

DFT study on stereoselective Rh-catalyzed intramolecular [2+2+2] cycloaddition of allene-ene-ynes

Xin-Rui Zhu^a and De-Cai Fang^{*,a}

^aCollege of Chemistry, Beijing Normal University, Beijing 100875, China

Email: dcfang@bnu.edu.cn

Figure S1 The main geometric parameters(Å) and $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$ for different directions of PhO₂S of **COM** and **COMa**, determined at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

..... s3

Figure S2 Proposed mechanism for the stereoselective rhodium-catalyzed intramolecular [2+2+2] Cycloaddition of Allene-Ene-Ynes coupling reaction(PhO₂S with downward direction), along with $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$, some numbering system and key geometric parametrs(Å) determined at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) in toluene solution.

..... s3

Figure S3 Proposed mechanism for the stereoselective rhodium-catalyzed intramolecular [2+2+2] Cycloaddition of Allene-Ene-Ynes coupling reaction, along with $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$, some numbering system and key geometric parametrs(Å) determined at B3LYP-D3b+IDSCRF/TZP-DKH(-dfg)(up,in blue) in toluene solution, and also $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$ determined at B3LYP+IDSCRF/TZP-DKH(-dfg) (middle,in black) and B3LYP-D3+IDSCRF/TZP-DKH(-dfg)(down, in magenta) for comparison.

..... s4

Table S1 The calculated total electronic energies, enthalpies, entropies and free energies in a.u. , in the toluene solvent with the temperature of 383.75 K.

..... s4-s6

Table S2 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

..... s6-s31

Table S3 Coordinates of some Stationary Points **CAT+1a**, Computed at B3LYP+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

..... s31-s45

Table S4 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

..... s46-s59

Table S5 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP-D3b+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

.... s59-s73

Table S6 Frequencies of all stationary points for the overall catalytic cycle, computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in toluene, and some of them computed at B3LYP+IDSCRF/TZP-DKH(-dfg), B3LYP-D3+IDSCRF/TZP-DKH(-dfg) and B3LYP-D3b+IDSCRF/TZP-DKH(-dfg).

..... s73-S101

Table S7 The calculated total electronic energies, enthalpies, entropies and free energies in a.u. , PhO₂S with downward direction of 1a in the toluene solvent with the temperature of 383.75 K.

..... s101-s102

Table S8 Coordinates of All Stationary Points **CAT+1a**(PhO₂S with downward direction of 1a), Computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

..... s102-s116

Table S9 Frequencies of all stationary points for the overall catalytic cycle, PhO₂S with downward direction of 1a computed at and some of them computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg).

..... s116-s122

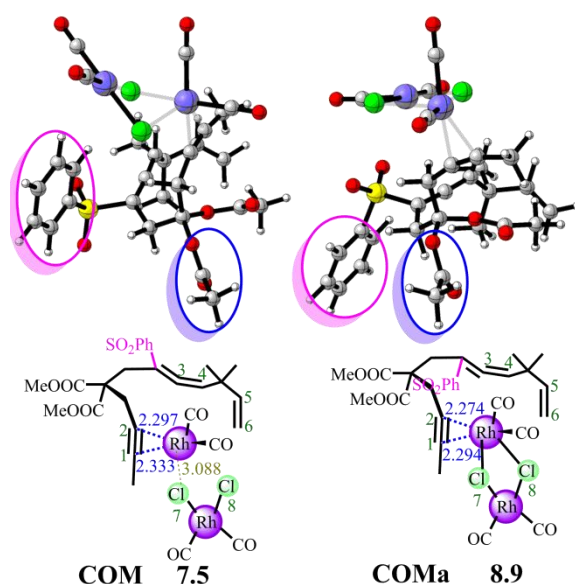


Figure S1 The main geometric parameters(Å) and $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$ for different directions of PhO_2S of **COM** and **COMa**, determined at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

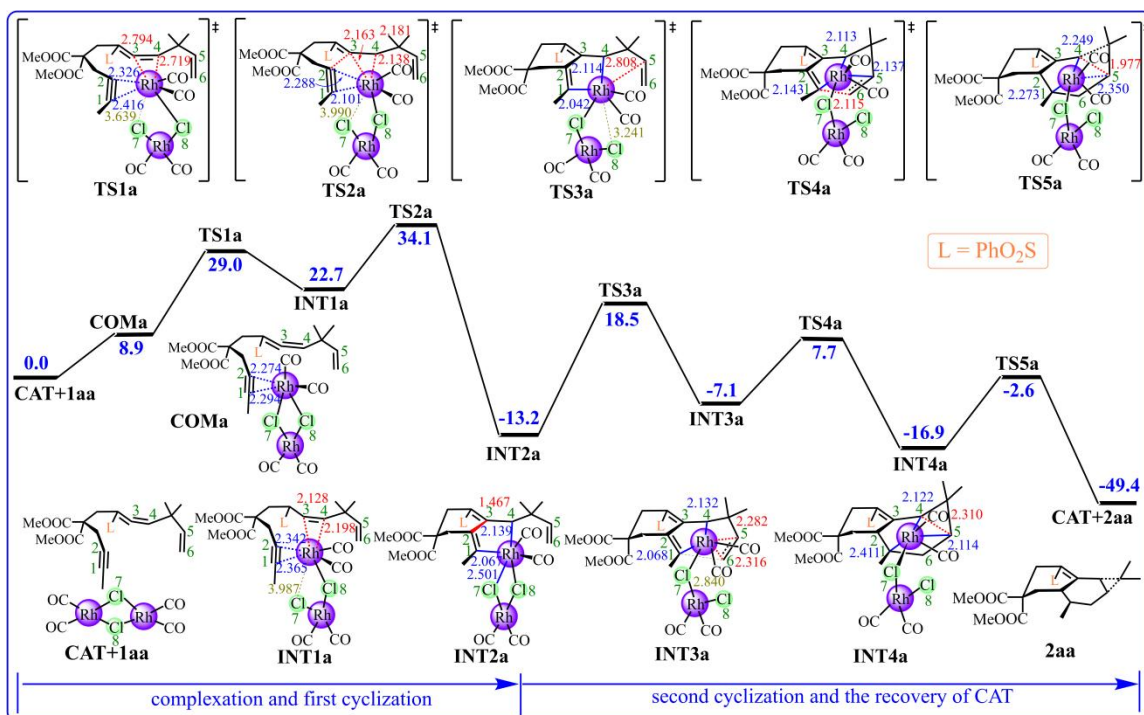


Figure S2 Proposed mechanism for the stereoselective rhodium-catalyzed intramolecular [2+2+2] Cycloaddition of Allene-Ene-Ynes coupling reaction(PhO_2S with downward direction), along with $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$, some numbering system and key geometric parameters(Å) determined at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) in toluene solution.

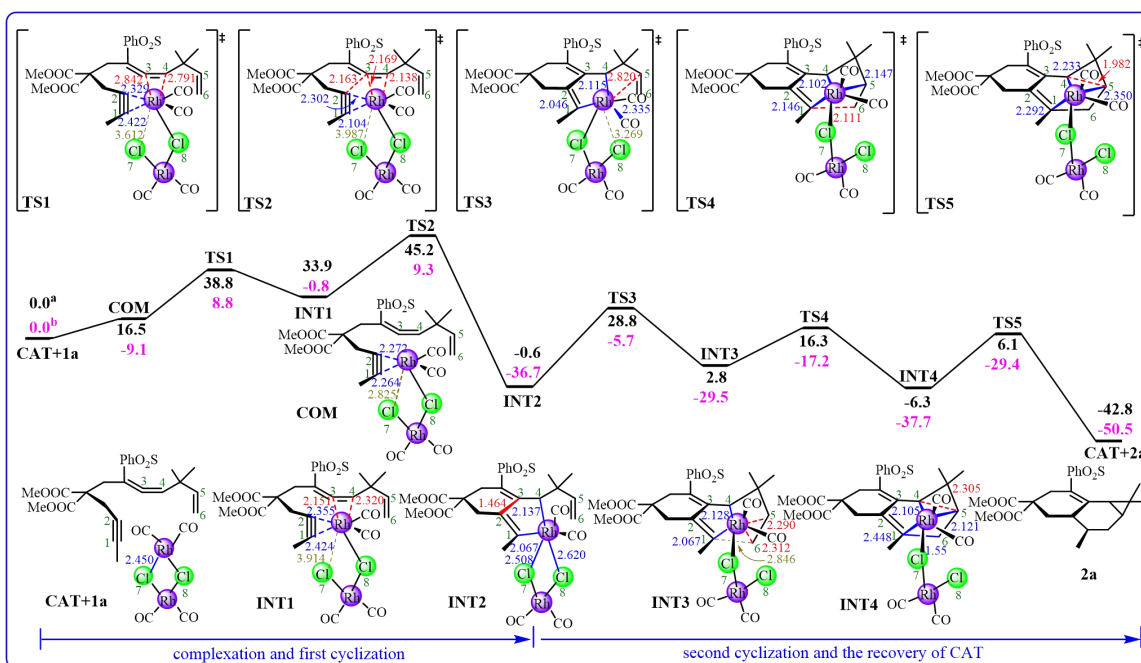


Figure S3 Proposed mechanism for the stereoselective rhodium-catalyzed intramolecular [2+2+2] Cycloaddition of Allene-Ene-Ynes coupling reaction, along with $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$, some numbering system and key geometric parametrs(Å) determined at $\Delta G(383.75\text{K}, \text{kcal mol}^{-1})$ determined at B3LYP+IDSCRF/TZP-DKH(-dft)(up,in black) and B3LYP-D3+IDSCRF/TZP-DKH(-dft)(down, in magenta) for comparison.

Table S1 The calculated total electronic energies, enthalpies, entropies and free energies in a.u. , in the toluene solvent with the temperature of 383.75 K.

Species	E _{elec} /a.u.	H/a.u.	S _g	S _l	G _g /a.u.	G _l /a.u.
CAT	-10590.41705 ^a	-10590.35690	144.5	120.8	-10590.44529	-10590.43081
	-10590.38879 ^b	-10590.32868	145.2	121.5	-10590.41749	-10590.40301
	-10590.41777 ^c	-10590.35762	145.2	121.5	-10590.44643	-10590.43195
	-10590.40725 ^d	-10590.34711	145.2	121.6	-10590.43593	-10590.42145
1a	-1781.23902 ^a	-1780.71344	251.8	230.2	-1780.86740	-1780.85425
	-1781.15370 ^b	-1780.62890	263.0	241.7	-1780.78972	-1780.77674
	-1781.28872 ^c	-1780.76421	253.9	232.3	-1780.91945	-1780.90625
	-1781.22033 ^d	-1780.69503	260.5	239.2	-1780.85432	-1780.84130
2a	-1781.33258 ^a	-1780.80367	231.9	210.3	-1780.94548	-1780.93225
	-1781.24037 ^b -17	-1780.71239	238.4	216.8	-1780.85816	-1780.84496
	81.38494 ^c	-1780.85592	235.4	213.8	-1780.99991	-1780.98665
	-1781.31219 ^d	-1780.78359	235.2	213.6	-1780.92746	-1780.91423

3a	-1781.28868 ^a	-1780.76161	237.9	216.3	-1780.90712	-1780.89392
	-1781.19831 ^b	-1780.67203	242.5	221.0	-1780.82035	-1780.80717
	-1781.33868 ^c	-1780.81140	240.3	218.7	-1780.95834	-1780.94512
	-1781.26811 ^d	-1780.74126	240.5	218.9	-1780.88833	-1780.87513
COM	-12371.65723 ^a	-12371.06947	354.2	332.9	-12371.28606	-12371.27304
	-12371.53127 ^b	-12370.94431	363.1	341.9	-12371.16634	-12371.15340
	-12371.73939 ^c	-12371.15135	350.7	329.2	-12371.36579	-12371.35265
	-12371.63260 ^d	-12371.04510	357.9	336.6	-12371.26396	-12371.25093
TS1	-12371.62995 ^a	-12371.04293	343.6	322.2	-12371.25308	-12371.24000
	-12371.49973 ^b	-12370.91379	355.1	333.8	-12371.13094	-12371.11792
	-12371.71484 ^c	-12371.12734	343.3	321.8	-12371.33726	-12371.32414
	-12371.60538 ^d	-12371.01863	348.3	326.9	-12371.23164	-12371.21855
INT1	-12371.64222 ^a	-12371.05403	348.2	326.8	-12371.26699	-12371.25388
	-12371.51121 ^b	-12370.92384	351.4	330.1	-12371.13875	-12371.12569
	-12371.73092 ^c	-12371.14231	343.9	322.3	-12371.35260	-12371.33943
	-12371.61894 ^d	-12371.03096	348.5	327.1	-12371.24409	-12371.23098
TS2	-12371.62557 ^a	-12371.03976	340.4	319.0	-12371.24792	-12371.23485
	-12371.49329 ^b	-12370.90830	347.5	326.2	-12371.12083	-12371.10779
	-12371.71272 ^c	-12371.12644	343.4	321.9	-12371.33646	-12371.32332
	-12371.60169 ^d	-12371.01610	346.0	324.6	-12371.22768	-12371.21460
INT2	-12371.70794 ^a	-12371.11888	335.5	314.1	-12371.32406	-12371.31096
	-12371.57410 ^b	-12370.98576	340.1	318.8	-12371.19377	-12371.18069
	-12371.79617 ^c	-12371.20638	332.8	311.3	-12371.40988	-12371.39673
	-12371.68360 ^d	-12371.09466	337.5	316.1	-12371.30104	-12371.28795
TS3	-12371.65424 ^a	-12371.06704	336.7	315.3	-12371.27295	-12371.25987
	-12371.52152 ^b	-12370.93529	346.0	324.6	-12371.14686	-12371.13380
	-12371.74130 ^c	-12371.15359	338.3	316.8	-12371.36049	-12371.34734
	-12371.62970 ^d	-12371.04284	344.0	322.7	-12371.25324	-12371.24017
INT3	-12371.69893 ^a	-12371.10936	334.8	313.5	-12371.31412	-12371.30106
	-12371.56704 ^b	-12370.97836	343.4	322.1	-12371.18840	-12371.17535
	-12371.78453 ^c	-12371.19422	333.8	312.3	-12371.39835	-12371.38523
	-12371.67406 ^d	-12371.08482	340.2	318.8	-12371.29286	-12371.27980
TS4	-12371.67802 ^a	-12371.09016	331.6	310.2	-12371.29293	-12371.27987
	-12371.54593 ^b	-12370.95899	339.9	318.6	-12371.16686	-12371.15385
	-12371.76596 ^c	-12371.17777	328.7	307.1	-12371.37877	-12371.36557
	-12371.65306 ^d	-12371.06554	336.9	315.6	-12371.27158	-12371.25852
INT4	-12371.71554 ^a	-12371.12484	331.4	310.0	-12371.32751	-12371.31443
	-12371.58572 ^b	-12370.99565	338.8	317.5	-12371.20286	-12371.18982
	-12371.80226 ^c	-12371.21089	328.0	306.4	-12371.41148	-12371.39828
	-12371.69051 ^d	-12371.09985	333.7	312.2	-12371.30391	-12371.29079

TS5	-12371.69434 ^a	-12371.10564	328.2	306.8	-12371.30637	-12371.29328
	-12371.56334 ^b	-12370.97541	339.5	318.2	-12371.18304	-12371.16999
	-12371.78579 ^c	-12371.19656	329.8	308.3	-12371.39822	-12371.38507
	-12371.66978 ^d	-12371.08126	336.8	315.4	-12371.28724	-12371.27417
TS6	-12371.70426 ^a	-12371.11484	331.7	310.2	-12371.31768	-12371.30457
	-12371.58986 ^b	-12371.00092	356.0	335.0	-12371.21866	-12371.20578
	-12371.79624 ^c	-12371.20596	339.7	318.1	-12371.41371	-12371.40052
	-12371.62536 ^d	-12371.03863	341.5	320.1	-12371.24749	-12371.23436
1b	-1899.23365 ^a	-1898.61659	277.9	256.7	-1898.78652	-1898.77355
2b	-1899.31894 ^a	-1898.69839	257.2	235.8	-1898.85566	-1898.84260
3b	-1899.28275 ^a	-1898.66424	261.1	239.8	-1898.82389	-1898.81088
1c	-1899.22687 ^a	-1898.60935	274.7	253.5	-1898.77734	-1898.76437
2c	-1899.31377 ^a	-1898.69296	257.6	236.2	-1898.85050	-1898.83741
3c	-1899.27511 ^a	-1898.65631	262.6	241.2	-1898.81688	-1898.80384
INT2-n-E	-12489.70321 ^a	-12489.02241	360.4	339.3	-12489.24280	-12489.22988
TS3-n-E	-12489.65092 ^a	-12488.97196	359.7	338.6	-12489.19192	-12489.17901
TS6-n-E	-12489.64480 ^a	-12488.96630	364.9	343.7	-12489.18945	-12489.17649
INT2-n-Z	-12489.69522 ^a	-12489.01425	359.8	338.6	-12489.23426	-12489.22131
TS3-n-Z	-12489.64112 ^a	-12488.96220	365.9	344.7	-12489.18595	-12489.17299
TS6-n-Z	-12489.63631 ^a	-12488.95737	363.2	341.9	-12489.17945	-12489.16647

Table S2 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dftg) level in toluene solvent.

CAT				1a			
Rh	-1.61780	-0.00000	0.09014	C	0.29214	-0.65552	0.53699
Cl	-0.00003	-1.66443	0.87352	C	1.25875	-1.07871	-0.22683
C	-2.81197	1.33788	-0.48262	C	-0.00499	0.75483	0.98574
O	-3.52530	2.15415	-0.81982	H	0.84221	1.12800	1.56174
Rh	1.61781	-0.00001	0.09027	H	-0.86496	0.75625	1.65017
Cl	-0.00002	1.66421	0.87396	C	-0.26727	1.78511	-0.12039
C	2.81192	-1.33779	-0.48285	C	0.89009	1.96858	-1.11482
O	3.52528	-2.15394	-0.82029	H	0.58022	2.72477	-1.83511
C	-2.81197	-1.33774	-0.48294	H	1.00207	1.03109	-1.66068
O	-3.52526	-2.15396	-0.82036	C	2.15015	2.33649	-0.48507
C	2.81195	1.33791	-0.48244	O	-0.50403	2.99289	0.61466
O	3.52539	2.15409	-0.81963	O	-1.37383	1.41697	-0.95283
				C	-0.90395	4.14316	0.01261
				C	-2.65598	1.43074	-0.49623
				O	-2.97077	1.65760	0.64235
				O	-1.13100	4.25602	-1.16448

C	-3.59921	1.14431	-1.62761
H	-3.53028	1.94792	-2.36231
H	-3.32083	0.21404	-2.12229
H	-4.61327	1.07396	-1.24674
C	-1.04076	5.23191	1.03753
H	-1.26794	6.17156	0.54269
H	-1.84303	4.97415	1.73057
H	-0.12165	5.32022	1.61667
C	4.47418	2.98675	0.62754
H	4.34152	3.71984	1.42570
H	4.96389	2.10874	1.05362
H	5.14924	3.41811	-0.11437
C	3.19753	2.63178	0.02285
C	2.21476	-1.57881	-0.94923
H	2.04691	-1.70547	-2.01643
C	3.56746	-2.05021	-0.42351
C	3.72305	-1.74236	1.06429
H	2.93898	-2.24037	1.63418
H	4.68600	-2.10176	1.42834
H	3.65876	-0.67046	1.25643
C	3.62950	-3.57950	-0.64880
H	2.83178	-4.07415	-0.09361
H	3.52109	-3.82893	-1.70630
H	4.59181	-3.96488	-0.30757
C	4.63144	-1.39757	-1.28259
H	4.52330	-1.58700	-2.34826
C	5.65590	-0.66473	-0.86806
H	5.82398	-0.43974	0.17717
H	6.37166	-0.26191	-1.57328
S	-0.68691	-1.98572	1.31027
O	-1.07996	-1.50696	2.63816
O	0.06710	-3.23180	1.17201
C	-2.18020	-2.15827	0.32864
C	-3.38285	-1.68769	0.83710
C	-2.11128	-2.81372	-0.89742
C	-4.54646	-1.88689	0.10191
H	-3.40197	-1.18492	1.79263
C	-3.27789	-2.99834	-1.62544
H	-1.16455	-3.18965	-1.25980
C	-4.49390	-2.53939	-1.12382
H	-5.49160	-1.53096	0.49011

				H	-3.24200	-3.51162	-2.57734
				H	-5.40233	-2.69487	-1.69140
2a				3a			
C	-0.39271	-0.58625	-0.14367	C	-0.95454	-0.59353	0.52623
C	0.76872	-1.10298	-0.61250	C	1.16593	0.59262	0.13443
C	-0.75259	0.88196	-0.12265	H	1.70502	0.77172	-0.79404
H	-1.20144	1.14500	0.83212	H	1.91058	0.44285	0.92022
H	-1.48020	1.11578	-0.90391	C	0.39062	1.88147	0.47076
C	0.46713	1.76081	-0.34753	C	-0.59989	1.70582	1.63490
C	1.28128	1.20825	-1.50676	H	-1.17787	2.61786	1.76279
H	2.09288	1.88789	-1.72919	H	-0.00667	1.56305	2.54212
H	0.61288	1.20321	-2.37300	C	-1.42253	0.50002	1.35313
C	1.75760	-0.19196	-1.22024	O	-0.29171	2.22756	-0.74268
O	1.18285	1.74810	0.89482	O	1.28387	2.91582	0.90154
O	0.11731	3.09923	-0.72805	C	-0.98543	3.38859	-0.87691
C	2.36800	2.39044	1.05125	C	2.21743	3.45538	0.06982
C	-0.61964	3.90189	0.08796	O	2.43172	3.07800	-1.05171
O	-1.07755	3.56301	1.14710	O	-1.08293	4.22970	-0.02077
O	2.91522	3.04022	0.19697	C	2.91205	4.59561	0.75781
C	-0.75264	5.26789	-0.52413	H	2.18842	5.38872	0.95202
H	0.22973	5.74143	-0.56225	H	3.30998	4.27375	1.72031
H	-1.11730	5.19203	-1.54833	H	3.71136	4.97093	0.12568
H	-1.42863	5.87135	0.07463	C	-1.58590	3.46519	-2.25097
C	2.87444	2.18511	2.45049	H	-2.16727	4.37769	-2.34490
H	3.85014	2.64947	2.55853	H	-0.78971	3.45041	-2.99625
H	2.17120	2.62699	3.15780	H	-2.21677	2.59416	-2.43127
H	2.93221	1.11973	2.67543	C	-3.69551	0.18338	2.60447
C	4.04251	0.32508	-2.13731	H	-3.82098	-0.61498	3.34194
H	3.95791	1.35802	-1.80623	H	-3.53157	1.12299	3.13294
H	5.04579	-0.02521	-1.88972	H	-4.63932	0.24404	2.05764
H	3.96486	0.31711	-3.22947	C	-2.57367	-0.12238	1.68903
C	3.01107	-0.58657	-1.52719	C	-2.28410	-1.34196	0.77571
C	1.10844	-2.54337	-0.52006	H	-2.14291	-2.28553	1.30886
H	0.29839	-3.20836	-0.76814	C	-3.27591	-1.56674	-0.40266
C	2.02733	-3.05456	0.58198	C	-3.53990	-0.26153	-1.15841
C	2.57623	-2.09077	1.60926	H	-4.20110	-0.44172	-2.00723
H	1.83052	-1.90147	2.38502	H	-4.00050	0.49822	-0.52596
H	3.45981	-2.51609	2.09250	H	-2.60336	0.14430	-1.54370
H	2.85704	-1.12938	1.18154	C	-2.71833	-2.60804	-1.39049

C	1.69122	-4.41618	1.14923	H	-3.47376	-2.83265	-2.14553
H	0.95012	-4.33304	1.94698	H	-1.82985	-2.23380	-1.89693
H	1.28155	-5.07641	0.38350	H	-2.44498	-3.53452	-0.88668
H	2.58497	-4.89104	1.56417	C	-4.53445	-2.15522	0.20146
C	2.50632	-3.00135	-0.84703	H	-4.36893	-3.07584	0.75761
H	2.57235	-3.96294	-1.34168	C	-5.77563	-1.69791	0.09578
C	3.51379	-1.98881	-1.32622	H	-6.01744	-0.79253	-0.44650
H	4.37654	-1.94234	-0.64881	H	-6.60388	-2.22568	0.55174
H	3.93229	-2.32081	-2.28294	C	0.27239	-0.62692	0.00316
S	-1.63221	-1.55744	0.72858	S	0.94648	-2.03979	-0.83978
O	-1.60040	-1.13814	2.13386	O	1.09013	-1.72960	-2.26641
C	-3.18953	-0.97751	0.03604	C	2.60447	-2.17753	-0.15865
C	-3.98103	-0.10828	0.77409	C	3.68544	-1.70939	-0.89373
H	-3.64518	0.22779	1.74474	H	3.52060	-1.27095	-1.86776
C	-5.20370	0.29808	0.25149	C	4.96446	-1.83424	-0.36329
H	-5.83357	0.96957	0.82006	H	5.81685	-1.48084	-0.92840
C	-5.61616	-0.16108	-0.99423	C	5.14702	-2.41681	0.88601
H	-6.56985	0.15522	-1.39689	H	6.14481	-2.51398	1.29430
C	-4.81208	-1.03306	-1.72374	C	4.05391	-2.88369	1.61140
H	-5.14074	-1.39660	-2.68850	C	2.77261	-2.76689	1.08964
H	-2.96728	-2.14384	-1.75339	H	1.91373	-3.14136	1.62943
C	-3.59190	-1.44902	-1.20889	H	4.20106	-3.34596	2.57873
O	-1.53670	-2.98500	0.41411	O	0.19738	-3.22966	-0.42954
COM				TS1			
C	2.44388	-0.70863	-1.34079	C	1.23748	0.86933	-0.72241
C	2.70202	-1.21851	1.14991	C	1.81756	-1.64249	-0.62518
H	3.75800	-1.39213	1.35275	H	2.71272	-2.15546	-0.96122
H	2.13835	-1.92991	1.75633	H	0.98506	-2.00552	-1.22553
C	2.34259	0.16963	1.68132	C	1.57989	-2.09869	0.82418
C	0.83666	0.53030	1.51925	C	0.11955	-1.98090	1.29870
H	0.51784	1.00271	2.44684	H	0.01472	-2.60178	2.18691
H	0.25898	-0.39035	1.42720	H	-0.52765	-2.39387	0.52898
C	0.51404	1.42945	0.41238	C	-0.31707	-0.63704	1.67487
O	3.21898	1.08933	1.04313	O	2.50268	-1.37157	1.62307
O	2.52095	0.15228	3.11140	O	1.78515	-3.52044	0.90646
C	3.27975	2.39241	1.43789	C	2.62671	-1.57201	2.96371
C	3.75223	0.05213	3.68976	C	2.99993	-4.10620	0.70685
O	4.78434	-0.05953	3.08321	O	3.99817	-3.51611	0.38840

O	2.58401	2.87027	2.29403	O	1.98512	-2.37091	3.59406
C	3.61808	0.12810	5.18332	C	2.89595	-5.58225	0.96096
H	3.23743	1.11224	5.46074	H	2.63903	-5.75058	2.00770
H	2.90063	-0.61184	5.53768	H	2.09793	-6.01433	0.35721
H	4.58812	-0.03650	5.64320	H	3.84448	-6.05850	0.73104
C	4.35137	3.10676	0.66845	C	3.67486	-0.64932	3.51276
H	4.29893	4.17239	0.87162	H	3.84978	-0.87510	4.56056
H	5.32364	2.72109	0.98051	H	4.59459	-0.74908	2.93695
H	4.25414	2.91221	-0.39989	H	3.33898	0.38382	3.40572
C	1.02582	3.12039	-1.58588	C	-0.72101	1.19659	3.56030
H	0.86401	4.16605	-1.32170	H	-1.72372	1.10189	3.97870
H	2.09275	2.96382	-1.75970	H	-0.00083	0.90244	4.32651
H	0.49154	2.92230	-2.51534	H	-0.54883	2.23778	3.29544
C	0.57293	2.23559	-0.51479	C	-0.55656	0.30741	2.41283
C	2.47658	-0.05485	-2.46171	C	0.82220	2.11971	-0.71775
H	1.55281	0.38097	-2.83371	H	0.28893	2.46500	-1.59996
C	3.71716	0.11829	-3.33356	C	1.22732	3.21915	0.26227
C	4.95210	-0.48929	-2.67085	C	2.09855	2.67096	1.39109
H	5.82435	-0.37202	-3.31448	H	2.40972	3.47557	2.05666
H	5.16500	-0.02005	-1.70965	H	1.56907	1.91798	1.97343
H	4.80024	-1.55456	-2.49975	H	2.99894	2.21122	0.98494
C	3.43565	-0.60489	-4.67093	C	2.05359	4.22907	-0.58115
H	4.29155	-0.49422	-5.33885	H	2.40275	5.03048	0.07044
H	3.25657	-1.66582	-4.49391	H	2.90656	3.73188	-1.03979
H	2.55875	-0.18734	-5.16886	H	1.44453	4.67468	-1.36958
C	3.86425	1.59990	-3.61462	C	-0.00597	3.95340	0.74606
H	3.01164	2.04438	-4.12388	H	-0.74814	4.14357	-0.02426
C	4.90616	2.37099	-3.32885	C	-0.21450	4.44697	1.95958
H	5.79063	1.99209	-2.83320	H	0.49404	4.32309	2.76830
H	4.91114	3.41973	-3.59784	H	-1.11176	5.00950	2.18271
Rh	-1.62303	2.08610	0.01112	Rh	-1.43767	0.78649	0.20559
Cl	-1.83903	0.18913	-1.58089	Cl	-1.43801	-1.11752	-1.62600
C	-1.38300	3.59701	1.08758	C	-2.74083	1.56404	1.33128
C	-3.31209	2.79929	-0.64740	C	-2.21690	1.76024	-1.21020
O	-1.21798	4.50838	1.74554	O	-3.55563	2.02098	1.97959
O	-4.27444	3.24157	-1.05212	O	-2.65337	2.34838	-2.07711
Rh	-3.80276	-0.49068	-0.25480	Rh	-3.83393	-1.20073	-0.99252
Cl	-2.64639	0.14113	1.77987	Cl	-3.37912	-2.10831	1.19823
C	-4.70840	-0.94752	-1.84101	C	-4.25682	-0.58982	-2.71796
O	-5.24876	-1.21084	-2.80583	O	-4.51188	-0.23746	-3.77092
C	-5.30698	-0.91513	0.79189	C	-5.64374	-1.32331	-0.51938

O	-6.20996	-1.15476	1.43771	O	-6.73723	-1.41699	-0.22165
C	2.42848	-1.49258	-0.30481	C	2.00289	-0.17139	-0.87976
S	2.21204	-3.26076	-0.68598	S	3.65453	0.27859	-1.57440
O	3.30548	-3.97939	-0.02364	O	4.65026	-0.04516	-0.55300
O	2.01576	-3.41105	-2.12610	O	3.57514	1.64088	-2.10239
C	0.68933	-3.69431	0.15688	C	3.88868	-0.83997	-2.95455
C	0.71083	-4.69542	1.11869	C	4.69733	-1.95786	-2.78915
C	-0.48267	-3.02666	-0.17927	C	3.27799	-0.54723	-4.16930
C	-0.47944	-5.04647	1.74630	C	4.90081	-2.80025	-3.87594
C	-1.65905	-3.37343	0.46806	C	3.48747	-1.39916	-5.24467
C	-1.65913	-4.38467	1.42435	C	4.29769	-2.52194	-5.09754
H	1.64285	-5.18630	1.36014	H	5.15563	-2.15477	-1.83025
H	-0.47870	-2.24294	-0.92467	H	2.66738	0.33891	-4.27116
H	-0.48128	-5.83128	2.49126	H	5.53265	-3.67161	-3.76634
H	-2.57000	-2.83544	0.23409	H	3.02580	-1.18317	-6.19886
H	-2.58126	-4.65264	1.92374	H	4.46065	-3.18066	-5.94077
INT1				TS2			
C	-1.31766	0.40838	-0.82430	C	-5.68881	-3.31295	3.14933
C	0.71027	1.20479	0.44031	C	-6.98742	-4.54665	4.93008
H	1.38754	2.04344	0.31106	H	-7.69997	-4.26605	5.69805
H	1.26761	0.29760	0.20567	H	-6.14482	-5.05007	5.40944
C	0.30635	1.16257	1.92060	C	-7.66979	-5.53819	3.98843
C	-0.16306	-0.21939	2.39553	C	-6.68330	-6.13821	2.99667
H	-0.27101	-0.17030	3.47975	H	-7.22259	-6.80634	2.32339
H	0.62836	-0.93335	2.16976	H	-5.98512	-6.75282	3.57898
C	-1.43107	-0.73119	1.87981	C	-5.88848	-5.22613	2.15603
O	-0.67910	2.17002	2.10533	O	-8.72857	-4.81832	3.35891
O	1.46847	1.36742	2.74048	O	-8.14422	-6.68016	4.71125
C	-1.18642	2.48504	3.32598	C	-9.59024	-5.40846	2.48851
C	2.12883	2.56003	2.77388	C	-9.12379	-6.58017	5.65486
O	1.82479	3.52351	2.12256	O	-9.66249	-5.55248	5.96988
O	-0.87071	1.94339	4.35450	O	-9.53924	-6.56643	2.16106
C	3.26502	2.48368	3.75227	C	-9.42516	-7.93971	6.21508
H	2.86685	2.33584	4.75720	H	-9.78789	-8.58926	5.41740
H	3.90288	1.63004	3.52279	H	-8.51535	-8.38829	6.61537
H	3.83891	3.40490	3.71471	H	-10.17596	-7.85390	6.99481
C	-2.18112	3.59796	3.18330	C	-10.60049	-4.40412	2.01843
H	-2.54551	3.89266	4.16299	H	-11.29787	-4.87885	1.33473
H	-1.71553	4.44008	2.67193	H	-11.13070	-3.98931	2.87610

H	-3.01095	3.26573	2.55771	H	-10.09186	-3.57511	1.52485
C	-3.83691	-1.77943	2.27379	C	-5.00361	-5.79682	-0.23228
H	-3.77688	-2.85651	2.43629	H	-4.10945	-6.42300	-0.24301
H	-4.12510	-1.30484	3.21330	H	-5.86675	-6.40567	-0.50691
H	-4.60667	-1.58639	1.52981	H	-4.87194	-5.01186	-0.97769
C	-2.53673	-1.25080	1.86322	C	-5.17715	-5.21501	1.10703
C	-2.49366	0.05749	-1.46369	C	-5.04959	-2.39709	2.27751
H	-2.38590	-0.25914	-2.49686	H	-4.46752	-1.65169	2.80899
C	-3.92144	0.54393	-1.18420	C	-5.63986	-1.81019	0.97122
C	-4.02423	1.38304	0.08831	C	-6.98591	-2.42579	0.58147
H	-5.04456	1.74322	0.21992	H	-7.41112	-1.87420	-0.25780
H	-3.73878	0.82183	0.97571	H	-6.90023	-3.47047	0.29541
H	-3.37516	2.25534	0.01843	H	-7.68773	-2.35638	1.41272
C	-4.33243	1.41870	-2.40029	C	-5.86044	-0.29585	1.22684
H	-5.35196	1.77530	-2.24999	H	-6.23896	0.16864	0.31580
H	-3.65914	2.26489	-2.50974	H	-6.56979	-0.13488	2.03467
H	-4.31033	0.83850	-3.32469	H	-4.92483	0.19640	1.49770
C	-4.84261	-0.65876	-1.20496	C	-4.60696	-1.89612	-0.13044
H	-4.61304	-1.37933	-1.98552	H	-3.63739	-1.48777	0.14198
C	-5.91156	-0.86352	-0.44648	C	-4.78775	-2.33044	-1.37066
H	-6.21287	-0.17442	0.33214	H	-5.73500	-2.72496	-1.71502
H	-6.53663	-1.73495	-0.59330	H	-3.98359	-2.29414	-2.09445
Rh	-1.57053	-1.63408	-0.30576	Rh	-3.85471	-4.16738	2.36365
Cl	1.92274	-1.13228	-1.97209	Cl	-3.77691	-5.68042	6.01680
C	-2.62764	-3.38099	-0.13788	C	-2.41605	-3.88140	0.98534
C	-1.01664	-2.22051	-2.04086	C	-2.73128	-3.42389	3.84644
O	-3.25483	-4.31950	-0.09562	O	-1.60137	-3.74480	0.21434
O	-0.79378	-2.65256	-3.06073	O	-2.04162	-2.98551	4.62451
Rh	2.75590	-2.40141	-0.10334	Rh	-3.79936	-7.64892	4.62783
Cl	0.49850	-3.07697	0.60914	Cl	-2.69120	-6.45957	2.78487
C	4.48064	-1.92722	-0.66388	C	-4.58501	-8.55673	6.06902
O	5.52218	-1.64374	-1.02293	O	-5.05546	-9.09335	6.95481
C	3.42553	-3.40378	1.33913	C	-3.77628	-9.20047	3.56369
O	3.82688	-4.02126	2.20798	O	-3.74510	-10.13820	2.91867
C	-0.43738	1.33092	-0.51628	C	-6.50432	-3.33985	4.18981
S	-0.61013	2.93879	-1.36353	S	-7.24433	-1.74621	4.69088
O	-1.00631	3.96532	-0.39750	O	-8.61204	-1.67078	4.17552
O	-1.43845	2.72496	-2.55372	O	-6.29180	-0.68577	4.35235
C	1.05813	3.30085	-1.90971	C	-7.31926	-1.86446	6.47700
C	1.76662	4.31990	-1.28675	C	-8.54646	-2.07764	7.09132
C	1.59708	2.56376	-2.95871	C	-6.14608	-1.71349	7.20838

C	3.04519	4.61837	-1.74264	C	-8.59672	-2.13228	8.47901
C	2.87793	2.86673	-3.39775	C	-6.21008	-1.77609	8.59312
C	3.59703	3.89489	-2.79405	C	-7.43311	-1.98293	9.22537
H	1.32126	4.85809	-0.46282	H	-9.43656	-2.19529	6.49002
H	1.02725	1.76919	-3.41897	H	-5.20611	-1.54168	6.70290
H	3.60889	5.41372	-1.27345	H	-9.54457	-2.29386	8.97456
H	3.31421	2.30001	-4.20926	H	-5.30774	-1.65983	9.17832
H	4.59439	4.12932	-3.14341	H	-7.47774	-2.02922	10.30571
INT2				TS3			
C	1.98093	-0.25539	-0.64038	C	8.15397	0.81486	-9.31768
C	1.01116	0.62571	-0.31162	C	6.81481	0.63831	-9.29864
C	2.88165	-0.88242	0.39699	C	9.06192	-0.03499	-10.17276
H	3.87037	-1.06078	-0.01951	H	10.02360	-0.17446	-9.68432
H	2.48355	-1.84115	0.73946	H	9.24301	0.44181	-11.13988
C	3.02447	0.01967	1.61986	C	8.45137	-1.40829	-10.44691
C	1.65674	0.38465	2.17833	C	7.03753	-1.28142	-10.99937
H	1.77814	1.14233	2.94939	H	6.58467	-2.26906	-11.03631
H	1.27790	-0.51306	2.67164	H	7.14159	-0.94006	-12.03249
C	0.68851	0.82845	1.10276	C	6.19003	-0.29637	-10.22640
O	3.75634	1.16754	1.16714	O	8.49063	-2.10354	-9.19109
O	3.69842	-0.65570	2.69096	O	9.18513	-2.10831	-11.46178
C	4.18126	2.13473	2.02199	C	8.17248	-3.42182	-9.09175
C	4.99770	-1.04820	2.58698	C	10.47320	-2.50585	-11.27051
O	5.67507	-0.91080	1.60263	O	11.12469	-2.25807	-10.29030
O	3.96826	2.14155	3.20695	O	7.77221	-4.09866	-10.00335
C	5.45418	-1.65026	3.88529	C	10.93692	-3.31710	-12.44615
H	5.48396	-0.87096	4.64858	H	10.40148	-4.26823	-12.45009
H	4.75025	-2.41105	4.22189	H	10.70589	-2.80776	-13.38115
H	6.44445	-2.07824	3.75965	H	12.00457	-3.49920	-12.36508
C	4.96859	3.16804	1.26847	C	8.42518	-3.90446	-7.69234
H	5.22885	3.98564	1.93424	H	8.08824	-4.93237	-7.59507
H	5.87449	2.70808	0.87090	H	9.49405	-3.84187	-7.48267
H	4.39336	3.53738	0.41947	H	7.91445	-3.26813	-6.96983
C	-1.15287	1.38542	2.72911	C	4.05053	-0.84687	-11.43398
H	-1.90600	0.61566	2.91457	H	3.53909	-0.15916	-12.11131
H	-0.39515	1.31808	3.51173	H	4.64437	-1.53827	-12.03469
H	-1.66772	2.34266	2.83490	H	3.27123	-1.42388	-10.92737
C	-0.56550	1.22731	1.36908	C	4.87633	-0.10036	-10.43954
C	0.15987	1.43518	-1.25116	C	5.83901	1.29329	-8.38033
H	-0.04544	0.88690	-2.16502	H	6.10405	2.31148	-8.12977

