1.65619700	1.78866700
C	-8.69493500	-1.03763900	0.01020600
H	-8.89205300	-0.43949800	0.90719400
H	-9.21550600	-0.56985600	-0.83107400
H	-9.14867400	-2.02366600	0.17432100
H	0.60430900	-1.69016300	4.41094700
H	-0.46158300	-4.39350200	-1.42866200
H	3.46495100	2.41247600	2.95063700
H	3.84281900	1.17548200	-3.60217200
H	-0.95553400	0.21325300	-1.96391400
C	0.00189400	3.11232300	1.76240900
C	0.13803900	4.54436200	1.27511900
C	-2.20229400	4.27672000	0.23285900
C	-2.23754300	2.91078300	0.88360100
H	0.71846400	5.10256200	2.01456800
H	-3.21652300	4.68314400	0.20502600
H	-1.80983300	4.21085700	-0.78767000
H	0.66449700	4.57150600	0.31753500
C	-0.88225900	2.15286400	0.93992600
C	-1.26818000	5.16827000	1.08992600
H	-1.16629800	6.14957000	0.61538800
H	-1.73004500	5.32995100	2.07161700
O	0.36300000	2.77941500	2.88121800
O	-3.21686400	2.48579300	1.47378400
H	-2.21319700	-0.25109600	0.73012300
H	-1.03773200	1.28938000	1.58423700
O	-2.16058200	-0.82106900	2.38255600
H	-1.21654400	-1.04572700	2.25630000

H	-2.16436600	-0.12217700	3.08198600
O	-2.08933700	1.39774400	4.00963000
H	-1.19917900	1.76870900	3.85738100
H	-2.65392400	1.84855300	3.35364200
TS3c-2w			
C	1.46459200	-1.04837400	0.41938000
C	0.52093400	-2.06124400	-0.08180200
C	0.76850700	-2.72313800	-1.29804200
C	-0.66551800	-2.39302600	0.61988900
C	-0.12438900	-3.66830700	-1.80311400
H	1.68472200	-2.50753400	-1.84076600
C	-1.54994600	-3.35668200	0.11176400
H	-0.85899000	-1.95881600	1.59460100
C	-1.28624000	-3.99345700	-1.10193300
H	0.09934900	-4.16349000	-2.74477400
H	-2.44802400	-3.59292400	0.67315900
H	-1.97850200	-4.73238500	-1.49417600
C	2.03540900	-0.13414700	-0.40370600
N	2.81535100	0.86918300	0.14463400
S	3.76800000	1.74195100	-0.86974300
O	3.08174600	2.01584300	-2.14559000
O	4.27648100	2.88223900	-0.06715400
C	5.21379900	0.74663300	-1.26246800
C	5.17870400	-0.10660000	-2.36771400
C	6.34938700	0.81244700	-0.45169300
C	6.28487500	-0.90882300	-2.64670000
H	4.30946000	-0.11637000	-3.01691400
C	7.44778500	0.00728600	-0.74783800
H	6.37442000	1.50610100	0.38189900
C	7.43213300	-0.87121500	-1.84177100
H	6.26091500	-1.56509900	-3.51338900
H	8.33744400	0.07005000	-0.12543700
C	8.61676200	-1.76071000	-2.13707500
H	8.67917300	-2.00488600	-3.20245400
H	9.55823600	-1.28628200	-1.84100800
H	8.54480300	-2.70982900	-1.58895600
H	1.83122000	-0.13444100	-1.47169400
C	1.63591700	-2.10906100	2.76649800

C	2.75744000	-3.10802400	2.53917800
C	4.26045800	-1.15269400	1.88589200
C	3.10133800	-0.23444500	2.16207100
H	2.61297200	-3.95146300	3.21895500
H	5.19390800	-0.62553100	2.09374000
H	4.24049400	-1.44129900	0.83134600
H	2.69402200	-3.47683000	1.50668100
C	1.70775600	-0.80667200	1.91231800
C	4.11972300	-2.42184200	2.76077900
H	4.93133700	-3.11430300	2.51449100
H	4.23230100	-2.15530200	3.81880200
O	0.75897200	-2.26230600	3.58754000
H	1.89546600	2.07069900	1.28802200
H	0.95386900	-0.12681200	2.32810200
O	1.77509800	2.44113600	2.20937900
H	2.26731500	3.32897100	2.18047900
H	2.48730700	1.58245900	2.78022600
O	3.28549500	0.73269600	2.96265000
Rh	-4.00026200	1.33691300	-0.39164100
Rh	-2.45404800	-0.48811400	-0.12864700
O	-1.15938400	0.55014200	-1.36023800
C	-1.50623000	1.68998400	-1.81496400
O	-2.60971500	2.27969800	-1.57281200
O	-3.86099500	-1.39663700	1.09407500
C	-4.97519400	-0.81076200	1.29543300
O	-5.32840100	0.30675900	0.80256900
O	-1.69024500	0.50694400	1.52014300
C	-2.22168200	1.61110200	1.87940400
O	-3.18206200	2.19824900	1.28691800
O	-4.76391800	0.39396400	-2.05216300
C	-4.26788300	-0.72695600	-2.39585200
O	-3.32832000	-1.34473300	-1.79787000
C	-0.53752400	2.38462700	-2.74344800
H	0.49098200	2.28107000	-2.38707200
H	-0.80175600	3.43861800	-2.84675300
C	-4.82433300	-1.37421800	-3.64452100
H	-5.80989500	-0.96787400	-3.87899600
H	-4.87598600	-2.45832000	-3.51661900

C	-1.65273000	2.27107900	3.11301200
H	-1.68697400	1.56728000	3.95121100
H	-2.21706500	3.17193000	3.35918200
C	-5.94952400	-1.49317500	2.22928200
H	-5.69773000	-1.22389500	3.26192000
H	-5.87138100	-2.57879500	2.13480200
H	-0.59471400	1.90962400	-3.73030900
H	-4.14934400	-1.16670400	-4.48310500
H	-0.60240100	2.52391600	2.93508600
H	-6.96923000	-1.16152400	2.02404400
O	3.21470700	4.59473600	1.78611800
H	3.96129400	4.69136000	2.39777500
H	3.60786500	4.17985400	0.98220800