C	0.74688	2.82294	-1.64283	C	5.46914	0.49465	-7.10153
C	1.20576	3.66626	-0.45201	C	5.55570	-1.02578	-7.24931
H	1.98843	3.14320	0.09455	H	6.57310	-1.31777	-7.50295
H	1.62185	4.61046	-0.80510	H	5.29395	-1.49559	-6.30017
H	0.41211	3.89339	0.25525	H	4.89675	-1.41517	-8.02214
C	1.99456	2.59217	-2.53927	C	6.41624	0.92510	-5.96153
H	2.77991	2.06851	-1.99551	H	7.44434	0.63423	-6.17677
H	1.75033	2.01366	-3.42738	H	6.39704	2.00352	-5.81074
H	2.38581	3.56093	-2.85170	H	6.10678	0.43581	-5.03527
C	-0.25956	3.52367	-2.52671	C	4.06919	0.94407	-6.73472
H	-0.62394	2.90933	-3.34691	H	3.99768	1.97048	-6.38903
C	-0.67735	4.78010	-2.44307	C	2.96465	0.19595	-6.74191
H	-0.34925	5.45193	-1.66052	H	2.97417	-0.84559	-7.03216
H	-1.37122	5.18423	-3.16876	H	2.01367	0.61064	-6.43365
Rh	-1.75755	1.37319	-0.31176	Rh	4.04920	1.50279	-9.48657
Cl	-1.73797	-1.12907	-0.55475	Cl	5.36818	2.88248	-10.97437
C	-1.91322	3.21071	0.10153	C	1.89121	0.52628	-9.53276
C	-2.88157	1.43269	-2.06985	C	3.31643	3.25616	-8.69138
O	-2.15740	4.25963	0.45505	O	0.81785	0.19190	-9.48562
O	-3.51824	1.46811	-2.99767	O	2.95265	4.25676	-8.31569
Rh	-3.72234	-1.48892	0.83893	Rh	3.96637	3.17839	-12.97077
Cl	-4.06160	0.92904	0.86069	Cl	1.98718	2.61809	-11.70514
C	-3.45221	-3.34831	0.78828	C	5.50104	3.61835	-13.96294
O	-3.28190	-4.47128	0.74442	O	6.43404	3.88786	-14.55722
C	-5.26099	-1.72492	1.89461	C	2.86732	3.45346	-14.47023
O	-6.19478	-1.85310	2.52840	O	2.19046	3.62474	-15.36660
S	2.34124	-0.83675	-2.29668	S	9.03330	2.06176	-8.38590
O	3.71656	-0.46523	-2.64171	O	10.01089	1.39778	-7.51920
O	1.25503	-0.48606	-3.21752	O	8.09815	3.02275	-7.79311
C	2.30942	-2.62387	-2.09648	C	9.94068	2.92239	-9.67608
C	3.50067	-3.33204	-2.17453	C	11.32277	2.80847	-9.72415
C	1.08920	-3.26368	-1.90850	C	9.23734	3.70592	-10.58552
C	3.46654	-4.71806	-2.06773	C	12.01962	3.50910	-10.70294
C	1.06901	-4.64697	-1.79458	C	9.94318	4.39153	-11.56405
C	2.25508	-5.37230	-1.87633	C	11.33186	4.29577	-11.61960
H	4.42924	-2.80112	-2.32909	H	11.83447	2.19039	-9.00002
H	0.17464	-2.68925	-1.85484	H	8.15930	3.77731	-10.52650
H	4.38625	-5.28399	-2.13650	H	13.09841	3.43823	-10.74784
H	0.12752	-5.15992	-1.64749	H	9.41109	5.00395	-12.28029
H	2.23285	-6.45120	-1.79292	H	11.87812	4.83692	-12.38134

INT3				TS4			
C	-2.26523	0.35610	-0.65848	C	-10.84461	-1.57723	-5.67302
C	-1.25688	-0.52043	-0.45799	C	-9.58465	-1.73149	-6.14127
C	-3.17248	0.83026	0.45214	C	-12.08679	-1.55138	-6.52962
H	-4.16828	1.03033	0.06502	H	-12.75138	-0.76101	-6.19121
H	-2.79132	1.75257	0.89873	H	-12.63126	-2.49611	-6.44091
C	-3.27492	-0.21190	1.55999	C	-11.75979	-1.33858	-8.00074
C	-1.89027	-0.62371	2.03608	C	-10.60648	-2.23843	-8.41749
H	-1.99051	-1.43693	2.74944	H	-10.40979	-2.10767	-9.47532
H	-1.48808	0.23347	2.58179	H	-10.93382	-3.27187	-8.26894
C	-0.96051	-0.97925	0.89741	C	-9.38713	-1.98536	-7.57496
O	-4.01198	-1.30418	0.99160	O	-11.43057	0.05582	-8.12191
O	-3.92399	0.31836	2.72375	O	-12.84779	-1.69820	-8.85569
C	-4.38754	-2.37898	1.73093	C	-11.08578	0.61163	-9.31274
C	-5.22847	0.70934	2.70215	C	-14.05162	-1.05785	-8.78696
O	-5.93382	0.67547	1.72905	O	-14.30294	-0.16740	-8.02059
O	-4.10108	-2.54792	2.88866	O	-11.00143	0.00862	-10.35169
C	-5.64622	1.16495	4.07125	C	-14.98849	-1.62622	-9.81358
H	-5.57162	0.32993	4.76925	H	-14.56413	-1.49487	-10.80968
H	-4.97812	1.94912	4.42781	H	-15.11385	-2.69729	-9.65103
H	-6.66856	1.52973	4.03716	H	-15.94888	-1.12366	-9.74723
C	-5.22905	-3.30131	0.89652	C	-10.84420	2.08366	-9.13706
H	-5.44163	-4.20811	1.45508	H	-10.51290	2.51445	-10.07733
H	-6.16154	-2.79617	0.64006	H	-11.76728	2.56495	-8.81162
H	-4.72120	-3.53816	-0.03824	H	-10.10006	2.25426	-8.35835
C	0.77532	-1.97620	2.42054	C	-7.84377	-2.57767	-9.48092
H	1.58724	-1.30768	2.72251	H	-8.02929	-3.64926	-9.59624
H	0.01866	-1.95185	3.20601	H	-8.46832	-2.04887	-10.20399
H	1.19124	-2.98527	2.38708	H	-6.80429	-2.39987	-9.74758
C	0.23673	-1.55757	1.09395	C	-8.14398	-2.17777	-8.07216
C	-0.35704	-1.09896	-1.50398	C	-8.33546	-1.78232	-5.31587
H	-0.12436	-0.39254	-2.28701	H	-8.49530	-2.25801	-4.36023
C	-0.74362	-2.47653	-2.10860	C	-7.48565	-0.47937	-5.14972
C	-2.00814	-3.10755	-1.52333	C	-8.25431	0.81814	-5.42478
H	-2.87798	-2.50162	-1.77606	H	-9.01992	0.96274	-4.66300
H	-2.15083	-4.10527	-1.94280	H	-7.56988	1.66851	-5.38876
H	-1.96526	-3.19308	-0.43897	H	-8.75302	0.81767	-6.39344
C	-0.87433	-2.39335	-3.63186	C	-6.88699	-0.40104	-3.74420
H	-1.72367	-1.77327	-3.90889	H	-7.67988	-0.29093	-3.00722
H	0.01729	-1.95249	-4.08256	H	-6.31091	-1.29165	-3.49245
H	-1.01218	-3.39250	-4.05274	H	-6.21933	0.45976	-3.66991

C	0.50582	-3.27713	-1.76312	C	-6.39943	-0.77728	-6.17374
H	1.17732	-3.50287	-2.58326	H	-5.35652	-0.75149	-5.88344
C	0.80457	-3.80790	-0.53680	C	-6.72092	-0.71002	-7.54399
H	0.07450	-3.84479	0.25626	H	-7.50506	-0.05116	-7.87768
H	1.66961	-4.44861	-0.43416	H	-5.92826	-0.85318	-8.26521
Rh	1.48043	-1.59557	-0.55638	Rh	-6.91155	-2.84304	-6.44386
Cl	1.81041	0.83102	-0.12229	Cl	-8.33851	-5.00026	-6.45768
C	3.17658	-2.25705	0.49116	C	-5.38162	-3.61194	-7.65427
C	2.59870	-1.31340	-2.28661	C	-6.04957	-3.52118	-4.78762
O	3.99429	-2.75341	1.08603	O	-4.54026	-3.85616	-8.36356
O	3.11555	-1.12223	-3.26816	O	-5.60253	-3.91701	-3.83009
Rh	3.98120	1.25934	0.97009	Rh	-7.20530	-7.06258	-7.18290
Cl	5.16317	-0.04462	-0.67157	Cl	-5.11577	-6.39626	-6.18777
C	3.08210	2.28418	2.26483	C	-8.82020	-7.60856	-7.97098
O	2.53504	2.90608	3.04682	O	-9.80128	-7.93706	-8.44893
C	5.64926	1.64122	1.74033	C	-6.34968	-8.65296	-7.68774
O	6.66793	1.87371	2.18719	O	-5.81958	-9.61588	-7.97960
S	-2.68829	1.08812	-2.23352	S	-11.24500	-1.43579	-3.92772
O	-4.12308	0.89179	-2.45902	O	-12.37412	-0.51176	-3.79962
C	-2.41920	2.83879	-1.93089	C	-11.84423	-3.08184	-3.52249
C	-3.50377	3.70378	-1.96251	C	-13.11699	-3.21445	-2.98459
H	-4.49392	3.31255	-2.14861	H	-13.73286	-2.33736	-2.84623
C	-3.28451	5.06301	-1.76472	C	-13.56819	-4.48164	-2.63101
H	-4.11895	5.75125	-1.79513	H	-14.55540	-4.59872	-2.20366
C	-1.99816	5.53377	-1.52953	C	-12.75597	-5.59197	-2.83044
H	-1.83139	6.59171	-1.37417	H	-13.11299	-6.57695	-2.55876
C	-0.92089	4.65139	-1.49175	C	-11.48682	-5.44424	-3.38471
H	0.07891	5.02172	-1.30754	H	-10.85737	-6.30843	-3.54996
H	-0.29419	2.60205	-1.66919	H	-10.03912	-4.07412	-4.17087
C	-1.12566	3.29416	-1.69499	C	-11.02145	-4.18411	-3.73161
O	-1.74952	0.66738	-3.27776	O	-10.03677	-1.17706	-3.13918
INT4				TS5			
C	2.23722	0.62197	0.88670	C	-2.17565	0.45169	-0.26978
C	1.47288	-0.48812	0.89006	C	-1.28394	-0.47910	-0.64052
C	3.04775	1.13340	-0.27398	C	-2.82047	0.54308	1.08680
H	4.07282	1.32619	0.03050	H	-3.90129	0.62317	0.99330
H	2.62780	2.08340	-0.61692	H	-2.46756	1.44806	1.58737
C	3.03649	0.17057	-1.45322	C	-2.47939	-0.64313	1.98569
C	1.65651	-0.47193	-1.60663	C	-1.02119	-1.06776	1.78866
H	1.64526	-1.04758	-2.52117	H	-0.78061	-1.84087	2.50675

H	0.92794	0.33541	-1.69500	H	-0.40016	-0.19425	1.99256
C	1.36754	-1.29380	-0.37538	C	-0.83907	-1.50171	0.35849
O	4.05380	-0.80202	-1.15486	O	-3.39784	-1.68266	1.60679
O	3.27979	0.83024	-2.69454	O	-2.58865	-0.31557	3.36909
C	4.39600	-1.78167	-2.03268	C	-3.44918	-2.87001	2.26932
C	4.45908	1.47833	-2.93098	C	-3.78015	0.06984	3.91413
O	5.34912	1.57197	-2.12967	O	-4.79834	0.19602	3.28843
O	3.86960	-1.95342	-3.10169	O	-2.72803	-3.17088	3.18434
C	4.47134	2.02212	-4.32964	C	-3.61722	0.28672	5.38975
H	4.43003	1.19368	-5.03840	H	-3.30353	-0.64602	5.86028
H	3.59252	2.64329	-4.50266	H	-2.83581	1.02387	5.57597
H	5.37808	2.59883	-4.48674	H	-4.55857	0.62154	5.81520
C	5.52101	-2.60019	-1.46824	C	-4.53743	-3.72851	1.69228
H	5.77331	-3.40070	-2.15743	H	-4.52929	-4.70168	2.17430
H	6.38888	-1.96099	-1.30220	H	-5.50203	-3.24356	1.84847
H	5.23258	-3.01220	-0.50021	H	-4.39950	-3.83677	0.61589
C	1.04008	-3.31803	-1.83078	C	-0.24852	-3.89326	0.99165
H	0.60113	-2.68821	-2.59880	H	0.03012	-3.53356	1.97639
H	2.03893	-3.60554	-2.16965	H	-1.14533	-4.51107	1.10284
H	0.44882	-4.22865	-1.76103	H	0.54236	-4.54559	0.62259
C	1.12931	-2.64753	-0.48023	C	-0.52903	-2.80611	-0.00545
C	0.48989	-0.88101	1.92340	C	-0.45967	-0.49097	-1.87858
H	0.09653	-0.05659	2.49668	H	0.04825	0.43432	-2.11667
C	0.77055	-2.14431	2.75899	C	-0.86513	-1.30971	-3.08573
C	2.25149	-2.32106	3.12440	C	-2.35191	-1.54788	-3.31054
H	2.54706	-1.53904	3.82368	H	-2.80617	-0.64627	-3.71920
H	2.41111	-3.28980	3.60371	H	-2.49802	-2.35982	-4.02597
H	2.91154	-2.25008	2.26083	H	-2.88804	-1.79488	-2.39557
C	-0.02973	-2.12660	4.06198	C	-0.19020	-0.80354	-4.35376
H	0.27272	-1.27862	4.67674	H	-0.63622	0.14249	-4.65943
H	-1.10417	-2.05838	3.89917	H	0.87884	-0.64115	-4.20269
H	0.15990	-3.04126	4.62665	H	-0.31209	-1.52530	-5.16350
C	0.21114	-3.16595	1.77546	C	-0.07404	-2.37062	-2.39563
H	-0.42408	-3.93563	2.20063	H	0.79327	-2.74863	-2.91714
C	1.13497	-3.64285	0.68759	C	-0.73376	-3.31270	-1.42486
H	2.16167	-3.80466	1.03087	H	-1.79904	-3.45827	-1.62579
H	0.78047	-4.59787	0.30598	H	-0.25325	-4.28603	-1.51271
Rh	-0.87172	-1.78015	0.58748	Rh	1.19247	-1.38918	-0.67996
Cl	-1.56174	0.39235	-0.68523	Cl	1.43382	1.19904	0.43514
C	-1.96193	-3.06940	-0.65237	C	2.43773	-2.13043	0.69185
C	-2.32730	-1.54282	1.82209	C	2.68326	-1.07676	-1.89904

O	-2.43767	-3.89945	-1.24872	O	3.05457	-2.63262	1.49425
O	-3.20000	-1.36882	2.51841	O	3.49658	-0.91607	-2.66774
Rh	-3.95104	0.87379	-1.06678	Rh	3.66418	2.17317	0.77529
Cl	-4.61028	-1.39521	-0.60936	Cl	4.77830	0.07400	0.35163
C	-3.47316	2.65265	-1.42440	C	2.83303	3.81712	1.10923
O	-3.17785	3.73368	-1.63399	O	2.32184	4.81741	1.31150
C	-5.76455	1.23476	-1.37740	C	5.37148	2.90215	1.03617
O	-6.86756	1.43626	-1.56687	O	6.41436	3.33012	1.19316
S	2.38685	1.70047	2.32255	S	-2.77068	1.69683	-1.42577
O	3.79471	2.09169	2.41774	O	-4.20730	1.46137	-1.58939
C	1.44817	3.15665	1.84658	C	-2.56484	3.25182	-0.56135
C	2.08024	4.39264	1.86901	C	-3.69677	3.99287	-0.24790
H	3.12517	4.45424	2.13773	H	-4.67528	3.60760	-0.49643
C	1.34585	5.52780	1.54389	C	-3.53714	5.22662	0.37214
H	1.82269	6.49888	1.56508	H	-4.40761	5.82204	0.61393
C	0.00746	5.41331	1.18574	C	-2.26330	5.69077	0.68005
H	-0.55902	6.29787	0.92497	H	-2.14332	6.65090	1.16521
C	-0.60725	4.16450	1.15244	C	-1.13977	4.92793	0.37169
H	-1.64416	4.07537	0.85881	H	-0.15111	5.28837	0.62100
H	-0.36880	2.05649	1.45532	H	-0.41517	3.09771	-0.49513
C	0.11021	3.02572	1.48946	C	-1.28312	3.69942	-0.25863
O	1.74664	1.09299	3.49143	O	-1.91184	1.70769	-2.61263
TS6				1b			
C	-2.19970	5.39546	-6.92007	C	-0.61615	-0.62397	0.71308
C	-4.37222	4.24811	-6.70080	C	0.38172	-1.12512	0.04334
H	-5.39864	4.57249	-6.85737	C	-0.88404	0.81479	1.08362
H	-4.36093	3.60145	-5.81956	H	-0.14871	1.13573	1.82257
C	-3.95483	3.39855	-7.91318	H	-1.85923	0.89674	1.55526
C	-2.46279	3.04210	-7.89966	C	-0.83346	1.83581	-0.05984
H	-2.18209	2.60332	-8.85465	C	0.53556	1.96520	-0.74690
H	-2.32226	2.26707	-7.13964	H	0.44063	2.73209	-1.51453
C	-1.63609	4.22651	-7.52652	H	0.73692	1.02231	-1.25567
O	-4.30209	4.19244	-9.05673	C	1.62318	2.27719	0.16982
O	-4.63062	2.13757	-7.90681	O	-1.19693	3.06235	0.58805
C	-4.21978	3.69891	-10.32411	O	-1.72117	1.48999	-1.13034
C	-5.98578	2.04592	-8.03312	C	-1.39492	4.21622	-0.10125
O	-6.72423	2.99061	-8.11885	C	-3.07302	1.50039	-0.97788
O	-3.81328	2.60051	-10.59945	O	-3.64122	1.78261	0.04417
C	-6.39641	0.60268	-8.06597	O	-1.31286	4.32094	-1.29790
H	-5.98371	0.13121	-8.95917	C	-3.73248	1.11322	-2.26939

H	-5.99224	0.07550	-7.20171	H	-3.37882	1.75687	-3.07470
H	-7.47999	0.53279	-8.07812	H	-3.46513	0.08547	-2.51995
C	-4.72594	4.71805	-11.30274	H	-4.81019	1.19378	-2.16506
H	-4.61270	4.33844	-12.31383	C	-1.74680	5.32258	0.85097
H	-5.77668	4.92654	-11.09690	H	-1.87229	6.25042	0.30080
H	-4.17958	5.65453	-11.18791	H	-2.66913	5.07083	1.37588
C	0.64001	3.77199	-8.56860	H	-0.96232	5.43194	1.60037
H	1.33245	3.13814	-8.01282	C	3.64229	2.81310	1.81265
H	0.08830	3.14939	-9.27887	H	3.31565	2.81349	2.85444
H	1.22977	4.49035	-9.14101	H	4.43261	2.06623	1.70979
C	-0.31509	4.47596	-7.65899	H	4.07530	3.79209	1.59804
C	-1.08081	6.38372	-7.07680	C	2.53167	2.52146	0.91643
H	-0.82833	6.95806	-6.18765	C	1.36290	-1.68707	-0.59517
C	-1.05320	7.28841	-8.32077	H	1.26332	-1.83680	-1.66825
C	-1.48592	6.59068	-9.61037	C	2.66481	-2.17971	0.03140
H	-1.55440	7.32155	-10.41633	C	2.68968	-1.90853	1.53477
H	-0.79001	5.81229	-9.91749	H	1.85327	-2.41362	2.01796
H	-2.47023	6.14207	-9.48492	H	3.61444	-2.28585	1.97296
C	-2.04354	8.45888	-8.05718	H	2.61457	-0.84193	1.75041
H	-1.96166	9.16900	-8.88058	C	2.73835	-3.70297	-0.21859
H	-3.07190	8.10331	-8.01086	H	1.89493	-4.20667	0.25558
H	-1.82030	8.97581	-7.12594	H	2.72115	-3.93013	-1.28640
C	0.31981	7.91254	-8.42483	H	3.66535	-4.10090	0.19712
H	0.66302	8.38997	-7.51075	C	3.79492	-1.50661	-0.72270
C	1.08241	7.97653	-9.50755	H	3.79219	-1.69364	-1.79553
H	0.79372	7.53236	-10.45111	C	4.75917	-0.74444	-0.21940
H	2.03963	8.48075	-9.48199	H	4.78338	-0.54699	0.84863
Rh	0.85480	5.28720	-5.95800	S	-1.74225	-1.86675	1.43047
Cl	-0.75440	4.50256	-4.21821	O	-2.30613	-1.28143	2.64958
C	2.24891	5.91928	-7.05781	O	-1.02451	-3.14033	1.48878
C	2.05774	5.49406	-4.44359	C	-3.07981	-2.06492	0.24963
O	3.18317	6.24080	-7.62054	C	-4.29783	-1.44304	0.48757
O	2.74429	5.57665	-3.54841	C	-2.87943	-2.87812	-0.86215
Rh	-0.59202	2.05764	-4.50014	C	-5.34106	-1.64578	-0.40951
Cl	1.66379	2.25803	-5.32680	H	-4.42440	-0.82227	1.36217
C	-2.33381	1.87747	-3.82357	C	-3.92625	-3.06742	-1.75316
O	-3.39087	1.77623	-3.41001	H	-1.92721	-3.36806	-1.00948
C	-0.39500	0.19746	-4.66853	C	-5.15570	-2.45332	-1.52521
O	-0.24989	-0.92566	-4.76224	H	-6.29730	-1.17146	-0.23306
C	-3.46586	5.43549	-6.48989	H	-3.78798	-3.70342	-2.61763
S	-4.14708	6.84424	-5.62736	H	-5.97187	-2.60985	-2.21867

O	-5.18993	7.44660	-6.46155	C	5.86400	-0.12528	-1.02105
C	-4.94573	6.10053	-4.20680	H	5.70816	-0.32754	-2.08487
C	-6.33199	6.01435	-4.18032	H	5.82648	0.96467	-0.90152
H	-6.90983	6.38974	-5.01285	C	7.25851	-0.61208	-0.60367
C	-6.94621	5.45774	-3.06467	H	7.31094	-1.69577	-0.74130
H	-8.02529	5.39116	-3.02390	H	7.39531	-0.43290	0.46743
C	-6.17566	4.99017	-2.00577	C	8.38274	0.06371	-1.38479
H	-6.65873	4.55600	-1.14002	H	8.37123	1.14614	-1.23557
C	-4.78688	5.07965	-2.05056	H	8.28465	-0.12202	-2.45726
C	-4.16053	5.64209	-3.15395	H	9.36112	-0.30564	-1.07170
H	-3.08379	5.72688	-3.19953				
H	-4.19102	4.71576	-1.22413				
O	-3.02873	7.66351	-5.15458				
2b				3b			
C	-0.67267	-0.55395	0.26581	C	-0.26497	-0.25956	0.45571
C	0.66715	-0.43803	0.07925	C	2.10087	0.33428	0.12384
C	-1.70382	0.44829	-0.20214	H	2.69026	0.38110	-0.79001
H	-2.48137	0.55948	0.54857	H	2.75972	-0.02050	0.92049
H	-2.18157	0.11656	-1.12792	C	1.68707	1.77591	0.47713
C	-1.07477	1.80548	-0.46589	C	0.66310	1.84574	1.62306
C	0.16903	1.62891	-1.31764	H	0.33893	2.87443	1.76193
H	0.57938	2.60279	-1.55080	H	1.18150	1.53915	2.53544
H	-0.17007	1.18891	-2.26038	C	-0.43924	0.90108	1.30557
C	1.18405	0.71691	-0.67394	O	1.14535	2.31109	-0.73787
O	-0.79537	2.36021	0.82745	O	2.81423	2.52730	0.94472
O	-1.93284	2.67012	-1.22475	C	0.77220	3.61252	-0.85352
C	-0.17633	3.55783	0.98061	C	3.87635	2.81111	0.14140
C	-3.15175	3.05791	-0.75836	O	3.99973	2.42278	-0.99000
O	-3.63331	2.69401	0.28160	O	0.88545	4.43592	0.01783
O	0.16792	4.27437	0.07494	C	4.84792	3.69022	0.87599
C	-3.78787	4.01267	-1.72926	H	4.37547	4.65162	1.08333
H	-3.16554	4.90342	-1.82444	H	5.11352	3.24323	1.83402
H	-3.85477	3.55563	-2.71690	H	5.73641	3.83862	0.26927
H	-4.77721	4.28710	-1.37531	C	0.21072	3.86031	-2.22406
C	0.00203	3.85429	2.44237	H	-0.70928	3.28667	-2.34922
H	0.46400	4.82963	2.56387	H	0.00448	4.91943	-2.34751
H	-0.96508	3.82823	2.94495	H	0.91411	3.51779	-2.98270
H	0.62518	3.08438	2.89974	C	-2.71444	1.14837	2.56498
C	2.99605	2.20939	-1.52156	H	-2.31592	2.00793	3.10486
H	2.82368	2.17667	-2.60080	H	-3.61994	1.45016	2.03390
H	2.49533	3.10125	-1.14287	H	-3.02461	0.39229	3.29258

H	4.06643	2.33900	-1.36752	C	-1.71311	0.58955	1.62955
C	2.50426	0.95999	-0.82912	C	-1.74664	-0.64079	0.68734
C	1.65241	-1.39133	0.63381	H	-1.85919	-1.59977	1.19963
H	1.33249	-2.41899	0.63280	C	-2.76659	-0.57370	-0.48655
C	2.51279	-1.01207	1.83915	C	-2.65586	0.75742	-1.23626
C	2.35583	0.33496	2.50741	H	-3.36069	0.78368	-2.06827
H	1.50352	0.32061	3.19120	H	-2.85912	1.61472	-0.59320
H	3.24839	0.56404	3.09577	H	-1.65151	0.87457	-1.64630
H	2.20341	1.14741	1.80035	C	-2.52492	-1.72212	-1.48306
C	2.78588	-2.13215	2.82018	H	-3.31451	-1.71914	-2.23665
H	1.96671	-2.22835	3.53603	H	-1.56640	-1.61356	-1.98776
H	2.89688	-3.09107	2.31224	H	-2.52566	-2.69159	-0.98528
H	3.70436	-1.93666	3.38113	C	-4.13641	-0.78951	0.12632
C	3.12898	-1.13340	0.47198	H	-4.22679	-1.71385	0.69601
H	3.72361	-2.02820	0.33344	C	-5.21050	-0.01492	0.01903
C	3.60378	0.03907	-0.35557	H	-5.15125	0.90727	-0.55273
H	4.28570	0.65657	0.24659	C	0.92045	-0.60320	-0.05320
S	-1.47081	-1.87538	1.19016	S	1.22076	-2.12116	-0.92633
O	-2.30339	-1.25080	2.22285	O	1.54848	-1.81407	-2.32272
C	-2.58447	-2.58929	-0.03119	C	2.71660	-2.76182	-0.16142
C	-3.93155	-2.25417	-0.00587	C	3.94495	-2.54932	-0.77424
H	-4.29893	-1.57187	0.74747	H	3.99315	-2.00188	-1.70507
C	-4.78552	-2.82296	-0.94470	C	5.09083	-3.07069	-0.18445
H	-5.83926	-2.57718	-0.93023	H	6.05330	-2.91910	-0.65514
C	-4.28758	-3.70843	-1.89357	C	4.99867	-3.79191	1.00088
H	-4.95536	-4.14996	-2.62199	H	5.89283	-4.20024	1.45400
C	-2.93424	-4.03633	-1.90705	C	3.76063	-4.00040	1.60247
H	-2.55148	-4.73318	-2.64118	C	2.60961	-3.48507	1.02151
H	-1.02457	-3.73712	-0.95851	H	1.63738	-3.65743	1.46230
C	-2.07423	-3.47757	-0.97191	H	3.69085	-4.57292	2.51813
O	-0.53303	-2.92862	1.58466	O	0.13686	-3.05810	-0.62427
C	4.42326	-0.47286	-1.56849	C	-6.54908	-0.31605	0.62434
H	3.84624	-1.26077	-2.06361	H	-6.48906	-1.23322	1.21784
H	4.54119	0.32685	-2.30241	H	-6.82133	0.48812	1.31973
C	5.81334	-0.99465	-1.20449	C	-7.66861	-0.44970	-0.41719
H	5.73615	-1.78778	-0.45595	H	-7.42025	-1.26566	-1.10183
H	6.38161	-0.18635	-0.73280	H	-7.70273	0.45971	-1.02551
C	6.57989	-1.51928	-2.41674	C	-9.03713	-0.69742	0.21286
H	6.70782	-0.73902	-3.17111	H	-9.31684	0.12126	0.88071
H	6.04986	-2.35000	-2.88890	H	-9.03892	-1.61807	0.80169
H	7.57257	-1.87554	-2.13561	H	-9.81561	-0.78760	-0.54702

1c				2c			
C	-0.68399	-0.77401	0.45605	C	-0.84532	-0.61098	-0.03823
C	0.07551	-1.40114	-0.39270	C	0.42551	-0.82918	-0.45451
C	-0.73357	0.68566	0.82726	C	-1.56175	0.71925	-0.06234
H	-0.17407	0.84331	1.75044	H	-2.08870	0.87903	0.87555
H	-1.76397	0.97256	1.02648	H	-2.30267	0.74739	-0.86510
C	-0.18400	1.66869	-0.21237	C	-0.59479	1.86833	-0.28914
C	1.34128	1.60036	-0.40352	C	0.37103	1.50793	-1.40630
H	1.60808	2.34710	-1.15020	H	0.98226	2.37326	-1.61856
H	1.57394	0.62392	-0.82972	H	-0.24563	1.31111	-2.28865
C	2.09566	1.80981	0.82485	C	1.18317	0.28218	-1.06326
O	-0.58313	2.94602	0.30709	O	0.06150	2.07974	0.96784
O	-0.70608	1.43361	-1.52395	O	-1.25910	3.06050	-0.73320
C	-0.37055	4.10279	-0.37539	C	1.02973	3.01871	1.12383
C	-2.03941	1.50573	-1.78576	C	-2.19508	3.68247	0.03438
O	-2.88006	1.78843	-0.97364	O	-2.57363	3.28592	1.10485
O	0.13533	4.17178	-1.46528	O	1.40660	3.76682	0.25842
C	-2.29036	1.19466	-3.23324	C	-2.66491	4.93519	-0.65011
H	-1.78076	1.92912	-3.85814	H	-1.82323	5.61698	-0.77873
H	-1.88101	0.21429	-3.47905	H	-3.04816	4.69939	-1.64332
H	-3.35827	1.21461	-3.42890	H	-3.43875	5.40867	-0.05320
C	-0.88188	5.26688	0.42419	C	1.54025	2.98896	2.53620
H	-0.64317	6.19366	-0.08928	H	2.29750	3.75609	2.66802
H	-1.96255	5.17679	0.54329	H	0.71343	3.15188	3.22795
H	-0.44022	5.26109	1.42078	H	1.95783	2.00567	2.75731
C	3.51620	2.18256	3.04047	C	3.27201	1.31296	-2.00291
H	2.96535	1.85498	3.92407	H	2.65209	2.12498	-2.36552
H	4.44894	1.61571	2.99925	H	4.00758	1.74137	-1.31762
H	3.76964	3.23600	3.17393	H	3.83294	0.91625	-2.85282
C	2.73220	1.97969	1.82946	C	2.50560	0.20142	-1.33774
C	0.83132	-2.07920	-1.20297	C	1.10999	-2.13360	-0.29941
H	0.50577	-2.20748	-2.23268	H	0.51146	-2.99271	-0.55265
C	2.16991	-2.72170	-0.83838	C	2.05853	-2.33232	0.87816
C	2.45919	-2.56717	0.65484	C	2.21760	-1.22391	1.89642
H	1.66226	-3.03825	1.23149	H	1.38516	-1.24651	2.60418
H	3.39620	-3.05889	0.91288	H	3.14090	-1.35682	2.46475
H	2.52000	-1.52280	0.95783	H	2.24031	-0.23399	1.44505
C	2.05637	-4.22532	-1.17659	C	2.06259	-3.71400	1.49618
H	1.26910	-4.69081	-0.58219	H	1.25274	-3.81404	2.22177
H	1.82524	-4.37663	-2.23286	H	1.92862	-4.48991	0.74088
H	3.00128	-4.72732	-0.96166	H	3.00784	-3.90348	2.01309

C	3.18991	-2.10006	-1.77862	C	2.59197	-2.21411	-0.52832
H	2.96701	-2.32596	-2.81934	H	2.93670	-3.15663	-0.93909
C	4.26399	-1.33616	-1.57438	C	3.35383	-1.02803	-1.07910
H	4.78518	-1.03241	-2.48005	S	-1.86092	-1.85196	0.78213
S	-1.81956	-1.82171	1.41561	O	-2.07443	-1.39910	2.16080
O	-1.75740	-1.35296	2.80303	C	-3.43846	-1.71854	-0.07463
O	-1.54066	-3.22173	1.10053	C	-4.50902	-1.10108	0.55655
C	-3.44221	-1.41510	0.77225	H	-4.38205	-0.69405	1.54979
C	-4.27036	-0.57268	1.50087	C	-5.73185	-1.03577	-0.10266
C	-3.83894	-1.95578	-0.44660	H	-6.57735	-0.56419	0.38042
C	-5.52760	-0.26496	0.99431	C	-5.86755	-1.57640	-1.37619
H	-3.93515	-0.18182	2.45087	H	-6.82130	-1.52342	-1.88536
C	-5.09445	-1.63753	-0.94372	C	-4.78401	-2.19205	-1.99791
H	-3.17980	-2.62524	-0.98210	H	-4.89485	-2.61949	-2.98600
C	-5.93586	-0.79226	-0.22465	H	-2.71553	-2.76083	-1.80607
H	-6.18652	0.38606	1.55331	C	-3.56115	-2.26863	-1.34582
H	-5.42077	-2.05394	-1.88773	O	-1.36953	-3.21269	0.55411
H	-6.91517	-0.54847	-0.61570	H	3.69328	-1.33255	-2.07791
C	4.88685	-0.79764	-0.31110	C	4.65325	-0.73940	-0.26275
H	4.27121	0.01665	0.08798	H	4.51936	0.14912	0.36050
H	4.91425	-1.55959	0.46856	H	4.79851	-1.56912	0.43269
C	6.30613	-0.27258	-0.54366	C	5.92605	-0.59601	-1.09972
H	6.28037	0.49431	-1.32412	H	5.83570	0.24731	-1.78803
H	6.93098	-1.08262	-0.93283	H	6.03677	-1.48744	-1.72579
C	6.93829	0.30330	0.72023	C	7.17755	-0.41778	-0.24321
H	7.00163	-0.45101	1.50866	H	7.32122	-1.26934	0.42626
H	6.34778	1.13744	1.10764	H	7.10809	0.48004	0.37584
H	7.94838	0.67087	0.53031	H	8.07269	-0.32590	-0.86119
3c				INT2-n-E			
C	-0.21311	-0.51894	0.63148	C	0.77474	-0.78414	0.01998
C	1.92765	0.57585	0.10891	C	3.23242	-0.29515	-0.06019
H	2.42036	0.73733	-0.84801	H	4.08507	-0.81958	0.36559
H	2.70752	0.38927	0.85166	H	3.41834	0.77803	0.03232
C	1.23159	1.89499	0.49590	C	3.15797	-0.62036	-1.54908
C	0.31735	1.75504	1.72571	C	1.90813	-0.01443	-2.17010
H	-0.21509	2.68818	1.89327	H	1.80531	-0.38167	-3.18887
H	0.96627	1.58744	2.58938	H	2.08775	1.06119	-2.23801
C	-0.57048	0.58399	1.50048	C	0.66474	-0.27843	-1.35002
O	0.48381	2.27269	-0.66806	O	3.17336	-2.05303	-1.63400
O	2.19604	2.88874	0.86479	O	4.25426	-0.03325	-2.26503

C	-0.17247	3.45925	-0.75376	C	3.24502	-2.70009	-2.82708
C	3.08957	3.39287	-0.03053	C	5.54206	-0.41679	-2.04761
O	3.20241	3.01761	-1.16747	O	5.88346	-1.22825	-1.22804
O	-0.17587	4.30263	0.10587	O	3.26085	-2.15453	-3.90034
C	3.88415	4.49459	0.61014	C	6.45572	0.30722	-2.99510
H	3.22344	5.34169	0.80246	H	6.23411	-0.00685	-4.01626
H	4.28622	4.16845	1.56897	H	6.28596	1.38251	-2.93946
H	4.68679	4.79967	-0.05496	H	7.48896	0.07472	-2.75447
C	-0.87121	3.55761	-2.07911	C	3.32050	-4.18251	-2.59891
H	-1.38940	4.50942	-2.14889	H	3.36302	-4.69652	-3.55464
H	-0.14296	3.46510	-2.88533	H	4.20676	-4.41373	-2.00724
H	-1.57947	2.73479	-2.18422	H	2.45356	-4.51891	-2.02939
C	-2.75210	0.34344	2.92080	C	-0.86869	0.80630	-3.02277
H	-2.51439	1.27239	3.44018	H	-0.93952	1.88867	-2.87361
H	-3.73271	0.44318	2.44935	H	-0.09928	0.62000	-3.77456
H	-2.85036	-0.45654	3.66042	H	-1.83158	0.49385	-3.42812
C	-1.71683	0.00445	1.91946	C	-0.55629	0.12937	-1.73216
C	-1.55274	-1.21186	0.97319	C	-0.51444	-1.32644	0.57311
H	-1.41548	-2.17004	1.48012	H	-0.60846	-1.10903	1.63202
C	-2.65296	-1.36720	-0.12076	C	-0.72964	-2.85629	0.37573
C	-2.88209	-0.03657	-0.84478	C	-0.47306	-3.33941	-1.05318
H	-3.64501	-0.14693	-1.61553	H	-0.61770	-4.41880	-1.11047
H	-3.18239	0.76518	-0.17145	H	-1.11916	-2.87492	-1.79383
H	-1.95744	0.27347	-1.33550	H	0.55576	-3.12812	-1.33982
C	-2.22574	-2.41083	-1.17086	C	0.27232	-3.60981	1.29204
H	-3.04425	-2.57497	-1.87457	H	0.09281	-4.68154	1.19848
H	-1.35560	-2.07143	-1.73079	H	1.30332	-3.41010	1.00180
H	-1.97004	-3.36428	-0.71013	H	0.15156	-3.32783	2.33545
C	-3.85865	-1.95184	0.59598	C	-2.10680	-3.20545	0.89502
H	-3.60743	-2.90651	1.05488	H	-2.31472	-2.81247	1.88889
C	-5.12841	-1.57465	0.75221	C	-3.02991	-3.96293	0.31236
H	-5.74773	-2.27367	1.31203	H	-2.83816	-4.37908	-0.67283
C	0.97289	-0.60050	0.02454	Rh	-1.97300	0.00745	-0.23540
S	1.51793	-2.02878	-0.88161	Cl	-0.85077	1.88988	0.98961
O	1.61116	-1.68948	-2.30585	C	-2.86995	-1.22725	-1.35154
C	3.19638	-2.29377	-0.29251	C	-3.29940	-0.11101	1.36689
C	4.26752	-1.87323	-1.06978	O	-3.49303	-1.81023	-2.09802
H	4.08343	-1.38603	-2.01676	O	-4.03513	-0.15897	2.21789
C	5.56107	-2.11162	-0.61926	Rh	-1.93354	3.59688	-0.39742
H	6.40459	-1.79632	-1.21915	Cl	-3.55694	1.91511	-1.09647
C	5.76864	-2.75903	0.59363	C	-0.68455	4.88196	0.16811

H	6.77735	-2.94575	0.93914	O	0.07193	5.65317	0.52177
C	4.68530	-3.17541	1.36292	C	-2.81494	4.88918	-1.44097
C	3.38949	-2.94495	0.92093	O	-3.36185	5.66260	-2.06779
H	2.53663	-3.28036	1.49446	C	1.96369	-0.69489	0.65540
H	4.85035	-3.68790	2.30162	S	2.23457	-0.98483	2.40358
O	0.71612	-3.18017	-0.46189	O	3.19564	-2.08087	2.55806
C	-5.89605	-0.37120	0.28784	C	3.06338	0.52413	2.92439
H	-6.33360	0.11485	1.16906	C	4.42294	0.48796	3.20326
H	-5.26081	0.37043	-0.18879	H	4.96953	-0.43718	3.08705
C	-7.04106	-0.74588	-0.66571	C	5.04910	1.64741	3.64743
H	-7.66243	-1.51452	-0.19600	H	6.10630	1.63159	3.87763
H	-6.61651	-1.20386	-1.56367	C	4.31792	2.82006	3.79870
C	-7.90605	0.45126	-1.05145	H	4.80898	3.72062	4.14447
H	-7.31311	1.22158	-1.55075	C	2.95540	2.84106	3.51190
H	-8.36329	0.90705	-0.16947	C	2.31750	1.68812	3.07537
H	-8.70959	0.15887	-1.72995	H	1.25781	1.68810	2.86130
				H	2.38791	3.75410	3.63525
				O	0.95970	-1.04403	3.12604
				C	-4.35515	-4.31890	0.91474
				H	-4.48690	-3.79166	1.86423
				H	-5.15732	-3.97485	0.24992
				C	-4.52732	-5.82823	1.13660
				H	-3.75371	-6.17409	1.82788
				H	-4.34966	-6.35171	0.19197
				C	-5.90822	-6.19456	1.67428
				H	-6.69455	-5.89153	0.97846
				H	-6.10386	-5.70044	2.62910
				H	-6.00022	-7.27063	1.83227
TS3-n-E				TS6-n-E			
C	8.47990	0.62554	-9.65715	C	-2.20816	5.46183	-6.86223
C	7.12961	0.62195	-9.70799	C	-4.41864	4.37329	-6.75078
C	9.31339	-0.38937	-10.40094	H	-5.41605	4.70906	-7.02643
H	10.22055	-0.61641	-9.84548	H	-4.50865	3.79096	-5.83028
H	9.60729	-0.00648	-11.38191	C	-3.91509	3.43144	-7.85789
C	8.54275	-1.68845	-10.62658	C	-2.44129	3.04417	-7.67873
C	7.18980	-1.41977	-11.27238	H	-2.08718	2.52459	-8.56643
H	6.61676	-2.34352	-11.28268	H	-2.39191	2.32978	-6.85100
H	7.39498	-1.16061	-12.31427	C	-1.62242	4.24005	-7.32636
C	6.43495	-0.29028	-10.60828	O	-4.13224	4.15201	-9.07938

O	8.42233	-2.29176	-9.32951	O	-4.62448	2.18942	-7.83219
O	9.23017	-2.54453	-11.55000	C	-3.94968	3.57278	-10.29878
C	7.92389	-3.54561	-9.16500	C	-5.96313	2.11826	-8.08509
C	10.44067	-3.09455	-11.25814	O	-6.66427	3.07030	-8.30244
O	11.05967	-2.88461	-10.24852	O	-3.54037	2.45365	-10.46514
O	7.48923	-4.23021	-10.05483	C	-6.40695	0.68450	-8.07032
C	10.86494	-4.00995	-12.37091	H	-5.94620	0.15889	-8.90832
H	10.17995	-4.85820	-12.41658	H	-6.07561	0.19378	-7.15532
H	10.81069	-3.49402	-13.32946	H	-7.48847	0.63719	-8.15607
H	11.87566	-4.36243	-12.18735	C	-4.36079	4.52661	-11.38207
C	8.02458	-3.94941	-7.72203	H	-3.88891	5.49813	-11.23695
H	7.56000	-4.92104	-7.58225	H	-4.09470	4.11461	-12.35104
H	9.07643	-3.99418	-7.43611	H	-5.44016	4.67801	-11.32854
H	7.54664	-3.20581	-7.08439	C	0.73135	3.65530	-8.09076
C	4.30561	-0.67107	-11.88933	H	1.33350	3.05246	-7.40910
H	3.95851	0.01496	-12.66719	H	0.23413	2.98944	-8.80206
H	4.82707	-1.49666	-12.37663	H	1.40808	4.30010	-8.65307
H	3.41152	-1.07493	-11.40639	C	-0.29108	4.46075	-7.35390
C	5.16453	0.04443	-10.89899	C	-1.04797	6.40711	-6.98719
C	6.20389	1.45594	-8.89105	H	-0.85998	7.03368	-6.11649
H	6.58695	2.44673	-8.68634	C	-0.88356	7.23356	-8.27452
C	5.65652	0.80251	-7.59716	C	-1.10584	6.43357	-9.55869
C	5.51840	-0.72071	-7.65555	H	-1.10083	7.10699	-10.41583
H	6.48642	-1.17509	-7.85803	H	-0.33860	5.67805	-9.71779
H	5.16803	-1.08730	-6.68964	H	-2.07520	5.93762	-9.53309
H	4.82653	-1.05638	-8.42489	C	-1.95464	8.36122	-8.22995
C	6.61713	1.14935	-6.43838	H	-1.79459	9.01650	-9.08648
H	7.59268	0.68658	-6.58832	H	-2.96275	7.95276	-8.29231
H	6.76581	2.22429	-6.35019	H	-1.88316	8.95222	-7.31948
H	6.19612	0.77408	-5.50298	C	0.46170	7.92451	-8.23114
C	4.32952	1.48135	-7.30492	H	0.65527	8.46986	-7.30935
H	4.40912	2.53347	-7.04506	C	1.35852	7.99362	-9.20895
C	3.12726	0.90104	-7.21736	H	1.17658	7.47089	-10.14369
H	3.03479	-0.15966	-7.42770	Rh	0.76373	5.39825	-5.62900
Rh	4.50475	1.80803	-10.09403	Cl	-0.98975	4.77617	-3.97180
Cl	6.02384	2.90240	-11.63049	C	2.24549	5.92056	-6.67208
C	2.31182	1.10606	-10.19569	C	1.87051	5.64863	-4.05427
C	3.99052	3.69500	-9.46187	O	3.22547	6.17014	-7.19242
O	1.21660	0.84682	-10.18204	O	2.49895	5.75920	-3.12016
O	3.75872	4.76135	-9.17192	Rh	-0.89558	2.31229	-4.05167
Rh	4.69662	2.74778	-13.69479	Cl	1.43880	2.36817	-4.64908

Cl	2.65459	3.12202	-12.45909	C	-2.70612	2.24563	-3.56119
C	6.27787	2.46752	-14.67052	O	-3.80625	2.21290	-3.26525
O	7.24058	2.30301	-15.25569	C	-0.75771	0.43934	-4.04791
C	3.66253	2.70997	-15.26376	O	-0.65008	-0.69186	-4.03414
O	3.02651	2.70362	-16.20526	C	-3.50310	5.55446	-6.53998
S	9.46616	1.80834	-8.74973	S	-4.21955	7.02491	-5.81999
O	10.30542	1.08267	-7.79191	O	-5.20524	7.57289	-6.75489
O	8.63634	2.91684	-8.26749	C	-5.10851	6.38771	-4.40118
C	10.54108	2.46109	-10.03331	C	-6.48945	6.25327	-4.47385
C	11.89580	2.16284	-9.99900	H	-7.00945	6.53068	-5.37957
C	9.99322	3.26949	-11.02423	C	-7.17501	5.77995	-3.36154
C	12.72547	2.69660	-10.97945	H	-8.25144	5.67819	-3.39799
C	10.83030	3.78992	-12.00107	C	-6.47921	5.44319	-2.20551
C	12.19379	3.50554	-11.97696	H	-7.01790	5.07474	-1.34209
H	12.28483	1.53292	-9.21168	C	-5.09505	5.58192	-2.14998
H	8.93333	3.48745	-11.02861	C	-4.39821	6.06023	-3.25093
H	13.78526	2.47912	-10.96186	H	-3.32472	6.18173	-3.22163
H	10.42046	4.42060	-12.77886	H	-4.55805	5.32181	-1.24755
H	12.84239	3.91782	-12.73926	O	-3.12403	7.86764	-5.33509
C	1.87882	1.58785	-6.76322	C	2.63642	8.77182	-9.14315
H	2.05762	2.66072	-6.65002	H	2.74745	9.22158	-8.15239
H	1.09568	1.47392	-7.52182	H	3.48281	8.08646	-9.27140
C	1.35207	1.00424	-5.44127	C	2.72634	9.86338	-10.21890
H	2.11722	1.12853	-4.67010	H	1.89432	10.56092	-10.08736
H	1.20786	-0.07395	-5.56051	H	2.59027	9.40706	-11.20447
C	0.04569	1.65004	-4.98790	C	4.05031	10.62270	-10.18252
H	-0.74240	1.51039	-5.73142	H	4.89559	9.94991	-10.34667
H	0.16915	2.72407	-4.83258	H	4.19868	11.10935	-9.21546
H	-0.30175	1.21647	-4.04862	H	4.08534	11.39587	-10.95221
INT2-n-Z				TS3-n-Z			
C	-0.77625	-0.73951	-0.22129	C	8.47741	0.54349	-9.72718
C	-3.16482	-0.17438	0.27612	C	7.12744	0.52120	-9.75474
H	-4.10412	-0.54779	-0.12495	C	9.30397	-0.48576	-10.45815
H	-3.26676	0.90388	0.42515	H	10.24838	-0.65360	-9.94645
C	-2.93850	-0.81047	1.64458	H	9.52615	-0.15070	-11.47497
C	-1.58565	-0.40275	2.21024	C	8.56695	-1.82001	-10.56412
H	-1.37999	-0.99143	3.10171	C	7.17869	-1.63871	-11.16608
H	-1.68965	0.63529	2.53381	H	6.61859	-2.56269	-11.04193
C	-0.47082	-0.51633	1.19418	H	7.32704	-1.50123	-12.23963
O	-3.04388	-2.22517	1.43034	C	6.43766	-0.44690	-10.60160
O	-3.89793	-0.34396	2.60423	O	8.52433	-2.33746	-9.22594

C	-3.02441	-3.11214	2.45941	O	9.24348	-2.71569	-11.45796
C	-5.22487	-0.62227	2.48878	C	8.08294	-3.59347	-8.95450
O	-5.71963	-1.22115	1.57039	C	10.48250	-3.20792	-11.18324
O	-2.87803	-2.81326	3.61657	O	11.14124	-2.90222	-10.22440
C	-5.96148	-0.09364	3.68663	O	7.64829	-4.35783	-9.77717
H	-5.67452	-0.67574	4.56421	C	10.88180	-4.19772	-12.24028
H	-5.68707	0.94312	3.87886	H	10.22549	-5.06749	-12.17978
H	-7.03181	-0.17986	3.52417	H	10.75960	-3.76541	-13.23322
C	-3.23729	-4.50333	1.93558	H	11.91234	-4.50279	-12.08398
H	-3.12525	-5.21920	2.74451	C	8.23054	-3.88145	-7.48770
H	-4.24006	-4.57539	1.51152	H	7.99265	-4.92381	-7.29681
H	-2.53024	-4.71951	1.13479	H	9.24642	-3.65527	-7.16510
C	1.31714	0.18631	2.82055	H	7.55568	-3.24084	-6.91769
H	1.45695	1.27164	2.85880	C	4.30726	-0.86235	-11.88606
H	0.62967	-0.09427	3.62103	H	3.95909	-0.21365	-12.69287
H	2.29313	-0.25142	3.03391	H	4.81509	-1.72163	-12.32885
C	0.80611	-0.21611	1.47992	H	3.41248	-1.22496	-11.37190
C	0.40481	-1.19393	-1.03216	C	5.18027	-0.10916	-10.93944
H	0.36831	-0.78599	-2.03650	C	6.19228	1.38816	-8.98000
C	0.58713	-2.73815	-1.14653	H	6.56810	2.39093	-8.82879
C	0.46694	-3.46759	0.19455	C	5.65569	0.79208	-7.64665
H	0.52984	-4.54381	0.04122	C	5.78048	-0.72960	-7.54726
H	1.22214	-3.18291	0.92258	H	6.82839	-1.01442	-7.62913
H	-0.50511	-3.25639	0.63801	H	5.42144	-1.06142	-6.57308
C	-0.55297	-3.29110	-2.04749	H	5.22819	-1.25382	-8.32157
H	-0.41731	-4.36733	-2.16130	C	6.47147	1.40337	-6.48630
H	-1.53010	-3.11713	-1.59700	H	7.51638	1.10119	-6.54412
H	-0.54459	-2.83279	-3.03362	H	6.43728	2.49221	-6.50465
C	1.86024	-2.98116	-1.93275	H	6.06107	1.05712	-5.53506
H	1.91017	-2.33169	-2.80383	C	4.23420	1.30720	-7.51272
C	2.85011	-3.86991	-1.83401	H	4.20183	2.37622	-7.32850
H	3.58817	-3.82053	-2.63212	C	3.04006	0.69365	-7.48965
Rh	2.00458	-0.05394	-0.19405	H	2.19740	1.36387	-7.33317
Cl	0.79700	2.05010	-0.83948	Rh	4.53852	1.69645	-10.26068
C	2.99056	-1.50692	0.50499	Cl	6.15412	2.69095	-11.78092
C	3.09580	0.15804	-1.95851	C	2.15834	1.03653	-10.29640
O	3.67484	-2.25270	1.01594	C	4.01276	3.60425	-9.70197
O	3.70873	0.29662	-2.89269	O	1.03343	1.07851	-10.27840
Rh	2.09614	3.40352	0.73645	O	3.76825	4.67711	-9.44689
Cl	3.76560	1.62476	0.79133	Rh	4.90162	3.34151	-13.78575
C	0.81048	4.77200	0.65594	Cl	2.86067	2.62676	-12.71424

O	0.03146	5.59728	0.59235	C	6.49548	3.90620	-14.60816
C	3.13942	4.42887	1.91841	O	7.46382	4.24869	-15.09928
O	3.78272	5.04249	2.62537	C	3.90304	3.84405	-15.29644
C	-2.02664	-0.48849	-0.66652	O	3.28559	4.14559	-16.20150
S	-2.53184	-0.44179	-2.38540	S	9.46461	1.75765	-8.86556
O	-3.58380	-1.44160	-2.59059	O	10.31699	1.06099	-7.89771
C	-3.30263	1.17681	-2.52546	O	8.63033	2.87069	-8.40311
C	-4.68793	1.27026	-2.54845	C	10.52384	2.38720	-10.17335
H	-5.28753	0.37496	-2.46528	C	11.87457	2.06853	-10.16547
C	-5.27442	2.52168	-2.70030	C	9.96865	3.20108	-11.15564
H	-6.35246	2.60881	-2.72731	C	12.69206	2.58690	-11.16413
C	-4.47813	3.65489	-2.82289	C	10.79352	3.70640	-12.15073
H	-4.93946	4.62660	-2.94414	C	12.15277	3.40166	-12.15289
C	-3.09032	3.54504	-2.79725	H	12.27065	1.43533	-9.38431
C	-2.49310	2.30068	-2.64972	H	8.91266	3.43545	-11.13828
H	-1.41714	2.19970	-2.64096	H	13.74862	2.35356	-11.16721
H	-2.47207	4.42734	-2.89973	H	10.37733	4.34031	-12.92271
O	-1.36496	-0.43756	-3.27370	H	12.79241	3.80261	-12.92863
C	3.13135	-4.96041	-0.83688	C	2.64125	-0.75208	-7.62798
H	2.70939	-4.73490	0.14074	H	2.77788	-1.08081	-8.66514
H	2.64038	-5.88273	-1.17313	H	3.29319	-1.39217	-7.03379
C	4.63114	-5.23810	-0.68826	C	1.18619	-0.98906	-7.21411
H	5.13161	-4.32837	-0.34389	H	0.52913	-0.36414	-7.82661
H	5.05154	-5.46487	-1.67308	H	1.05157	-0.65173	-6.18193
C	4.92977	-6.38499	0.27300	C	0.76670	-2.45036	-7.33699
H	4.46062	-7.31296	-0.06373	H	1.38686	-3.09261	-6.70732
H	4.55196	-6.16882	1.27523	H	0.86314	-2.80345	-8.36659
H	6.00300	-6.56562	0.35517	H	-0.27188	-2.59095	-7.03376
TS6-n-Z							
C	-2.02255	5.44262	-6.85047				
C	-4.17608	4.38981	-6.27130				
H	-5.20053	4.75522	-6.29172				
H	-4.06461	3.76554	-5.38111				
C	-3.96948	3.49473	-7.50474				
C	-2.50734	3.06765	-7.68334				
H	-2.38123	2.57816	-8.64693				
H	-2.29174	2.31867	-6.91467				
C	-1.59486	4.23100	-7.48369				
O	-4.43131	4.28253	-8.61133				
O	-4.69587	2.26987	-7.37304				

C	-4.55840	3.76006	-9.86266
C	-6.05920	2.24366	-7.33124
O	-6.75660	3.22269	-7.34484
O	-4.25316	2.63584	-10.16368
C	-6.53983	0.82274	-7.28853
H	-6.28419	0.33066	-8.22832
H	-6.04116	0.27731	-6.48760
H	-7.61614	0.80692	-7.14498
C	-5.14536	4.78814	-10.78516
H	-5.23594	4.37204	-11.78404
H	-6.12430	5.09286	-10.41363
H	-4.51408	5.67713	-10.80385
C	0.50200	3.62922	-8.78778
H	1.23717	2.99738	-8.28714
H	-0.16479	2.99184	-9.37561
H	1.03742	4.28065	-9.48030
C	-0.29880	4.42582	-7.80652
C	-0.89206	6.36836	-7.19755
H	-0.49008	6.94152	-6.36374
C	-0.98762	7.25861	-8.45187
C	-1.51078	6.51645	-9.68185
H	-1.67963	7.22125	-10.49512
H	-0.83141	5.74232	-10.02942
H	-2.46702	6.04850	-9.44847
C	-2.01187	8.38805	-8.13377
H	-2.02588	9.07935	-8.97675
H	-3.01586	7.98534	-8.00296
H	-1.74448	8.93798	-7.23481
C	0.34786	7.95947	-8.60771
H	0.64569	8.44117	-7.67917
C	1.17073	8.15732	-9.63746
H	2.04265	8.76678	-9.40748
Rh	1.15962	5.25793	-6.33530
Cl	-0.18668	4.61560	-4.33958
C	2.37867	5.76775	-7.68088
C	2.60454	5.42309	-5.05230
O	3.21316	5.99365	-8.41964
O	3.43302	5.48360	-4.28422
Rh	-0.23755	2.15940	-4.56760
Cl	1.90924	2.16263	-5.66233
C	-1.89408	2.12961	-3.68512

O	-2.89927	2.11870	-3.14806
C	-0.19636	0.28638	-4.69777
O	-0.14445	-0.84644	-4.77117
C	-3.20441	5.54396	-6.23175
S	-3.69918	6.99431	-5.31283
O	-4.87586	7.57614	-5.96250
C	-4.22191	6.32270	-3.73670
C	-5.57980	6.17133	-3.48256
H	-6.30325	6.45757	-4.23278
C	-5.97784	5.67273	-2.24799
H	-7.03132	5.55704	-2.03046
C	-5.02467	5.33027	-1.29487
H	-5.33941	4.94301	-0.33448
C	-3.66836	5.48870	-1.56520
C	-3.25649	5.99051	-2.79194
H	-2.20785	6.12883	-3.01365
H	-2.93069	5.22611	-0.81867
O	-2.50589	7.81284	-5.08681
C	1.15439	7.70125	-11.06562
H	2.05043	7.08968	-11.23211
H	0.30249	7.06734	-11.29475
C	1.19166	8.87957	-12.05074
H	2.05215	9.51439	-11.81859
H	0.30461	9.50107	-11.89709
C	1.26345	8.42663	-13.50667
H	0.39552	7.81914	-13.77466
H	2.15643	7.82337	-13.68735
H	1.29453	9.27935	-14.18699

Table S3 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP+IDSCRF/TZP-DKH(-dft) level in toluene solvent

CAT				1a			
Rh	-1.62619	-0.00001	0.09014	C	-0.39265	-0.63315	0.41461
Cl	-0.00002	-1.66334	0.86843	C	0.11422	-1.51715	-0.39400
C	-2.82283	1.33874	-0.48010	C	0.00356	0.79355	0.70006
O	-3.53624	2.15554	-0.81621	H	0.38256	0.85812	1.72118
Rh	1.62619	-0.00001	0.09022	H	-0.88103	1.42773	0.64891
Cl	-0.00002	1.66312	0.86886	C	1.06207	1.42616	-0.21304
C	2.82286	-1.33861	-0.48033	C	2.46132	0.79141	-0.09645
O	3.53626	-2.15533	-0.81664	H	3.11815	1.32296	-0.78442

C	-2.82284	-1.33861	-0.48045	H	2.38502	-0.23352	-0.46189
O	-3.53624	-2.15533	-0.81679	C	3.00769	0.80958	1.25505
C	2.82286	1.33874	-0.47996	O	1.07243	2.79635	0.22006
O	3.53628	2.15554	-0.81603	O	0.74712	1.30887	-1.60627
				C	1.83647	3.74847	-0.38157
				C	-0.37800	1.85556	-2.14302
				O	-1.21160	2.45677	-1.51784
				O	2.53475	3.56047	-1.34360
				C	-0.40475	1.61277	-3.62602
				H	0.42404	2.14749	-4.09363
				H	-0.27115	0.55183	-3.83948
				H	-1.34776	1.96475	-4.03498
				C	1.66060	5.06256	0.32638
				H	2.26897	5.82082	-0.15872
				H	0.60977	5.35507	0.30564
				H	1.95223	4.96110	1.37278
				C	4.02052	0.81940	3.71383
				H	3.89807	1.79668	4.18593
				H	3.52674	0.07744	4.34496
				H	5.08802	0.58863	3.69586
				C	3.46479	0.81539	2.36633
				C	0.56959	-2.44794	-1.18024
				H	0.17208	-2.49651	-2.19269
				C	1.61700	-3.50391	-0.83067
				C	2.02867	-3.42883	0.64003
				H	1.16062	-3.58337	1.28158
				H	2.76050	-4.20521	0.86778
				H	2.46775	-2.46327	0.89522
				C	0.98551	-4.88611	-1.12119
				H	0.10627	-5.04221	-0.49409
				H	0.68132	-4.97137	-2.16671
				H	1.70856	-5.67698	-0.91333
				C	2.77675	-3.29635	-1.78892
				H	2.50264	-3.34988	-2.84069
				C	4.04752	-3.07597	-1.47585
				H	4.39478	-3.01061	-0.45256
				H	4.79507	-2.95403	-2.25001
				S	-1.78980	-1.22209	1.43946
				O	-1.59029	-0.66305	2.78001
				O	-1.92105	-2.66709	1.25841
				C	-3.24697	-0.44474	0.73156

				C	-3.74395	0.72122	1.30127
				C	-3.86037	-1.03879	-0.36715
				C	-4.87929	1.30653	0.75190
				H	-3.25757	1.14767	2.16761
				C	-4.99258	-0.44406	-0.90689
				H	-3.46578	-1.95910	-0.77576
				C	-5.49892	0.72748	-0.34973
				H	-5.27913	2.21312	1.18770
				H	-5.48438	-0.89808	-1.75777
				H	-6.38301	1.18695	-0.77368
2a				3a			
C	-0.36598	-0.43790	-0.23162	C	-0.98876	-0.54945	0.48259
C	-0.38095	0.79353	0.33683	C	1.16722	0.58476	0.10901
C	0.76639	-1.43259	-0.13601	H	1.71911	0.75277	-0.81412
H	0.93805	-1.90108	-1.10058	H	1.90173	0.40865	0.89982
H	0.52263	-2.23588	0.56627	C	0.43506	1.89828	0.45271
C	2.05185	-0.77711	0.34838	C	-0.57408	1.74017	1.60422
C	1.75461	0.12850	1.53357	H	-1.13319	2.66461	1.73004
H	2.68416	0.53363	1.91348	H	0.00534	1.58204	2.51859
H	1.34246	-0.51880	2.31515	C	-1.42341	0.55329	1.31423
C	0.75180	1.20248	1.18907	O	-0.21255	2.29407	-0.76531
O	2.57361	-0.06019	-0.78196	O	1.36485	2.88962	0.91368
O	2.99629	-1.74246	0.83705	C	-0.86417	3.48203	-0.89137
C	3.72732	0.65359	-0.71757	C	2.35777	3.38215	0.12093
C	3.51715	-2.71169	0.03296	O	2.57257	3.02494	-1.00723
O	3.23894	-2.85950	-1.12714	O	-0.96841	4.30133	-0.01517
O	4.41231	0.76581	0.26733	C	3.12306	4.44120	0.86406
C	4.49305	-3.54949	0.81230	H	2.45967	5.27864	1.08704
H	5.30170	-2.91969	1.18641	H	3.48521	4.04853	1.81502
H	3.99784	-3.99353	1.67721	H	3.95676	4.78152	0.25617
H	4.89458	-4.32983	0.17182	C	-1.40895	3.61951	-2.28501
C	4.03093	1.25701	-2.06067	H	-1.96053	4.55181	-2.36913
H	4.90001	1.90434	-1.98102	H	-0.58568	3.60648	-3.00110
H	4.22930	0.45830	-2.77780	H	-2.05768	2.77484	-2.52013
H	3.17123	1.81735	-2.42909	C	-3.65404	0.26480	2.63996
C	1.99931	2.88165	2.58820	H	-3.73647	-0.52033	3.39866
H	2.95462	2.44128	2.30677	H	-3.46845	1.21394	3.14478
H	2.10930	3.96694	2.55654	H	-4.62569	0.31323	2.14309
H	1.80686	2.61196	3.63246	C	-2.57478	-0.05250	1.67536
C	0.85799	2.44622	1.70507	C	-2.32814	-1.27658	0.75763

C	-1.51043	1.73974	0.16315	H	-2.18605	-2.21817	1.29611
H	-2.48688	1.27965	0.19353	C	-3.35840	-1.50651	-0.39161
C	-1.42489	2.95386	-0.75632	C	-3.61930	-0.21541	-1.17490
C	-0.17575	3.20887	-1.56976	H	-4.30869	-0.40355	-1.99977
H	-0.20685	2.63258	-2.49729	H	-4.04594	0.57206	-0.55179
H	-0.10909	4.26732	-1.83816	H	-2.68800	0.16041	-1.60174
H	0.73796	2.93927	-1.04211	C	-2.85386	-2.58612	-1.37031
C	-2.70099	3.32034	-1.48538	H	-3.63341	-2.80492	-2.10302
H	-2.81003	2.72566	-2.39439	H	-1.96652	-2.25114	-1.90534
H	-3.58192	3.14928	-0.86305	H	-2.59711	-3.51137	-0.85418
H	-2.69209	4.37783	-1.76649	C	-4.61355	-2.05801	0.25831
C	-1.41546	3.13300	0.74043	H	-4.44783	-2.96040	0.84454
H	-2.33434	3.52374	1.16225	C	-5.85436	-1.59738	0.15504
C	-0.17234	3.52271	1.50096	H	-6.10308	-0.71112	-0.41563
H	0.32202	4.38116	1.02668	H	-6.67792	-2.10448	0.64300
H	-0.45774	3.88523	2.49545	C	0.24192	-0.61148	-0.03445
S	-1.73226	-1.04973	-1.25106	S	0.89616	-2.03710	-0.88105
O	-1.27855	-2.32060	-1.82597	O	1.08560	-1.70778	-2.29842
C	-3.06707	-1.45583	-0.10448	C	2.53675	-2.25212	-0.16647
C	-4.25637	-0.74047	-0.15982	C	3.65098	-1.80905	-0.86841
H	-4.36583	0.06179	-0.87634	H	3.52514	-1.33710	-1.83313
C	-5.29751	-1.08930	0.69492	C	4.91418	-2.00119	-0.31907
H	-6.23105	-0.54249	0.65353	H	5.79059	-1.66542	-0.85865
C	-5.14134	-2.13907	1.59239	C	5.04997	-2.62716	0.91539
H	-5.95336	-2.40806	2.25624	H	6.03556	-2.77658	1.33845
C	-3.94680	-2.85434	1.63293	C	3.92512	-3.07029	1.60670
H	-3.83117	-3.68097	2.32244	C	2.65906	-2.88545	1.06637
H	-1.98632	-3.09049	0.78527	H	1.77738	-3.24195	1.58191
C	-2.90492	-2.51919	0.77915	H	4.03484	-3.56739	2.56221
O	-2.22855	-0.00155	-2.14558	O	0.09802	-3.20804	-0.51011

COM				TS1			
C	-2.58097	0.76157	-1.30839	C	1.36417	1.03432	-0.54100
C	-2.60234	1.16227	1.22273	C	1.82218	-1.51675	-0.44273
H	-3.63449	1.34110	1.52326	H	2.72610	-2.05168	-0.72089
H	-1.98025	1.84827	1.80109	H	1.01428	-1.86491	-1.08687
C	-2.22030	-0.24344	1.70169	C	1.49679	-1.98305	0.98712
C	-0.73420	-0.63112	1.42575	C	0.03436	-1.76411	1.43015
H	-0.36434	-1.11978	2.32580	H	-0.13959	-2.40436	2.29449
H	-0.14640	0.28052	1.30742	H	-0.61774	-2.10713	0.62944
C	-0.49745	-1.51822	0.28568	C	-0.31352	-0.40121	1.83488
O	-3.16343	-1.14430	1.13457	O	2.45734	-1.36731	1.83698
O	-2.27674	-0.23139	3.14420	O	1.57248	-3.42208	1.01719
C	-3.22594	-2.44827	1.53524	C	2.55595	-1.66626	3.16389
C	-3.44363	-0.09219	3.83844	C	2.73288	-4.11832	0.84030
O	-4.52836	0.03316	3.33505	O	3.80284	-3.61714	0.61872
O	-2.46391	-2.94911	2.31836	O	1.81581	-2.41373	3.74757
C	-3.16265	-0.14067	5.31374	C	2.46338	-5.58988	0.97986
H	-2.74530	-1.11494	5.57361	H	2.11552	-5.80161	1.99236
H	-2.42254	0.61442	5.58146	H	1.67324	-5.89504	0.29273
H	-4.08500	0.02605	5.86302	H	3.37456	-6.14592	0.77752
C	-4.39019	-3.13049	0.87809	C	3.72549	-0.94065	3.76282
H	-4.33975	-4.19940	1.06667	H	3.75031	-1.11200	4.83541
H	-5.31541	-2.72883	1.29669	H	4.64644	-1.30577	3.30494
H	-4.40270	-2.92816	-0.19306	H	3.66042	0.12640	3.54782
C	-1.04043	-3.10670	-1.78959	C	-0.57526	1.47332	3.70935
H	-0.90633	-4.16872	-1.57962	H	-1.58399	1.47240	4.12509
H	-2.10210	-2.91796	-1.96645	H	0.11013	1.12393	4.48488
H	-0.49021	-2.87156	-2.70140	H	-0.31285	2.49442	3.43878
C	-0.58633	-2.28475	-0.66872	C	-0.48302	0.56447	2.56762
C	-2.71032	0.15836	-2.45281	C	0.97855	2.29452	-0.55143
H	-1.81651	-0.25428	-2.91580	H	0.40166	2.61736	-1.41561
C	-4.00957	0.00322	-3.24199	C	1.46516	3.42851	0.35423
C	-5.20397	0.58236	-2.48315	C	2.37165	2.91247	1.47179
H	-6.11571	0.47576	-3.07262	H	2.74210	3.74078	2.07601
H	-5.35436	0.08542	-1.52370	H	1.84771	2.21352	2.12410
H	-5.05212	1.64472	-2.29128	H	3.23657	2.39968	1.05162
C	-3.82284	0.76412	-4.57771	C	2.28125	4.36944	-0.57786
H	-4.71750	0.65614	-5.19393	H	2.67078	5.20206	0.00970
H	-3.64968	1.82416	-4.38888	H	3.10853	3.82891	-1.03546
H	-2.97310	0.37375	-5.14185	H	1.65433	4.78084	-1.37169
C	-4.16528	-1.47266	-3.55850	C	0.27759	4.22800	0.85442

H	-3.33830	-1.89558	-4.12594	H	-0.47442	4.43783	0.09800
C	-5.18698	-2.26177	-3.24778	C	0.11695	4.75464	2.06217
H	-6.04980	-1.91002	-2.69643	H	0.83467	4.61692	2.86124
H	-5.19672	-3.30119	-3.55261	H	-0.74956	5.36278	2.29009
Rh	1.63718	-2.28848	-0.10366	Rh	-1.38085	1.06083	0.40005
Cl	2.00351	-0.36436	-1.64861	Cl	-1.31054	-0.67206	-1.67266
C	1.29904	-3.83277	0.90373	C	-2.77946	1.66536	1.51160
C	3.36909	-2.99296	-0.62486	C	-2.19004	2.06190	-0.99419
O	1.08087	-4.76587	1.51490	O	-3.64614	2.01204	2.16082
O	4.37151	-3.41152	-0.94693	O	-2.66598	2.64846	-1.84011
Rh	3.86146	0.56354	-0.31231	Rh	-3.42600	-1.95814	-1.58638
Cl	2.82715	-0.31901	1.69427	Cl	-3.61501	-1.69293	0.80492
C	4.67713	1.21171	-1.88057	C	-3.30346	-2.17614	-3.44937
O	5.16637	1.59289	-2.83438	O	-3.22475	-2.30466	-4.57906
C	5.26442	1.21747	0.75538	C	-5.01347	-2.95274	-1.50518
O	6.10463	1.60258	1.41654	O	-5.97656	-3.55475	-1.44023
C	-2.45690	1.49408	-0.24109	C	2.06082	-0.05257	-0.71683
S	-2.30606	3.29138	-0.56355	S	3.66606	0.26709	-1.58295
O	-3.39220	3.93748	0.18129	O	4.72844	-0.23955	-0.71350
O	-2.18770	3.50158	-2.00489	O	3.68809	1.66296	-2.02025
C	-0.75865	3.78088	0.20953	C	3.59790	-0.77504	-3.04489
C	-0.79702	4.58176	1.34479	C	4.35435	-1.94039	-3.08060
C	0.44524	3.37710	-0.35920	C	2.80699	-0.38133	-4.12014
C	0.40137	4.99122	1.91954	C	4.31606	-2.72831	-4.22590
C	1.63382	3.78653	0.22919	C	2.77372	-1.18024	-5.25477
C	1.61197	4.59171	1.36490	C	3.52684	-2.35068	-5.30677
H	-1.75034	4.88506	1.75490	H	4.96512	-2.21304	-2.23086
H	0.45355	2.75743	-1.24600	H	2.23790	0.53711	-4.07324
H	0.38632	5.62085	2.80005	H	4.90449	-3.63570	-4.27141
H	2.57741	3.47207	-0.19747	H	2.16443	-0.88697	-6.09995
H	2.54313	4.90803	1.81797	H	3.49904	-2.96860	-6.19549
INT1				TS2			
C	-1.37359	-0.60220	-0.78527	C	-5.72978	-3.29814	3.16710
C	-0.51038	1.44369	0.42460	C	-7.08687	-4.56143	4.88184
H	-0.70242	2.50791	0.32041	H	-7.84471	-4.28901	5.60764
H	0.51942	1.26758	0.10735	H	-6.26524	-5.05003	5.40606
C	-0.61766	1.11518	1.92217	C	-7.70413	-5.54821	3.89885
C	0.07466	-0.19448	2.33388	C	-6.65995	-6.12726	2.96082
H	0.06295	-0.23536	3.42441	H	-7.14193	-6.82600	2.27609