Int5c-2w

C	1.45419300	-0.65095200	1.04742400
C	0.49065400	-1.70167200	1.39158100
C	0.70136200	-3.02405600	0.96759400
C	-0.68534100	-1.41222500	2.12551900
C	-0.22967500	-4.02561600	1.24469900
H	1.61551400	-3.27307000	0.43531600
C	-1.61169400	-2.42696500	2.40426100
H	-0.82881200	-0.42277300	2.54453400
C	-1.39007600	-3.73365700	1.96129200
H	-0.03906400	-5.04102400	0.90671300
H	-2.50318500	-2.18408600	2.97313500
H	-2.11297000	-4.51410500	2.17945300
C	2.12455800	-0.58615400	-0.11709900
N	2.87431100	0.59917800	-0.26236500
S	3.99760900	0.70916700	-1.52024600
O	3.27273000	0.23789700	-2.70382500
O	4.56456100	2.06270900	-1.46217200
C	5.34528200	-0.44050000	-1.23262800
C	5.17250500	-1.79318600	-1.54034200
C	6.55967800	0.02900600	-0.72703800
C	6.22135500	-2.68065400	-1.30989200
H	4.24629900	-2.14067200	-1.98482800
C	7.59894200	-0.87325300	-0.51035300
H	6.69093600	1.08738900	-0.53116200

C	7.44582000	-2.23996700	-0.78607600
H	6.09128500	-3.73164600	-1.55501900
H	8.54877300	-0.50726400	-0.12880200
C	8.56717400	-3.21417200	-0.51632100
H	8.53191200	-4.06650900	-1.20235800
H	9.54665400	-2.73551000	-0.61574400
H	8.50126200	-3.61388300	0.50437500
H	2.04534900	-1.26193300	-0.95688800
C	1.74081400	0.59899200	3.31678900
C	3.09236900	0.35666100	3.96175600
C	4.25529500	0.95563400	1.81594300
C	2.94125400	1.29190800	1.09656000
H	2.98949100	0.52918600	5.03669000
H	5.04790100	1.54959200	1.35159900
H	4.48685900	-0.10399000	1.65560800
H	3.35237300	-0.70335300	3.81600700
C	1.67037200	0.67040600	1.78443900
C	4.17813100	1.23438900	3.31904700
H	5.14796300	1.02970900	3.78648700
H	3.95555900	2.29433800	3.48873800
O	0.73142200	0.74665800	3.97989900
H	0.95033900	2.88347000	-1.46817800
H	0.81260600	1.32094800	1.56154100
O	1.04303300	3.57281700	-0.79199900
H	1.81837900	4.12399600	-1.08349300
H	2.03562400	2.90927900	0.47769400
O	2.85071600	2.67139000	0.99833800
Rh	-3.97494300	0.70683000	-1.20450700
Rh	-2.49331000	-0.49947100	0.25799600
O	-1.10431800	-0.48017000	-1.27836500
C	-1.40683400	0.08206900	-2.38218700
O	-2.50297600	0.67655100	-2.63862600
O	-3.99020800	-0.43344900	1.68505100
C	-5.09478600	0.13739300	1.40255300
O	-5.38921600	0.67931300	0.29008100
O	-1.80366800	1.33444000	0.92293600
C	-2.32429100	2.40563700	0.45984200
O	-3.22956100	2.45717300	-0.43399700

O	-4.67556400	-1.09818800	-1.90227400
C	-4.19274300	-2.17020800	-1.41376600
O	-3.29652300	-2.24411000	-0.51175400
C	-0.38444800	0.01084300	-3.49442200
H	0.62907700	0.14703200	-3.10747300
H	-0.60483700	0.75553700	-4.26161600
C	-4.70734400	-3.47737500	-1.97434400
H	-5.68758400	-3.33647100	-2.43359600
H	-4.75635700	-4.23291100	-1.18652600
C	-1.80029200	3.71526300	0.99343200
H	-1.53924700	3.61377500	2.04998800
H	-2.54376700	4.50295700	0.85500600
C	-6.13312900	0.19551100	2.49990200
H	-5.85906000	0.98768700	3.20633800
H	-6.15451100	-0.74892300	3.04983400
H	-0.43198600	-0.98468200	-3.95214500
H	-4.00985400	-3.83453500	-2.74119700
H	-0.89337400	3.97775200	0.43539700
H	-7.11713300	0.41881400	2.08401800
O	3.50898500	4.65962500	-1.07965200
H	3.66047100	4.34963900	-0.16798200
H	3.93671900	3.94430000	-1.58614200

Int6c

C	0.93353300	1.62503600	-0.49007200
C	2.02590500	2.44900700	-1.02507100
C	1.83700200	3.21040200	-2.19489100
C	3.29117800	2.47456400	-0.40881500
C	2.88130700	3.94918200	-2.74387100
H	0.85641900	3.23466400	-2.66293800
C	4.33178500	3.22177800	-0.95936900
H	3.46285500	1.90705200	0.49934200
C	4.13548600	3.95829100	-2.12833300
H	2.71207600	4.52974600	-3.64703400
H	5.30186200	3.22354800	-0.46984300
H	4.94862800	4.54139500	-2.55191000
C	-0.02260500	1.02614500	-1.22557200
N	-0.95491500	0.32015900	-0.43553700
S	-1.85227800	-0.95262500	-1.03111900

O	-1.76276600	-0.83738400	-2.49790800
O	-1.45195500	-2.23064800	-0.40679900
C	-3.53895100	-0.64712800	-0.53711800
C	-4.38533700	0.02243000	-1.42315800
C	-3.99093100	-1.08888900	0.70889300
C	-5.70556000	0.25493200	-1.04522500
H	-4.01704800	0.33996100	-2.39266000
C	-5.31364600	-0.83975100	1.06662600
H	-3.31543500	-1.60084400	1.38420300
C	-6.19086600	-0.17042500	0.19981400
H	-6.37130600	0.77190100	-1.73147800
H	-5.67240000	-1.17666000	2.03582800
C	-7.63173600	0.05801200	0.58730400
H	-7.73725700	0.21081700	1.66623000
H	-8.05215300	0.92914900	0.07518500
H	-8.24989600	-0.80900300	0.31954700
H	-0.14198900	1.02226500	-2.29993200
C	1.12467700	2.21173900	2.05110900
C	0.08717800	3.25921700	2.40151400
C	-1.70985100	1.82672700	1.37543700
C	-0.72108200	0.70013400	1.02895600
H	0.44027500	3.80688700	3.27943400
H	-2.69651300	1.37368300	1.50869700
H	-1.76831100	2.50910000	0.52007600
H	0.02025200	3.96953400	1.56348500
C	0.76561000	1.18212000	0.96937400
C	-1.28768100	2.60567900	2.62347700
H	-2.03376600	3.37532300	2.85078300
H	-1.24742700	1.93175900	3.48746600
O	2.20309200	2.15199900	2.60920500
H	1.42836600	0.32450500	1.15378200
H	-0.22687000	-1.00836800	1.82685600
O	-0.94304200	-0.34163700	1.91570900
C	4.48343400	-2.61975400	1.35784100
C	4.76235200	-3.48472900	0.12758800
C	2.30353400	-3.42862600	-0.48646300
C	2.08400700	-2.66919900	0.79365000
H	5.78720900	-3.28505400	-0.19975400