H	1.11560	-0.12918	2.01636	H	-5.96845	-6.70316	3.58973
C	-0.48000	-1.46699	1.87242	C	-5.85547	-5.20756	2.14615
O	-2.00169	1.14081	2.25287	O	-8.73229	-4.82977	3.22304
O	0.15087	2.07760	2.66764	O	-8.19965	-6.70225	4.58394
C	-2.45305	1.03019	3.53280	C	-9.50851	-5.40596	2.27018
C	-0.19462	3.39410	2.75332	C	-9.19965	-6.61194	5.50644
O	-1.16337	3.88011	2.23297	O	-9.76998	-5.59346	5.79225
O	-1.74517	0.84475	4.48957	O	-9.42293	-6.55785	1.92849
C	0.80628	4.12525	3.60240	C	-9.46638	-7.96731	6.09157
H	0.80032	3.71222	4.61244	H	-9.69591	-8.67633	5.29548
H	1.81013	3.98924	3.19791	H	-8.57130	-8.32525	6.60349
H	0.55333	5.18140	3.63207	H	-10.29448	-7.90499	6.79157
C	-3.94544	1.18650	3.56227	C	-10.46707	-4.39199	1.72144
H	-4.30518	1.05607	4.57910	H	-11.17828	-4.87951	1.06090
H	-4.21320	2.17648	3.19020	H	-10.97983	-3.88334	2.53733
H	-4.41222	0.45917	2.89717	H	-9.90810	-3.63391	1.16969
C	-1.30559	-3.94748	2.33438	C	-4.82151	-5.82020	-0.16213
H	-0.45720	-4.62168	2.46635	H	-3.93431	-6.45190	-0.08167
H	-1.80424	-3.83158	3.29880	H	-5.66763	-6.43463	-0.47519
H	-2.00070	-4.40219	1.63158	H	-4.63200	-5.06409	-0.92320
C	-0.84523	-2.63352	1.88122	C	-5.08754	-5.19366	1.14050
C	-1.94200	-1.70392	-1.40809	C	-5.10844	-2.35743	2.31254
H	-1.67819	-1.83126	-2.45455	H	-4.57010	-1.58327	2.84723
C	-3.25826	-2.43457	-1.08637	C	-5.72338	-1.81951	1.00073
C	-3.89543	-1.96868	0.22269	C	-7.09625	-2.42674	0.70543
H	-4.84753	-2.47638	0.38127	H	-7.54175	-1.92811	-0.15596
H	-3.25500	-2.16193	1.08132	H	-7.03900	-3.49166	0.49627
H	-4.09850	-0.89828	0.18803	H	-7.76244	-2.28123	1.55530
C	-4.23195	-2.13064	-2.26073	C	-5.89761	-0.29229	1.18606
H	-5.17150	-2.65555	-2.08233	H	-6.30879	0.13698	0.27181
H	-4.42033	-1.06326	-2.34403	H	-6.56385	-0.07835	2.01836
H	-3.82501	-2.48316	-3.21094	H	-4.93786	0.18784	1.38739
C	-2.99943	-3.92868	-1.14444	C	-4.74176	-1.99612	-0.13321
H	-2.36443	-4.23724	-1.97169	H	-3.75843	-1.57990	0.06638
C	-3.52796	-4.86645	-0.36755	C	-4.98288	-2.51832	-1.32753
H	-4.19101	-4.63553	0.45709	H	-5.94728	-2.92996	-1.59560
H	-3.32319	-5.91494	-0.54564	H	-4.21276	-2.54484	-2.08815
Rh	-0.02210	-2.18824	-0.34207	Rh	-3.85526	-4.07895	2.43061
Cl	2.29848	0.81951	-1.80232	Cl	-3.88369	-5.20718	6.12970
C	0.55388	-4.17337	-0.25787	C	-2.41802	-3.78229	1.07197
C	0.73431	-2.09149	-2.09394	C	-2.79037	-3.23478	3.89433

O	0.84235	-5.26454	-0.27896	O	-1.62063	-3.62993	0.28538
O	1.18206	-2.12325	-3.13084	O	-2.12123	-2.71684	4.64098
Rh	3.93412	0.06727	-0.20049	Rh	-3.99425	-7.26449	4.88219
Cl	2.53258	-1.83440	0.52216	Cl	-2.69403	-6.32061	3.02731
C	5.00503	1.50493	-0.74991	C	-4.97560	-7.97141	6.31508
O	5.64330	2.38117	-1.09579	O	-5.58528	-8.37515	7.18648
C	5.22169	-0.50752	1.04436	C	-4.04495	-8.88692	3.93112
O	5.99872	-0.86087	1.79888	O	-4.06702	-9.86256	3.34547
C	-1.43466	0.67434	-0.47779	C	-6.58431	-3.34948	4.17057
S	-2.77969	1.63963	-1.27067	S	-7.33456	-1.78682	4.71068
O	-3.75552	2.03751	-0.25372	O	-8.74732	-1.76075	4.33272
O	-3.23584	0.88158	-2.43954	O	-6.46012	-0.68865	4.29262
C	-1.96377	3.12353	-1.87117	C	-7.21764	-1.96306	6.48476
C	-2.18974	4.33067	-1.22130	C	-8.37843	-2.11499	7.22938
C	-1.15112	3.03737	-2.99740	C	-5.95607	-1.98630	7.06794
C	-1.58825	5.48107	-1.71943	C	-8.26881	-2.27845	8.60491
C	-0.55207	4.19257	-3.48026	C	-5.86065	-2.16134	8.44017
C	-0.77162	5.41101	-2.84284	C	-7.01498	-2.30414	9.20561
H	-2.82393	4.36105	-0.34658	H	-9.33862	-2.11239	6.73333
H	-0.99710	2.08730	-3.49036	H	-5.06858	-1.87893	6.46017
H	-1.75716	6.42968	-1.22615	H	-9.16239	-2.39585	9.20352
H	0.08501	4.14135	-4.35364	H	-4.88704	-2.19244	8.91044
H	-0.30267	6.30923	-3.22480	H	-6.93464	-2.44257	10.27608
INT2				TS3			
C	1.99831	-0.31848	-0.62948	C	8.13215	0.79983	-9.33753
C	1.07001	0.61668	-0.32192	C	6.79264	0.61305	-9.30377
C	2.91448	-0.91396	0.41550	C	9.03687	-0.05390	-10.19425
H	3.87708	-1.16517	-0.02420	H	10.01100	-0.16894	-9.72458
H	2.48890	-1.82948	0.83663	H	9.19017	0.40883	-11.17366
C	3.14976	0.05343	1.57457	C	8.44960	-1.44551	-10.43556
C	1.82284	0.52579	2.15497	C	7.01953	-1.35533	-10.95793
H	2.01062	1.33960	2.85235	H	6.57777	-2.34892	-10.94605
H	1.43313	-0.30929	2.74191	H	7.09746	-1.05692	-12.00690
C	0.81724	0.91941	1.09095	C	6.17129	-0.34785	-10.21001
O	3.93416	1.12675	1.03167	O	8.54057	-2.12636	-9.17378
O	3.82241	-0.59584	2.66528	O	9.17498	-2.14006	-11.46298
C	4.44143	2.11934	1.81203	C	8.23712	-3.44684	-9.04158
C	5.08470	-1.09341	2.54658	C	10.49034	-2.46821	-11.32832
O	5.73973	-1.06225	1.53814	O	11.16650	-2.20113	-10.36992

O	4.24805	2.22550	2.99567	O	7.80879	-4.14190	-9.92627
C	5.53192	-1.66655	3.86243	C	10.95459	-3.21960	-12.54453
H	5.57349	-0.87207	4.60950	H	10.39288	-4.15089	-12.63392
H	4.81438	-2.40891	4.21426	H	10.76242	-2.63434	-13.44476
H	6.51337	-2.11808	3.74717	H	12.01603	-3.43373	-12.45599
C	5.29420	3.03742	0.98212	C	8.54422	-3.90627	-7.64395
H	5.59349	3.89441	1.57932	H	8.18459	-4.92262	-7.50833
H	6.17942	2.49461	0.64520	H	9.62414	-3.87283	-7.48732
H	4.75540	3.36281	0.09220	H	8.08982	-3.24067	-6.91010
C	-0.93440	1.62354	2.76259	C	4.02920	-0.95537	-11.39125
H	-1.68949	0.88303	3.03903	H	3.49110	-0.30032	-12.08032
H	-0.14068	1.59692	3.51200	H	4.62673	-1.65188	-11.98318
H	-1.42688	2.59663	2.82788	H	3.27156	-1.53661	-10.85585
C	-0.41603	1.36139	1.38849	C	4.85562	-0.16481	-10.42833
C	0.19528	1.38875	-1.27659	C	5.81253	1.28174	-8.39624
H	-0.06643	0.78479	-2.14022	H	6.07522	2.30662	-8.16798
C	0.78311	2.73902	-1.79691	C	5.42737	0.51512	-7.09741
C	1.31325	3.66220	-0.69537	C	5.50686	-1.01104	-7.20018
H	2.12264	3.17399	-0.15403	H	6.52231	-1.31857	-7.44568
H	1.71768	4.57429	-1.13707	H	5.24625	-1.45234	-6.23656
H	0.56055	3.95010	0.03495	H	4.84286	-1.42226	-7.95791
C	1.98155	2.42639	-2.73876	C	6.36775	0.97125	-5.95702
H	2.78553	1.92134	-2.20397	H	7.39641	0.66523	-6.14829
H	1.68393	1.80097	-3.57803	H	6.35677	2.05390	-5.83504
H	2.37256	3.36695	-3.12956	H	6.04140	0.51138	-5.02095
C	-0.25546	3.39347	-2.68424	C	4.02850	0.98162	-6.73759
H	-0.67729	2.72343	-3.43051	H	3.96353	2.02276	-6.43647
C	-0.63665	4.66503	-2.69474	C	2.92334	0.23611	-6.67739
H	-0.25418	5.39714	-1.99453	H	2.92016	-0.81921	-6.91546
H	-1.35674	5.02204	-3.42073	H	1.98163	0.66926	-6.36348
Rh	-1.68670	1.41390	-0.24436	Rh	4.02399	1.46781	-9.52330
Cl	-1.73973	-1.11345	-0.30190	Cl	5.32890	2.81672	-11.06584
C	-1.80183	3.27920	0.04517	C	1.85877	0.50920	-9.53973
C	-2.89455	1.37497	-1.95420	C	3.29336	3.25041	-8.77786
O	-2.01930	4.35483	0.32982	O	0.78290	0.18487	-9.48246
O	-3.57133	1.36119	-2.85403	O	2.93589	4.26407	-8.43200
Rh	-3.88633	-1.36469	0.86109	Rh	3.91014	3.22301	-13.04506
Cl	-3.95927	1.07222	1.05569	Cl	1.93906	2.54798	-11.81915
C	-3.80046	-3.23593	0.68758	C	5.43539	3.75061	-14.01224
O	-3.73742	-4.36532	0.57439	O	6.35994	4.07066	-14.59489
C	-5.54036	-1.50671	1.74767	C	2.80534	3.56526	-14.52634

O	-6.54061	-1.57774	2.28142	O	2.12376	3.77237	-15.41180
S	2.28755	-1.01517	-2.26260	S	9.02132	2.04798	-8.40313
O	3.66368	-0.70846	-2.66502	O	9.97269	1.37019	-7.51725
O	1.18579	-0.68000	-3.17112	O	8.08885	3.02453	-7.83106
C	2.20663	-2.79248	-1.97092	C	9.97299	2.89979	-9.67231
C	3.38222	-3.53295	-1.97507	C	11.34409	2.69072	-9.74751
C	0.96537	-3.39642	-1.79727	C	9.31961	3.77868	-10.53123
C	3.31080	-4.91069	-1.79816	C	12.07744	3.38049	-10.70740
C	0.90751	-4.77218	-1.61717	C	10.06192	4.45701	-11.48853
C	2.07767	-5.52734	-1.61735	C	11.43784	4.25799	-11.57587
H	4.33000	-3.03592	-2.12943	H	11.82292	2.01008	-9.05707
H	0.06203	-2.80190	-1.81053	H	8.25215	3.93400	-10.44613
H	4.21908	-5.49972	-1.80581	H	13.14772	3.23195	-10.77316
H	-0.05172	-5.25584	-1.48301	H	9.56781	5.14501	-12.16261
H	2.02600	-6.60039	-1.48092	H	12.01236	4.79242	-12.32211
INT3				TS4			
C	-2.20444	0.41849	-0.66170	C	-10.73347	-1.67488	-5.68609
C	-1.27804	-0.54131	-0.43594	C	-9.47948	-1.77216	-6.18942
C	-3.15907	0.90761	0.40417	C	-11.99622	-1.66395	-6.51753
H	-4.10869	1.19115	-0.04265	H	-12.69232	-0.92844	-6.12274
H	-2.75407	1.78530	0.91599	H	-12.48804	-2.64041	-6.47427
C	-3.41738	-0.16123	1.46270	C	-11.72218	-1.35194	-7.98335
C	-2.10238	-0.70757	2.00268	C	-10.53751	-2.16906	-8.48001
H	-2.31539	-1.54178	2.66559	H	-10.36368	-1.95092	-9.52791
H	-1.67456	0.08753	2.61950	H	-10.82717	-3.22243	-8.40988
C	-1.11978	-1.08427	0.91333	C	-9.30908	-1.94099	-7.64004
O	-4.21713	-1.16308	0.81500	O	-11.48136	0.06511	-8.03766
O	-4.08686	0.38488	2.61033	O	-12.81395	-1.72763	-8.83092
C	-4.71599	-2.23668	1.48346	C	-11.21603	0.71104	-9.20498
C	-5.33058	0.93604	2.53114	C	-14.06050	-1.18974	-8.68428
O	-5.97199	1.03247	1.51843	O	-14.35532	-0.37433	-7.85222
O	-4.50411	-2.48150	2.64360	O	-11.09865	0.17238	-10.27569
C	-5.77590	1.38568	3.89478	C	-14.98607	-1.76161	-9.72074
H	-5.84263	0.52285	4.55965	H	-14.61567	-1.51883	-10.71799
H	-5.04404	2.07211	4.32263	H	-15.01369	-2.84913	-9.63872
H	-6.74506	1.87082	3.81870	H	-15.98246	-1.35099	-9.58365
C	-5.58516	-3.05122	0.56673	C	-11.11926	2.19093	-8.96027
H	-5.90388	-3.95643	1.07630	H	-10.75608	2.68615	-9.85668
H	-6.45716	-2.46068	0.27979	H	-12.10968	2.57392	-8.70609

H	-5.04731	-3.29908	-0.34855	H	-10.46564	2.40149	-8.11375
C	0.40862	-2.28868	2.50922	C	-7.79779	-2.34962	-9.61977
H	1.23642	-1.69707	2.91299	H	-7.99977	-3.40457	-9.82771
H	-0.40703	-2.24645	3.23296	H	-8.42596	-1.75257	-10.28537
H	0.75251	-3.32433	2.45765	H	-6.76074	-2.16188	-9.89010
C	0.01202	-1.76646	1.16680	C	-8.07115	-2.06552	-8.17486
C	-0.34282	-1.13887	-1.44329	C	-8.20599	-1.82830	-5.39711
H	0.00000	-0.41249	-2.16596	H	-8.33302	-2.37227	-4.47302
C	-0.77250	-2.45578	-2.15468	C	-7.38245	-0.51486	-5.16484
C	-2.11342	-3.03980	-1.69950	C	-8.17886	0.78667	-5.33793
H	-2.92940	-2.37652	-1.98686	H	-8.92624	0.87682	-4.54936
H	-2.27656	-4.00759	-2.17913	H	-7.50585	1.64465	-5.26578
H	-2.16025	-3.18070	-0.62097	H	-8.70230	0.84178	-6.29220
C	-0.78697	-2.28583	-3.67866	C	-6.75044	-0.51018	-3.76897
H	-1.57831	-1.60338	-3.98210	H	-7.52655	-0.46384	-3.00689
H	0.15804	-1.87778	-4.04424	H	-6.14853	-1.40050	-3.58399
H	-0.95089	-3.25236	-4.16301	H	-6.09977	0.35994	-3.65447
C	0.39709	-3.35492	-1.76891	C	-6.31527	-0.72313	-6.23247
H	1.11420	-3.57836	-2.55111	H	-5.26508	-0.68149	-5.96837
C	0.56758	-3.97583	-0.55994	C	-6.67374	-0.58842	-7.58905
H	-0.22290	-4.01421	0.17349	H	-7.48622	0.06286	-7.86623
H	1.37853	-4.68168	-0.43778	H	-5.89410	-0.66109	-8.33533
Rh	1.38527	-1.81454	-0.38578	Rh	-6.77777	-2.78574	-6.62043
Cl	1.84471	0.54631	0.27316	Cl	-8.13651	-4.99885	-6.73853
C	2.94807	-2.63720	0.75772	C	-5.25530	-3.45869	-7.90659
C	2.64177	-1.51335	-2.01991	C	-5.85288	-3.54783	-5.02948
O	3.68424	-3.19421	1.40318	O	-4.42134	-3.65993	-8.63751
O	3.22015	-1.29243	-2.96042	O	-5.36828	-4.00335	-4.11769
Rh	4.13698	1.28887	0.87270	Rh	-7.08271	-7.20065	-7.12589
Cl	5.20314	-0.57727	-0.20778	Cl	-4.86761	-6.38588	-6.63559
C	3.34773	2.76286	1.73751	C	-8.79613	-7.86856	-7.51525
O	2.86935	3.65411	2.26149	O	-9.83731	-8.26847	-7.75063
C	5.85973	1.88923	1.30816	C	-6.29444	-8.87851	-7.40623
O	6.91141	2.23909	1.56079	O	-5.80072	-9.89009	-7.57121
S	-2.47497	1.23894	-2.23491	S	-11.10916	-1.53028	-3.92922
O	-3.88749	1.07283	-2.59155	O	-12.10090	-0.46137	-3.78286
C	-2.21726	2.97781	-1.84392	C	-11.92817	-3.08484	-3.53995
C	-3.31408	3.82770	-1.78036	C	-13.29927	-3.08666	-3.31530
H	-4.30700	3.43682	-1.95508	H	-13.85495	-2.16146	-3.38015
C	-3.10593	5.17605	-1.50849	C	-13.92687	-4.28579	-2.99396
H	-3.95151	5.85043	-1.46244	H	-14.99349	-4.29974	-2.80949

C	-1.81715	5.65427	-1.30021	C	-13.18633	-5.45939	-2.90831
H	-1.65911	6.70442	-1.08850	H	-13.67883	-6.39100	-2.65926
C	-0.72670	4.79002	-1.36652	C	-11.81269	-5.44306	-3.13867
H	0.27606	5.16612	-1.20894	H	-11.23752	-6.35729	-3.06890
H	-0.07848	2.76737	-1.70717	H	-10.10611	-4.23328	-3.62633
C	-0.92099	3.44326	-1.64182	C	-11.17397	-4.25181	-3.45419
O	-1.45170	0.85213	-3.21112	O	-9.87666	-1.46121	-3.13905
INT4				TS5			
C	2.00549	0.67570	0.73911	C	-2.18898	0.42182	-0.34867
C	1.37577	-0.49676	0.92779	C	-1.30820	-0.51617	-0.73673
C	2.69096	1.08960	-0.53831	C	-2.78430	0.54227	1.02928
H	3.69065	1.46166	-0.32148	H	-3.86719	0.62920	0.97107
H	2.13481	1.90428	-1.00854	H	-2.40809	1.45583	1.49695
C	2.78994	-0.04533	-1.55486	C	-2.42157	-0.62510	1.94601
C	1.48368	-0.84180	-1.57765	C	-0.97829	-1.07567	1.69788
H	1.53397	-1.58610	-2.36439	H	-0.72508	-1.84399	2.41688
H	0.70069	-0.12754	-1.83914	H	-0.34157	-0.20678	1.87613
C	1.20685	-1.43763	-0.21645	C	-0.82996	-1.52440	0.26513
O	3.91495	-0.83920	-1.14199	O	-3.38353	-1.65397	1.65097
O	2.94665	0.44852	-2.88730	O	-2.45477	-0.25523	3.32530
C	4.37070	-1.88435	-1.88701	C	-3.43278	-2.82159	2.35159
C	4.01686	1.21809	-3.24530	C	-3.59129	0.22767	3.91103
O	4.89685	1.54371	-2.49403	O	-4.63606	0.37705	3.33612
O	3.85390	-2.27435	-2.90117	O	-2.64308	-3.14006	3.20177
C	3.92570	1.57277	-4.70173	C	-3.33084	0.52425	5.35969
H	3.94317	0.66171	-5.30204	H	-3.02052	-0.38783	5.87181
H	2.98152	2.07972	-4.90562	H	-2.51572	1.24353	5.45203
H	4.76066	2.21291	-4.97244	H	-4.23292	0.92076	5.81699
C	5.60927	-2.45818	-1.25873	C	-4.62211	-3.63000	1.91590
H	5.93937	-3.32263	-1.82795	H	-4.57840	-4.61647	2.36926
H	6.39394	-1.70009	-1.24312	H	-5.53442	-3.12063	2.23262
H	5.41167	-2.74057	-0.22364	H	-4.65722	-3.70917	0.82915
C	1.41719	-3.88112	-1.03088	C	-0.14255	-3.88154	0.92954
H	1.19486	-3.55110	-2.04142	H	0.15123	-3.49826	1.90135
H	2.47121	-4.17778	-1.00598	H	-1.02172	-4.51836	1.07499
H	0.82862	-4.77533	-0.82297	H	0.65446	-4.52432	0.55536
C	1.17226	-2.84401	0.02954	C	-0.47491	-2.82026	-0.08380
C	0.65523	-0.92904	2.16834	C	-0.53516	-0.54097	-2.00904
H	-0.21635	-0.33669	2.41518	H	-0.07407	0.39427	-2.29851
C	1.34864	-1.53301	3.36695	C	-0.96210	-1.40584	-3.18161

C	2.86045	-1.51516	3.45299	C	-2.44706	-1.71776	-3.33060
H	3.18662	-0.58047	3.91073	H	-2.96427	-0.84520	-3.72916
H	3.21032	-2.33841	4.08067	H	-2.58864	-2.54557	-4.02961
H	3.35479	-1.58836	2.48582	H	-2.92927	-1.97887	-2.38937
C	0.66606	-1.28615	4.69827	C	-0.37592	-0.90298	-4.49690
H	0.93915	-0.30362	5.08360	H	-0.88003	0.01287	-4.80589
H	-0.42129	-1.32320	4.60816	H	0.69143	-0.68847	-4.41002
H	0.97065	-2.04262	5.42574	H	-0.50563	-1.65245	-5.28056
C	0.65450	-2.49481	2.44523	C	-0.08885	-2.41077	-2.50559
H	-0.24180	-2.94222	2.85327	H	0.77548	-2.75229	-3.05793
C	1.40935	-3.34399	1.44072	C	-0.65813	-3.36930	-1.49408
H	2.48589	-3.36490	1.64112	H	-1.71149	-3.60535	-1.67494
H	1.06482	-4.37595	1.51676	H	-0.10514	-4.30521	-1.56504
Rh	-0.83306	-1.99500	0.32924	Rh	1.19070	-1.34903	-0.85095
Cl	-1.94712	0.49392	0.41256	Cl	1.41626	1.26969	0.32056
C	-1.41674	-2.44118	-1.39659	C	2.53730	-2.01838	0.46912
C	-2.45700	-2.94456	1.11125	C	2.62472	-0.92130	-2.09534
O	-1.70864	-2.71992	-2.45552	O	3.23459	-2.46675	1.23634
O	-3.28105	-3.54308	1.59829	O	3.42221	-0.68999	-2.86248
Rh	-4.16175	0.85717	-0.61182	Rh	3.52293	2.12254	1.26583
Cl	-4.54035	-1.50566	-0.93332	Cl	4.84193	0.44321	0.13101
C	-3.90118	2.69932	-0.37253	C	2.51990	3.43352	2.15580
O	-3.73618	3.81835	-0.22429	O	1.90163	4.22819	2.69290
C	-5.84731	1.12713	-1.38695	C	5.13683	2.76519	1.97007
O	-6.87259	1.27399	-1.85844	O	6.12524	3.14454	2.38928
S	2.19117	1.90850	2.04837	S	-2.84024	1.65501	-1.50003
O	3.62916	2.04267	2.30080	O	-4.28627	1.42798	-1.56556
C	1.62409	3.44106	1.30044	C	-2.57047	3.23717	-0.69605
C	2.55588	4.42608	0.99567	C	-3.66621	3.92212	-0.18324
H	3.60562	4.25169	1.18695	H	-4.65412	3.48917	-0.25610
C	2.10860	5.62966	0.46196	C	-3.46405	5.16626	0.40313
H	2.82148	6.40955	0.22654	H	-4.30821	5.71486	0.80079
C	0.75117	5.82909	0.23418	C	-2.18255	5.70175	0.47670
H	0.40702	6.76755	-0.18238	H	-2.02891	6.66996	0.93656
C	-0.16963	4.83006	0.54034	C	-1.09492	5.00061	-0.03737
H	-1.22539	4.98834	0.36285	H	-0.09876	5.41901	0.02371
H	-0.44653	2.84470	1.32290	H	-0.44023	3.21011	-1.02961
C	0.26220	3.62597	1.08095	C	-1.28232	3.76019	-0.63245
O	1.29456	1.59135	3.16058	O	-2.05589	1.62854	-2.73733

TS6			
C	-2.24641	5.39483	-7.00787
C	-4.43596	4.27650	-6.79509
H	-5.45948	4.61836	-6.93259
H	-4.42243	3.61060	-5.92759
C	-4.04614	3.44329	-8.03008
C	-2.55753	3.06287	-8.03579
H	-2.28804	2.65020	-9.00620
H	-2.43092	2.25783	-7.30582
C	-1.70612	4.22131	-7.62748
O	-4.40022	4.26182	-9.15529
O	-4.74075	2.19051	-8.04016
C	-4.34110	3.79674	-10.43636
C	-6.10136	2.11295	-8.12075
O	-6.83506	3.06456	-8.16200
O	-3.93040	2.70921	-10.74621
C	-6.52681	0.67313	-8.16392
H	-6.12637	0.20261	-9.06351
H	-6.12234	0.13461	-7.30597
H	-7.61167	0.61508	-8.16663
C	-4.88655	4.82894	-11.38142
H	-4.71062	4.51257	-12.40587
H	-5.95905	4.93788	-11.20844
H	-4.42825	5.80077	-11.19817
C	0.58269	3.68280	-8.59704
H	1.22712	3.01960	-8.01668
H	0.02998	3.08169	-9.32552
H	1.22769	4.36696	-9.15168
C	-0.37511	4.43285	-7.72113
C	-1.09860	6.35610	-7.13292
H	-0.84740	6.90226	-6.22513
C	-1.02270	7.30006	-8.35143
C	-1.34050	6.62971	-9.68991
H	-1.38731	7.38364	-10.47648
H	-0.59286	5.89118	-9.97505
H	-2.31165	6.13751	-9.64968
C	-2.07319	8.42950	-8.12494
H	-1.97087	9.15756	-8.93069
H	-3.08874	8.03529	-8.14606
H	-1.92556	8.93917	-7.17476
C	0.32710	7.98696	-8.34586

H	0.60178	8.42432	-7.38867
C	1.13744	8.16243	-9.38142
H	0.92384	7.76861	-10.36692
H	2.06248	8.71437	-9.27237
Rh	0.80271	5.18689	-5.99284
Cl	-0.80230	4.26013	-4.31137
C	2.21472	5.84292	-7.05992
C	1.96554	5.41606	-4.44836
O	3.16007	6.16113	-7.60553
O	2.62327	5.52805	-3.53464
Rh	-0.28472	1.83670	-4.17620
Cl	1.81181	2.15578	-5.32690
C	-1.89803	1.56080	-3.25077
O	-2.87326	1.39532	-2.68516
C	0.14898	0.01358	-4.06708
O	0.43049	-1.08589	-4.00468
C	-3.50996	5.44731	-6.56535
S	-4.17353	6.85051	-5.66707
O	-5.22921	7.46230	-6.47820
C	-4.95239	6.10918	-4.22948
C	-6.33524	5.96680	-4.20760
H	-6.92491	6.29338	-5.05298
C	-6.93505	5.42140	-3.07832
H	-8.01117	5.31014	-3.04384
C	-6.15477	5.02619	-1.99673
H	-6.62639	4.60197	-1.11918
C	-4.77102	5.17796	-2.03273
C	-4.15875	5.72459	-3.15278
H	-3.08639	5.85818	-3.18984
H	-4.16799	4.87573	-1.18623
O	-3.04396	7.66122	-5.20468

Table S4 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level in toluene solvent

CAT				1a			
Rh	-1.60008	-0.00003	0.09751	C	0.11306	-0.70298	0.57315
Cl	-0.00003	-1.66216	0.91587	C	0.89973	-1.24786	-0.30522
C	-2.77479	1.33938	-0.50842	C	-0.01815	0.73785	0.98766
O	-3.47466	2.15855	-0.86608	H	0.73666	0.96639	1.74069
Rh	1.60007	-0.00000	0.09765	H	-0.98580	0.90124	1.45452
Cl	-0.00005	1.66187	0.91639	C	0.12551	1.76794	-0.13267
C	2.77485	-1.33921	-0.50859	C	1.49814	1.79536	-0.82270
O	3.47483	-2.15820	-0.86646	H	1.50363	2.64607	-1.50308
C	-2.77473	-1.33928	-0.50891	H	1.58194	0.89567	-1.43098
O	-3.47456	-2.15834	-0.86688	C	2.60839	1.85911	0.11494
C	2.77469	1.33943	-0.50842	O	-0.12388	3.00957	0.53710
O	3.47456	2.15857	-0.86616	O	-0.79800	1.50570	-1.19453
				C	-0.29243	4.17065	-0.14505
				C	-2.14144	1.60353	-1.01154
				O	-2.66474	1.99604	-0.00183
				O	-0.22113	4.27599	-1.34224
				C	-2.85868	1.14038	-2.24438
				H	-2.41119	1.57958	-3.13512
				H	-2.76272	0.05524	-2.31699
				H	-3.91035	1.40168	-2.17271
				C	-0.60293	5.28135	0.81481
				H	-0.63805	6.22659	0.28064
				H	-1.56771	5.08437	1.28563
				H	0.14749	5.31773	1.60482
				C	4.63538	1.86902	1.83152
				H	4.50366	2.62805	2.60530
				H	4.72720	0.89895	2.32568
				H	5.57671	2.07431	1.31715
				C	3.52074	1.87253	0.89492
				C	1.69600	-1.84888	-1.13376
				H	1.37076	-2.00555	-2.15962
				C	3.09130	-2.34663	-0.77646
				C	3.42268	-2.04799	0.68404
				H	2.70893	-2.54854	1.33843
				H	4.42250	-2.41047	0.92491
				H	3.37947	-0.97834	0.88971
				C	3.12051	-3.86930	-1.01956
				H	2.40013	-4.36889	-0.37061

				H	2.87512	-4.10873	-2.05630
				H	4.11714	-4.25978	-0.80666
				C	4.03820	-1.67559	-1.75089
				H	3.86846	-1.93793	-2.79300
				C	5.01215	-0.82606	-1.45571
				H	5.22329	-0.51640	-0.44109
				H	5.63407	-0.40198	-2.23390
				S	-0.93272	-1.87055	1.48412
				O	-1.15465	-1.30517	2.81699
				O	-0.37048	-3.21178	1.33448
				C	-2.48189	-1.81856	0.58992
				C	-3.48820	-0.96358	1.01607
				C	-2.63401	-2.62829	-0.53156
				C	-4.67823	-0.91979	0.29937
				H	-3.34087	-0.34911	1.89203
				C	-3.82728	-2.57693	-1.23699
				H	-1.83551	-3.29393	-0.82802
				C	-4.84659	-1.72276	-0.82184
				H	-5.46914	-0.25391	0.61740
				H	-3.96554	-3.20622	-2.10651
				H	-5.77551	-1.68519	-1.37631
2a				3a			
C	-0.34140	-0.64712	-0.22169	C	-0.93344	-0.62786	0.59358
C	0.86404	-1.04138	-0.68741	C	1.17123	0.56660	0.17616
C	-0.82526	0.77933	-0.13867	H	1.70854	0.73607	-0.75447
H	-1.27363	0.97028	0.83302	H	1.91525	0.43859	0.96605
H	-1.58801	0.97722	-0.89525	C	0.37542	1.84628	0.48577
C	0.31138	1.76371	-0.35319	C	-0.59285	1.68333	1.66934
C	1.16190	1.30811	-1.52900	H	-1.17281	2.59379	1.79551
H	1.88835	2.07294	-1.76588	H	0.01702	1.55030	2.56708
H	0.48532	1.21870	-2.38403	C	-1.41174	0.47215	1.40668
C	1.78521	-0.02654	-1.22614	O	-0.33198	2.13636	-0.72643
O	1.04171	1.77500	0.87977	O	1.25217	2.91036	0.86706
O	-0.15617	3.07342	-0.69136	C	-1.07255	3.26429	-0.87296
C	2.18168	2.49392	1.02476	C	2.16306	3.43086	0.00026
C	-0.95535	3.77475	0.15718	O	2.35088	3.02699	-1.11676
O	-1.35902	3.36146	1.21200	O	-1.18488	4.12125	-0.03439
O	2.63996	3.22902	0.18765	C	2.87188	4.58622	0.64519
C	-1.23853	5.13294	-0.41718	H	2.15293	5.38433	0.83772
H	-0.30303	5.68526	-0.51946	H	3.29064	4.28357	1.60542

H	-1.67084	5.03526	-1.41373	H	3.65733	4.94606	-0.01323
H	-1.91861	5.67121	0.23679	C	-1.71143	3.27848	-2.23072
C	2.77011	2.24205	2.38261	H	-2.24575	4.21351	-2.37270
H	3.66112	2.84928	2.51361	H	-0.94840	3.15504	-2.99961
H	2.03492	2.47615	3.15328	H	-2.40153	2.43786	-2.31739
H	3.01804	1.18423	2.48258	C	-3.73292	0.19334	2.57705
C	4.08101	0.73820	-1.91978	H	-3.88660	-0.58579	3.33003
H	3.77449	1.76792	-1.76034	H	-3.58802	1.14715	3.08569
H	5.04644	0.59703	-1.42866	H	-4.65374	0.23785	1.99127
H	4.25139	0.59398	-2.99212	C	-2.57896	-0.13600	1.71415
C	3.09649	-0.27643	-1.41115	C	-2.27134	-1.36449	0.81497
C	1.32446	-2.44745	-0.63134	H	-2.15920	-2.31050	1.35001
H	0.61430	-3.16750	-1.00343	C	-3.21731	-1.56423	-0.40042
C	2.15951	-2.91311	0.54901	C	-3.40659	-0.25150	-1.16372
C	2.47544	-1.93249	1.65334	H	-4.03169	-0.41015	-2.04335
H	1.63777	-1.86972	2.35155	H	-3.87132	0.52167	-0.55061
H	3.35785	-2.25743	2.21122	H	-2.43927	0.12248	-1.50065
H	2.66355	-0.92730	1.27871	C	-2.64417	-2.61866	-1.36324
C	1.90435	-4.32116	1.03370	H	-3.37997	-2.84078	-2.13825
H	1.05720	-4.34249	1.72240	H	-1.73879	-2.25667	-1.84759
H	1.67484	-4.99133	0.20363	H	-2.39559	-3.54380	-0.84411
H	2.78078	-4.71530	1.55644	C	-4.51413	-2.11472	0.14940
C	2.78780	-2.74662	-0.81249	H	-4.39961	-3.04087	0.70921
H	3.00790	-3.67263	-1.32937	C	-5.73301	-1.61461	-0.00391
C	3.72806	-1.61466	-1.13984	H	-5.91993	-0.70013	-0.55254
H	4.47135	-1.47913	-0.34340	H	-6.59722	-2.11283	0.41740
H	4.31596	-1.87991	-2.02494	C	0.28689	-0.65815	0.06089
S	-1.48008	-1.77300	0.58830	S	0.95323	-2.06510	-0.78656
O	-1.39637	-1.52147	2.03120	O	1.03388	-1.77871	-2.22310
C	-3.07969	-1.18218	0.02788	C	2.63131	-2.12675	-0.15934
C	-3.85813	-0.40623	0.87422	C	3.66715	-1.61892	-0.93065
H	-3.49918	-0.17214	1.86652	H	3.45639	-1.21845	-1.91222
C	-5.09236	0.04730	0.42369	C	4.96005	-1.64862	-0.42153
H	-5.71231	0.65060	1.07384	H	5.77905	-1.26041	-1.01277
C	-5.52668	-0.27333	-0.85750	C	5.19879	-2.17746	0.84206
H	-6.48793	0.08280	-1.20532	H	6.20722	-2.19882	1.23508
C	-4.73463	-1.05492	-1.69463	C	4.14915	-2.68541	1.60316
H	-5.08017	-1.30916	-2.68819	C	2.85447	-2.66239	1.10358
H	-2.88010	-2.13632	-1.88385	H	2.02688	-3.06215	1.67347
C	-3.50256	-1.51655	-1.25297	H	4.34097	-3.10391	2.58259
O	-1.33355	-3.14561	0.09841	O	0.25141	-3.26527	-0.32597

COM				TS1			
C	-1.98666	1.33969	-0.79201	C	1.22699	0.87160	-0.78799
C	-2.55020	0.93242	1.65939	C	1.81358	-1.63253	-0.70387
H	-3.55532	1.29498	1.87177	H	2.70954	-2.14120	-1.04188
H	-1.94337	1.16520	2.53372	H	0.98356	-1.99428	-1.30685
C	-2.60353	-0.58704	1.55456	C	1.57761	-2.08010	0.74448
C	-1.20377	-1.22486	1.36948	C	0.11006	-2.00234	1.19841
H	-1.16181	-2.12239	1.98525	H	-0.00030	-2.64615	2.06883
H	-0.45443	-0.53854	1.76183	H	-0.52023	-2.39959	0.40798
C	-0.86651	-1.59853	0.00074	C	-0.33850	-0.67360	1.60633
O	-3.51213	-0.89600	0.50710	O	2.46539	-1.31039	1.54018
O	-3.03908	-1.10618	2.82289	O	1.83681	-3.48932	0.84688
C	-3.88170	-2.18212	0.26390	C	2.56779	-1.48446	2.88345
C	-4.31009	-0.92123	3.27766	C	3.08121	-4.01470	0.66993
O	-5.16269	-0.30927	2.69095	O	4.05660	-3.37476	0.37797
O	-3.45736	-3.13125	0.86812	O	1.92316	-2.27905	3.51676
C	-4.47790	-1.61443	4.59797	C	3.04011	-5.49546	0.90851
H	-4.34852	-2.68912	4.45947	H	2.75424	-5.68675	1.94406
H	-3.71229	-1.27894	5.29818	H	2.28528	-5.95662	0.27070
H	-5.46797	-1.40719	4.99359	H	4.01796	-5.92356	0.70747
C	-4.89936	-2.21631	-0.83594	C	3.60076	-0.54542	3.43029
H	-5.05651	-3.24169	-1.15866	H	3.70976	-0.70109	4.49967
H	-5.83685	-1.80401	-0.45709	H	4.54980	-0.71128	2.91949
H	-4.58346	-1.59142	-1.67104	H	3.30359	0.48419	3.22651
C	-1.36825	-2.30120	-2.51990	C	-0.72031	1.09736	3.55241
H	-1.28979	-3.37675	-2.68482	H	-1.72125	0.99378	3.97293
H	-2.41010	-2.00085	-2.64770	H	0.00327	0.77542	4.30418
H	-0.77162	-1.79831	-3.28048	H	-0.54383	2.14473	3.31786
C	-0.92369	-1.94787	-1.17573	C	-0.56630	0.24432	2.37889
C	-1.95689	1.18009	-2.07780	C	0.80434	2.11416	-0.75831
H	-1.07209	0.73737	-2.52527	H	0.27450	2.48547	-1.63152
C	-3.07183	1.61380	-3.02047	C	1.19487	3.16594	0.27359
C	-4.29216	2.10456	-2.24487	C	2.03875	2.55325	1.38876
H	-5.07774	2.41960	-2.93234	H	2.33154	3.31382	2.11163
H	-4.69117	1.32582	-1.59357	H	1.49334	1.76448	1.90370
H	-4.01999	2.95748	-1.62393	H	2.94882	2.11849	0.97700
C	-2.50666	2.76304	-3.88488	C	2.04345	4.20498	-0.50610