H	1.59118300	-3.09793300	-1.25522400
H	2.08857100	-4.49297700	-0.29720200
H	4.73256500	-4.53578400	0.45489300
C	3.08099700	-2.27885200	1.61865800
C	3.74266900	-3.25869800	-0.99388000
H	3.92162800	-3.94605800	-1.82767500
H	3.85731000	-2.24263800	-1.39215700
O	5.38687700	-2.26622500	2.10586000
O	0.79160200	-2.40508400	1.13926500
H	0.16448900	-2.59155200	0.40720600
H	2.86698400	-1.72501200	2.52816800
O	0.28310100	-2.83569400	-3.19614300
H	-0.28503100	-3.58436600	-2.96007200
H	-0.33412700	-2.08284400	-3.17056200

TS4c

C	-0.38475900	-1.11232700	-0.17623000
C	-1.44473700	-2.12361300	-0.20841600
C	-1.41553400	-3.16528400	-1.15467600
C	-2.52604100	-2.05504800	0.68742100
C	-2.44226000	-4.10111100	-1.21309500
H	-0.57424900	-3.25171400	-1.83733300
C	-3.55557100	-2.99241100	0.62082100
H	-2.57522400	-1.26387600	1.42921500
C	-3.52011500	-4.01527200	-0.32692900
H	-2.40128300	-4.90048200	-1.94801100
H	-4.39283100	-2.91404400	1.30787400
H	-4.32545100	-4.74287600	-0.37534600
C	0.50975800	-0.82269900	-1.14147200
N	1.34181000	0.26887500	-0.72193000
S	2.62901100	0.89676000	-1.74401200
O	2.41969500	0.20630400	-3.01115000
O	2.56126900	2.34845600	-1.61569900
C	4.11764900	0.29418500	-0.97522500
C	4.44238700	-1.06239500	-1.09014700
C	4.95114000	1.18862300	-0.30246700
C	5.61311900	-1.52165500	-0.49909300
H	3.79639600	-1.74049800	-1.63785900

C	6.12416500	0.70512800	0.27616200
H	4.69030700	2.23979800	-0.24602600
C	6.47167900	-0.64947300	0.19244800
H	5.87038100	-2.57450300	-0.57942600
H	6.78117800	1.39551400	0.79783500
C	7.74517800	-1.16750800	0.81374300
H	8.24309400	-0.39882300	1.41128500
H	7.54749600	-2.02846500	1.46248300
H	8.44972400	-1.50088500	0.04171700
H	0.65593700	-1.22164700	-2.13262200
C	0.28592700	-0.71986300	2.32779000
C	0.72799800	0.31937000	3.34760800
C	1.73464900	1.60389400	1.40020800
C	0.90371400	0.79539900	0.44397800
H	-0.08140500	0.38276500	4.08310800
H	1.94710100	2.58459400	0.97340200
H	2.69373300	1.08055400	1.53437100
H	1.61100900	-0.08734900	3.85535400
C	-0.16247000	-0.13579900	0.95222200
C	0.99980300	1.70826800	2.74495700
H	1.59794600	2.30483700	3.44102200
H	0.05716600	2.24416800	2.59701200
O	0.26841300	-1.90687400	2.54622300
H	-1.08339600	0.43115700	1.17402300
H	-0.17744800	2.60941400	-1.05163400
O	-0.25594900	2.46349800	-0.09531300
C	-5.98180800	0.88075700	-0.24787900
C	-5.91877300	1.20152000	-1.74654600
C	-3.48659000	1.83877900	-1.50790300
C	-3.60154700	1.58709200	-0.01182100
H	-6.64772100	0.56469700	-2.25798600
H	-2.46329500	1.59250100	-1.82260500
H	-3.61603000	2.91723000	-1.69055700
H	-6.25698600	2.24092900	-1.88031100
C	-4.78103200	1.12597300	0.52234100
C	-4.50868300	1.03578000	-2.32135600
H	-4.47859500	1.34138700	-3.37493600
H	-4.22996600	-0.02588700	-2.28930200

O	-7.02967000	0.46565000	0.25183900
O	-2.54201300	1.84639100	0.71337700
H	-1.26408200	2.28136100	0.13253200
H	-4.84921900	0.94824200	1.59283500
O	-2.36670000	0.77467100	3.19400300
H	-3.22922100	0.53992100	3.56586000
H	-2.57575400	1.29504700	2.37680000

Int7c

C	0.29241900	1.01634200	-0.06566800
C	1.31064900	2.05753800	0.08042300
C	1.21413900	3.26427000	-0.63904200
C	2.41806600	1.86046800	0.92397300
C	2.20065600	4.23755000	-0.52884500
H	0.35409700	3.44758500	-1.27765800
C	3.40900100	2.83525000	1.02407300
H	2.51638800	0.94276700	1.49350500
C	3.30589800	4.02354300	0.30051500
H	2.10880700	5.16400300	-1.08905700
H	4.26863200	2.65719200	1.66291900
H	4.08111700	4.78042500	0.38126700
C	-0.66348700	0.92179200	-1.02176300
N	-1.42327400	-0.26530900	-0.81211400
S	-2.81996000	-0.67256000	-1.85673900
O	-2.60810200	0.16908100	-3.02618100
O	-2.87105700	-2.12453900	-1.91052600
C	-4.19128300	-0.05602100	-0.90505900
C	-4.44707600	1.31945300	-0.88309100
C	-5.00455700	-0.96083700	-0.21988800
C	-5.52531100	1.78620900	-0.14065500
H	-3.82412300	2.00573400	-1.44663000
C	-6.08300600	-0.46845400	0.51331100
H	-4.80736000	-2.02561500	-0.28014400
C	-6.35606500	0.90479100	0.57222700
H	-5.73206400	2.85285300	-0.11834500
H	-6.72615900	-1.16575300	1.04292500
C	-7.51019200	1.43472300	1.38618600
H	-8.17931100	0.63128200	1.70669500
H	-7.14828100	1.94713200	2.28655800

H	-8.09796500	2.16221900	0.81564200
H	-0.88509100	1.52848600	-1.88517900
C	-0.08441600	-0.04704500	2.32997200
C	-0.54211900	-1.31295700	3.03789300
C	-1.50527900	-2.19651600	0.84129700
C	-0.94905800	-0.96600200	0.21395300
H	0.20604500	-1.51444100	3.80974900
H	-1.44090200	-3.01142000	0.11428000
H	-2.56867500	-2.03797600	1.07373900
H	-1.48644000	-1.06522500	3.54214500
C	0.17667400	-0.21275700	0.78783200
C	-0.69862400	-2.52513600	2.11013900
H	-1.18945400	-3.34341600	2.64624700
H	0.28957800	-2.89060300	1.81309700
O	0.01729500	1.02801800	2.86286200
H	1.12970500	-0.84049700	0.69759700
H	0.92216200	-3.18558400	-1.97084100
O	0.59918100	-2.89008700	-1.10787800
C	5.95898900	-0.49556500	-0.26486600
C	5.89645000	-0.42737300	-1.79550100
C	3.51215900	-1.25353800	-1.73304500
C	3.61993300	-1.36730500	-0.21816300
H	6.58063600	0.36119400	-2.12517500
H	2.47023900	-1.02572100	-1.98866600
H	3.72824000	-2.24336600	-2.16805500
H	6.29476800	-1.37636900	-2.18758600
C	4.78270100	-0.99545700	0.41679500
C	4.47161100	-0.20880200	-2.31389800
H	4.44768500	-0.23898000	-3.41070600
H	4.12866800	0.79077600	-2.01517800
O	6.98524100	-0.15676300	0.32878100
O	2.57416500	-1.84451900	0.41208100
H	1.41383100	-2.64538300	-0.59616200
H	4.85813200	-1.08808500	1.49735200
O	2.47068800	-1.34245900	3.06350500
H	3.32063400	-1.01284900	3.38873800
H	2.65621400	-1.66108600	2.14377100

TS5c

C	-0.01230500	1.53087400	0.06674300
C	-0.93787600	2.52589200	-0.48168600
C	-0.44272700	3.65736000	-1.15671100
C	-2.32593600	2.38893600	-0.31742100
C	-1.31077200	4.62822500	-1.64591300
H	0.62661400	3.76011100	-1.32201800
C	-3.19078200	3.36682600	-0.80455900
H	-2.74366500	1.54051500	0.21176400
C	-2.69015500	4.48699300	-1.46906000
H	-0.91257400	5.49124200	-2.17271700
H	-4.25945000	3.24613200	-0.65360500
H	-3.36848900	5.24486200	-1.85165700
C	1.26434200	1.75591700	0.46289800
N	1.83009400	0.53954300	0.93445800
S	3.50648400	0.46642700	1.54869800
O	3.82946000	1.86652000	1.78736000
O	3.51165400	-0.54708000	2.59161400
C	4.40175700	-0.12970100	0.13077800
C	4.69039500	0.75021000	-0.91718600
C	4.82865200	-1.45938600	0.10553500
C	5.40008200	0.27348200	-2.01392400
H	4.38107500	1.78877600	-0.86716400
C	5.54251400	-1.91208000	-1.00201600
H	4.62569200	-2.11350200	0.94649400
C	5.83153700	-1.06163100	-2.07866600
H	5.63103100	0.95089300	-2.83155900
H	5.88671100	-2.94242800	-1.02561100
C	6.57636400	-1.56976600	-3.28794900
H	7.19488500	-2.43830100	-3.04302600
H	5.87429800	-1.87660100	-4.07417700
H	7.22299500	-0.79610900	-3.71405100
H	1.84884000	2.66020200	0.52236500
C	-0.78358700	-0.83388200	-0.83858500
C	-0.61484700	-2.32490500	-0.59485500
C	1.11827600	-1.87854100	1.25373900
C	0.93283600	-0.44292500	0.91063700
H	-1.57725800	-2.81783400	-0.80994000
H	1.27979200	-1.95315900	2.33525000

H	2.02779300	-2.25873700	0.76903900
H	0.09382700	-2.67816500	-1.35855600
C	-0.30584200	0.08785300	0.34238500
C	-0.12419400	-2.68028700	0.81548400
H	0.10054400	-3.74980700	0.86775400
H	-0.92866700	-2.50093100	1.53651900
O	-1.21165000	-0.35309000	-1.85593200
H	-1.14942900	-0.03902000	1.14469400
H	0.38129900	0.88687100	4.15486400
O	0.15604800	0.15675000	3.56110200
C	-4.38598000	-2.61206000	-0.72585500
C	-5.75636800	-2.47341900	-1.39246400
C	-6.13239200	-0.30556400	-0.13347600
C	-4.79633200	-0.51086600	0.55776000
H	-5.70809900	-2.95681900	-2.37364300
H	-6.30860800	0.77216400	-0.22582800
H	-6.92076000	-0.68950200	0.53258200
H	-6.48238000	-3.04339300	-0.79172200
C	-4.03808200	-1.63082300	0.26018500
C	-6.20214700	-1.00890300	-1.49543500
H	-7.21864900	-0.94381000	-1.90371600
H	-5.54318000	-0.48473700	-2.20058000
O	-3.63453700	-3.55256200	-1.03761300
H	-0.79083700	0.29375000	3.32278700
H	-3.09608300	-1.77922900	0.77522900
O	-2.27225600	-0.06712600	2.39068300
H	-2.37494100	-0.97188900	2.72823300
O	-4.45389900	0.40565000	1.41089700
H	-3.32388400	0.17938100	1.96442400
Int4c-2w'			
C	-1.67126000	-0.46135100	-0.13569800
C	-2.84978700	-1.35433300	0.04048500
C	-2.85638200	-2.35350500	1.02888400
C	-3.96670500	-1.26196400	-0.81186700
C	-3.93467100	-3.23071700	1.16006700
H	-2.00535500	-2.43757200	1.69971200
C	-5.04865300	-2.12951800	-0.67309000
H	-3.97795000	-0.51475900	-1.60159900