H	-3.26010	3.09479	-4.60141	H	2.38271	4.97762	0.18459
H	-2.22754	3.60263	-3.24757	H	2.90337	3.71992	-0.96566
H	-1.62385	2.44147	-4.44116	H	1.45459	4.68440	-1.29020
C	-3.37305	0.43686	-3.92222	C	-0.04453	3.87761	0.76970
H	-2.51863	0.08360	-4.49546	H	-0.77991	4.09299	-0.00022
C	-4.54166	-0.17055	-4.08170	C	-0.26736	4.32242	1.99886
H	-5.43167	0.13649	-3.54790	H	0.43553	4.17161	2.80801
H	-4.64813	-0.99971	-4.77005	H	-1.17100	4.86896	2.23639
Rh	1.26257	-2.03907	-0.60917	Rh	-1.47714	0.77810	0.18457
Cl	1.46455	0.35026	-1.21424	Cl	-1.41539	-1.06329	-1.65679
C	1.00426	-3.85625	-0.25647	C	-2.66810	1.65190	1.35361
C	2.97229	-2.42088	-1.45922	C	-2.25427	1.78517	-1.20444
O	0.81388	-4.95409	-0.03282	O	-3.42979	2.16834	2.02156
O	3.92873	-2.69664	-2.00435	O	-2.67790	2.40399	-2.05651
Rh	3.46602	0.10902	0.19930	Rh	-3.79336	-1.06409	-0.95070
Cl	2.15601	-1.00336	1.90835	Cl	-3.32528	-2.04887	1.20006
C	4.48955	0.91456	-1.15643	C	-4.23706	-0.42260	-2.65767
O	5.08825	1.40827	-1.98821	O	-4.50145	-0.05273	-3.70205
C	4.98320	-0.20445	1.26343	C	-5.59102	-1.11555	-0.42575
O	5.88593	-0.40280	1.92442	O	-6.67668	-1.16097	-0.09091
C	-2.00831	1.66494	0.46401	C	1.99668	-0.16276	-0.94403
S	-1.42823	3.35390	0.81278	S	3.65216	0.30365	-1.59241
O	-1.93564	3.69433	2.14545	O	4.62707	0.02490	-0.53867
O	-1.74908	4.20128	-0.33583	O	3.56562	1.64978	-2.15867
C	0.35397	3.23955	0.91426	C	3.91474	-0.85896	-2.92325
C	0.93942	2.73388	2.06840	C	4.74742	-1.95000	-2.71292
C	1.11633	3.69740	-0.15222	C	3.25736	-0.65291	-4.13059
C	2.32304	2.69335	2.15532	C	4.92878	-2.85716	-3.74993
C	2.49962	3.67020	-0.04584	C	3.44513	-1.56861	-5.15589
C	3.10062	3.16938	1.10401	C	4.27902	-2.66742	-4.96460
H	0.32512	2.39916	2.89213	H	5.22977	-2.08130	-1.75481
H	0.62521	4.08379	-1.03323	H	2.62173	0.21182	-4.26228
H	2.79509	2.29233	3.04154	H	5.57566	-3.71249	-3.60591
H	3.10802	4.03557	-0.86270	H	2.94484	-1.42394	-6.10431
H	4.17877	3.16223	1.19023	H	4.42230	-3.37839	-5.76812
INT1				TS2			
C	-1.06983	0.42887	-0.93248	C	-5.72978	-3.29814	3.16710
C	1.05303	0.74989	0.39548	C	-7.08687	-4.56143	4.88184
H	1.99478	1.23949	0.17340	H	-7.84471	-4.28901	5.60764
H	1.26123	-0.32260	0.45295	H	-6.26524	-5.05003	5.40606

C	0.60820	1.22409	1.77960	C	-7.70413	-5.54821	3.89885
C	-0.34762	0.26077	2.49008	C	-6.65995	-6.12726	2.96082
H	-0.45037	0.60107	3.52015	H	-7.14193	-6.82600	2.27609
H	0.11428	-0.72449	2.49913	H	-5.96845	-6.70316	3.58973
C	-1.69660	0.16578	1.94044	C	-5.85547	-5.20756	2.14615
O	0.04766	2.51443	1.59474	O	-8.73229	-4.82977	3.22304
O	1.73656	1.22494	2.66514	O	-8.19965	-6.70225	4.58394
C	-0.36525	3.28534	2.63221	C	-9.50851	-5.40596	2.27018
C	2.77743	2.08895	2.49895	C	-9.19965	-6.61194	5.50644
O	2.84229	2.91369	1.62698	O	-9.76998	-5.59346	5.79225
O	-0.31970	2.95020	3.78827	O	-9.42293	-6.55785	1.92849
C	3.80324	1.85463	3.56822	C	-9.46638	-7.96731	6.09157
H	3.35530	2.02649	4.54794	H	-9.69591	-8.67633	5.29548
H	4.14018	0.81755	3.53915	H	-8.57130	-8.32525	6.60349
H	4.64332	2.52666	3.41882	H	-10.29448	-7.90499	6.79157
C	-0.87127	4.59464	2.10740	C	-10.46707	-4.39199	1.72144
H	-1.14829	5.24112	2.93502	H	-11.17828	-4.87951	1.06090
H	-0.10239	5.06040	1.49080	H	-10.97983	-3.88334	2.53733
H	-1.73323	4.41798	1.46207	H	-9.90810	-3.63391	1.16969
C	-4.33125	0.42516	2.16376	C	-4.82151	-5.82020	-0.16213
H	-4.75453	-0.44552	2.66706	H	-3.93431	-6.45190	-0.08167
H	-4.43213	1.28867	2.82425	H	-5.66763	-6.43463	-0.47519
H	-4.89584	0.60952	1.25307	H	-4.63200	-5.06409	-0.92320
C	-2.91494	0.21507	1.88453	C	-5.08754	-5.19366	1.14050
C	-2.24385	0.40336	-1.64657	C	-5.10844	-2.35743	2.31254
H	-2.23642	-0.20943	-2.54248	H	-4.57010	-1.58327	2.84723
C	-3.35766	1.44687	-1.67270	C	-5.72338	-1.81951	1.00073
C	-3.13533	2.55848	-0.65029	C	-7.09625	-2.42674	0.70543
H	-3.93113	3.29988	-0.71816	H	-7.54175	-1.92811	-0.15596
H	-3.10196	2.17584	0.36709	H	-7.03900	-3.49166	0.49627
H	-2.19269	3.06786	-0.84643	H	-7.76244	-2.28123	1.55530
C	-3.35119	2.05912	-3.09860	C	-5.89761	-0.29229	1.18606
H	-4.14376	2.80520	-3.16232	H	-6.30879	0.13698	0.27181
H	-2.39102	2.52104	-3.31286	H	-6.56385	-0.07835	2.01836
H	-3.54367	1.29434	-3.85343	H	-4.93786	0.18784	1.38739
C	-4.68145	0.72638	-1.52851	C	-4.74176	-1.99612	-0.13321
H	-4.73056	-0.22526	-2.05084	H	-3.75843	-1.57990	0.06638
C	-5.76982	1.17657	-0.91926	C	-4.98288	-2.51832	-1.32753
H	-5.79386	2.12695	-0.40104	H	-5.94728	-2.92996	-1.59560
H	-6.68946	0.60546	-0.92987	H	-4.21276	-2.54484	-2.08815
Rh	-2.13509	-1.13698	0.03878	Rh	-3.85526	-4.07895	2.43061

Cl	0.92145	-2.31526	-1.96721	Cl	-3.88369	-5.20718	6.12970
C	-3.64868	-2.26701	0.72238	C	-2.41802	-3.78229	1.07197
C	-2.07174	-2.34936	-1.44421	C	-2.79037	-3.23478	3.89433
O	-4.51858	-2.87892	1.10607	O	-1.62063	-3.62993	0.28538
O	-2.19539	-3.11389	-2.26705	O	-2.12123	-2.71684	4.64098
Rh	1.78477	-2.59933	0.26022	Rh	-3.99425	-7.26449	4.88219
Cl	-0.45649	-2.89901	1.21413	Cl	-2.69403	-6.32061	3.02731
C	3.49645	-2.40445	-0.48362	C	-4.97560	-7.97141	6.31508
O	4.52669	-2.28807	-0.95081	O	-5.58528	-8.37515	7.18648
C	2.47276	-2.85193	1.98955	C	-4.04495	-8.88692	3.93112
O	2.87857	-3.00280	3.04311	O	-4.06702	-9.86256	3.34547
C	0.08081	1.01215	-0.70634	C	-6.58431	-3.34948	4.17057
S	0.58775	2.28237	-1.90718	S	-7.33456	-1.78682	4.71068
O	0.55762	3.59781	-1.26460	O	-8.74732	-1.76075	4.33272
O	-0.18160	2.07148	-3.13558	O	-6.46012	-0.68865	4.29262
C	2.29135	1.84386	-2.21918	C	-7.21764	-1.96306	6.48476
C	3.30344	2.63881	-1.69859	C	-8.37843	-2.11499	7.22938
C	2.55586	0.68349	-2.93681	C	-5.95607	-1.98630	7.06794
C	4.62272	2.26124	-1.91676	C	-8.26881	-2.27845	8.60491
C	3.87751	0.31407	-3.13799	C	-5.86065	-2.16134	8.44017
C	4.90707	1.10196	-2.63105	C	-7.01498	-2.30414	9.20561
H	3.05363	3.51827	-1.12338	H	-9.33862	-2.11239	6.73333
H	1.74717	0.07051	-3.30622	H	-5.06858	-1.87893	6.46017
H	5.42598	2.86782	-1.51961	H	-9.16239	-2.39585	9.20352
H	4.10168	-0.59361	-3.68201	H	-4.88704	-2.19244	8.91044
H	5.93637	0.80593	-2.78832	H	-6.93464	-2.44257	10.27608
INT2				TS3			
C	-1.67471	-0.30583	-0.75409	C	8.07856	0.94601	-9.34493
C	-0.49784	-0.78980	-0.31223	C	6.73991	0.80172	-9.29854
C	-2.68644	0.29245	0.19022	C	8.92159	0.16305	-10.31681
H	-3.69338	0.15303	-0.19317	H	9.91974	0.00543	-9.91770
H	-2.52075	1.36475	0.32362	H	9.01490	0.69390	-11.26745
C	-2.59536	-0.37130	1.56033	C	8.29271	-1.19759	-10.60140
C	-1.18526	-0.26650	2.11968	C	6.85290	-1.05501	-11.07533
H	-1.09767	-0.90480	2.99647	H	6.38451	-2.03592	-11.07448
H	-1.05979	0.76303	2.46519	H	6.90172	-0.72925	-12.11704
C	-0.13448	-0.59010	1.08800	C	6.06592	-0.05247	-10.26666
O	-2.99290	-1.73093	1.34272	O	8.39163	-1.92016	-9.36644
O	-3.43290	0.28456	2.51768	O	8.97213	-1.87014	-11.66649
C	-3.14634	-2.60609	2.36836	C	8.05746	-3.23307	-9.27906

C	-4.78763	0.29292	2.38946	C	10.26950	-2.26323	-11.54744
O	-5.38838	-0.19925	1.47126	O	10.95671	-2.06170	-10.58118
O	-2.93743	-2.34600	3.52543	O	7.60167	-3.88350	-10.18398
C	-5.40356	0.98698	3.56917	C	10.69278	-2.99336	-12.78853
H	-5.18024	0.42132	4.47528	H	10.09415	-3.89948	-12.89500
H	-4.97178	1.98123	3.68848	H	10.51072	-2.37505	-13.66819
H	-6.47862	1.05665	3.43047	H	11.74599	-3.24974	-12.71922
C	-3.63216	-3.92385	1.83901	C	8.37012	-3.74585	-7.90371
H	-3.65539	-4.65458	2.64238	H	7.97688	-4.75214	-7.79070
H	-4.63335	-3.79341	1.42460	H	9.45335	-3.75386	-7.76909
H	-2.98837	-4.26729	1.02922	H	7.95374	-3.08479	-7.14412
C	1.73532	-0.48677	2.75094	C	3.85343	-0.64154	-11.29424
H	1.25214	0.31191	3.32052	H	3.11766	-0.03175	-11.81474
H	1.55226	-1.42237	3.29183	H	4.41080	-1.21065	-12.04086
H	2.80623	-0.30036	2.75796	H	3.30408	-1.35803	-10.67228
C	1.17864	-0.58439	1.36615	C	4.74927	0.17945	-10.42120
C	0.53252	-1.54857	-1.09698	C	5.81415	1.38293	-8.28952
H	0.56115	-1.22319	-2.13018	H	6.11951	2.35671	-7.93512
C	0.36030	-3.08810	-1.08084	C	5.43393	0.46375	-7.10608
C	0.17245	-3.68563	0.31277	C	5.45875	-1.03134	-7.42273
H	-0.71460	-3.26494	0.78196	H	6.45689	-1.32434	-7.74026
H	0.02993	-4.76421	0.23763	H	5.20585	-1.59518	-6.52387
H	1.01163	-3.50356	0.97915	H	4.76595	-1.30927	-8.21303
C	-0.91146	-3.43053	-1.90134	C	6.42645	0.73370	-5.95789
H	-1.80166	-3.00994	-1.43550	H	7.43541	0.43227	-6.23979
H	-0.84733	-3.04876	-2.91818	H	6.45370	1.79027	-5.69428
H	-1.02437	-4.51440	-1.94244	H	6.12711	0.15893	-5.07865
C	1.52046	-3.68297	-1.84030	C	4.05910	0.92484	-6.66986
H	1.68425	-3.22693	-2.81381	H	4.03513	1.90276	-6.19895
C	2.29593	-4.69353	-1.47219	C	2.91928	0.24190	-6.78375
H	2.18292	-5.19638	-0.52028	H	2.88151	-0.75037	-7.21195
H	3.08252	-5.05620	-2.12165	H	1.98601	0.66105	-6.43010
Rh	2.35479	-0.73044	-0.33923	Rh	4.02476	1.77822	-9.35908
Cl	1.55688	1.43528	-1.33514	Cl	5.45753	3.32061	-10.57072
C	3.05786	-2.26926	0.49347	C	1.88265	0.98638	-9.52889
C	3.42868	-0.89864	-2.09931	C	3.39721	3.46233	-8.39964
O	3.59252	-3.08801	1.06604	O	0.79793	0.69117	-9.56285
O	4.02387	-0.99448	-3.05023	O	3.08631	4.42831	-7.90396
Rh	2.28557	2.24432	0.84159	Rh	4.66742	2.36920	-12.66873
Cl	4.24700	0.79573	0.60395	Cl	2.38695	2.79691	-11.97570
C	0.74506	3.30919	0.96104	C	6.44794	2.04722	-13.16132

O	-0.20879	3.92634	1.00910	O	7.54022	1.84404	-13.41413
C	2.93152	2.89978	2.47977	C	4.00821	1.73346	-14.30866
O	3.33921	3.28853	3.46649	O	3.59085	1.35931	-15.29748
S	-2.20366	-0.26008	-2.45713	S	9.01956	2.06451	-8.32884
O	-3.41519	-1.07180	-2.60181	O	9.99622	1.29254	-7.55650
O	-1.07205	-0.49638	-3.35848	O	8.13336	2.99707	-7.62637
C	-2.68503	1.45951	-2.61788	C	9.90450	2.98321	-9.58552
C	-4.03324	1.78678	-2.64334	C	11.26209	2.76127	-9.76359
C	-1.69275	2.43010	-2.68581	C	9.19429	3.87777	-10.37835
C	-4.39528	3.12524	-2.74080	C	11.92838	3.46352	-10.76155
C	-2.06651	3.76325	-2.77625	C	9.86893	4.56660	-11.37537
C	-3.41502	4.10945	-2.80271	C	11.23316	4.35964	-11.56559
H	-4.77552	1.00276	-2.59201	H	11.77782	2.05524	-9.12794
H	-0.65141	2.14337	-2.66226	H	8.13519	4.02445	-10.21797
H	-5.44234	3.39741	-2.76594	H	12.98859	3.30707	-10.91134
H	-1.30589	4.53131	-2.82861	H	9.33133	5.26523	-12.00300
H	-3.70177	5.15086	-2.87371	H	11.75508	4.90007	-12.34483
INT3				TS4			
C	-2.25356	0.54540	-0.55702	C	-11.19940	-1.61002	-5.81221
C	-1.15529	-0.23281	-0.64559	C	-9.93381	-1.85797	-6.20738
C	-3.20891	0.48582	0.60868	C	-12.37711	-1.52099	-6.74179
H	-4.22217	0.68328	0.26948	H	-13.04616	-0.72637	-6.42600
H	-2.95314	1.23178	1.36539	H	-12.95431	-2.44977	-6.74068
C	-3.16952	-0.88435	1.27158	C	-11.91016	-1.26043	-8.16670
C	-1.74370	-1.26178	1.63374	C	-10.82517	-2.25194	-8.55809
H	-1.73713	-2.26810	2.04018	H	-10.52209	-2.06800	-9.58288
H	-1.43884	-0.58537	2.43634	H	-11.27191	-3.24977	-8.51698
C	-0.79913	-1.11274	0.46571	C	-9.66179	-2.18693	-7.60755
O	-3.74784	-1.78616	0.31767	O	-11.43059	0.09302	-8.16436
O	-3.88748	-0.89551	2.50981	O	-12.95495	-1.44896	-9.11985
C	-3.94285	-3.09687	0.60565	C	-10.93677	0.67883	-9.28333
C	-5.23547	-0.70805	2.55092	C	-14.06652	-0.65715	-9.11596
O	-5.91917	-0.46824	1.59153	O	-14.26311	0.23085	-8.33127
O	-3.62482	-3.62547	1.64032	O	-10.81790	0.12976	-10.34890
C	-5.72756	-0.87207	3.95947	C	-14.97528	-1.05642	-10.24137
H	-5.59110	-1.91060	4.26539	H	-14.46149	-0.90833	-11.19253
H	-5.14504	-0.25201	4.64024	H	-15.22255	-2.11586	-10.16434
H	-6.77958	-0.60786	4.01128	H	-15.87981	-0.45600	-10.20911
C	-4.63291	-3.77327	-0.54274	C	-10.58432	2.10879	-8.99302
H	-4.72609	-4.83573	-0.33871	H	-10.09853	2.54974	-9.85876

H	-5.62118	-3.33122	-0.67533	H	-11.49680	2.65954	-8.75825
H	-4.07773	-3.61001	-1.46597	H	-9.93661	2.17017	-8.11817
C	1.00769	-2.52634	1.50435	C	-8.07217	-3.00515	-9.37904
H	1.84158	-2.04650	2.02029	H	-8.82347	-3.67629	-9.79361
H	0.26945	-2.81095	2.25412	H	-8.01515	-2.13621	-10.04252
H	1.40678	-3.44122	1.06019	H	-7.11473	-3.51817	-9.42257
C	0.44084	-1.62809	0.45763	C	-8.42954	-2.59529	-7.98593
C	-0.22355	-0.31840	-1.80985	C	-8.76973	-1.94750	-5.28623
H	-0.07314	0.63019	-2.30125	H	-9.04955	-2.29452	-4.30503
C	-0.47754	-1.43741	-2.84959	C	-7.76549	-0.76207	-5.19661
C	-1.63121	-2.37793	-2.50770	C	-8.32913	0.56360	-5.71445
H	-2.57212	-1.82934	-2.52724	H	-9.14694	0.88604	-5.07150
H	-1.68434	-3.18263	-3.24293	H	-7.55169	1.33073	-5.70994
H	-1.52446	-2.81870	-1.51892	H	-8.72491	0.47613	-6.72548
C	-0.68698	-0.85222	-4.24564	C	-7.29794	-0.57863	-3.75412
H	-1.61668	-0.28995	-4.28815	H	-8.13582	-0.26877	-3.13173
H	0.12389	-0.17080	-4.51018	H	-6.88484	-1.50004	-3.34149
H	-0.71975	-1.65333	-4.98778	H	-6.52323	0.18881	-3.70144
C	0.87098	-2.14105	-2.80205	C	-6.64430	-1.33206	-6.05493
H	1.54223	-1.95487	-3.63217	H	-5.64688	-1.43970	-5.64758
C	1.26821	-3.04253	-1.85084	C	-6.81282	-1.35971	-7.45191
H	0.56415	-3.46284	-1.15110	H	-7.43459	-0.62003	-7.92891
H	2.20690	-3.56439	-1.97281	H	-5.99516	-1.71260	-8.06530
Rh	1.66448	-0.92034	-1.04261	Rh	-7.46398	-3.31194	-6.18724
Cl	1.64217	1.31495	0.07776	Cl	-9.30819	-5.13571	-5.86571
C	3.42858	-1.75612	-0.25890	C	-5.94937	-4.37510	-7.15716
C	2.73099	0.08710	-2.50428	C	-6.87640	-3.92670	-4.39824
O	4.29094	-2.43518	0.00733	O	-4.97879	-4.67165	-7.65817
O	3.20631	0.68991	-3.32752	O	-6.60806	-4.25106	-3.35129
Rh	3.53964	0.63137	1.45123	Rh	-7.85232	-6.50632	-7.24848
Cl	5.06602	0.99142	-0.37341	Cl	-6.40753	-7.00493	-5.38348
C	2.34853	0.42404	2.89264	C	-9.05130	-6.22199	-8.66474
O	1.60944	0.32000	3.75214	O	-9.81330	-6.06100	-9.49660
C	5.03825	0.18300	2.49320	C	-6.75696	-7.65158	-8.26017
O	5.95665	-0.07299	3.11050	O	-6.08621	-8.35185	-8.85288
S	-2.72215	1.78689	-1.74953	S	-11.60169	-1.37656	-4.07826
O	-4.16068	1.66647	-1.99693	O	-13.04029	-1.11071	-4.01850
C	-2.44835	3.28929	-0.81398	C	-11.29963	-2.98481	-3.34780
C	-3.53726	3.98618	-0.31029	C	-12.05582	-4.06784	-3.77897
H	-4.53810	3.62813	-0.50471	H	-12.83915	-3.93100	-4.51163
C	-3.30868	5.14337	0.42596	C	-11.78557	-5.32441	-3.25936

H	-4.14648	5.70454	0.81782	H	-12.35597	-6.17912	-3.59738
C	-2.00834	5.57750	0.65574	C	-10.77350	-5.48790	-2.31835
H	-1.83540	6.47736	1.23148	H	-10.55536	-6.47345	-1.92884
C	-0.92620	4.86204	0.14877	C	-10.03792	-4.39323	-1.88174
H	0.08487	5.20167	0.32927	H	-9.25418	-4.52193	-1.14704
H	-0.31009	3.14734	-0.99230	H	-9.73755	-2.26401	-2.07364
C	-1.14165	3.71029	-0.59291	C	-10.29773	-3.12950	-2.39793
O	-1.80462	1.79411	-2.89203	O	-10.66730	-0.42577	-3.46592
INT4				TS5			
C	2.04909	0.69569	1.20963	C	-2.35826	0.43937	-0.15561
C	1.58720	-0.49098	0.76829	C	-1.41102	-0.44257	-0.50076
C	2.82109	1.69575	0.40005	C	-3.08855	0.45281	1.15676
H	3.71565	2.00954	0.92975	H	-4.16108	0.50996	0.99339
H	2.21774	2.59054	0.22746	H	-2.79247	1.34106	1.72075
C	3.19061	1.11820	-0.95454	C	-2.76443	-0.76313	2.01328
C	1.99889	0.36533	-1.54187	C	-1.27757	-1.10167	1.91991
H	2.22145	0.11583	-2.56810	H	-1.05078	-1.88939	2.62517
H	1.14161	1.04058	-1.52051	H	-0.72734	-0.20491	2.20390
C	1.72082	-0.84172	-0.68416	C	-0.97063	-1.46937	0.49426
O	4.30873	0.25215	-0.70001	O	-3.58857	-1.82077	1.49646
O	3.50966	2.12186	-1.91293	O	-3.00925	-0.52732	3.39665
C	4.88394	-0.47990	-1.68622	C	-3.59666	-3.05440	2.06273
C	4.56322	2.96896	-1.71577	C	-4.26181	-0.22736	3.84698
O	5.27634	2.94565	-0.74985	O	-5.22728	-0.12497	3.13923
O	4.53433	-0.46650	-2.83884	O	-2.92849	-3.37319	3.01208
C	4.68867	3.90089	-2.88455	C	-4.23876	-0.06766	5.33824
H	4.86602	3.32391	-3.79339	H	-3.93425	-1.00897	5.79853
H	3.75744	4.45165	-3.02336	H	-3.50476	0.68752	5.62181
H	5.51021	4.59031	-2.71316	H	-5.22651	0.21648	5.68928
C	6.01464	-1.29018	-1.12378	C	-4.55674	-3.94498	1.32970
H	6.44160	-1.91448	-1.90338	H	-4.56898	-4.92791	1.79169
H	6.77648	-0.61994	-0.72278	H	-5.55461	-3.50547	1.35093
H	5.65783	-1.90529	-0.29664	H	-4.26047	-4.02603	0.28251
C	1.66873	-2.21632	-2.77602	C	-0.21469	-3.80851	1.12670
H	1.15752	-1.40710	-3.29058	H	0.00308	-3.43704	2.12253
H	2.70762	-2.22282	-3.11661	H	-1.06889	-4.48815	1.20405
H	1.21298	-3.15348	-3.08793	H	0.63459	-4.39708	0.78087
C	1.61912	-2.08430	-1.27179	C	-0.53350	-2.73484	0.12833
C	0.67582	-1.35717	1.53065	C	-0.50873	-0.35873	-1.67588
H	0.15664	-0.85917	2.32795	H	-0.01956	0.59123	-1.85417

C	1.13005	-2.78008	1.88174	C	-0.75874	-1.18937	-2.91145
C	2.62988	-2.86556	2.18988	C	-2.20558	-1.53282	-3.23499
H	2.84139	-2.30386	3.10010	H	-2.69403	-0.65876	-3.66141
H	2.93264	-3.90401	2.34278	H	-2.24668	-2.34728	-3.96173
H	3.24356	-2.43801	1.39746	H	-2.77710	-1.82531	-2.35492
C	0.36309	-3.30764	3.09224	C	-0.04135	-0.60524	-4.11966
H	0.57793	-2.69512	3.96852	H	-0.54215	0.30742	-4.44093
H	-0.71427	-3.30977	2.93569	H	0.99311	-0.35055	-3.88447
H	0.66739	-4.33304	3.30978	H	-0.04613	-1.31968	-4.94537
C	0.68054	-3.46176	0.59593	C	0.05847	-2.22393	-2.20758
H	0.13716	-4.39285	0.71458	H	0.96673	-2.54297	-2.69770
C	1.64722	-3.44001	-0.55153	C	-0.60342	-3.22938	-1.30653
H	2.67582	-3.66649	-0.25020	H	-1.63834	-3.43928	-1.58916
H	1.36236	-4.20013	-1.27524	H	-0.05289	-4.16635	-1.37140
Rh	-0.53227	-1.87196	-0.10394	Rh	1.11095	-1.17997	-0.41028
Cl	-1.29568	0.54133	-0.62389	Cl	1.06003	1.24740	0.99754
C	-1.44597	-2.71453	-1.77500	C	2.31957	-1.72011	1.07459
C	-1.98937	-2.21077	1.08652	C	2.69051	-0.87159	-1.51130
O	-1.84999	-3.27314	-2.66694	O	2.98064	-2.00109	1.94840
O	-2.83435	-2.37812	1.81908	O	3.64719	-0.82375	-2.11378
Rh	-3.66893	0.95008	-1.04332	Rh	2.76027	2.63540	-0.07495
Cl	-4.20864	-1.39437	-1.02178	Cl	2.00662	2.09704	-2.31569
C	-3.27832	2.78139	-1.12872	C	3.35428	3.07317	1.64887
O	-3.03746	3.89365	-1.19709	O	3.69902	3.33404	2.70287
C	-5.48659	1.26011	-1.37477	C	4.05989	3.70798	-0.89249
O	-6.59288	1.42976	-1.57779	O	4.84106	4.35852	-1.40434
S	1.67696	1.26932	2.87766	S	-2.84868	1.78041	-1.24717
O	2.52635	2.43863	3.10730	O	-4.30571	1.88267	-1.14079
C	-0.01729	1.83111	2.72587	C	-2.12556	3.21590	-0.47690
C	-0.26266	3.01726	2.04303	C	-2.84222	3.89420	0.50429
H	0.56109	3.62070	1.68872	H	-3.84924	3.58714	0.74959
C	-1.57429	3.41737	1.83937	C	-2.24553	4.97712	1.13488
H	-1.77758	4.33540	1.30512	H	-2.78790	5.51988	1.89803
C	-2.62415	2.63502	2.30949	C	-0.95635	5.36699	0.78051
H	-3.64670	2.94034	2.13151	H	-0.49586	6.21169	1.27688
C	-2.36575	1.46595	3.01412	C	-0.26149	4.68411	-0.21102
H	-3.18345	0.86708	3.39227	H	0.73813	4.98792	-0.49247
H	-0.83873	0.16904	3.80337	H	-0.30334	3.05886	-1.61172
C	-1.05594	1.06006	3.23217	C	-0.84356	3.59673	-0.84694
O	1.71211	0.15044	3.82286	O	-2.22582	1.59167	-2.55759

TS6			
C	-2.20519	5.39435	-6.90447
C	-4.36411	4.22377	-6.72628
H	-5.38672	4.54121	-6.91307
H	-4.37261	3.57766	-5.84694
C	-3.90742	3.38478	-7.92824
C	-2.41658	3.03819	-7.87932
H	-2.10967	2.59030	-8.82122
H	-2.28774	2.27792	-7.10280
C	-1.61356	4.23331	-7.49966
O	-4.23054	4.18492	-9.07285
O	-4.57511	2.12196	-7.94919
C	-4.10093	3.70266	-10.33871
C	-5.92586	2.03202	-8.10806
O	-6.66224	2.97767	-8.20252
O	-3.66512	2.61423	-10.60915
C	-6.33325	0.58958	-8.16310
H	-5.88872	0.12452	-9.04459
H	-5.95661	0.05889	-7.28814
H	-7.41596	0.51813	-8.21160
C	-4.60462	4.71660	-11.32254
H	-5.67666	4.85517	-11.17215
H	-4.12545	5.68093	-11.15425
H	-4.41363	4.36957	-12.33392
C	0.68111	3.84440	-8.52994
H	1.39201	3.23060	-7.97621
H	0.15124	3.20889	-9.24536
H	1.24406	4.58995	-9.09443
C	-0.29761	4.50781	-7.62231
C	-1.10459	6.39965	-7.05561
H	-0.87363	6.99671	-6.17608
C	-1.07872	7.27180	-8.31745
C	-1.52245	6.54436	-9.58540
H	-1.59350	7.25581	-10.40814
H	-0.83512	5.75395	-9.87925
H	-2.50699	6.10467	-9.43806
C	-2.06326	8.44896	-8.07882
H	-1.98370	9.14097	-8.91786
H	-3.09076	8.09269	-8.02103
H	-1.83848	8.98391	-7.15843
C	0.30019	7.87427	-8.43685

H	0.64268	8.38710	-7.54181
C	1.07499	7.86847	-9.51201
H	0.78595	7.38335	-10.43510
H	2.04239	8.35336	-9.50062
Rh	0.80411	5.35182	-5.89023
Cl	-0.87538	4.73394	-4.14742
C	2.21973	5.95687	-6.97154
C	1.99266	5.49228	-4.36489
O	3.15956	6.27462	-7.52744
O	2.67146	5.52062	-3.46037
Rh	-1.02722	2.32116	-4.55101
Cl	1.26469	2.28936	-5.29202
C	-2.79312	2.31058	-3.91772
O	-3.86542	2.29299	-3.53275
C	-1.05682	0.46452	-4.82928
O	-1.05174	-0.65924	-4.99755
C	-3.47658	5.41893	-6.49727
S	-4.18503	6.80669	-5.63709
O	-5.30412	7.32058	-6.42976
C	-4.84823	6.03588	-4.16909
C	-6.16573	5.59329	-4.16957
H	-6.78855	5.75031	-5.03885
C	-6.66057	4.96983	-3.03167
H	-7.68462	4.62097	-3.01341
C	-5.84315	4.80051	-1.91887
H	-6.23308	4.31184	-1.03532
C	-4.52941	5.25825	-1.93218
C	-4.02099	5.88052	-3.06327
H	-3.00455	6.24271	-3.09506
H	-3.89861	5.12877	-1.06267
O	-3.09620	7.69951	-5.23615

Table S5 Coordinates of All Stationary Points **CAT+1a**, Computed at B3LYP-D3b+IDSCRF/TZP-DKH(-dfg) level in toluene solvent.

CAT				1a			
Rh	-1.60957	-0.00002	0.09490	C	-0.23966	-0.74439	0.41608
Cl	0.00001	-1.66230	0.89914	C	0.40659	-1.46824	-0.44797
C	-2.79285	1.33852	-0.49828	C	-0.09505	0.70904	0.77899
O	-3.49835	2.15616	-0.84839	H	0.36558	0.78768	1.76459
Rh	1.60963	-0.00002	0.09502	H	-1.08149	1.16427	0.84855
Cl	0.00001	1.66203	0.89963	C	0.73142	1.57031	-0.18012
C	2.79279	-1.33845	-0.49869	C	2.22742	1.21319	-0.22737

O	3.49814	-2.15611	-0.84906	H	2.71072	1.92258	-0.89830
C	-2.79274	-1.33840	-0.49890	H	2.31536	0.23005	-0.69036
O	-3.49816	-2.15595	-0.84938	C	2.86754	1.21426	1.08071
C	2.79276	1.33864	-0.49821	O	0.53159	2.89677	0.33154
O	3.49803	2.15649	-0.84831	O	0.30486	1.44780	-1.54067
				C	1.00848	3.99931	-0.30503
				C	-0.95820	1.77052	-1.92814
				O	-1.81098	2.19498	-1.19344
				O	1.60990	3.98232	-1.34743
				C	-1.11376	1.52997	-3.40242
				H	-0.40764	2.15511	-3.95097
				H	-0.88114	0.49007	-3.63579
				H	-2.13107	1.76288	-3.70388
				C	0.65508	5.23004	0.48024
				H	1.04882	6.10854	-0.02311
				H	-0.42928	5.30595	0.57340
				H	1.06691	5.15766	1.48775
				C	4.02617	1.18336	3.47291
				H	3.60121	1.95090	4.12334
				H	3.89042	0.21656	3.96226
				H	5.09884	1.37151	3.38995
				C	3.39088	1.20096	2.16185
				C	1.04717	-2.24331	-1.26979
				H	0.68402	-2.33239	-2.29139
				C	2.29886	-3.04719	-0.92747
				C	2.64327	-2.93952	0.55788
				H	1.81731	-3.31715	1.16114
				H	3.52990	-3.53362	0.78304
				H	2.83661	-1.90979	0.86131
				C	2.01564	-4.52127	-1.28929
				H	1.18416	-4.90455	-0.69580
				H	1.76165	-4.62819	-2.34614
				H	2.89913	-5.13025	-1.08962
				C	3.39763	-2.52607	-1.83426
				H	3.19237	-2.63923	-2.89667
				C	4.54133	-1.96548	-1.46281
				H	4.80786	-1.81919	-0.42401
				H	5.25935	-1.63001	-2.20072
				S	-1.48945	-1.62834	1.39939
				O	-1.36385	-1.14635	2.77789
				O	-1.38752	-3.05731	1.10785

	C	-3.04598	-1.03037	0.74408			
	C	-3.70712	0.00231	1.39564			
	C	-3.55159	-1.60544	-0.41710			
	C	-4.90275	0.47300	0.86582			
	H	-3.29476	0.41569	2.30532			
	C	-4.74657	-1.12716	-0.93549			
	H	-3.02207	-2.42044	-0.89110			
	C	-5.41803	-0.08760	-0.29696			
	H	-5.43001	1.27693	1.36269			
	H	-5.15733	-1.56830	-1.83455			
	H	-6.34886	0.28310	-0.70701			
2a	3a						
C	-0.34742	-0.62697	-0.13882	C	-0.96860	-0.58605	0.54992
C	0.84133	-1.06445	-0.61677	C	1.16791	0.56804	0.15872
C	-0.79413	0.81556	-0.08438	H	1.71831	0.73029	-0.76588
H	-1.23506	1.03776	0.88463	H	1.90260	0.41840	0.95417
H	-1.55553	1.01329	-0.84302	C	0.40546	1.86943	0.47260
C	0.35974	1.77507	-0.32882	C	-0.58904	1.71927	1.63697
C	1.19615	1.27481	-1.49631	H	-1.15582	2.63959	1.75493
H	1.95109	2.01081	-1.73748	H	0.00140	1.57685	2.54654
H	0.51797	1.20915	-2.35307	C	-1.42615	0.52133	1.36377
C	1.77507	-0.08348	-1.20128	O	-0.26657	2.20466	-0.74924
O	1.09244	1.81828	0.90333	O	1.30962	2.89942	0.89035
O	-0.09012	3.08254	-0.70949	C	-0.96080	3.36323	-0.89954
C	2.22997	2.54594	1.03758	C	2.26884	3.39679	0.06150
C	-0.88519	3.82663	0.10706	O	2.47586	3.00485	-1.05649
O	-1.29429	3.46300	1.17802	O	-1.07210	4.20869	-0.04942
O	2.71283	3.23111	0.17226	C	3.00594	4.51017	0.74957
C	-1.15844	5.16151	-0.52660	H	2.31496	5.33142	0.94733
H	-0.21870	5.69812	-0.66664	H	3.39301	4.16926	1.71047
H	-1.60539	5.02339	-1.51204	H	3.81897	4.85460	0.11666
H	-1.82449	5.73766	0.10951	C	-1.54468	3.42985	-2.28147
C	2.77683	2.38226	2.42715	H	-2.10017	4.35619	-2.39785
H	3.71399	2.92433	2.51676	H	-0.74356	3.37600	-3.01995
H	2.05382	2.76473	3.14952	H	-2.20048	2.57442	-2.44932
H	2.92653	1.32489	2.64836	C	-3.71332	0.25205	2.59883
C	4.04458	0.59624	-2.05246	H	-3.83394	-0.52173	3.36374
H	3.84318	1.62887	-1.77660	H	-3.55266	1.20939	3.09630
H	5.05537	0.35219	-1.71950	H	-4.65771	0.29045	2.05123
H	4.04991	0.53492	-3.14623	C	-2.59015	-0.07964	1.69407