C	-5.03742000	-3.11929800	0.31339400
H	-3.91357300	-3.99638800	1.93117600
H	-5.89651800	-2.04184400	-1.34736300
H	-5.87991500	-3.79731900	0.41783200
C	-0.46507200	-1.04719600	-0.32548500
N	0.74673200	-0.40152200	-0.54361500
S	2.03067700	-1.27362900	-1.25465200
O	1.77186900	-2.69561200	-1.01205300
O	2.21547000	-0.76662300	-2.62139200
C	3.43454100	-0.75996900	-0.27402700
C	4.06579200	-1.69909500	0.53894600
C	3.89691300	0.55753900	-0.36178100
C	5.18122200	-1.30786600	1.28009500
H	3.68940900	-2.71529900	0.58284600
C	5.00603900	0.92574400	0.39276700
H	3.38844700	1.28080400	-0.99263300
C	5.66826800	0.00313700	1.21918800
H	5.68054100	-2.03601900	1.91437900
H	5.36739100	1.94982600	0.33763500
C	6.88767500	0.41873300	2.00702100
H	6.72539300	1.37349500	2.52001400
H	7.15402800	-0.32997400	2.75925800
H	7.75591700	0.55053300	1.34845000
H	-0.38549800	-2.12935700	-0.31997500
C	-3.16735300	1.72250100	-0.22369800
C	-4.04086800	1.57540900	1.01188600
C	-1.86470900	1.40059400	2.38068500
C	-1.15161000	1.71748800	1.08432000
H	-4.94782700	2.16705800	0.86252600
H	-1.30377300	1.82415900	3.21722700
H	-1.95599800	0.31727300	2.51515200
H	-4.32645500	0.52511800	1.12783900
C	-1.77436300	1.06707900	-0.17543200
C	-3.27436800	2.03733100	2.27567000
H	-3.85854200	1.77927100	3.16485300
H	-3.16965300	3.12898200	2.26378100
O	-3.45693500	2.46082000	-1.15153000
O	-0.27020900	2.55527200	0.99577600

H	0.76653200	0.57688700	-0.88848800
H	-1.22746700	1.45343000	-1.03762300
O	1.26447600	1.94891200	-1.98566600
H	1.36494900	1.48343600	-2.83073500
H	0.59461600	2.66264700	-2.11022800
O	-0.70474400	3.83358700	-1.68104000
H	-1.62472300	3.52797000	-1.78720600
H	-0.51473300	3.69105100	-0.73383700
TS3c-2w'			
C	-1.78721400	0.11884400	-0.39315500
C	-3.00348000	-0.60903600	-0.80635600
C	-2.89979600	-1.82450100	-1.51262800
C	-4.29492200	-0.11643700	-0.53596400
C	-4.03388000	-2.50459400	-1.94924900
H	-1.91521900	-2.24246000	-1.70487100
C	-5.42935200	-0.80695900	-0.96260600
H	-4.41604700	0.81952300	-0.00058800
C	-5.30744600	-2.00092600	-1.67408700
H	-3.92257900	-3.43930700	-2.49308000
H	-6.41357600	-0.40134500	-0.74309300
H	-6.19301400	-2.53613600	-2.00562800
C	-0.68918500	0.21767600	-1.18329600
N	0.36723400	1.00973100	-0.76543500
S	1.81698000	0.83672400	-1.52634400
O	1.63830600	0.45886300	-2.93786100
O	2.59727500	2.05503800	-1.20303500
C	2.69553900	-0.51486500	-0.72880600
C	2.50500300	-1.82129900	-1.18459700
C	3.53783300	-0.25617500	0.35441900
C	3.15283700	-2.87182300	-0.53664700
H	1.87566300	-2.00707600	-2.04881300
C	4.18282000	-1.31788600	0.98664900
H	3.69354200	0.76631700	0.68154000
C	4.00105600	-2.63985300	0.55551600
H	3.00628200	-3.88870200	-0.89324400
H	4.84517500	-1.11527200	1.82510000
C	4.72965300	-3.78059100	1.22557700
H	5.69180000	-3.97580100	0.73371500

H	4.94148200	-3.55966400	2.27684700
H	4.14966300	-4.70842700	1.18219600
H	-0.64278600	-0.25873000	-2.16070800
C	-2.59605300	0.40463400	2.04523300
C	-2.11485000	-0.89665100	2.66087900
C	0.26122200	-0.24913300	1.98595000
C	-0.29831400	1.03194400	1.43173200
H	-2.78194600	-1.15653600	3.48660300
H	1.27952700	-0.07523800	2.33862400
H	0.28244600	-1.00198700	1.19321800
H	-2.17735000	-1.68667900	1.90064500
C	-1.72362100	0.96519000	0.88236700
C	-0.65463700	-0.74423200	3.13121800
H	-0.27792400	-1.70572400	3.49522700
H	-0.60757100	-0.04046700	3.97121200
O	-3.55933300	1.02138700	2.44359800
H	-0.01974800	2.85700100	-0.58151700
H	-2.07908900	1.98886200	0.70881000
O	-0.15660600	3.64387300	0.01744100
H	0.67514600	4.19781400	-0.12477500
H	-0.04534100	2.98897500	1.10294600
O	0.19338000	2.12553700	1.85078100
O	2.19851800	4.69929600	-0.54019700
H	2.52806500	3.80404200	-0.78266900
H	2.18948400	5.18938300	-1.37686300

Int5c-2w'

C	-1.80003100	-0.28339800	-0.30117800
C	-2.90677700	-1.16703600	-0.68977300
C	-2.65035100	-2.36558600	-1.38514200
C	-4.24550900	-0.83910400	-0.40392000
C	-3.69114900	-3.18964900	-1.80258900
H	-1.62197300	-2.65938700	-1.57906600
C	-5.28472600	-1.67230400	-0.81748800
H	-4.47293000	0.06812900	0.14509900
C	-5.01634300	-2.84667200	-1.52135000
H	-3.46725700	-4.10950500	-2.33675800
H	-6.31073200	-1.39763400	-0.58724200
H	-5.82885700	-3.49427200	-1.83926500