C	3.06065	-0.38650	-1.47612	C	-2.31116	-1.31172	0.79354
C	1.26300	-2.48498	-0.56192	H	-2.19080	-2.25330	1.33592
H	0.50299	-3.18592	-0.86550	C	-3.29037	-1.52869	-0.39679
C	2.17490	-2.98213	0.55074	C	-3.51078	-0.22704	-1.17293
C	2.63438	-2.02349	1.62556	H	-4.15690	-0.40257	-2.03440
H	1.87142	-1.93101	2.40228	H	-3.96780	0.55072	-0.55958
H	3.54915	-2.39260	2.09786	H	-2.55726	0.15298	-1.54237
H	2.83354	-1.02391	1.24147	C	-2.74064	-2.59519	-1.36277
C	1.90488	-4.38137	1.05845	H	-3.49120	-2.81752	-2.12376
H	1.12617	-4.37231	1.82431	H	-1.83995	-2.24478	-1.86475
H	1.57139	-5.03995	0.25472	H	-2.49072	-3.51951	-0.84230
H	2.80911	-4.81365	1.49752	C	-4.57132	-2.08145	0.19315
C	2.69592	-2.84466	-0.85848	H	-4.43505	-2.99614	0.76722
H	2.83685	-3.77961	-1.38771	C	-5.80102	-1.60207	0.05553
C	3.65354	-1.75280	-1.26529	H	-6.01540	-0.70143	-0.50608
H	4.47312	-1.65718	-0.54078	H	-6.64836	-2.10607	0.50392
H	4.14587	-2.03743	-2.20187	C	0.25928	-0.64002	0.03155
S	-1.53324	-1.69721	0.69178	S	0.91335	-2.06503	-0.80631
O	-1.50731	-1.35686	2.11856	O	1.02508	-1.77660	-2.24064
C	-3.11507	-1.14158	0.03683	C	2.58515	-2.18762	-0.15841
C	-3.93616	-0.34438	0.82213	C	3.64763	-1.71771	-0.91892
H	-3.61651	-0.06059	1.81511	H	3.46132	-1.29481	-1.89627
C	-5.16447	0.06330	0.31382	C	4.93660	-1.81681	-0.40747
H	-5.81661	0.68109	0.91758	H	5.77478	-1.45901	-0.99138
C	-5.55240	-0.32275	-0.96427	C	5.14697	-2.37702	0.84781
H	-6.50928	-0.00284	-1.35703	H	6.15245	-2.45328	1.24212
C	-4.71922	-1.12473	-1.74027	C	4.07207	-2.84728	1.59801
H	-5.02840	-1.43097	-2.73140	C	2.78092	-2.75515	1.09590
H	-2.84322	-2.17963	-1.82419	H	1.93552	-3.12933	1.65723
C	-3.49320	-1.54189	-1.24024	H	4.24088	-3.29179	2.57042
O	-1.37829	-3.09923	0.29623	O	0.17281	-3.24839	-0.36233
COM				TS1			
C	-2.44529	0.66980	-1.37150	C	1.27716	0.87541	-0.70308
C	-2.68971	1.27837	1.09590	C	1.86617	-1.63533	-0.59594
H	-3.74561	1.46098	1.29197	H	2.77489	-2.13936	-0.90832
H	-2.12478	2.01096	1.67510	H	1.05163	-2.01149	-1.21266
C	-2.32949	-0.08791	1.68042	C	1.60492	-2.08805	0.84934
C	-0.82763	-0.46148	1.51377	C	0.13549	-1.98415	1.29726
H	-0.49619	-0.89251	2.45719	H	0.01946	-2.60710	2.18293
H	-0.24856	0.45173	1.37134	H	-0.49425	-2.40120	0.51537

C	-0.52437	-1.40968	0.44344	C	-0.31540	-0.64333	1.66688
O	-3.21818	-1.02957	1.09269	O	2.50533	-1.34909	1.66319
O	-2.48731	-0.00958	3.11013	O	1.82400	-3.50690	0.93522
C	-3.27629	-2.31464	1.54267	C	2.61584	-1.55935	3.00312
C	-3.70751	0.13182	3.70195	C	3.05106	-4.07529	0.76193
O	-4.74897	0.21995	3.10747	O	4.05096	-3.46741	0.48531
O	-2.56936	-2.75803	2.40812	O	1.96888	-2.36432	3.62034
C	-3.54623	0.13694	5.19490	C	2.95521	-5.55738	0.98187
H	-3.14844	-0.82622	5.51900	H	2.65291	-5.75212	2.01217
H	-2.83102	0.90404	5.49377	H	2.19142	-5.98476	0.33115
H	-4.50969	0.31702	5.66327	H	3.91961	-6.01700	0.78471
C	-4.36186	-3.05864	0.82262	C	3.65889	-0.64207	3.57048
H	-4.27966	-4.12078	1.03626	H	3.79440	-0.85114	4.62781
H	-5.32862	-2.69036	1.17266	H	4.59684	-0.77192	3.02986
H	-4.31260	-2.87468	-0.25056	H	3.34711	0.39462	3.43099
C	-1.06369	-3.18037	-1.47654	C	-0.74581	1.18766	3.54888
H	-0.90450	-4.21484	-1.16859	H	-1.74900	1.07900	3.96354
H	-2.13164	-3.02512	-1.64530	H	-0.02481	0.90286	4.31828
H	-0.53867	-3.02626	-2.41968	H	-0.58598	2.23113	3.28530
C	-0.59516	-2.25200	-0.44987	C	-0.56506	0.30080	2.40203
C	-2.49218	-0.03352	-2.46132	C	0.85627	2.12321	-0.70476
H	-1.57625	-0.50060	-2.81417	H	0.32708	2.46435	-1.59110
C	-3.73791	-0.23156	-3.32000	C	1.24708	3.22420	0.27879
C	-4.96819	0.40245	-2.67270	C	2.10393	2.67635	1.41886
H	-5.84608	0.25822	-3.30361	H	2.40149	3.47865	2.09364
H	-5.17305	-0.02668	-1.69103	H	1.56917	1.91748	1.98882
H	-4.81728	1.47442	-2.54598	H	3.01267	2.22315	1.02378
C	-3.46148	0.44140	-4.68459	C	2.08209	4.23564	-0.55431
H	-4.31602	0.29919	-5.34880	H	2.41445	5.04414	0.09793
H	-3.29123	1.50991	-4.54871	H	2.94720	3.74176	-0.99417
H	-2.58015	0.01298	-5.16619	H	1.48540	4.67224	-1.35758
C	-3.88809	-1.72257	-3.54521	C	0.00407	3.95327	0.74591
H	-3.04135	-2.18445	-4.04889	H	-0.72561	4.14569	-0.03602
C	-4.92382	-2.48535	-3.21780	C	-0.22761	4.43984	1.95817
H	-5.80347	-2.09204	-2.72447	H	0.46629	4.31449	2.77968
H	-4.92802	-3.54362	-3.44819	H	-1.13080	4.99878	2.16805
Rh	1.60744	-2.08938	0.04956	Rh	-1.41989	0.77593	0.18644
Cl	1.82081	-0.23412	-1.58969	Cl	-1.36265	-1.11825	-1.65644
C	1.36590	-3.57102	1.16529	C	-2.75035	1.53136	1.29371
C	3.29081	-2.82206	-0.59857	C	-2.18011	1.75850	-1.23438
O	1.19638	-4.46513	1.84555	O	-3.58358	1.97276	1.92926

O	4.25104	-3.27371	-0.99825	O	-2.60421	2.35397	-2.10254
Rh	3.78205	0.47386	-0.27162	Rh	-3.76866	-1.20701	-1.06451
Cl	2.62546	-0.10273	1.78027	Cl	-3.35447	-2.12445	1.13119
C	4.69240	0.88575	-1.86698	C	-4.15716	-0.59532	-2.79759
O	5.23535	1.12088	-2.83766	O	-4.38851	-0.24232	-3.85581
C	5.27976	0.93063	0.77023	C	-5.58652	-1.31748	-0.61989
O	6.17597	1.19443	1.41612	O	-6.68478	-1.39931	-0.33653
C	-2.41308	1.49384	-0.36788	C	2.04390	-0.16455	-0.85496
S	-2.15753	3.24040	-0.81491	S	3.68609	0.27347	-1.57399
O	-3.25532	4.00144	-0.20949	O	4.70161	-0.08262	-0.58343
O	-1.91947	3.32941	-2.25382	O	3.61779	1.64334	-2.08327
C	-0.64982	3.67772	0.05093	C	3.85126	-0.83825	-2.96877
C	-0.69725	4.63111	1.05951	C	4.66097	-1.96073	-2.84701
C	0.53618	3.04578	-0.30490	C	3.16489	-0.54963	-4.14347
C	0.48024	4.96704	1.71901	C	4.78602	-2.81392	-3.93735
C	1.69991	3.37928	0.37124	C	3.29600	-1.41235	-5.22262
C	1.67344	4.33965	1.37833	C	4.10463	-2.54137	-5.11860
H	-1.63903	5.09777	1.31226	H	5.17846	-2.15368	-1.91742
H	0.55060	2.29923	-1.08729	H	2.55205	0.33869	-4.21182
H	0.46157	5.71296	2.50313	H	5.41602	-3.69060	-3.86159
H	2.62230	2.86811	0.12275	H	2.77180	-1.20167	-6.14565
H	2.58556	4.59362	1.90321	H	4.20461	-3.20994	-5.96421
INT1				TS2			
C	-1.14509	0.44900	-0.91640	C	-5.68109	-3.30922	3.13660
C	0.95700	0.82745	0.44440	C	-6.97098	-4.53661	4.92508
H	1.88070	1.35710	0.23222	H	-7.67777	-4.25531	5.69771
H	1.20129	-0.23735	0.47430	H	-6.12481	-5.03853	5.39973
C	0.50696	1.25123	1.84895	C	-7.65954	-5.52958	3.99004
C	-0.43428	0.25193	2.53540	C	-6.67972	-6.13155	2.99342
H	-0.56205	0.57992	3.56720	H	-7.22163	-6.80143	2.32405
H	0.06212	-0.71751	2.54467	H	-5.98018	-6.74568	3.57509
C	-1.77320	0.10485	1.96739	C	-5.88483	-5.22345	2.14940
O	-0.06647	2.54386	1.71440	O	-8.72454	-4.81176	3.36889
O	1.63916	1.23080	2.73330	O	-8.12594	-6.67032	4.72029
C	-0.45758	3.28681	2.78379	C	-9.58998	-5.40357	2.50336
C	2.67441	2.11002	2.61284	C	-9.08835	-6.56747	5.68095
O	2.74472	2.96671	1.77249	O	-9.63603	-5.54206	5.98818
O	-0.40218	2.91332	3.92748	O	-9.52960	-6.55766	2.16394

C	3.68791	1.84856	3.68909	C	-9.35506	-7.91992	6.27511
H	3.22700	1.99232	4.66750	H	-9.66850	-8.61138	5.49180
H	4.03044	0.81428	3.63688	H	-8.43913	-8.31654	6.71606
H	4.52691	2.52808	3.56952	H	-10.12836	-7.83741	7.03347
C	-0.94577	4.62434	2.31384	C	-10.62470	-4.41045	2.06341
H	-1.28759	5.20922	3.16301	H	-11.25809	-4.85560	1.30134
H	-0.13578	5.14010	1.79638	H	-11.22690	-4.11655	2.92485
H	-1.75184	4.49299	1.59097	H	-10.14431	-3.50785	1.68548
C	-4.42283	0.20599	2.15871	C	-5.00378	-5.79919	-0.23909
H	-4.80578	-0.70317	2.62553	H	-4.11627	-6.43527	-0.25149
H	-4.57749	1.03759	2.84957	H	-5.87373	-6.39812	-0.51565
H	-4.99001	0.39312	1.24969	H	-4.86313	-5.01480	-0.98374
C	-2.99211	0.08257	1.89246	C	-5.17255	-5.21710	1.10093
C	-2.29763	0.35030	-1.65416	C	-5.04195	-2.39600	2.26245
H	-2.22637	-0.26910	-2.54330	H	-4.45906	-1.64968	2.79197
C	-3.49361	1.30288	-1.71076	C	-5.63119	-1.81116	0.95589
C	-3.38033	2.44075	-0.69761	C	-6.96406	-2.44421	0.54922
H	-4.22909	3.11822	-0.79185	H	-7.39412	-1.88874	-0.28518
H	-3.34206	2.07377	0.32626	H	-6.86014	-3.48322	0.24961
H	-2.47582	3.02021	-0.88018	H	-7.67137	-2.39761	1.37741
C	-3.50163	1.89772	-3.14679	C	-5.87906	-0.30184	1.21884
H	-4.34634	2.58146	-3.23716	H	-6.25095	0.16267	0.30475
H	-2.57510	2.42965	-3.34806	H	-6.60471	-0.15657	2.01550
H	-3.62054	1.11258	-3.89609	H	-4.95638	0.20444	1.50864
C	-4.76634	0.48834	-1.58654	C	-4.58472	-1.87565	-0.13429
H	-4.74167	-0.46444	-2.10879	H	-3.62305	-1.45738	0.15220
C	-5.89581	0.85970	-0.99789	C	-4.74569	-2.30528	-1.37891
H	-6.00016	1.80533	-0.48057	H	-5.68422	-2.70873	-1.73726
H	-6.77154	0.22357	-1.02661	H	-3.93326	-2.25616	-2.09307
Rh	-2.10743	-1.21632	0.04647	Rh	-3.84915	-4.16796	2.35599
Cl	1.06068	-2.19419	-2.03275	Cl	-3.76916	-5.67364	6.04641
C	-3.45783	-2.49619	0.78600	C	-2.40968	-3.88858	0.97807
C	-1.98861	-2.41304	-1.44692	C	-2.72748	-3.41761	3.83608
O	-4.22446	-3.20635	1.21791	O	-1.59525	-3.75381	0.20647
O	-2.05523	-3.17854	-2.27563	O	-2.03935	-2.97532	4.61328
Rh	1.98539	-2.64404	0.14642	Rh	-3.84613	-7.62819	4.63912
Cl	-0.23685	-2.89152	1.17007	Cl	-2.69390	-6.45865	2.80906
C	3.67628	-2.48519	-0.64948	C	-4.67635	-8.51582	6.06788
O	4.69336	-2.39290	-1.15097	O	-5.18015	-9.03555	6.94550
C	2.72356	-3.02700	1.83094	C	-3.87926	-9.16659	3.55613
O	3.16309	-3.26578	2.85460	O	-3.88940	-10.09332	2.89468

C	-0.02424	1.07987	-0.65971	C	-6.49298	-3.33154	4.17968
S	0.41867	2.41304	-1.83360	S	-7.22377	-1.73309	4.67910
O	0.28286	3.70702	-1.16100	O	-8.58340	-1.63831	4.14538
O	-0.32626	2.17679	-3.07276	O	-6.25469	-0.68183	4.35932
C	2.15667	2.12828	-2.16055	C	-7.32104	-1.86661	6.46220
C	3.09529	3.01459	-1.64800	C	-8.55430	-2.09225	7.05967
C	2.52185	1.02326	-2.92181	C	-6.15474	-1.73157	7.20759
C	4.43992	2.79019	-1.91875	C	-8.61763	-2.17988	8.44510
C	3.86896	0.80688	-3.17553	C	-6.23164	-1.82784	8.58978
C	4.82389	1.68981	-2.67803	C	-7.46041	-2.05093	9.20547
H	2.77245	3.85166	-1.04622	H	-9.43876	-2.19736	6.44758
H	1.77261	0.33736	-3.29023	H	-5.20992	-1.54721	6.71530
H	5.18538	3.47184	-1.53026	H	-9.57047	-2.35405	8.92744
H	4.17177	-0.05303	-3.75837	H	-5.33403	-1.72718	9.18561
H	5.87320	1.51568	-2.88072	H	-7.51452	-2.12510	10.28415
INT2				TS3			
C	-1.93906	0.01698	-0.68481	C	8.15326	0.84835	-9.30153
C	-0.88334	-0.72754	-0.29137	C	6.81303	0.68510	-9.28189
C	-2.85320	0.70364	0.30209	C	9.04303	0.02451	-10.19869
H	-3.87054	0.72627	-0.08132	H	10.01538	-0.12652	-9.73662
H	-2.54021	1.73565	0.48223	H	9.19966	0.52631	-11.15773
C	-2.85718	-0.01745	1.64631	C	8.42587	-1.34183	-10.48982
C	-1.43767	-0.17869	2.17002	C	7.00689	-1.19979	-11.02584
H	-1.45245	-0.81370	3.05293	H	6.54589	-2.18356	-11.06492
H	-1.11714	0.81314	2.49827	H	7.10425	-0.85293	-12.05781
C	-0.48652	-0.70329	1.11767	C	6.17465	-0.21437	-10.23616
O	-3.50546	-1.27474	1.40664	O	8.47848	-2.05602	-9.24582
O	-3.54048	0.74857	2.64816	O	9.14645	-2.02594	-11.52404
C	-3.79237	-2.13944	2.41510	C	8.13780	-3.36903	-9.15668
C	-4.86838	1.03318	2.55414	C	10.44501	-2.40380	-11.36658
O	-5.57467	0.70291	1.63827	O	11.10517	-2.18512	-10.38522
O	-3.49460	-1.96721	3.56888	O	7.70925	-4.02742	-10.06897
C	-5.31019	1.80076	3.76764	C	10.91107	-3.14170	-12.58904
H	-5.18010	1.18009	4.65574	H	10.32850	-4.05741	-12.70275
H	-4.69185	2.68993	3.89619	H	10.74578	-2.53577	-13.48066
H	-6.35431	2.08097	3.66085	H	11.96540	-3.38320	-12.48819
C	-4.55510	-3.31503	1.87486	C	8.40480	-3.87228	-7.76698
H	-4.68981	-4.05446	2.65930	H	8.01346	-4.88046	-7.66316
H	-5.52743	-2.97288	1.51563	H	9.48229	-3.87369	-7.59168
H	-4.03124	-3.75256	1.02496	H	7.95658	-3.21099	-7.02564

C	1.45484	-0.86012	2.71047	C	4.02882	-0.72062	-11.44723
H	1.99396	0.08964	2.79655	H	3.55437	-0.01836	-12.13811
H	0.72551	-0.90872	3.52192	H	4.60832	-1.43350	-12.03724
H	2.19743	-1.64348	2.86678	H	3.22212	-1.26976	-10.95276
C	0.80646	-0.96111	1.37199	C	4.86354	0.00455	-10.44304
C	-0.00409	-1.58572	-1.15824	C	5.84817	1.32211	-8.34256
H	0.11218	-1.15223	-2.14603	H	6.13415	2.32310	-8.04908
C	-0.48434	-3.05615	-1.33438	C	5.44916	0.48389	-7.09882
C	-0.82740	-3.76246	-0.02104	C	5.47268	-1.03144	-7.31020
H	-1.62628	-3.22821	0.49062	H	6.47360	-1.35266	-7.59240
H	-1.18147	-4.77428	-0.22339	H	5.20725	-1.53071	-6.37699
H	0.01058	-3.83294	0.66794	H	4.78752	-1.36293	-8.08727
C	-1.77731	-3.04664	-2.19537	C	6.42027	0.82680	-5.94814
H	-2.58146	-2.51088	-1.69241	H	7.43377	0.50071	-6.18245
H	-1.61163	-2.58256	-3.16537	H	6.44920	1.89810	-5.75352
H	-2.10059	-4.07615	-2.35409	H	6.09472	0.31363	-5.04025
C	0.54701	-3.78708	-2.16300	C	4.07139	0.97590	-6.70246
H	0.82954	-3.26041	-3.07179	H	4.04490	1.99561	-6.33054
C	1.07155	-4.98444	-1.93674	C	2.93786	0.27289	-6.71293
H	0.82800	-5.57134	-1.06016	H	2.90052	-0.76038	-7.03033
H	1.77332	-5.42457	-2.63414	H	2.00813	0.71802	-6.38162
Rh	1.93837	-1.24619	-0.33388	Rh	4.06981	1.60793	-9.45123
Cl	1.69420	1.17801	-0.92884	Cl	5.40966	3.00052	-10.90488
C	2.26417	-2.98921	0.32283	C	1.91448	0.71513	-9.54661
C	2.98387	-1.45256	-2.12439	C	3.39666	3.36170	-8.61064
O	2.60595	-3.95534	0.80696	O	0.84013	0.38249	-9.51146
O	3.57591	-1.55210	-3.07681	O	3.07431	4.36517	-8.20610
Rh	3.34021	1.80615	0.77257	Rh	4.04639	2.82489	-12.94048
Cl	4.23985	-0.46185	0.64334	Cl	2.02297	2.93967	-11.62486
C	2.63791	3.54834	0.83060	C	5.61729	2.73594	-13.96875
O	2.20448	4.59897	0.84923	O	6.57521	2.68171	-14.58171
C	4.64536	2.26043	2.04865	C	2.97041	2.76433	-14.48058
O	5.44389	2.52226	2.81274	O	2.30693	2.74124	-15.40259
S	-2.40602	0.34886	-2.38292	S	9.05576	2.04197	-8.32417
O	-3.75517	-0.17468	-2.61666	O	10.03471	1.32630	-7.50129
O	-1.32616	-0.02318	-3.30299	O	8.13817	2.98578	-7.67851
C	-2.52033	2.14336	-2.39463	C	9.95651	2.94641	-9.58725
C	-3.77214	2.74291	-2.42177	C	11.32412	2.75016	-9.72007
C	-1.34969	2.89392	-2.39512	C	9.26046	3.83393	-10.40166
C	-3.85125	4.13091	-2.45069	C	12.01281	3.46676	-10.69291
C	-1.44149	4.27877	-2.41844	C	9.95809	4.53893	-11.37226

C	-2.68990	4.89549	-2.44596	C	11.33139	4.35553	-11.51675
H	-4.66112	2.12787	-2.43036	H	11.83289	2.05650	-9.06522
H	-0.38716	2.40195	-2.37964	H	8.19491	3.97062	-10.27478
H	-4.82019	4.61247	-2.47812	H	13.08058	3.32964	-10.80475
H	-0.53908	4.87654	-2.42071	H	9.43156	5.23453	-12.01284
H	-2.75607	5.97598	-2.46706	H	11.87111	4.91012	-12.27390
INT3				TS4			
C	-2.24679	0.36621	-0.69691	C	-10.82384	-1.59070	-5.63802
C	-1.27393	-0.54144	-0.46392	C	-9.56481	-1.75472	-6.10449
C	-3.13449	0.91023	0.39610	C	-12.06767	-1.59684	-6.49234
H	-4.11677	1.14759	-0.00259	H	-12.73802	-0.80413	-6.17169
H	-2.71217	1.82351	0.82480	H	-12.60324	-2.54460	-6.38166
C	-3.29170	-0.10045	1.52628	C	-11.74302	-1.41453	-7.96748
C	-1.93031	-0.55748	2.02799	C	-10.58943	-2.32229	-8.36522
H	-2.07159	-1.35655	2.75048	H	-10.39468	-2.21727	-9.42628
H	-1.50439	0.29154	2.56884	H	-10.91523	-3.35228	-8.18969
C	-0.99803	-0.96377	0.90830	C	-9.36975	-2.04527	-7.53144
O	-4.06853	-1.17429	0.97491	O	-11.41767	-0.02224	-8.11706
O	-3.93154	0.48130	2.66958	O	-12.83089	-1.79259	-8.81372
C	-4.48330	-2.22249	1.73124	C	-11.07315	0.51016	-9.31827
C	-5.20979	0.94858	2.61644	C	-14.03621	-1.15454	-8.75394
O	-5.89925	0.93897	1.63140	O	-14.28881	-0.25091	-8.00346
O	-4.21407	-2.37673	2.89521	O	-10.97429	-0.11567	-10.34247
C	-5.62226	1.45441	3.96950	C	-14.97227	-1.74280	-9.77004
H	-5.61814	0.62768	4.68188	H	-14.56185	-1.59825	-10.77073
H	-4.90929	2.19821	4.32716	H	-15.07176	-2.81713	-9.60975
H	-6.61736	1.88593	3.90841	H	-15.94245	-1.26043	-9.69250
C	-5.33869	-3.13999	0.90492	C	-10.85416	1.98940	-9.17540
H	-5.62182	-4.00609	1.49648	H	-10.50367	2.39964	-10.11830
H	-6.23043	-2.60331	0.57709	H	-11.79288	2.46623	-8.88828
H	-4.80085	-3.45229	0.00947	H	-10.13397	2.19139	-8.38167
C	0.70793	-1.93879	2.47710	C	-7.83192	-2.67367	-9.42950
H	1.52653	-1.27369	2.76950	H	-8.05346	-3.73959	-9.53734
H	-0.05731	-1.87937	3.25278	H	-8.43319	-2.13044	-10.16234
H	1.10855	-2.95502	2.48160	H	-6.78523	-2.53482	-9.69151
C	0.18870	-1.55343	1.13213	C	-8.12759	-2.24614	-8.02715
C	-0.38973	-1.18390	-1.48325	C	-8.31500	-1.78182	-5.27946
H	-0.14939	-0.52363	-2.30287	H	-8.47351	-2.23650	-4.31350
C	-0.79286	-2.58487	-2.01642	C	-7.46597	-0.47580	-5.14486
C	-2.04676	-3.18503	-1.37815	C	-8.23869	0.81418	-5.44401

H	-2.91831	-2.58481	-1.63921	H	-9.00266	0.97398	-4.68323
H	-2.20308	-4.19889	-1.75225	H	-7.55722	1.66786	-5.42952
H	-1.98228	-3.22571	-0.29233	H	-8.74116	0.79036	-6.41047
C	-0.95590	-2.56825	-3.53878	C	-6.86186	-0.37000	-3.74326
H	-1.80927	-1.95708	-3.82477	H	-7.65226	-0.25140	-3.00452
H	-0.07304	-2.15087	-4.02800	H	-6.28088	-1.25425	-3.47895
H	-1.10567	-3.58450	-3.91274	H	-6.19740	0.49483	-3.68500
C	0.46376	-3.36881	-1.66016	C	-6.38352	-0.79450	-6.16756
H	1.12982	-3.61069	-2.48064	H	-5.33895	-0.75980	-5.88292
C	0.78048	-3.86287	-0.42287	C	-6.71046	-0.75931	-7.53782
H	0.06019	-3.88479	0.38006	H	-7.49781	-0.11071	-7.88383
H	1.65095	-4.49565	-0.31431	H	-5.91955	-0.91538	-8.25875
Rh	1.44328	-1.64901	-0.50746	Rh	-6.89467	-2.86808	-6.38396
Cl	1.75834	0.79518	-0.17862	Cl	-8.33601	-5.01392	-6.27428
C	3.12905	-2.26864	0.57741	C	-5.36015	-3.65798	-7.57234
C	2.57237	-1.41568	-2.23565	C	-6.02429	-3.52141	-4.72236
O	3.94348	-2.74371	1.19392	O	-4.50169	-3.90251	-8.26097
O	3.09628	-1.23616	-3.21574	O	-5.56782	-3.92161	-3.77106
Rh	3.88205	1.23310	0.99067	Rh	-7.21052	-6.90795	-7.36414
Cl	5.12288	-0.06100	-0.61456	Cl	-5.17455	-6.49782	-6.14275
C	2.92523	2.24698	2.25249	C	-8.79524	-7.24007	-8.31511
O	2.33669	2.85970	3.01129	O	-9.76365	-7.43155	-8.88513
C	5.51983	1.61616	1.82288	C	-6.34631	-8.38057	-8.13976
O	6.52165	1.84708	2.30718	O	-5.81083	-9.27611	-8.59222
S	-2.62057	1.08131	-2.29281	S	-11.22495	-1.39283	-3.89916
O	-4.07283	1.03423	-2.48240	O	-12.32495	-0.43068	-3.80007
C	-2.15366	2.79952	-2.05837	C	-11.87500	-3.01114	-3.46753
C	-3.14535	3.76224	-1.92751	C	-13.19265	-3.11513	-3.04368
H	-4.18547	3.47076	-1.97317	H	-13.80909	-2.22876	-2.98915
C	-2.77215	5.09096	-1.75468	C	-13.68797	-4.36706	-2.69400
H	-3.53393	5.85384	-1.65833	H	-14.71157	-4.46292	-2.35554
C	-1.42633	5.43656	-1.70832	C	-12.87281	-5.48957	-2.78343
H	-1.14015	6.47187	-1.57274	H	-13.26398	-6.46266	-2.51483
C	-0.44313	4.45821	-1.83729	C	-11.55589	-5.37040	-3.22161
H	0.60405	4.72952	-1.80252	H	-10.92345	-6.24512	-3.29844
H	-0.04576	2.36489	-2.11979	H	-10.02842	-4.03489	-3.91394
C	-0.80281	3.12997	-2.01469	C	-11.04789	-4.12594	-3.56447
O	-1.75454	0.52296	-3.33563	O	-10.01287	-1.15571	-3.10999

INT4				TS5			
C	2.11683	0.75824	1.10184	C	-2.21849	0.48239	-0.41610
C	1.58790	-0.45146	0.82605	C	-1.31769	-0.43607	-0.79459
C	2.87566	1.63045	0.14162	C	-2.75868	0.64517	0.97818
H	3.80822	1.96886	0.58379	H	-3.84547	0.68436	0.96540
H	2.28926	2.52333	-0.09224	H	-2.40080	1.59303	1.38761
C	3.15176	0.90899	-1.16803	C	-2.30455	-0.46375	1.92294
C	1.92640	0.10107	-1.59297	C	-0.85074	-0.84925	1.63961
H	2.09713	-0.27981	-2.58914	H	-0.52228	-1.55954	2.38690
H	1.07917	0.78919	-1.62286	H	-0.25512	0.06016	1.73099
C	1.66833	-0.98387	-0.57601	C	-0.75558	-1.37149	0.23102
O	4.29702	0.07876	-0.90804	O	-3.21075	-1.55467	1.68803
O	3.38926	1.81102	-2.24787	O	-2.31720	-0.04616	3.28595
C	4.86205	-0.69278	-1.87311	C	-3.15371	-2.70368	2.41403
C	4.43926	2.68503	-2.22386	C	-3.46824	0.37562	3.88785
O	5.22299	2.77451	-1.31810	O	-4.53501	0.43317	3.33748
O	4.43978	-0.79893	-2.99591	O	-2.34527	-2.92443	3.27747
C	4.46225	3.48467	-3.49398	C	-3.19113	0.73353	5.31836
H	4.60058	2.81442	-4.34392	H	-2.82865	-0.14731	5.85068
H	3.50839	3.99520	-3.63259	H	-2.40746	1.49061	5.36834
H	5.27254	4.20693	-3.45380	H	-4.10061	1.10234	5.78386
C	6.08729	-1.37121	-1.33162	C	-4.24414	-3.63759	1.97400
H	6.48154	-2.06066	-2.07285	H	-4.18686	-4.56050	2.54406
H	6.83824	-0.61663	-1.09090	H	-5.21526	-3.16370	2.12319
H	5.85174	-1.89901	-0.40686	H	-4.14605	-3.84677	0.90741
C	1.61249	-2.64306	-2.45887	C	0.01633	-3.67514	0.97525
H	1.11408	-1.91126	-3.08880	H	0.34341	-3.23474	1.91134
H	2.65112	-2.71387	-2.79404	H	-0.83987	-4.32175	1.19279
H	1.14744	-3.61082	-2.63546	H	0.81117	-4.31732	0.59654
C	1.56736	-2.29650	-0.98794	C	-0.38716	-2.67485	-0.07040
C	0.65994	-1.18403	1.70655	C	-0.58579	-0.48993	-2.08748
H	0.15543	-0.56194	2.42615	H	-0.16252	0.44397	-2.43128
C	1.07022	-2.56281	2.24912	C	-1.02856	-1.41280	-3.20374
C	2.56191	-2.65939	2.60254	C	-2.50977	-1.75637	-3.28280
H	2.77586	-2.00407	3.44686	H	-3.05560	-0.90995	-3.69839
H	2.82323	-3.68288	2.88277	H	-2.66313	-2.61777	-3.93688
H	3.20973	-2.35046	1.78261	H	-2.94923	-1.97969	-2.31161
C	0.26755	-2.91193	3.50347	C	-0.49486	-0.95399	-4.55446
H	0.49551	-2.20662	4.30360	H	-1.02477	-0.05904	-4.88054
H	-0.80830	-2.89469	3.33450	H	0.57066	-0.71916	-4.50757
H	0.53124	-3.91340	3.84913	H	-0.63552	-1.73556	-5.30378

C	0.62234	-3.39294	1.05063	C	-0.11231	-2.36649	-2.51403
H	0.06164	-4.29335	1.27945	H	0.74509	-2.71087	-3.07411
C	1.60205	-3.53475	-0.08079	C	-0.62876	-3.28796	-1.44235
H	2.62814	-3.71279	0.25818	H	-1.68678	-3.53747	-1.56618
H	1.32534	-4.39346	-0.68873	H	-0.07013	-4.22127	-1.49879
Rh	-0.56375	-1.88628	0.14398	Rh	1.20057	-1.20156	-0.95154
Cl	-1.38852	0.45570	-0.63649	Cl	1.33415	1.48559	-0.06139
C	-1.48453	-2.94288	-1.40825	C	2.58901	-1.86091	0.31567
C	-2.05762	-2.07407	1.33230	C	2.58428	-0.77132	-2.25085
O	-1.87491	-3.63706	-2.20609	O	3.30284	-2.34674	1.04527
O	-2.94607	-2.15319	2.02669	O	3.35352	-0.52410	-3.04120
Rh	-3.76260	0.82034	-1.15782	Rh	3.16907	1.61912	1.55383
Cl	-4.28320	-1.52784	-1.03346	Cl	4.71945	0.63583	-0.01554
C	-3.38468	2.65587	-1.26690	C	1.96591	2.38197	2.77154
O	-3.14839	3.76903	-1.33398	O	1.21802	2.84362	3.49925
C	-5.56912	1.09876	-1.57070	C	4.60070	1.72256	2.76026
O	-6.66810	1.24861	-1.82346	O	5.48161	1.78469	3.47848
S	1.89550	1.53105	2.72210	S	-2.93867	1.64723	-1.58616
O	2.88118	2.61057	2.79641	O	-4.38281	1.40266	-1.57760
C	0.26662	2.27640	2.61744	C	-2.64528	3.24913	-0.84306
C	0.10678	3.43249	1.85944	C	-3.70859	3.92217	-0.25373
H	0.96319	3.90635	1.40029	H	-4.69342	3.47666	-0.25383
C	-1.16136	3.97840	1.72257	C	-3.47705	5.16840	0.31604
H	-1.29971	4.87302	1.12977	H	-4.29519	5.70940	0.77346
C	-2.25103	3.37717	2.34524	C	-2.19824	5.71544	0.29864
H	-3.23969	3.80221	2.22939	H	-2.02164	6.68460	0.74770
C	-2.07395	2.23966	3.12362	C	-1.14328	5.02520	-0.29210
H	-2.91979	1.78415	3.62177	H	-0.14871	5.45133	-0.30156
H	-0.65326	0.81006	3.88429	H	-0.54668	3.23898	-1.32703
C	-0.80955	1.68141	3.26438	C	-1.36178	3.78360	-0.87254
O	1.86348	0.50760	3.76980	O	-2.20808	1.58201	-2.85420
TS6							
C	-2.19986	5.40034	-6.92821				
C	-4.37049	4.25339	-6.70447				
H	-5.39677	4.57662	-6.86203				
H	-4.35852	3.60978	-5.82126				
C	-3.95345	3.40263	-7.91552				
C	-2.46216	3.04363	-7.89993				
H	-2.17972	2.60124	-8.85275				

H	-2.32430	2.27089	-7.13705
C	-1.63537	4.22778	-7.52689
O	-4.30138	4.19742	-9.05808
O	-4.63157	2.14317	-7.91090
C	-4.21509	3.70823	-10.32668
C	-5.98846	2.05491	-8.02126
O	-6.72626	3.00104	-8.09828
O	-3.79291	2.61686	-10.60655
C	-6.40211	0.61234	-8.04724
H	-5.98132	0.13155	-8.93195
H	-6.00790	0.09207	-7.17356
H	-7.48610	0.54509	-8.06836
C	-4.74686	4.71936	-11.30019
H	-4.56481	4.37818	-12.31539
H	-5.81945	4.83959	-11.13668
H	-4.28243	5.69157	-11.13547
C	0.64731	3.76216	-8.54871
H	1.32847	3.12356	-7.98425
H	0.09894	3.14282	-9.26471
H	1.24967	4.47434	-9.11564
C	-0.31308	4.47411	-7.65073
C	-1.07919	6.38550	-7.08417
H	-0.83119	6.96446	-6.19670
C	-1.04250	7.28394	-8.33199
C	-1.44321	6.57438	-9.62576
H	-1.51230	7.30073	-10.43591
H	-0.73067	5.80612	-9.92021
H	-2.42184	6.11004	-9.51349
C	-2.05532	8.44081	-8.09201
H	-1.97169	9.14753	-8.91850
H	-3.07830	8.06789	-8.06082
H	-1.85726	8.96715	-7.16029
C	0.32333	7.92727	-8.41297
H	0.64459	8.41033	-7.49339
C	1.10340	8.00274	-9.48246
H	0.83866	7.55460	-10.43142
H	2.05231	8.52185	-9.44019
Rh	0.84170	5.28999	-5.93951
Cl	-0.78620	4.53042	-4.20435
C	2.24554	5.90872	-7.03377
C	2.02985	5.49939	-4.41546

O	3.18261	6.22246	-7.59626
O	2.70711	5.58177	-3.51308
Rh	-0.68702	2.08748	-4.52238
Cl	1.59380	2.24337	-5.28855
C	-2.44802	1.94114	-3.88775
O	-3.51707	1.85730	-3.50174
C	-0.54273	0.22721	-4.73569
O	-0.43337	-0.89675	-4.86266
C	-3.46557	5.44216	-6.49827
S	-4.14991	6.84909	-5.63605
O	-5.21430	7.42846	-6.45921
C	-4.91201	6.09974	-4.19974
C	-6.28519	5.88625	-4.19524
H	-6.87992	6.18475	-5.04719
C	-6.86741	5.30370	-3.07599
H	-7.93618	5.13512	-3.05384
C	-6.07864	4.94233	-1.98875
H	-6.53656	4.48711	-1.11978
C	-4.70469	5.16611	-2.00838
C	-4.11028	5.75031	-3.11826
H	-3.04609	5.93587	-3.14823
H	-4.09551	4.88812	-1.15823
O	-3.03621	7.68649	-5.18463

Table S6 Frequencies of all stationary points for the overall catalytic cycle, computed at B3LYP+IDSCRF/TZP-DKH(-dfg) level in toluene, and some of them computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg), B3LYP-D3+IDSCRF/TZP-DKH(-dfg) and B3LYP-D3b+IDSCRF/TZP-DKH(-dfg).

Species	Frequencies(cm ⁻¹)												
CAT D3a	35	41	52	89	90	93	96	101	117	143	243	277	
	283	300	415	416	432	434	459	466	467	468	469	470	
	610	613	2096	2098	2152	2168							
CAT	30	41	49	87	89	92	95	100	116	142	240	274	
	281	297	413	414	431	433	457	465	465	466	467	469	
	609	612	2095	2097	2151	2167							
CATD3	29	41	48	87	88	90	95	99	116	143	241	279	
	282	302	416	416	431	432	457	465	467	467	469	470	

	610 614 2096 20992152 2169
CATD3b	29 41 48 87 88 91 95 99 116 142 241 277 282 300 415 415 431 432 457 465 467 467 469 469 610 613 2096 2098 2152 2168
1aD3a	14 25 27 38 39 44 52 58 69 78 81 83 85 97101 112 123 140 144 148 160 171 180 196 219 233 260 267270 283 286 293 300 306 320 330 355 358 370 399 401 404414 415 438 446 457 481 516 533 549 553 599 601 606 610 633 668 694 705 706 727 742 759 774 776 812 847 856 860 861 886 930 945 954 954 958 970 996 1002 1019 1022 1023 1024 1030 1037 1044 1049 1055 1058 1066 1068 1070 1081 1104 1110 1128 1168 1171 1186 1187 1201 1204 1215 1224 1251 1282 1283 1289 1304 1335 1348 1352 1359 1379 1398 1401 1401 1413 1416 1431 1455 1467 1468 1472 1473 1474 1476 1478 1485 1487 1488 1494 1504 1513 1517 1627 1629 1702 17821793 2025 2355 3034 3035 3045 3061 3063 3075 3084 3091 3092 3099 3111 3115 3117 3118 3121 3122 3124 3125 3148 3151 3165 3170 3182 3193 3202 3211 3226 3228
1a	12 18 21 22 31 33 37 44 49 52 58 64 67 7682 93 96 101 134 146 160 171 180 189 216 228 254 258 263 276 281 284 297 303 322 331 346 355 364 396 399 402411 415 433 439 456 476 516 521 542 556 594 601 603 608632 674 694 700 704 722 751 754 772 773 809 842 853 859875 882 928 943 951 957 959 963 980 999 1013 1020 1021 10211026 1036 1038 1046 1056 1056 1064 1066 1069 1078 1099 1102 1125 11631170 1180 1186 1199 1205 1218 1224 1248 1280 1285 1287 1300 1334 13471350 1360 1385 1399 1400 1401 1417 1418 1434 1457 1468 1469 1473 14741475 1476 1477 1478 1485 1488 1493 1505 1515 1516 1626 1629 1697 17831792 2029 2349 3031 3031 3044 3057 3057 3073 3075 3088 3089 3097 31063108 3113 3114 3114 3115 3116 3117 3119 3148 3161 3162 3178 3189 31983209 3213 3225
1a D3	-37 9 11 29 36 38 45 47 50 61 64 71 72 7884 94 99 100 140 147 160 171 181 190 221 234 251 259267 281 287 292 305 318 325 329 354 360 370 395 401 406413 419 437 441 459 483 518 530 543 554 597 599 607 610633 672 691 705 706 730 752 759 774 776 816 847 859 862871 887 936 950 953 954 961 971 1001 1002 1020 1021 1024 10261027 1036 1038 1050 1055 1057 1064 1068 1070 1084 1105 1110 1134 11691178 1189 1190 1203 1206 1219 1230 1253 1278 1286 1289 1303 1336

	13461353 1359 1386 1399 1400 1402 1413 1418 1436 1458 1467 1468 1473 14741475 1477 1479 1484 1486 1489 1492 1504 1518 1521 1629 1630 1703 17841793 2043 2359 3030 3031 3047 3057 3059 3081 3084 3085 3090 3097 31083115 3118 3119 3119 3120 3122 3125 3143 3153 3163 3166 3181 3193 32023212 3223 3232
1a D3b	18 21 23 28 29 31 41 44 50 51 59 63 73 75 81 92 99 107 135 145 161 171 181 191 219 231 257 258 263 281 285 286 303 306 325 331 350 361 366 396 397 403 414 417 434 440 456 479 517 523 543 557 596 601 605 609 633 677 695 702 707 726 753 756 773 774 813 846 856 861 878 885 933 946 954 958 961 968 988 1002 1018 1020 1023 1024 1027 1037 1040 1048 1055 1056 1064 1068 1069 1081 1104 1105 1130 1165 1173 1184 1187 1200 1206 1218 1227 1251 1280 1284 1287 1304 1336 1345 1352 1360 1389 1400 1401 1403 1417 1418 1435 1458 1468 1469 1473 1473 1476 1477 1479 1483 1486 1489 1493 1505 1515 1517 1628 1630 1699 1783 1793 2040 2353 3031 3032 3043 3057 3057 3078 3079 3089 3089 3097 3107 3109 3115 3115 3116 3117 3120 3123 3124 3150 3162 3163 3179 3190 3199 3209 3214 3228
2a D3a	19 31 39 43 43 50 66 70 79 85 95 106 122 128 140 152 169 180 185 191 196 209 222 228 246 253 269 293 296 310 316 344 352 362 383 412 413 433 438 453 463 469 491 510 532 539 564 568 589 604 610 633 637 666 685 709 715 743 752 766 775 797 801 807 863 878 906 917 924 929 953 956 976 979 991 1003 1016 1019 1020 1022 1024 1028 1043 1046 1051 1061 1066 1070 1076 1085 1095 1105 1126 1131 1151 1160 1169 1176 1186 1201 1219 1223 1238 1255 1264 1271 1304 1306 1320 1334 1336 1347 1354 1374 1384 1398 1401 1402 1412 1416 1429 1448 1468 1468 1469 1471 1472 1474 1480 1481 1485 1489 1492 1502 1509 1513 1518 1615 1629 1630 1677 1780 1794 2997 3021 3023 3025 3031 3040 3052 3060 3060 3080 3083 3085 3101 3118 3120 3120 3128 3131 3144 3163 3167 3179 3191 3192 3200 3210 3219 3222
2a	13 23 32 37 45 49 52 58 67 73 78 87 92 95 108 139 165 177 187 193 206 207 229 233 243 249 282 284 300 305 308 344 346 358 373 403 413 419 435 442 458 476 489 510 530 545 551 570 586 602 609 631 635 664 683 708 714 737 752 762 771 791 797 802 861 877 901 912 919 926 948 952 967 977 988 1000 1014 1016 1018 1018 1022 1026 1040 1041 1048

		1059 1067 1068 1075 1082 1091 1103 1121 1127 1146 1154 1166 1174 1186 1202 1215 1218 1237 1251 1262 1274 1299 1306 1317 1331 1335 1350 1352 1376 1383 1399 1400 1402 1412 1413 1423 1445 1468 1468 1468 1473 1473 1474 1480 1483 1484 1490 1494 1503 1507 1512 1516 1605 1626 1628 1669 1778 1794 2989 3015 3020 3020 3027 3028 3034 3056 3056 3077 3079 3079 3097 3114 3116 3117 3119 3139 3146 3160 3161 3177 3179 3187 3188 3197 3205 3212
2a	D3	17 29 32 38 44 50 54 64 68 78 91 94 98 103 111 134 170 176 185 195 204 213 221 227 246 256 266 291 299 312 321 341 349 363 396 412 412 424 433 453 465 471 490 510 531 537 564 572 592 601 611 634 639 670 688 708 719 745 749 768 777 801 807 810 863 880 908 917 924 930 954 956 972 979 990 1002 1018 1019 1021 1022 1026 1031 1044 1048 1052 1062 1068 1069 1078 1086 1095 1104 1129 1136 1152 1162 1169 1176 1188 1201 1222 1225 1241 1258 1259 1271 1303 1306 1325 1336 1336 1348 1353 1371 1386 1400 1401 1404 1414 1416 1426 1448 1467 1468 1468 1472 1473 1474 1480 1483 1486 1490 1492 1502 1512 1513 1520 1629 1631 1632 1687 1782 1795 2991 3020 3021 3026 3029 3039 3053 3057 3059 3071 3079 3083 3097 3116 3117 3118 3132 3147 3148 3163 3164 3179 3190 3197 3198 3207 3213 3214
2a	D3b	16 30 34 39 44 51 60 69 74 78 92 94 94 103 107 135 169 178 184 194 197 209 221 225 247 256 266 289 298 309 316 342 349 360 386 411 413 428 435 451 464 469 490 508 531 538 563 569 590 603 610 633 635 667 686 708 715 743 750 766 776 797 803 807 864 877 905 915 923 928 953 955 971 977 986 1003 1017 1018 1020 1021 1024 1028 1041 1045 1050 1061 1068 1069 1076 1084 1092 1104 1126 1132 1150 1159 1168 1178 1187 1201 1219 1222 1238 1255 1262 1270 1303 1307 1321 1334 1335 1348 1353 1370 1385 1400 1401 1403 1414 1415 1428 1446 1469 1469 1471 1473 1473 1474 1480 1481 1485 1490 1494 1501 1514 1514 1518 1618 1629 1630 1678 1780 1793 2992 3019 3019 3022 3028 3034 3049 3057 3058 3076 3077 3079 3096 3115 3116 3117 3129 3133 3142 3162 3163 3178 3189 3193 3197 3205 3214 3214
3a	D3a	16 36 41 44 47 49 54 68 76 80 86 94 94 109 115 150 161 164 171 187 195 201 212 235 236 257 275 279 296 299 307 318 319 339 342 355 360 394 415 425 438 458 467 487 490 529 538 554 562 585 602 610 621 632 643 669 703 710 717

		732 760 776 789 798 821 860 868 880 902 918 935 951 954 958 959 982 1007 1018 1020 1022 1023 1026 1031 1042 1046 1048 1051 1060 1069 1073 1076 1083 1103 1113 1130 1135 1162 1175 1187 1195 1202 1208 1215 1222 1250 1253 1266 1275 1305 1318 1325 1335 1349 1353 1359 1377 1401 1401 1408 1412 1425 1457 1464 1468 1469 1471 1471 1475 1478 1484 1485 1487 1496 1509 1512 1517 1629 1629 1672 1700 1745 1783 1794 3027 3039 3044 3046 3049 3052 3061 3061 3075 3103 3106 3110 3111 3117 3120 3120 3122 3129 3135 3148 3165 3167 3181 3192 3201 3213 3219 3225
3a		13 30 32 37 42 47 55 64 67 69 79 90 98 104 108 114 135 161 168 183 193 197 210 231 232 254 269 279 289 296 301 310 319 335 339 353 358 391 413 422 436 456 466 485 488 528 538 554 560 584 601 608 619 631 639 667 701 708 714 730 757 774 785 795 818 856 863 876 899 915 933 948 950 952 955 979 1002 1016 1017 1019 1021 1021 1028 1040 1045 1046 1048 1055 1068 1069 1072 1080 1101 1107 1125 1132 1160 1173 1186 1191 1200 1207 1212 1220 1247 1250 1263 1274 1304 1317 1324 1332 1347 1350 1357 1376 1401 1402 1406 1412 1423 1457 1467 1468 1469 1473 1473 1474 1478 1481 1483 1487 1495 1504 1511 1515 1626 1627 1664 1697 1742 1781 1792 3022 3037 3041 3042 3044 3046 3057 3058 3072 3100 3102 3106 3107 3112 3116 3117 3122 3128 3130 3144 3161 3162 3177 3188 3197 3206 3213 3220
3a	D3	18 35 38 41 48 49 51 57 61 69 78 89 93 97 105 117 134 166 171 188 200 202 217 235 238 258 278 292 301 305 310 321 323 338 344 356 361 395 413 427 438 458 468 487 490 529 539 556 562 586 599 608 623 634 644 670 703 708 720 734 761 775 793 801 824 863 864 886 904 918 938 948 956 958 959 984 1003 1020 1021 1022 1025 1026 1032 1045 1045 1050 1052 1065 1068 1069 1075 1085 1104 1116 1134 1139 1163 1175 1188 1194 1202 1209 1218 1223 1254 1256 1268 1275 1304 1317 1323 1337 1348 1353 1358 1380 1401 1401 1410 1414 1426 1457 1466 1469 1469 1472 1473 1474 1478 1484 1485 1487 1503 1512 1515 1519 1630 1632 1679 1702 1751 1783 1795 3026 3041 3046 3047 3052 3056 3058 3059 3075 3105 3109 3109 3112 3117 3117 3119 3128 3130 3138 3146 3163 3164 3179 3190 3199 3209 3215 3222
3a	D3b	19 32 36 41 46 49 51 60 66 70 79 91 93 99 108 116 137 164 170 186 197 200 214 233 235 256 276 288 298 300 306 318 323 337 342 354 359 393 414 426 437 458 467 486 489 529 538 555

	562 585 601 608 621 632 642 669 702 709 717 732 759 774 789 798 821 860 864 881 902 917 936 948 954 955 956 982 1003 1019 1020 1021 1023 1024 1031 1042 1045 1048 1050 1061 1068 1070 1074 1083 1103 1112 1130 1136 1162 1174 1188 1193 1202 1208 1215 1222 1251 1253 1266 1273 1304 1317 1324 1334 1348 1352 1358 1378 1401 1401 1409 1413 1425 1457 1467 1468 1469 1473 1473 1474 1479 1483 1485 1487 1501 1509 1514 1517 1628 1630 1673 1700 1746 1783 1794 3024 3039 3044 3045 3049 3049 3057 3058 3073 3103 3105 3108 3109 3115 3116 3118 3125 3129 3134 3145 3162 3162 3178 3189 3198 3208 3214 3221
COM D3a	11 16 21 27 31 32 34 37 38 42 49 52 53 58 62 66 71 78 79 83 87 88 92 94 99 101 102 111 117 125 138 141 145 146 150 154 161 175 193 199 216 225 242 254 258 263 272 278 288 292 299 301 302 313 317 323 353 358 372 375 380 388 399 404 412 425 438 440 444 445 458 469 471 473 473 474 489 500 509 530 550 559 587 595 601 607 609 611 633 664 699 700 711 727 756 758 772 784 803 853 857 868 877 886 931 946 951 958 960 966 977 1009 1018 1021 1024 1027 1039 1041 1041 1049 1050 1064 1066 1068 1069 1082 1105 1110 1129 1151 1169 1172 1187 1204 1208 1217 1223 1248 1283 1285 1296 1318 1337 1346 1354 1358 1391 1398 1399 1402 1415 1418 1440 1459 1461 1467 1467 1468 1471 1477 1481 1483 1486 1486 1493 1506 1512 1520 1629 1630 1698 1788 1798 2040 2090 2096 2144 2158 2173 3036 3038 3049 3056 3061 3068 3078 3103 3104 3109 3114 3115 3116 3117 3118 3119 3121 3122 3133 3152 3164 3164 3165 3186 3199 3202 3216 3230
COM	12 13 15 21 22 26 29 31 33 40 44 47 51 52 56 61 65 70 70 76 80 82 87 89 92 94 99 100 104 114 119 130 132 137 142 152 160 176 184 194 210 218 235 249 256 260 265 272 285 290 297 298 301 307 309 321 350 354 369 376 385 387 398 400 411 423 434 440 442 443 457 464 469 471 472 474 478 489 505 527 548 555 589 593 602 604 608 611 630 660 696 698 705 723 750 752 762 776 798 847 857 857 875 880 925 942 947 954 955 962 973 997 1014 1018 1019 1021 1027 1038 1041 1046 1048 1064 1064 1068 1070 1079 1104 1106 1125 1146 1164 1169 1188 1201 1205 1212 1218 1243 1283 1284 1298 1321 1334 1345 1353 1359 1395 1400 1402 1403 1414 1416 1437 1454 1458 1466 1468 1471 1473 1475 1481 1481 1484 1488 1493 1506 1513 1517 1626 1628 1696 1787

	1798 2029 2083 2097 2145 2156 2189 3032 3037 3045 3055 3057 3063 3075 3097 3102 3108 3108 3112 3112 3115 3116 3116 3116 3117 3125 3146 3161 3162 3179 3189 3198 3205 3214 3224
COM D3	15 24 27 29 31 37 39 42 46 51 51 54 56 59 62 66 72 75 81 83 86 90 92 94 97 99 100 107 110 116 121 129 135 143 149 160 164 174 182 199 213 222 246 247 255 263 276 284 290 299 305 305 309 318 322 326 351 357 370 372 390 395 397 407 424 424 431 442 445 451 455 468 470 472 475 477 479 497 509 532 549 558 588 593 600 607 609 610 633 669 698 701 706 729 759 764 771 785 808 856 861 867 884 890 935 949 951 956 958 970 979 998 1020 1021 1023 1029 1031 1041 1042 1046 1050 1064 1066 1068 1070 1082 1106 1118 1130 1157 1172 1180 1189 1201 1203 1219 1226 1253 1283 1287 1296 1316 1337 1345 1352 1363 1390 1400 1401 1402 1417 1419 1440 1457 1463 1468 1468 1470 1473 1476 1481 1483 1486 1488 1493 1508 1514 1517 1628 1629 1701 1788 1799 2049 2084 2092 2137 2154 2183 3032 3041 3045 3055 3058 3079 3083 3098 3105 3111 3111 3114 3116 3117 3118 3119 3121 3122 3143 3149 3162 3164 3183 3195 3204 3215 3221 3227
COM D3b	10 17 21 23 27 28 34 36 38 41 47 51 54 55 60 65 67 70 76 80 83 85 90 93 95 98 100 102 105 116 121 125 139 141 145 150 159 177 195 198 215 223 243 249 253 257 271 278 289 292 297 299 303 314 317 323 353 356 371 373 384 390 398 403 411 424 438 440 443 446 459 468 470 472 473 473 485 499 508 530 549 558 588 594 602 606 609 610 633 663 697 699 707 728 755 757 769 782 804 850 856 864 876 885 931 945 951 956 957 967 978 1006 1019 1022 1024 1027 1029 1040 1042 1045 1050 1064 1065 1068 1069 1082 1105 1110 1130 1152 1170 1173 1188 1201 1206 1216 1222 1248 1283 1284 1297 1321 1337 1345 1354 1361 1394 1402 1402 1402 1415 1417 1440 1458 1459 1467 1468 1470 1473 1476 1481 1483 1486 1487 1492 1506 1513 1519 1629 1630 1698 1787 1798 2041 2089 2096 2144 2158 2174 3033 3037 3046 3054 3058 3066 3077 3098 3102 3107 3110 3112 3114 3115 3117 3117 3117 3117 3133 3149 3161 3163 3164 3184 3197 3205 3214 3227
TS1 D3a	-62 15 20 24 28 29 34 44 46 50 53 55 58 60 66 71 73 78 80 86 90 92 94 102 102 106 109 115 118 124 132 136 149 154 158

		171	177	186	191	195	211	214	225	238	244	256	270
		275	287	297	305	308	316	322	332	341	348	358	374
		383	386	394	401	407	415	417	423	431	448	461	464
		471	474	477	478	482	483	495	506	517	550	562	595
		598	601	609	611	616	632	659	683	699	707	725	741
		752	773	778	797	849	864	877	890	912	927	930	952
		956	958	973	988	1000	1009	1020	1023	1027	1035	1040	1043
		1049	1066	1066	1070	1073	1081	1106	1114	1129	1140	1156	1171
		1189	1204	1209	1219	1220	1250	1282	1287	1303	1325	1336	1348
		1351	1355	1398	1401	1404	1406	1415	1416	1429	1455	1458	1466
		1467	1469	1473	1475	1481	1485	1486	1487	1495	1511	1514	1517
		1627	1629	1699	1786	1794	1968	2073	2090	2136	2152	2215	3043
		3048	3058	3060	3061	3092	3096	3109	3111	3121	3121	3123	3123
		3130	3131	3132	3138	3140	3151	3157	3164	3168	3182	3196	3203
		3213	3221	3228									
TS1		-66	8	12	17	21	25	31	38	40	44	46	48
		49	52	59	61	63	65	71	74	85	90	94	95
		99	100	101	105	106	112	118	126	134	140	150	161
		165	173	183	188	192	205	223	237	242	251	261	273
		279	280	302	304	313	316	329	339	346	350	371	380
		384	390	397	403	411	414	423	427	443	454	459	469
		473	475	476	477	478	494	498	514	550	559	593	595
		601	606	611	612	630	657	685	697	706	721	744	751
		771	772	792	842	862	867	884	901	924	926	952	952
		956	969	981	993	1003	1019	1020	1023	1031	1037	1038	1044
		1045	1063	1064	1067	1069	1078	1104	1108	1125	1138	1154	1170
		1188	1202	1205	1214	1218	1245	1281	1287	1301	1331	1334	1347
		1349	1353	1400	1401	1402	1406	1412	1421	1430	1455	1456	1466
		1468	1468	1472	1473	1480	1481	1484	1485	1495	1510	1512	1516
		1625	1627	1696	1786	1794	1963	2070	2091	2137	2152	2205	3037
		3043	3052	3057	3059	3079	3087	3101	3103	3113	3116	3117	3118
		3121	3127	3129	3133	3133	3143	3146	3162	3162	3179	3190	3198
		3209	3213	3223									
TS1	D3	-49	11	20	25	29	32	38	45	47	48	53	55
		57	58	66	72	74	78	83	89	93	93	99	99
		103	105	109	114	120	122	127	134	139	152	158	171
		178	187	191	198	204	211	220	243	250	261	272	278
		284	291	308	310	320	323	336	346	352	362	379	388
		390	395	401	410	412	417	424	430	443	461	469	472
		473	479	482	484	488	497	506	519	553	563	597	601
		603	609	612	619	633	662	688	699	706	729	743	758
		772	783	802	854	862	880	891	912	934	935	952	956
		961	972	992	1003	1008	1023	1024	1026	1036	1041	1043	1049
		1050											

		1067 1068 1069 1073 1084 1106 1119 1134 1145 1161 1176 1189 1204 1212 1222 1224 1255 1284 1288 1304 1328 1337 1350 1352 1356 1401 1403 1406 1411 1413 1419 1436 1457 1461 1468 1468 1471 1473 1476 1482 1487 1487 1489 1498 1513 1516 1518 1629 1631 1701 1787 1795 1990 2074 2091 2135 2154 2222 3039 3045 3058 3059 3061 3099 3104 3106 3106 3117 3120 3122 3123 3132 3132 3133 3137 3148 3149 3163 3163 3165 3181 3192 3200 3209 3217 3226
TS1	D3b	-62 10 18 23 25 28 33 40 44 47 49 51 55 55 62 66 69 73 76 82 88 91 93 96 99 101 104 107 115 119 123 131 137 153 158 167 174 186 190 194 203 211 223 237 239 256 269 276 280 285 305 306 317 321 331 342 347 356 374 383 385 393 400 407 412 415 423 429 444 460 463 470 472 476 479 481 483 495 505 516 551 561 595 599 602 609 611 616 631 659 685 698 706 725 743 753 772 779 797 849 863 876 889 910 928 930 953 956 958 970 988 1001 1005 1021 1023 1024 1034 1039 1040 1045 1047 1066 1068 1068 1071 1081 1105 1114 1130 1140 1156 1174 1190 1203 1208 1219 1220 1250 1283 1288 1303 1329 1335 1349 1351 1354 1401 1402 1403 1409 1413 1418 1430 1456 1460 1468 1468 1470 1473 1473 1482 1485 1486 1487 1495 1511 1512 1517 1627 1629 1698 1786 1794 1972 2073 2090 2135 2152 2214 3038 3045 3056 3057 3058 3093 3097 3104 3105 3116 3117 3119 3121 3128 3131 3131 3133 3140 3148 3156 3162 3164 3180 3191 3199 3209 3213 3225
INT1	D3a	5 14 20 33 35 38 41 44 46 51 54 58 61 66 71 72 81 86 89 91 92 97 98 105 109 111 120 123 125 132 142 144 157 167 177 178 179 189 195 198 218 224 231 248 253 266 272 276 282 286 290 306 309 311 321 333 346 350 362 369 379 394 397 405 412 415 419 428 436 445 450 467 474 477 479 480 493 505 514 543 548 554 567 601 609 612 623 631 635 662 688 704 706 728 745 752 772 787 802 854 856 879 898 925 931 946 953 956 964 984 1000 1006 1013 1021 1024 1027 1036 1040 1044 1049 1063 1067 1068 1069 1072 1080 1105 1112 1126 1138 1157 1179 1187 1196 1203 1221 1231 1253 1272 1276 1305 1324 1335 1345 1351 1356 1381 1396 1401 1405 1407 1416 1425 1459 1459 1466 1467 1469 1470 1471 1484 1485 1489 1495 1496 1513 1514 1518 1628 1629 1698 1782 1795 1827 2074 2137 2141 2172 2220 3043 3045 3061 3061 3064 3072 3079 3104 3107 3117 3119 3122 3122 3124 3129 3134 3142 3149 3151 3154 3166 3168 3182 3196 3204 3219 3225 3228

INT1	11	13	19	24	32	37	38	41	45	47	50	55
	61	64	69	73	77	79	87	88	90	92	96	98
	101	109	111	120	121	123	137	139	152	164	167	173
	175	179	189	192	211	215	227	243	247	258	267	271
	276	279	283	304	307	309	317	329	341	347	358	366
	374	393	397	404	410	413	417	427	434	443	446	466
	474	475	476	481	491	500	513	542	547	552	566	600
	607	611	620	628	631	658	684	704	705	725	745	750
	773	783	797	848	859	876	894	922	929	943	953	954
	960	983	998	1002	1008	1020	1022	1023	1031	1037	1041	1059
	1067	1068	1069	1069	1077	1105	1108	1122	1132	1157	1177	1188
	1203	1217	1227	1248	1267	1275	1302	1328	1334	1348	1351	1385
	1398	1403	1404	1405	1416	1425	1456	1457	1468	1469	1470	1473
	1483	1485	1487	1496	1504	1511	1514	1516	1626	1628	1695	1780
	1793	1809	2071	2137	2143	2173	2214	3040	3043	3056	3057	3059
	3065	3069	3100	3102	3111	3113	3116	3116	3118	3126	3133	3135
	3143	3146	3152	3162	3163	3179	3191	3199	3211	3219	3222	
INT1 D3	14	18	27	30	32	38	40	44	47	50	57	61
	64	69	73	74	79	85	86	91	94	98	99	105
	108	113	121	129	132	141	144	148	153	166	173	175
	180	184	193	197	216	224	230	245	252	267	273	277
	282	286	306	310	313	316	323	339	348	353	366	373
	387	397	398	410	412	416	423	432	439	448	456	467
	477	478	480	487	494	503	514	536	546	554	568	600
	609	612	623	632	636	665	693	705	706	732	748	755
	774	788	806	859	863	883	904	931	933	952	954	957
	966	988	1005	1011	1016	1021	1027	1033	1037	1041	1044	1050
	1062	1067	1068	1069	1071	1082	1108	1117	1131	1143	1159	1182
	1188	1202	1206	1223	1233	1256	1276	1281	1306	1329	1338	1351
	1351	1357	1386	1400	1405	1407	1409	1414	1429	1458	1464	1468
	1468	1469	1469	1473	1475	1483	1487	1487	1488	1498	1513	1516
	1519	1630	1631	1701	1783	1795	1845	2076	2132	2142	2171	2229
	2297	3042	3043	3058	3061	3064	3083	3104	3105	3117	3121	3122
	3128	3130	3131	3134	3148	3149	3154	3155	3164	3166	3181	3195
	3203	3223	3225	3226								
INT1 D3b	9	17	22	27	34	37	43	44	47	49	53	56
	61	64	72	73	77	81	83	87	91	94	96	100
	106	110	114	119	125	127	137	142	149	162	164	171
	173	174	191	195	213	221	230	248	249	264	270	277
	285	289	304	307	311	316	323	339	348	354	362	372
	386	394	398	408	410	412	422	430	437	446	456	466
	476	476	480	486	492	498	512	535	545	554	567	601

		608	612	620	628	632	661	687	703	703	729	745	752
		772	784	801	852	858	877	900	925	929	945	953	953
		964	983	1001	1006	1011	1020	1024	1026	1035	1039	1041	1048
		1067	1068	1070	1070	1080	1108	1112	1127	1138	1157	1177	1189
		1206	1220	1231	1251	1274	1278	1303	1325	1335	1351	1355	1358
		1399	1404	1405	1406	1414	1427	1458	1459	1466	1467	1468	1471
		1484	1485	1488	1489	1498	1515	1515	1519	1628	1629	1699	1782
		1839	2072	2131	2139	2170	2223	3039	3042	3042	3058	3061	3061
		3102	3104	3117	3120	3120	3121	3130	3131	3133	3140	3145	3147
		3164	3164	3179	3193	3201	3220	3223	3226				
TS2	D3a	-252	15	20	24	32	36	40	42	44	47	51	55
		56	64	66	69	76	79	82	84	88	90	95	100
		101	106	110	119	124	130	130	137	150	163	172	180
		182	193	200	205	220	226	231	248	271	275	278	281
		294	305	306	310	316	321	332	336	343	362	365	367
		386	397	411	411	419	429	431	438	447	448	464	473
		476	477	479	489	495	511	518	528	552	565	590	600
		604	612	616	632	633	664	688	707	708	731	749	760
		774	804	823	856	862	897	905	928	934	952	956	957
		961	977	1003	1012	1017	1023	1027	1028	1034	1041	1048	1049
		1057	1069	1070	1072	1080	1092	1106	1125	1128	1158	1169	1189
		1203	1220	1225	1251	1260	1279	1295	1326	1335	1336	1348	1353
		1395	1397	1402	1403	1407	1425	1448	1454	1465	1469	1469	1470
		1479	1486	1487	1490	1499	1508	1516	1517	1627	1630	1698	1735
		1794	1925	2077	2141	2144	2174	2976	3035	3043	3054	3055	3061
		3091	3102	3103	3107	3111	3121	3121	3131	3135	3148	3149	3149
		3166	3167	3186	3197	3204	3214	3220	3227				
TS2		-277	11	15	19	26	28	36	38	40	45	48	51
		51	61	63	64	68	72	79	82	83	85	91	94
		98	100	101	109	117	119	128	130	158	159	170	174
		178	189	193	200	216	224	234	256	266	273	275	278
		287	300	303	306	312	317	327	329	341	357	362	363
		383	394	408	412	414	427	428	434	444	446	463	472
		473	475	477	486	494	504	516	526	551	564	585	598
		602	611	612	629	630	662	683	704	705	726	745	757
		773	800	817	849	860	893	901	921	930	948	953	955
		956	976	1003	1008	1013	1020	1023	1023	1030	1038	1046	1049
		1057	1067	1068	1070	1077	1087	1105	1120	1123	1153	1164	1190
		1203	1216	1219	1247	1257	1278	1292	1324	1334	1335	1345	1353
		1392	1399	1402	1403	1407	1425	1450	1456	1468	1468	1469	1472
		1481	1484	1488	1489	1496	1506	1514	1516	1625	1628	1695	1724
													1780

		1793 1919 2074 2139 2144 2173 2997 3032 3041 3043 3053 3057 3059 3091 3096 3102 3102 3108 3116 3119 3122 3128 3145 3146 3146 3158 3162 3162 3180 3192 3200 3211 3218 3223
TS2	D3	-221 11 14 21 23 32 35 37 43 44 48 50 55 58 62 67 73 78 81 83 88 92 94 99 101 108 110 112 117 129 137 137 161 167 171 181 185 193 205 211 224 232 245 262 272 278 280 283 294 307 309 312 315 322 336 338 349 363 367 371 384 397 409 411 423 430 432 440 447 453 465 474 476 476 478 489 498 519 521 531 553 566 593 599 603 612 615 632 635 667 696 704 710 734 753 764 773 806 829 858 864 899 911 933 938 951 952 960 963 981 999 1016 1019 1021 1026 1031 1037 1042 1046 1049 1050 1063 1069 1071 1071 1084 1098 1108 1130 1134 1164 1174 1190 1203 1206 1224 1231 1255 1264 1281 1300 1320 1337 1338 1354 1356 1365 1395 1399 1403 1404 1407 1425 1446 1455 1467 1468 1469 1473 1474 1486 1487 1490 1495 1497 1508 1519 1519 1630 1631 1702 1752 1783 1797 1935 2079 2140 2144 2174 2953 3035 3040 3055 3056 3060 3072 3095 3098 3102 3114 3114 3116 3121 3131 3143 3145 3146 3148 3164 3165 3167 3182 3194 3201 3212 3216 3225
TS2	D3b	-251 6 15 24 27 29 35 39 41 44 48 51 53 62 63 66 69 75 80 83 85 90 93 97 99 102 104 110 117 127 131 134 155 162 172 178 181 191 200 206 221 228 239 257 269 275 277 281 289 303 306 309 314 320 331 336 342 359 365 366 385 397 410 411 418 429 431 436 446 448 464 473 475 476 478 488 495 511 518 528 552 565 590 600 602 612 613 631 633 665 688 704 707 731 749 760 773 804 823 856 859 897 906 926 934 952 953 954 960 979 1001 1012 1017 1023 1023 1026 1032 1040 1047 1048 1050 1059 1068 1068 1070 1080 1092 1106 1126 1128 1157 1169 1190 1199 1203 1221 1225 1251 1261 1278 1295 1326 1335 1336 1348 1354 1365 1394 1398 1403 1403 1407 1425 1449 1456 1467 1469 1469 1471 1473 1482 1486 1489 1489 1497 1507 1515 1517 1627 1629 1699 1736 1781 1794 1925 2076 2140 2144 2174 2969 3033 3042 3052 3054 3057 3059 3092 3099 3103 3105 3110 3116 3119 3126 3135 3146 3147 3149 3163 3164 3165 3181 3193 3201 3211 3218 3224
INT2	D3a	16 24 27 31 39 40 45 48 50 53 61 63 64 68 71 75 77 82 85 89 95 98 99 106 112 118 123 125 132 138 141 165 167 173 187

	193 206 212 228 236 246 255 260 270 272 273 282 284 291 296 300 309 318 322 333 349 361 369 396 407 415 421 421 427 433 442 455 469 470 472 475 476 492 508 514 522 537 545 567 569 575 602 609 616 627 632 658 664 693 706 709 717 740 770 776 779 802 832 864 884 900 912 926 931 956 956 958 971 1004 1017 1019 1019 1020 1026 1031 1037 1043 1046 1049 1052 1063 1067 1070 1078 1089 1104 1109 1124 1127 1140 1162 1176 1187 1203 1204 1218 1248 1252 1268 1292 1304 1313 1333 1335 1344 1354 1369 1387 1400 1402 1403 1408 1425 1457 1467 1467 1468 1471 1472 1473 1477 1484 1485 1489 1495 1510 1513 1518 1611 1628 1630 1645 1701 1782 1793 2089 2131 2154 2190 3029 3044 3049 3057 3061 3061 3063 3078 3097 3114 3120 3121 3121 3123 3123 3133 31373144 3147 3150 3165 3166 3181 3193 3201 3211 3215 3228
INT2	9 18 23 27 33 38 40 45 47 55 59 61 63 67 71 73 75 82 83 90 93 95 99 100 108 114 120 121 129 135 141 163 167 173 185 189 201 206 228 233 244 253 255 268 269 270 282 282 294 299 306 308 316 320 331 347 362 367 394 405 413 418 420 426 433 440 454 467 468 470 472 475 490 508 513 522 536 544 565 570 573 603 609 615 625 631 652 660 689 703 706 713 736 767 771 775 798 825 861 878 900 908 926 928 953 954 956 967 1002 1014 1016 1019 1019 1021 1032 1033 1040 1044 1049 1051 1061 1067 1069 1075 1084 1102 1104 1119 1122 1133 1158 1177 1187 1198 1203 1215 1245 1249 1267 1289 1301 1313 1332 1333 1341 1354 1367 1386 1400 1400 1402 1411 1426 1458 1468 1469 1470 1473 1473 1474 1478 1482 1483 1490 1496 1509 1514 1517 1600 1626 1628 1639 1698 1781 1792 2088 2129 2153 2188 3028 3040 3048 3053 3057 3057 3058 3076 3094 3111 3116 3116 3118 3119 3121 3131 3133 3138 3139 3146 3161 3162 3177 3188 3197 3209 3213 3222
INT2 D3	22 25 26 31 36 43 46 49 49 56 58 59 60 64 65 69 80 83 83 89 95 99 102 104 112 126 132 134 145 146 164 174 175 179 188 199 206 216 233 246 247 259 261 273 274 282 284 288 298 305 310 317 320 324 338 352 366 372 404 411 414 425 427 429 438 443 463 464 468 473 475 475 492 513 518 523 539 550 570 573 577 603 609 617 630 635 660 668 698 705 708 722 745 772 778 783 805 839 865 892 905 919 930 933 955 958 965 977 1005 1009 1019 1022 1022 1026 1027 1041 1047 1049 1053 1059 1068

		1070 1070 1085 1091 1108 1112 1129 1132 1147 1166 1179 1189 1207 1209 1221 1255 1256 1271 1294 1310 1315 1332 1338 1348 1359 1373 1389 1397 1401 1402 1404 1425 1459 1467 1468 1473 1473 1474 1476 1484 1487 1491 1498 1501 1511 1515 1521 1628 1631 1632 1645 1705 1783 1795 2087 2135 2152 2190 3008 3045 3050 3051 3057 3058 3059 3063 3117 3118 3119 3119 3122 3125 3131 3139 3142 3148 3149 3155 3164 3164 3179 3191 3200 3214 3219 3225
INT2	D3b	14 20 23 26 35 39 40 46 48 51 61 62 64 64 69 75 76 83 85 92 95 96 99 100 109 110 121 126 132 136 141 168 171 179 189 194 205 215 230 242 248 258 261 270 273 276 281 283 295 298 304 310 319 326 334 349 363 371 398 407 412 422 424 429 436 442 456 467 468 471 473 474 491 509 514 521 537 545 567 570 575 602 608 616 628 633 658 664 692 704 706 717 740 770 773 777 802 834 860 883 903 912 928 931 954 956 958 972 1001 1017 1018 1020 1021 1023 1026 1038 1042 1046 1053 1058 1065 1067 1069 1079 1089 1105 1108 1124 1127 1140 1162 1177 1188 1202 1204 1218 1247 1252 1268 1292 1306 1314 1331 1335 1343 1355 1365 1387 1400 1401 1402 1407 1424 1459 1467 1468 1468 1472 1473 1474 1477 1485 1486 1489 1498 1512 1514 1519 1614 1628 1630 1645 1702 1782 1793 2089 2132 2154 2190 3011 3044 3050 3051 3057 3058 3060 3068 3100 3115 3116 3118 3120 3122 3125 3132 3137 3141 3144 3149 3163 3163 3179 3190 3199 3213 3214 3226
TS3	D3a	-163 17 22 24 27 31 37 40 45 49 50 53 58 64 68 73 79 82 85 90 93 94 99 101 102 112 113 121 131 138 151 161 163 169 171 176 190 195 209 226 240 250 258 263 267 269 280 284 288 293 296 304 308 309 313 322 337 348 355 362 376 403 410 419 425 441 443 446 460 470 472 474 477 478 493 516 525 541 559 566 574 605 610 612 629 633 647 661 693 705 705 717 740 767 775 779 802 833 863 873 901 910 926 940 952 955 970 973 1002 1016 1019 1021 1022 1023 1027 1031 1044 1044 1050 1059 1068 1070 1072 1080 1093 1102 1105 1124 1128 1149 1175 1177 1187 1202 1205 1217 1252 1253 1270 1290 1307 1315 1329 1335 1348 1354 1361 1388 1401 1401 1403 1404 1422 1455 1468 1468 1472 1472 1473 1474 1479 1481 1485 1490 1494 1506 1516 1519 1612 1628 1630 1634 1669 1782 1793 2080 2147 2155 2191 3019 3039 3045 3050 3056 3060 3062 3069 3093 3108 3120 3122 3123 3126 3130 3133 3138 3140 3155

		3165 3167 3180 3181 3191 3198 3205 3214 3238
TS3		-166 8 15 22 26 28 34 37 41 44 46 53 56 59 61 62 66 70 77 81 84 89 93 95 97 98 102 111 112 117 132 147 149 157 171 173 185 192 205 223 232 243 254 256 262 266 273 276 282 286 290 301 303 306 309 319 332 342 349 364 374 401 411 417 424 439 440 441 459 468 470 472 472 477 491 515 523 541 558 565 573 602 608 611 625 631 640 659 690 700 706 714 736 763 773 774 798 825 861 867 897 906 925 934 950 954 967 970 1001 1011 1015 1020 1020 1021 1023 1030 1039 1042 1047 1054 1064 1067 1069 1077 1089 1097 1103 1118 1123 1142 1170 1176 1188 1199 1202 1214 1248 1249 1268 1287 1306 1312 1328 1333 1345 1353 1359 1386 1401 1401 1402 1404 1422 1455 1467 1468 1469 1473 1474 1475 1480 1483 1484 1490 1493 1505 1514 1517 1602 1626 1626 1628 1666 1781 1792 2078 2145 2153 2193 3016 3034 3039 3047 3051 3056 3057 3067 3090 3103 3114 3115 3117 3123 3127 3132 3133 3137 3150 3161 3161 3171 3178 3188 3196 3204 3212 3232
TS3	D3	-198 15 22 25 31 34 37 41 44 47 48 51 52 59 61 67 71 75 78 83 89 90 94 95 97 103 105 112 119 131 147 162 168 172 178 180 188 201 209 225 241 252 264 267 274 274 279 282 288 293 300 304 307 310 315 328 340 354 359 366 377 405 410 421 430 442 447 449 468 468 472 473 479 479 493 517 527 543 559 567 575 602 607 615 629 634 648 663 697 706 708 722 743 767 774 783 806 837 863 879 903 916 931 944 955 962 970 975 1002 1017 1020 1021 1023 1026 1030 1032 1046 1048 1057 1059 1067 1068 1069 1084 1099 1106 1108 1128 1133 1154 1178 1180 1188 1204 1210 1220 1255 1258 1272 1293 1310 1316 1330 1337 1351 1356 1365 1391 1401 1402 1402 1405 1424 1456 1467 1468 1468 1473 1474 1478 1483 1486 1490 1494 1501 1507 1520 1520 1622 1630 1631 1637 1670 1783 1794 2075 2142 2152 2195 3007 3037 3051 3055 3057 3058 3059 3070 3106 3116 3116 3120 3123 3126 3130 3135 3143 3147 3153 3163 3164 3179 3190 3190 3199 3209 3213 3236
TS3	D3b	-172 11 15 17 26 28 36 37 44 46 48 50 56 58 60 67 67 70 79 81 85 90 94 97 97 98 103 109 111 117 143 154 159 160 171 175 186 195 207 225 242 248 260 263 267 269 270 279 284 289 296 304 305 306 310 322 336 348 352 365