C	-0.64384800	-0.13709900	-0.97759300
N	0.20368900	0.83628500	-0.41588300
S	1.75458800	1.06834100	-1.01238800
O	1.60764200	0.95028300	-2.47424500
O	2.26867600	2.30660300	-0.41985300
C	2.82646700	-0.26818700	-0.48233700
C	2.76490200	-1.50578300	-1.12896100
C	3.71366800	-0.05375000	0.57356500
C	3.59113800	-2.53855500	-0.69441800
H	2.09988300	-1.65107600	-1.97358000
C	4.53619400	-1.09889600	0.98996000
H	3.76457800	0.92124800	1.04610200
C	4.48790100	-2.35454600	0.36917500
H	3.54635600	-3.50209100	-1.19603800
H	5.23114600	-0.93314700	1.80923600
C	5.40092200	-3.47372300	0.80850900
H	6.28657300	-3.53356500	0.16239300
H	5.75308800	-3.32511000	1.83390500
H	4.89726700	-4.44490600	0.75760500
H	-0.35993600	-0.60326200	-1.91155600
C	-2.53449500	0.41026500	2.11292600
C	-1.76310200	-0.40426600	3.13145700
C	0.40337600	0.25381900	2.02481300
C	-0.30724200	1.15217100	0.99885000
H	-2.35182300	-0.44474900	4.05204800
H	1.40596400	0.66261700	2.17977100
H	0.50716900	-0.75558700	1.60960600
H	-1.66819400	-1.43092200	2.74551600
C	-1.82069900	0.77304000	0.80569400
C	-0.35888100	0.18549500	3.35102800
H	0.19392900	-0.43207100	4.06806200
H	-0.43704600	1.19010200	3.78198300
O	-3.67236200	0.79289300	2.31374400
H	-2.02142400	4.00067400	-0.90966800
H	-2.33608200	1.66721600	0.42829100
O	-1.13395000	4.08855400	-0.53420200
H	-0.50985600	4.02100400	-1.30066800
H	-0.55494400	3.06535200	0.72347100

O	-0.11539900	2.45576100	1.37629500
O	0.81330500	3.88867600	-2.46959200
H	1.53880000	3.84562200	-1.82073500
H	0.86529300	3.00829000	-2.88367100

1cc + 2H₂O + 1c

C	-0.01604300	1.13567500	-0.61322000
C	-0.80932600	2.35942400	-0.86155700
C	-0.19338800	3.61977900	-0.75947500
C	-2.18937900	2.30772800	-1.12827100
C	-0.93087200	4.79265400	-0.91310300
H	0.87714400	3.67339600	-0.57966200
C	-2.92394400	3.48393200	-1.27796700
H	-2.67913700	1.34685100	-1.23081400
C	-2.30105900	4.72883900	-1.17107600
H	-0.43295800	5.75582200	-0.83710100
H	-3.98955700	3.42388100	-1.48146000
H	-2.87791500	5.64162400	-1.29293700
C	0.90087600	1.03539600	0.39845400
N	1.44215400	-0.25703700	0.39350800
S	2.62612100	-0.74655700	1.53738300
O	2.45774600	0.19477000	2.65572100
O	2.49054300	-2.18461600	1.73304500
C	4.19099200	-0.40593300	0.75330700
C	4.71467500	0.88920900	0.78912600
C	4.86970900	-1.44691400	0.11799300
C	5.93281200	1.13705400	0.16444400
H	4.18871600	1.67992600	1.31299100
C	6.08859500	-1.17528600	-0.50032900
H	4.45920300	-2.45067300	0.12767200
C	6.63510800	0.11541400	-0.49442200
H	6.35015200	2.14017900	0.19424600
H	6.62651300	-1.98275100	-0.98985800
C	7.94055400	0.40815400	-1.19262300
H	8.54346000	-0.49689600	-1.31330600
H	7.76213200	0.82087300	-2.19417900
H	8.53378800	1.14402200	-0.63991100
H	1.17629200	1.73763000	1.16875300

C	-0.75975100	-0.59981800	-2.48419400
C	-0.41281700	-2.00225400	-2.98121900
C	1.18742500	-2.40103200	-1.03536600
C	0.87222700	-0.98925300	-0.64496700
H	-1.28862500	-2.38238300	-3.51404000
H	1.35864300	-3.02047400	-0.15205300
H	2.12002800	-2.42238900	-1.62318300
H	0.39295800	-1.88735700	-3.72446400
C	-0.03169500	-0.15466800	-1.27885500
C	0.01849500	-2.96103000	-1.86503000
H	0.30712700	-3.92910900	-2.29045700
H	-0.84000900	-3.12611700	-1.20760800
O	-1.54488300	0.11385300	-3.09114200
H	-1.97527700	1.90786000	1.48129800
H	0.60958800	0.08848300	3.30631100
O	-0.34244500	-0.12327900	3.30020600
C	-3.99170800	-2.05672300	-0.24420200
C	-5.41686400	-2.58249300	-0.42861200
C	-6.28256900	-0.77759400	1.10896300
C	-4.85449500	-0.33448600	1.30153300
H	-5.47841300	-3.04487500	-1.41861500
H	-6.93029200	0.10186200	1.19568400
H	-6.55371700	-1.44301300	1.94305600
H	-5.56625600	-3.38817600	0.30716400
C	-3.80872900	-0.93390000	0.65885800
C	-6.47819300	-1.49547400	-0.23122800
H	-7.48593500	-1.92386100	-0.28585600
H	-6.39992300	-0.76188700	-1.04431800
O	-3.05377100	-2.60681700	-0.82547600
H	-0.50000400	-0.65502800	4.09349400
H	-2.79039000	-0.59824200	0.83112500
O	-2.26592900	1.63503200	2.36688000
H	-1.56732900	1.02613000	2.70308700
O	-4.73893700	0.67290100	2.16349500
H	-3.78538900	0.97571800	2.25863500

TS2a_{C-H}

Rh	3.40351500	-1.53984400	-0.00595100
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Rh	1.49881100	0.01790000	-0.02842700
O	2.32650700	0.89488200	1.68168600
C	3.42395900	0.42257600	2.14909000
O	4.05874300	-0.57477100	1.70361900
O	0.91611600	-0.97082000	-1.74976000
C	1.58755300	-1.95742800	-2.20879100
O	2.66069000	-2.41570000	-1.71537300
O	2.69209600	1.25329800	-1.20529100
C	3.87858600	0.89019400	-1.50956900
O	4.45571900	-0.17881200	-1.14571500
O	2.22147900	-2.84114600	1.07792600
C	1.02549600	-2.51465400	1.34336200
O	0.48862000	-1.37787200	1.10365200
C	4.01809900	1.15438300	3.33504100
H	3.23189000	1.48256500	4.02036900
H	4.54197300	2.04805400	2.97554300
C	0.13245200	-3.54395200	1.99766600
H	-0.78970100	-3.63172900	1.41469600
H	-0.14295000	-3.21397600	3.00567600
C	4.65301100	1.82139900	-2.41852600
H	4.39775200	1.59162600	-3.45981500
H	5.72704000	1.67572100	-2.28644600
C	1.04542600	-2.59888400	-3.46528600
H	1.35538800	-2.00237400	-4.33174000
H	-0.04703800	-2.61032700	-3.43624800
C	-0.24067000	1.28511300	-0.17224900
C	-0.09515100	2.63933900	-0.71548600
C	-1.01598800	3.16728100	-1.64950200
C	1.00009800	3.44515800	-0.33175300
C	-0.83242200	4.43399100	-2.19822300
H	-1.87585200	2.57490000	-1.94901900
C	1.16241200	4.72298900	-0.85762800
H	1.71493600	3.04874400	0.38022800
C	0.25334000	5.21808200	-1.79920700
H	-1.54229400	4.81443900	-2.92744300
H	2.00744800	5.33125400	-0.54648000
H	0.39038200	6.21120700	-2.21857700
C	-1.25410000	0.40914400	-0.73068700

N	-2.17807400	-0.22616200	-0.09496800
S	-2.92842900	-1.47465200	-0.99822600
O	-2.70127000	-1.31369700	-2.44729700
O	-2.56387200	-2.73661200	-0.33945800
C	-4.65473000	-1.15161900	-0.66028400
C	-5.47190700	-0.64480300	-1.66808100
C	-5.16803100	-1.44480700	0.60698300
C	-6.82320100	-0.42322900	-1.39691400
H	-5.05460200	-0.44327600	-2.64882100
C	-6.51599900	-1.21254900	0.85983300
H	-4.52032700	-1.86087500	1.37184100
C	-7.36436500	-0.69895400	-0.13548900
H	-7.46739100	-0.03444300	-2.18158000
H	-6.92140600	-1.44059000	1.84285700
C	-8.82610000	-0.45619500	0.15747400
H	-9.36331200	-0.11893300	-0.73413300
H	-9.31561000	-1.36797000	0.52065300
H	-8.95308400	0.30821700	0.93431600
H	4.73455700	0.51615700	3.85515100
H	0.64343700	-4.50597000	2.06129300
H	4.37730000	2.86097400	-2.22633500
H	1.44271400	-3.60955000	-3.57651200
H	-1.07326400	0.20212600	-1.79472400
C	-2.19859500	2.62880800	1.60617900
O	-3.33492400	2.13339200	1.54215600
C	-1.01862300	1.79767100	1.90466900
C	-1.26290400	0.65402800	2.70875500
C	-0.24694000	0.09736700	3.64829900
H	-0.36335200	0.60728800	4.61575100
H	-0.41829200	-0.96866700	3.80573500
H	0.75980500	0.27471200	3.27260800
H	-0.08073700	2.30134400	2.10355300
C	-2.03310900	4.12719500	1.48903600
H	-2.12210600	4.55305200	2.49824000
H	-1.06105700	4.42022700	1.08881100
H	-2.83851600	4.53943400	0.87709300
O	-2.44173000	0.11157600	2.78828300
H	-3.04796400	0.63609800	2.16914600

TS2b_{C-H}

Rh	-3.58080100	-1.48742200	0.17168200
Rh	-1.53616600	-0.15151400	0.00852500
O	-1.90777700	-0.08636200	-2.01536800
C	-2.95061800	-0.62917400	-2.50418900
O	-3.83361700	-1.27452200	-1.85546200
O	-1.36025400	-0.39040700	2.06977200
C	-2.23037400	-1.07793200	2.70496500
O	-3.25220000	-1.63643100	2.20414000
O	-2.77878300	1.51165400	0.25058600
C	-4.03787800	1.35556300	0.39692100
O	-4.65226700	0.24807900	0.44378600
O	-2.44087000	-3.17523000	-0.13117900
C	-1.18773200	-3.05098200	-0.28644300
O	-0.54401900	-1.94569700	-0.28503900
C	-3.12798800	-0.50389100	-4.00050700
H	-2.78548000	0.48012700	-4.32935900
H	-4.17196600	-0.66551400	-4.27613000
C	-0.36380500	-4.30300200	-0.46939200
H	-1.01147300	-5.16446900	-0.64024100
H	0.23734100	-4.46526800	0.43204300
C	-4.86467300	2.61893000	0.50361300
H	-4.86345000	3.12863200	-0.46634200
H	-4.42040500	3.30021100	1.23566900
C	-1.99441800	-1.25039000	4.18979700
H	-2.89212400	-1.63413900	4.67741100
H	-1.69447800	-0.29805800	4.63576800
C	0.45248600	0.97427900	0.21671000
C	0.60555700	1.95586300	1.30668000
C	1.82164900	2.05557900	2.02884500
C	-0.46105900	2.79348800	1.70200000
C	1.95809200	2.93286100	3.10182700
H	2.66671000	1.43743500	1.73873800
C	-0.31861200	3.67433300	2.77215600
H	-1.40719000	2.71224800	1.18145800
C	0.88553600	3.74603800	3.47792600
H	2.89831200	2.98118800	3.64437300

H	-1.15665200	4.30107400	3.06528500
H	0.98757200	4.42910900	4.31701100
C	1.36073600	-0.14816800	0.30260300
N	2.32164600	-0.50711000	-0.49476300
S	3.01201300	-2.05605000	-0.19165500
O	2.54216400	-2.57963800	1.10086900
O	2.84806700	-2.83407000	-1.42271200
C	4.74270600	-1.62929800	-0.02720800
C	5.29482000	-1.47463900	1.24547200
C	5.52180800	-1.47328500	-1.17569900
C	6.64498700	-1.14932300	1.36165100
H	4.67677800	-1.62508900	2.12437000
C	6.86885400	-1.14488500	-1.03884500
H	5.08118600	-1.62519500	-2.15560300
C	7.45139900	-0.97983500	0.22665600
H	7.08189600	-1.03191600	2.35031200
H	7.48038100	-1.02224500	-1.92927800
C	8.92160600	-0.66295600	0.36378600
H	9.28677400	-0.07773500	-0.48644300
H	9.12742700	-0.10010200	1.28004700
H	9.51800200	-1.58404200	0.40584500
H	-2.51270700	-1.26295400	-4.49800400
H	0.33813500	-4.17077000	-1.29693900
H	-5.89156900	2.38206300	0.78629200
H	-1.17384200	-1.96131800	4.34061200
H	1.11737900	-0.78930700	1.15969500
C	-0.17128800	2.96364700	-2.01455400
C	-0.03870300	4.33443400	-1.36381700
C	2.38518400	3.89192300	-0.90790400
C	2.17678200	2.48162000	-1.37423300
H	-0.78182300	4.98685200	-1.83016100
H	3.42540200	4.16015500	-1.12337900
H	2.29460600	3.88066000	0.19051400
H	-0.28759000	4.25136400	-0.29819600
C	0.94105200	1.96079300	-1.81430200
C	1.38555100	4.88192500	-1.50941900
H	1.47880700	5.85410400	-1.01346900
H	1.61609400	5.04230100	-2.57053100

O	-1.11968800	2.70994000	-2.73760300
O	3.27695600	1.76107700	-1.31758800
H	3.03388500	0.77415700	-1.27459500
C	0.92503900	0.78875200	-2.78824100
H	1.93606500	0.51537400	-3.10190400
H	0.43798300	-0.09629300	-2.38508800
H	0.34793800	1.09532200	-3.66401800

TS2c_{O-H}

Rh	-3.19954500	-1.39559500	-0.87210400
Rh	-1.28972100	-0.35054800	0.24072300
O	-2.28084400	1.47416200	-0.02512300
C	-3.43140500	1.48085500	-0.58596300
O	-4.05265100	0.47385800	-1.03343700
O	-0.53206300	-2.27195000	0.43083600
C	-1.15477700	-3.26962700	-0.07036300
O	-2.27175100	-3.22020300	-0.66780900
O	-2.31138900	-0.63052900	2.02755300
C	-3.44736000	-1.21410300	2.01349500
O	-4.06931600	-1.62562900	0.98645300
O	-2.21241500	-1.12285800	-2.66342300
C	-1.04995300	-0.61317900	-2.65682200
O	-0.42235100	-0.19636800	-1.62250600
C	-4.10256200	2.82829100	-0.75910100
H	-3.83114600	3.23872200	-1.73918700
H	-3.77849400	3.52942400	0.01355700
C	-0.32561300	-0.46726800	-3.97509000
H	0.66559900	-0.92452300	-3.89117600
H	-0.18507100	0.59585700	-4.20354200
C	-4.09432800	-1.46198400	3.35957900
H	-3.71894900	-2.41003600	3.76295300
H	-5.17823000	-1.53911900	3.25235000
C	-0.49789200	-4.61995700	0.10074700
H	-0.85496000	-5.31383000	-0.66283300
H	-0.76221300	-5.02154800	1.08649900
C	0.49707300	0.62778000	1.25462300
C	0.34247100	1.21100700	2.61061700
C	1.38684100	1.11465300	3.55006300

C	-0.83832200	1.87655900	2.98250900
C	1.25210600	1.65639000	4.82713000
H	2.31226600	0.61600700	3.27319200
C	-0.96433500	2.43443800	4.25339300
H	-1.65264000	1.93823600	2.27089600
C	0.07600600	2.32207600	5.17937400
H	2.06520100	1.56592100	5.54219700
H	-1.88258300	2.94692100	4.52768700
H	-0.03017400	2.75003900	6.17273100
C	1.42331100	-0.44435900	1.01343100
N	2.31143900	-0.30773500	0.06263500
S	3.16842200	-1.67176700	-0.50321900
O	2.92764200	-2.79794800	0.40987600
O	2.88771500	-1.78457600	-1.93551900
C	4.86115500	-1.12738700	-0.30460900
C	5.56445700	-1.47407800	0.84978900
C	5.45865400	-0.37014300	-1.31483700
C	6.88223300	-1.04302600	0.99277600
H	5.08900000	-2.08272800	1.61172200
C	6.77544400	0.05329100	-1.15192200
H	4.90317800	-0.13307800	-2.21612100
C	7.50723300	-0.27527200	-0.00036900
H	7.43663600	-1.31283300	1.88811700
H	7.24576500	0.64279200	-1.93505000
C	8.94575600	0.15986200	0.14761800
H	9.62043300	-0.53723900	-0.36671500
H	9.11177700	1.15110500	-0.28750800
H	9.24928200	0.19301300	1.19874000
H	-5.18817600	2.71172500	-0.73425800
H	-0.89366700	-0.94083900	-4.77735900
H	-3.83075300	-0.66842800	4.06261700
H	0.58870100	-4.51494000	0.05596200
H	1.30291700	-1.37444400	1.56589500
C	0.21329900	3.59059800	-2.79347100
C	-0.53263000	4.76622100	-2.16785700
C	-0.02409400	3.86479300	0.15293300
C	0.65702500	2.72477500	-0.53941600
H	-0.45739200	5.61894500	-2.84969100

H	0.48895500	4.07420600	1.09746400
H	-1.04623200	3.55338500	0.40288000
H	-1.59581600	4.48426800	-2.13242700
C	-0.03633900	5.10604400	-0.75630800
H	-0.66435100	5.88445700	-0.30935400
H	0.98119200	5.51333500	-0.81723400
O	0.27034800	3.43235300	-4.00570000
O	1.25682900	1.78767000	0.30044200
H	1.91167200	1.06969300	-0.19839500
C	0.80732400	2.60949700	-1.86875400
H	1.29773100	1.75006900	-2.31170000