		376	402	411	418	426	440	442	445	461	469	469	472
		474	477	493	515	525	541	560	566	574	602	608	612
		627	632	646	661	694	704	706	717	739	767	773	778
		802	831	862	873	901	910	927	940	954	956	969	972
		1002	1014	1018	1021	1021	1023	1027	1030	1043	1043	1050	1055
		1067	1069	1080	1094	1102	1105	1123	1128	1149	1174	1177	1188
		1203	1217	1252	1253	1270	1291	1308	1313	1329	1335	1348	1355
		1361	1386	1400	1401	1402	1405	1423	1455	1467	1468	1471	1473
		1474	1475	1479	1482	1485	1490	1493	1507	1515	1518	1615	1628
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		3235											
INT3	D3a	14	17	22	26	27	38	41	44	46	50	56	60
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		121	131	136	142	143	144	165	170	179	193	198	204
		227	232	244	246	252	263	266	277	279	280	288	289
		300	306	308	312	316	321	345	353	362	364	386	394
		408	412	418	426	430	437	442	454	468	471	475	476
		480	494	498	510	537	549	560	571	574	603	610	612
		628	633	662	670	705	706	718	741	769	772	777	803
		807	836	861	881	908	912	932	952	959	960	979	1003
		1013	1020	1020	1020	1022	1024	1034	1036	1045	1046	1051	1056
		1068	1071	1072	1082	1094	1099	1107	1123	1128	1150	1180	1188
		1201	1205	1218	1220	1253	1254	1271	1297	1303	1310	1317	1334
		1339	1354	1357	1389	1401	1403	1405	1411	1422	1448	1468	1469
		1472	1473	1473	1479	1480	1484	1485	1491	1492	1499	1516	1519
		1582	1618	1628	1630	1644	1781	1795	2077	2145	2172	2194	3022
		3033	3044	3047	3054	3062	3062	3071	3091	3099	3111	3121	3123
		3127	3138	3139	3143	3158	3165	3166	3167	3182	3186	3193	3200
		3207	3217	3258									
INT3		5	10	20	25	27	34	35	40	46	52	54	56
		62	63	66	67	75	79	85	87	91	98	99	106
		109	114	118	127	131	139	165	170	180	192	198	201
		223	226	235	241	246	254	264	265	276	277	288	291
		302	304	306	314	314	318	342	349	360	366	384	391
		406	412	419	424	427	435	439	452	468	472	472	473
		476	494	500	507	535	548	558	569	573	604	610	611
		626	631	661	662	702	706	714	737	765	769	774	794
		799	829	862	876	903	909	929	952	954	955	973	1003
		1004	1017	1018	1019	1019	1021	1030	1032	1041	1043	1047	1053
		1067	1068	1069	1078	1090	1093	1104	1117	1124	1143	1178	1188
		1197	1203										

	1213 1216 1248 1250 1269 1295 1302 1308 1314 1332 1336 1351 1353 1387 1401 1402 1406 1408 1422 1449 1468 1469 1473 1473 1475 1480 1483 1484 1486 1489 1493 1499 1516 1517 1581 1607 1626 1628 1633 1780 1792 2075 2143 2171 2192 3021 3029 3040 3044 3047 3057 3059 3069 3086 3094 3107 3115 3119 3128 3136 3137 3138 3155 3161 3162 3163 3178 3182 3189 3197 3205 3214 3251
INT3 D3	15 16 20 24 31 34 42 46 54 54 56 60 65 68 71 77 84 90 97 99 100 102 105 114 116 117 126 134 144 151 172 176 188 195 201 202 230 232 246 249 258 265 271 278 282 285 288 290 302 308 311 313 320 326 348 356 358 371 382 398 405 413 418 429 433 438 452 454 473 473 475 477 481 495 508 510 540 549 559 570 578 604 610 612 632 634 664 673 706 708 722 742 771 772 778 807 809 842 862 886 909 915 933 954 963 964 984 1001 1013 1021 1022 1025 1026 1027 1036 1040 1046 1049 1052 1058 1069 1072 1073 1085 1097 1101 1108 1127 1134 1154 1179 1188 1204 1205 1223 1224 1257 1258 1275 1301 1305 1309 1318 1336 1343 1355 1359 1389 1402 1403 1412 1414 1425 1448 1467 1470 1472 1472 1474 1479 1483 1486 1486 1492 1495 1500 1518 1519 1578 1627 1630 1631 1652 1782 1796 2083 2142 2154 2190 3032 3038 3047 3052 3053 3061 3065 3076 3097 3107 3117 3121 3126 3134 3142 3144 3151 3162 3167 3168 3169 3184 3195 3197 3203 3215 3218 3263
INT3 D3b	10 15 17 22 25 32 38 42 44 49 53 61 62 63 69 70 77 81 86 95 99 100 103 104 111 116 122 128 138 143 168 170 177 193 198 200 224 231 238 241 247 260 266 272 278 280 286 289 293 305 308 312 316 320 342 350 359 367 385 394 406 411 417 426 429 434 443 453 469 471 474 475 476 493 499 509 537 547 558 569 575 602 610 612 628 632 662 668 705 706 718 739 769 770 775 803 808 835 862 880 905 912 930 953 955 959 979 1003 1014 1019 1020 1020 1021 1023 1034 1036 1044 1045 1050 1056 1068 1070 1073 1083 1095 1099 1106 1122 1129 1150 1178 1188 1200 1204 1218 1219 1253 1254 1271 1296 1303 1308 1315 1334 1338 1353 1356 1387 1401 1402 1407 1408 1422 1447 1468 1469 1473 1474 1475 1480 1483 1483 1485 1491 1493 1497 1515 1518 1582 1618 1628 1629 1642 1780 1795 2076 2144 2171 2193 3021 3030 3041 3044 3050 3057 3059 3069 3088 3095 3108 3116 3120 3126 3134 3138 3145 3156 3162 3162 3165 3179 3190 3190 3198 3209 3213 3256

TS4	D3a	-299	13	20	21	27	31	41	42	43	46	50	54
		61	66	68	73	76	79	86	89	92	100	105	114
		116	121	126	132	136	155	158	163	174	189	193	200
		203	218	224	235	252	255	261	266	273	280	284	289
		304	307	309	315	338	341	354	357	364	371	387	405
		410	413	425	429	441	444	453	474	474	476	480	485
		491	494	506	513	543	556	565	571	599	605	613	613
		615	633	661	669	707	716	720	736	769	774	787	802
		829	848	865	878	898	910	917	932	955	957	957	965
		1007	1011	1016	1023	1023	1028	1029	1029	1044	1044	1050	1061
		1071	1075	1083	1090	1105	1109	1121	1127	1150	1173	1188	1205
		1210	1215	1225	1242	1249	1272	1293	1302	1309	1332	1334	1355
		1391	1398	1402	1402	1406	1412	1433	1465	1469	1470	1471	1481
		1483	1485	1491	1495	1496	1502	1510	1519	1525	1597	1611	1627
		1783	1798	2072	2141	2157	2182	3029	3039	3041	3046	3048	3060
		3083	3105	3108	3119	3120	3122	3126	3139	3142	3164	3164	3169
		3179	3182	3189	3194	3200	3209	3217	3258				
TS4		-310	7	10	20	22	25	27	35	38	47	51	52
		58	63	66	67	73	74	81	84	87	93	98	105
		109	111	118	122	131	132	151	156	168	187	191	195
		205	214	223	233	244	251	254	261	271	274	282	289
		297	303	307	309	331	339	350	356	365	370	384	408
		409	411	424	428	440	442	451	471	473	474	475	478
		488	492	505	511	543	556	564	567	597	603	609	611
		612	631	657	667	705	713	715	733	765	771	783	799
		822	848	861	875	896	906	917	929	952	953	955	960
		1003	1007	1017	1020	1022	1022	1024	1025	1041	1042	1048	1059
		1069	1073	1079	1084	1102	1104	1115	1124	1145	1172	1188	1191
		1205	1212	1221	1238	1247	1272	1289	1300	1307	1330	1332	1341
		1390	1398	1401	1402	1407	1411	1432	1468	1468	1472	1473	1481
		1483	1483	1490	1494	1497	1502	1510	1516	1523	1588	1601	1625
		1781	1796	2069	2138	2156	2182	3027	3036	3036	3041	3044	3056
		3078	3101	3104	3115	3116	3117	3121	3133	3138	3160	3161	3162
		3168	3178	3187	3189	3197	3207	3212	3250				
TS4	D3	-287	17	20	25	31	33	37	43	49	54	58	59
		61	65	72	73	76	82	87	96	98	100	101	104
		113	120	120	123	137	147	157	162	165	192	196	207
		216	219	229	237	247	258	261	265	277	282	287	288
		304	307	315	325	340	346	356	358	361	372	390	404
		409	420	422	432	442	450	455	471	474	477	478	485
		487	495	508	518	539	554	560	580	597	604	610	611

		614 633 663 670 703 720 724 737 764 772 788 805 833 850 855 888 904 906 920 931 946 961 963 971 993 1009 1015 1020 1025 1026 1029 1042 1045 1048 1054 1064 1068 1070 1082 1084 1102 1104 1108 1128 1131 1162 1167 1191 1203 1206 1216 1219 1228 1248 1253 1275 1295 1303 1311 1333 1338 1354 1355 1388 1398 1402 1403 1412 1415 1433 1468 1469 1472 1472 1473 1481 1483 1487 1488 1497 1498 1505 1513 1519 1532 1598 1628 1630 1633 1782 1800 2075 2124 2144 2171 3026 3039 3040 3044 3046 3057 3058 3100 3102 3108 3116 3117 3127 3131 3136 3149 3161 3163 3164 3165 3178 3183 3192 3201 3209 3210 3213 3252
TS4	D3b	-299 7 15 17 24 27 29 37 43 48 54 55 58 63 68 68 70 76 86 92 93 95 98 104 111 114 119 126 133 138 155 158 159 190 195 199 207 218 224 234 249 253 257 266 273 280 283 289 303 305 309 311 339 340 354 357 364 371 388 406 409 410 425 430 441 445 452 473 474 476 478 481 491 493 505 513 544 556 564 571 598 604 613 613 614 632 660 669 705 717 720 736 767 771 787 803 829 847 858 877 898 909 916 931 952 956 957 964 1002 1009 1019 1021 1023 1023 1025 1027 1044 1044 1050 1059 1068 1070 1076 1083 1090 1105 1107 1121 1128 1151 1170 1188 1195 1205 1209 1215 1224 1242 1250 1272 1293 1301 1307 1331 1334 1345 1355 1390 1397 1402 1403 1407 1412 1432 1468 1468 1472 1473 1473 1480 1483 1484 1490 1494 1498 1502 1511 1519 1526 1597 1612 1627 1629 1782 1798 2071 2140 2156 2181 3027 3036 3038 3042 3044 3057 3057 3080 3102 3105 3116 3116 3119 3124 3135 3141 3162 3163 3165 3167 3173 3179 3191 3191 3198 3208 3214 3258
INT4	D3a	12 15 25 28 35 36 39 44 48 53 56 61 65 72 74 75 80 84 92 98 103 108 114 122 127 130 135 140 141 146 152 160 187 195 199 199 207 208 228 235 247 254 264 272 284 287 294 304 310 315 332 343 351 363 369 379 383 400 409 412 420 429 432 443 454 456 475 475 481 483 490 490 500 503 529 532 552 564 574 590 603 610 614 629 632 668 684 706 706 715 732 755 772 785 800 807 864 864 894 909 911 939 948 952 956 957 978 988 1007 1013 1018 1020 1022 1023 1028 1038 1046 1047 1060 1067 1072 1081 1089 1097 1107 1114 1122 1129 1164 1180 1186 1198 1204 1216 1218 1228 1249 1256 1272 1282 1288 1309 1320 1335 1337 1353 1357 1385 1391 1400 1401 1404 1422 1430 1466 1467 1470 1471 1474 1480 1482 1484 1485 1493 1496 1504 1514 1518 1519 1570 1628 1630 1638

		1785 1800 2070 2140 2151 2180 3026 3037 3046 3049 3051 3061 3061 3078 3103 3108 3109 3118 3120 3120 3122 3131 3140 3144 3151 3165 3166 3181 3195 3200 3201 3205 3211 3219
INT4		10 19 20 27 28 31 36 37 44 45 54 56 59 62 64 69 73 82 83 87 94 97 106 110 114 116 123 127 133 142 157 158 169 180 187 192 196 208 218 224 228 243 249 263 270 283 295 301 305 307 310 342 344 352 361 374 379 391 412 417 429 437 443 443 448 459 470 475 475 476 480 486 495 504 525 543 548 561 575 593 602 610 613 621 630 664 678 706 706 714 736 758 770 779 795 799 837 863 875 908 914 940 947 954 957 973 982 1005 1014 1015 1020 1020 1023 1029 1034 1044 1046 1053 1057 1068 1071 1077 1087 1106 1117 1125 1132 1144 1162 1175 1189 1197 1205 1207 1215 1245 1252 1276 1285 1289 1316 1323 1333 1333 1345 1356 1363 1390 1402 1403 1404 1417 1424 1434 1442 1468 1471 1472 1473 1474 1476 1483 1484 1486 1495 1498 1506 1513 1518 1519 1626 1628 1651 1785 1796 2063 2128 2134 2168 3023 3029 3034 3042 3054 3057 3058 3068 3084 3091 3094 3103 3116 3116 3117 3124 3125 3148 3162 3163 3167 3169 3171 3179 3192 3197 3206 3214
INT4	D3	18 20 24 27 38 42 43 50 54 57 62 63 68 71 76 80 81 91 92 95 96 104 106 113 118 120 128 131 135 152 162 173 175 192 198 201 215 222 234 240 248 252 271 280 293 294 296 304 318 323 335 345 357 362 373 377 392 405 409 417 429 431 439 444 447 456 475 477 478 485 488 491 501 502 533 535 551 555 575 593 602 611 615 633 634 672 689 707 713 719 735 751 766 791 805 811 861 871 901 912 914 947 951 956 960 965 977 992 1001 1018 1020 1021 1022 1027 1030 1041 1049 1051 1062 1069 1070 1084 1096 1104 1109 1118 1127 1132 1165 1188 1191 1204 1206 1220 1227 1232 1253 1258 1280 1287 1298 1308 1324 1337 1344 1355 1359 1388 1393 1402 1403 1405 1421 1427 1467 1469 1473 1473 1473 1476 1478 1485 1487 1497 1499 1505 1517 1518 1519 1568 1629 1630 1640 1783 1802 2069 2139 2147 2180 3017 3037 3048 3050 3056 3058 3058 3070 3103 3104 3108 3117 3117 3117 3118 3133 3144 3145 3148 3164 3165 3185 3196 3203 3212 3215 3219 3263
INT4	D3b	13 18 20 25 34 36 39 44 51 55 58 60 65 68 72 74 76 80 90 95 96 97 101 105 110 118 126 128 132 143 146 161 172 192 192 196 207 213 232 237 246 249 265 279 287 290 294 303

		312	319	335	346	358	361	370	376	391	401	409	416
		424	429	437	443	446	456	473	475	476	480	489	493
		500	504	531	532	550	554	574	592	604	611	614	630
		632	670	686	707	710	715	733	750	768	788	801	808
		860	867	897	910	911	944	949	954	955	960	975	996
		1001	1018	1019	1022	1023	1025	1029	1040	1046	1048	1059	1068
		1081	1091	1096	1106	1115	1123	1129	1164	1182	1191	1201	1204
		1221	1228	1249	1255	1277	1285	1293	1307	1321	1335	1341	1353
		1386	1389	1402	1403	1405	1422	1429	1468	1468	1471	1473	1473
		1479	1484	1485	1496	1498	1504	1515	1517	1520	1566	1627	1628
		1783	1800	2069	2139	2149	2180	3019	3037	3044	3047	3057	3057
		3069	3102	3104	3106	3113	3115	3116	3120	3127	3139	3143	3162
		3164	3182	3193	3201	3211	3212	3214	3232				
TS5	D3a	-232	19	25	30	34	37	39	43	47	49	52	
		57	61	65	66	71	73	74	83	90	97	103	109
		114	118	125	127	128	135	144	154	159	165	169	179
		194	202	208	213	225	232	245	252	265	273	274	297
		306	308	314	327	336	344	350	355	374	382	390	398
		415	416	432	435	442	445	446	458	462	475	477	478
		484	493	504	516	527	547	559	566	586	594	602	608
		614	620	632	669	686	708	718	729	751	773	780	799
		801	851	868	878	908	912	918	939	946	956	958	965
		975	1003	1008	1020	1023	1025	1028	1030	1033	1049	1049	1058
		1071	1080	1090	1104	1109	1123	1128	1140	1163	1188	1189	1195
		1210	1217	1248	1252	1273	1282	1283	1300	1301	1312	1334	1337
		1360	1385	1388	1400	1402	1407	1422	1428	1466	1466	1468	1470
		1473	1480	1482	1486	1489	1497	1503	1504	1517	1521	1557	1628
		1660	1786	1798	2061	2133	2136	2167	3034	3037	3038	3046	3052
		3061	3076	3097	3099	3102	3111	3118	3121	3121	3129	3130	3165
		3165	3168	3183	3189	3192	3193	3198	3212	3216			
TS5		-231	9	14	19	24	30	32	35	36	42	45	
		53	55	58	59	62	68	70	79	88	91	94	95
		97	103	110	112	119	121	126	143	146	158	168	180
		190	198	199	206	223	229	243	249	263	269	273	298
		303	306	311	327	334	345	353	354	369	380	388	395
		411	413	430	436	440	445	446	457	466	468	475	477
		480	491	501	516	529	547	556	565	587	590	602	606
		613	616	630	667	686	703	715	727	747	766	774	795
		797	848	859	873	906	909	916	936	942	951	954	963
		973	1002	1002	1016	1020	1023	1023	1027	1030	1044	1045	1067

		1069 1077 1085 1102 1106 1118 1124 1134 1164 1185 1189 1189 1203 1205 1212 1245 1250 1273 1281 1283 1297 1299 1313 1334 1336 1354 1355 1385 1387 1402 1402 1409 1421 1430 1467 1468 1468 1472 1472 1474 1479 1484 1484 1489 1497 1505 1506 1516 1517 1557 1625 1627 1648 1785 1797 2060 2131 2137 2169 3027 3032 3036 3042 3053 3057 3057 3068 3092 3096 3099 3106 3115 3116 3117 3124 3129 3159 3161 3163 3168 3180 3180 3192 3192 3199 3210 3214
TS5	D3	-218 9 16 25 34 36 39 42 47 51 54 58 59 69 71 73 79 84 90 91 95 98 101 106 109 118 121 133 136 141 146 152 167 183 188 191 195 210 217 231 233 250 254 270 279 281 299 306 310 321 332 336 348 355 366 372 381 400 403 414 417 432 434 444 446 448 453 470 473 475 476 481 493 505 523 531 549 554 568 591 599 602 613 614 622 633 672 687 703 724 732 753 765 780 804 805 860 865 887 913 915 924 945 953 959 960 970 980 998 1007 1013 1021 1026 1027 1030 1037 1048 1049 1061 1069 1075 1083 1096 1106 1110 1126 1135 1144 1167 1187 1192 1199 1206 1214 1222 1253 1259 1279 1288 1291 1298 1312 1316 1337 1339 1357 1357 1388 1390 1402 1408 1410 1424 1430 1464 1468 1471 1473 1476 1479 1479 1481 1486 1492 1498 1503 1508 1519 1520 1562 1629 1630 1668 1785 1800 2071 2124 2139 2159 3037 3038 3040 3044 3053 3057 3058 3086 3097 3103 3104 3108 3116 3116 3121 3133 3143 3148 3158 3164 3165 3178 3189 3190 3198 3199 3211 3218
TS5	D3b	-235 11 14 15 27 28 32 36 38 46 50 53 55 58 60 65 68 76 88 90 94 95 99 100 110 115 116 123 125 128 145 148 160 170 182 192 199 206 211 226 231 244 251 265 276 278 298 307 307 315 328 336 346 353 357 369 381 390 396 412 414 432 437 440 447 449 458 465 470 475 478 480 491 504 517 530 547 557 565 586 593 601 609 614 620 631 669 687 703 718 729 750 769 778 799 801 851 858 877 908 911 916 936 946 954 957 965 974 1002 1006 1019 1023 1023 1024 1028 1033 1047 1048 1058 1069 1071 1079 1090 1105 1107 1122 1129 1139 1165 1188 1188 1194 1206 1206 1217 1248 1249 1275 1284 1284 1299 1302 1313 1335 1336 1355 1356 1387 1389 1402 1403 1409 1422 1430 1464 1468 1469 1472 1475 1476 1480 1484 1485 1489 1498 1506 1506 1518 1518 1562 1627 1629 1662 1787 1798 2062 2133 2134 2167 3027 3035 3036 3044 3054 3056 3057 3077 3095 3096 3101 3109 3115 3116 3118 3125 3132 3161 3162 3164 3173 3180 3189 3192 3194 3201 3214 3218

TS6	D3a	-218	14	23	24	29	33	35	41	42	47	49
		55	56	59	68	69	72	75	79	84	87	90
		99	100	102	104	110	121	126	130	131	141	153
		171	178	186	198	203	210	220	241	243	249	258
		273	277	293	295	305	308	309	317	328	334	340
		355	360	368	390	399	413	416	425	428	429	434
		444	456	463	468	472	477	479	487	491	513	526
		549	559	574	579	595	600	607	613	617	632	655
		672	701	708	717	735	762	775	785	799	830	867
		872	891	904	920	928	950	959	961	963	999	1007
		1018	1020	1023	1026	1028	1030	1037	1046	1048	1049	1064
		1068	1071	1076	1082	1098	1107	1120	1127	1140	1155	1166
		1189	1204	1206	1212	1247	1252	1268	1277	1300	1315	1329
		1336	1354	1357	1374	1391	1397	1401	1401	1406	1425	1459
		1465	1466	1467	1470	1471	1474	1482	1483	1485	1486	1498
		1512	1514	1519	1628	1629	1630	1691	1703	1786	1797	2075
		2098	2145	2156	3021	3034	3049	3051	3057	3060	3061	3088
		3098	3100	3116	3119	3121	3122	3128	3131	3133	3135	3138
		3155	3166	3167	3183	3195	3202	3215	3217	3232		
TS6		-241	10	13	18	23	28	32	37	40	43	48
		51	53	57	62	64	68	71	76	81	87	94
		96	98	100	103	105	117	121	128	132	147	168
		172	177	185	194	200	213	234	237	241	253	269
		273	284	290	303	304	307	314	322	325	335	350
		359	368	388	398	410	413	421	425	426	429	440
		450	457	464	472	474	478	484	489	512	524	546
		558	571	578	591	599	605	612	614	630	652	669
		698	705	714	731	758	772	780	796	822	862	867
		885	897	917	920	946	953	957	960	993	1004	1016
		1018	1020	1022	1024	1025	1033	1043	1045	1046	1059	1067
		1069	1070	1076	1093	1104	1110	1123	1135	1149	1163	1188
		1201	1203	1208	1243	1247	1266	1276	1301	1315	1328	1333
		1354	1356	1374	1390	1397	1402	1402	1403	1421	1457	1463
		1463	1466	1468	1468	1473	1474	1479	1482	1484	1485	1496
		1509	1512	1516	1624	1625	1627	1678	1700	1785	1795	2074
		2097	2143	2155	3017	3042	3047	3048	3055	3057	3057	3082
		3092	3096	3113	3116	3118	3118	3121	3124	3129	3131	3138
		3150	3162	3162	3179	3191	3199	3212	3213	3226		
TS6	D3	-197	16	22	27	29	33	39	39	40	48	51
		52	59	60	63	66	73	76	76	81	87	90
		92	97	99	102	103	110	119	128	131	142	158
		175	185	189	191	195	203	222	243	246	254	263
		277	281	290	299	307	309	312	316	328	333	342
		354	366	374	389	401	415	417	424	429	430	434
		444	454	462	465	474	478	483	485	492	511	527
		549	560	576	579	597	600	606				

		613	617	633	656	675	700	706	721	737	764	773	789
		803	836	862	876	895	905	922	933	955	957	959	962
		1000	1004	1020	1022	1023	1026	1028	1031	1041	1047	1047	1051
		1065	1068	1070	1078	1085	1103	1108	1128	1133	1146	1158	1171
		1191	1205	1210	1215	1250	1256	1272	1282	1301	1319	1329	1338
		1355	1356	1376	1391	1399	1402	1402	1406	1425	1459	1464	1466
		1468	1468	1473	1473	1479	1482	1485	1487	1498	1513	1516	1519
		1630	1630	1639	1706	1708	1786	1797	2077	2097	2146	2156	3022
		3025	3049	3058	3060	3061	3074	3088	3102	3106	3117	3119	3120
		3124	3128	3132	3139	3140	3141	3153	3164	3164	3181	3193	3202
		3213	3229	3230									
TS6	D3b	-219	15	18	21	26	28	34	37	39	45	49	50
		54	58	59	68	68	71	75	82	86	89	91	95
		98	100	102	108	117	125	127	140	152	170	179	186
		188	197	201	217	240	240	249	257	272	276	286	294
		304	307	309	316	326	329	338	352	361	370	389	399
		412	414	424	427	428	432	442	453	460	465	473	476
		480	486	491	512	526	547	559	573	579	594	599	605
		613	615	632	654	672	699	705	718	734	761	773	784
		799	829	863	872	891	902	919	926	951	956	958	960
		997	1004	1018	1020	1022	1023	1025	1029	1037	1045	1045	1048
		1062	1067	1069	1074	1080	1099	1105	1119	1128	1140	1154	1166
		1188	1203	1206	1211	1247	1252	1268	1278	1302	1315	1328	1336
		1354	1355	1375	1392	1398	1401	1402	1405	1423	1458	1465	1467
		1467	1467	1469	1473	1473	1480	1483	1485	1486	1498	1511	1514
		1517	1627	1629	1631	1693	1703	1785	1796	2075	2097	2144	2156
		3020	3031	3048	3055	3057	3058	3058	3085	3096	3101	3116	3116
		3118	3120	3125	3126	3134	3134	3138	3151	3163	3163	3179	3192
		3200	3213	3218	3228								
1b	D3a	10	21	27	31	39	41	46	56	60	67	68	74
		74	80	86	88	93	99	105	117	146	147	152	171
		174	182	192	209	220	234	252	262	268	272	281	284
		290	290	306	320	328	339	354	361	390	394	400	413
		416	421	431	449	461	482	503	524	540	550	557	599
		605	608	633	643	670	702	705	725	748	762	774	775
		782	812	831	849	858	859	862	882	908	917	932	951
		952	961	989	998	1004	1015	1016	1021	1022	1022	1024	1036
		1040	1050	1057	1058	1059	1068	1070	1081	1104	1109	1115	1127
		1128	1167	1174	1185	1187	1203	1207	1214	1226	1250	1256	1281
		1283	1287	1299	1302	1328	1335	1345	1353	1357	1359	1377	1388
		1397	1399	1402	1412	1415	1417	1434	1465	1466	1470	1474	1475
		1478	1478	1483	1484	1486	1487	1491	1494	1499	1501	1509	1511
		1517	1627	1629	1726	1783	1793	2025	2354	2997	3022	3028	3033
		3034	3041	3044	3059	3060	3061	3078					

		3078 3089 3090 3092 3093 3098 31093111 3112 3116 3117 3120 3121 3121 3142 3150 3166 3169 3180 3195 32033215 3231
2b	D3a	13 23 31 43 46 48 50 60 70 71 76 80 87 98 124 137 143 146 147 172 172 183 187 199 207 222 231 233 241 245 264 276 290 301 305 313 336 351 358 369 377 401 414 418 444 455 462 474 503 520 534 545 561 569 589 598 605 614 633 639 666 691 708 716 741 746 761 771 786 795 804 822 863 877 891 905 911 920 936 953 954 969 977 989 1002 1011 1017 1020 1022 1023 1024 1028 1043 1046 1047 1054 1059 1068 1073 1074 1088 1095 1104 1118 1121 1129 1135 1150 1160 1181 1188 1188 1202 1220 1224 1245 1255 1258 1273 1293 1312 1314 1322 1333 1334 1335 1345 1353 1358 1378 1392 1396 1401 1403 1409 1412 1413 1415 1425 1448 1466 1468 1471 1471 1476 1481 1484 1486 1491 1493 1494 1496 1499 1503 1508 1510 1515 1518 1606 1628 1630 1659 1779 1794 2971 3014 3022 3025 3028 3029 3036 3042 3044 3049 3060 3061 3072 3074 3082 3087 3089 3092 3101 3119 3120 3120 3130 3141 3146 3165 3165 3182 3188 3192 3200 3210 3218 3229
3b	D3a	18 29 33 42 44 51 55 60 68 77 84 86 88 95 100 112 123 138 143 146 167 174 186 195 201 209 214 229 237 249 260 266 279 290 294 306 313 321 337 346 354 362 377 414 426 430 441 454 467 475 490 495 538 553 562 574 585 602 612 632 633 665 675 709 718 733 746 759 775 797 803 821 833 859 866 879 901 907 913 918 945 957 958 958 1003 1004 1010 1018 1020 1021 1022 1026 1026 1037 1043 1049 1054 1056 1059 1069 1071 1083 1104 1110 1115 1127 1130 1134 1160 1174 1189 1191 1201 1208 1214 1220 1245 1253 1260 1265 1277 1298 1305 1316 1321 1331 1334 1344 1350 1352 1361 1374 1387 1400 1402 1406 1412 1412 1430 1462 1469 1469 1471 1473 1474 1477 1481 1482 1485 1488 1493 1496 1498 1506 1511 1512 1517 1628 1629 1669 1725 1744 1783 1794 2996 3023 3025 3027 3041 3043 3046 3048 3051 3053 3058 3061 3062 3074 3085 3093 3102 3106 3109 3109 3112 3121 3123 3123 3131 3133 3143 3165 3166 3183 3193 3201 3210 3215
1c	D3a	20 25 31 33 38 39 44 47 52 58 69 76 83 86 87 95 100 109 116 132 140 145 166 168 174 184 193 218 233 248 249 250 262 265 281 284 286 304 313 332 336 345 362 368 389 399 402 413 417 420 431 452 469 483 516 525 547 559 591 602 607 611 632 677 683 703 707 718 726 754 761 769 774 775 813 847 857 861 871 881 893 916 931 948

	956 961 969 990 1002 1015 1017 1023 1024 1024 1029 1040 1044 1048 1057 1060 1063 1069 1073 1082 1104 1106 1122 1124 1131 1165 1170 1183 1187 1202 1203 1216 1227 1251 1263 1272 1284 1288 1304 1311 1336 1339 1351 1353 1362 1388 1390 1399 1401 1403 1413 1418 1423 1432 1457 1467 1468 1473 1473 1476 1477 1478 1480 1483 1486 1489 1494 1495 1496 1509 1510 1517 1519 1628 1630 1707 1785 1795 2034 2352 3013 3021 3027 3033 3034 3046 3052 3060 3062 3076 3077 3081 3088 3090 3094 3096 3097 3107 3110 3115 3116 3120 3121 3123 3127 3129 3129 3168 3169 3182 3192 3202 3210 3219
2c D3a	11 26 32 39 42 47 49 60 71 72 77 82 88 102 105 108 126 142 159 170 182 185 195 203 220 234 234 246 249 260 263 270 280 306 316 321 338 348 356 365 377 400 416 418 450 461 467 476 497 505 520 548 563 574 594 603 608 618 633 663 673 696 710 715 737 746 752 771 778 798 803 814 863 864 893 903 908 922 934 950 956 963 980 993 1006 1016 1019 1020 1023 1026 1030 1034 1040 1044 1048 1051 1058 1068 1070 1078 1087 1096 1105 1118 1127 1129 1137 1157 1164 1179 1185 1189 1203 1220 1228 1242 1255 1261 1271 1298 1304 1316 1323 1335 1335 1337 1347 1351 1354 1378 1383 1395 1398 1401 1402 1412 1414 1427 1429 1452 1467 1468 1469 1471 1477 1481 1483 1485 1491 1495 1496 1498 1499 1504 1505 1512 1517 1518 1615 1629 1630 1659 1782 1794 2977 3019 3022 3026 3033 3034 3036 3038 3051 3055 3061 3061 3071 3076 3081 3084 3090 3093 3100 3120 3120 3128 3129 3133 3165 3166 3170 3181 3193 3201 3206 3208 3215 3216
3c D3a	20 22 29 33 40 45 47 52 56 71 74 83 87 97 109 114 120 136 144 147 171 174 186 196 201 209 228 238 250 259 271 274 285 294 303 311 318 328 351 354 366 368 383 406 415 429 438 450 467 487 489 534 550 558 569 586 603 612 617 632 634 666 686 710 717 732 739 762 769 778 794 798 820 859 865 871 892 901 907 917 936 952 955 958 979 1005 1010 1018 1019 1021 1023 1024 1034 1037 1043 1049 1049 1053 1060 1067 1073 1084 1102 1111 1114 1126 1130 1135 1162 1175 1185 1191 1201 1206 1215 1220 1238 1252 1263 1266 1275 1304 1306 1314 1316 1331 1335 1347 1352 1363 1377 1379 1398 1400 1407 1411 1412 1423 1454 1462 1466 1467 1472 1473 1473 1476 1480 1484 1486 1486 1493 1497 1498 1508 1512 1517 1519 1628 1629 1670 1717 1744 1782 1794 2995 3023 3027 3028 3040 3044 3049 3051 3051 3051 3060 3062 3074 3086 3088 3094 3100 3107 3108 3115 3119 3121 3122 3123 3129 3133 3139 3167 3167 3180 3191 3201 3212 3218

INT2-n-E	D3a	14	20	21	24	29	29	35	41	47	50	52	55
		62	65	67	71	73	78	82	85	90	92	96	98
		99	102	110	111	121	124	129	132	137	169	172	178
		189	196	206	209	214	223	235	239	250	254	257	269
		271	273	274	280	286	293	296	302	307	312	323	337
		351	364	367	388	398	414	419	420	426	434	445	451
		458	469	470	472	474	476	485	493	507	516	529	546
		546	569	576	603	607	614	616	631	634	661	675	705
		709	720	743	752	770	776	794	802	834	837	866	881
		905	907	911	917	931	942	957	958	989	1003	1016	1019
		1019	1022	1022	1024	1025	1029	1043	1045	1051	1056	1060	1071
		1071	1086	1093	1108	1115	1119	1127	1141	1143	1165	1174	1190
		1205	1219	1240	1253	1259	1269	1292	1300	1304	1313	1323	1335
		1337	1348	1350	1356	1367	1386	1389	1399	1400	1403	1405	1416
		1432	1465	1467	1468	1471	1472	1474	1477	1481	1482	1485	1488
		1491	1496	1498	1510	1510	1516	1520	1613	1628	1630	1644	1726
		1782	1793	2089	2129	2154	2189	2998	3018	3022	3028	3041	3044
		3050	3054	3060	3061	3062	3063	3073	3088	3093	3103	3108	3114
		3121	3123	3123	3123	3129	3138	3142	3144	3144	3166	3166	3183
		3194	3201	3213	3216								
TS3-n-E	D3a	-173	21	23	25	27	28	34	38	40	43	48	
		50	55	58	63	68	71	71	74	78	83	85	97
		99	102	104	107	110	110	116	119	139	145	152	158
		163	164	171	177	186	194	208	223	226	239	247	254
		263	266	269	271	276	283	287	297	301	305	306	308
		312	322	336	347	351	361	370	389	413	415	427	432
		441	443	452	462	471	471	475	478	479	479	495	525
		540	542	567	574	590	604	610	612	630	633	658	669
		706	706	722	742	755	764	774	793	802	833	843	862
		877	901	904	913	922	926	945	954	956	993	1003	1015
		1020	1022	1023	1024	1024	1033	1036	1042	1045	1047	1051	1055
		1068	1072	1079	1088	1095	1105	1112	1118	1128	1136	1150	1177
		1179	1189	1204	1207	1218	1244	1252	1262	1269	1290	1302	1310
		1314	1325	1335	1339	1345	1352	1355	1366	1386	1386	1400	1401
		1403	1404	1417	1430	1466	1467	1469	1471	1472	1476	1479	1483
		1485	1486	1490	1493	1498	1500	1507	1515	1515	1519	1611	1628
		1630	1632	1681	1782	1793	2081	2147	2153	2186	3011	3017	3029
		3035	3039	3044	3049	3050	3055	3060	3061	3063	3070	3093	3095
		3098	3109	3120	3120	3122	3129	3130	3131	3132	3139	3155	3164
		3167	3176	3182	3193	3199	3206	3216					
TS6-n-E	D3a	-220	8	13	21	25	27	31	37	40	44	48	54
		56	57	61	62	66	69	69	73	79	82	87	88
		93	99	101	105	107	109	113	126	130	140	140	158

		170	180	187	192	199	205	207	219	233	242	248	253
		259	267	273	278	295	301	305	311	314	323	333	343
		352	362	369	380	386	405	418	423	427	427	436	441
		447	453	457	468	472	474	477	481	487	490	528	541
		556	570	577	582	598	599	607	614	618	632	662	688
		710	721	736	752	764	777	797	799	830	832	870	872
		888	900	904	912	920	941	951	963	988	1002	1010	1016
		1020	1021	1023	1024	1029	1030	1038	1039	1047	1050	1055	1065
		1075	1082	1092	1107	1113	1116	1126	1132	1142	1160	1165	1189
		1207	1212	1238	1247	1261	1266	1278	1297	1299	1314	1321	1335
		1348	1357	1360	1374	1385	1393	1399	1400	1401	1405	1412	1429
		1466	1467	1470	1471	1472	1478	1482	1482	1485	1486	1492	1495
		1508	1511	1514	1519	1628	1629	1635	1693	1725	1785	1796	2075
		2096	2144	2156	3003	3021	3022	3025	3034	3040	3050	3053	3058
		3059	3061	3061	3086	3087	3090	3095	3101	3115	3117	3121	3121
		3122	3126	3128	3134	3140	3144	3167	3167	3184	3196	3204	3217
		3219											
INT2-n-Z	D3a	13	17	24	27	28	33	38	39	49	51	53	58
		60	65	66	69	74	78	81	82	86	89	91	98
		101	110	119	122	124	124	130	133	143	148	167	169
		178	189	192	205	210	233	234	240	251	253	262	265
		271	274	274	283	294	298	300	308	314	326	334	339
		351	366	371	386	399	415	422	422	427	434	439	450
		457	468	469	472	474	475	491	508	515	527	542	548
		554	570	576	602	608	615	625	632	650	662	679	708
		713	719	737	742	766	772	774	779	802	833	868	878
		890	901	912	914	928	931	957	959	978	1005	1012	1019
		1020	1022	1024	1026	1029	1043	1044	1047	1051	1056	1062	1067
		1068	1079	1088	1093	1104	1119	1120	1127	1134	1142	1163	1176
		1187	1199	1205	1219	1233	1253	1263	1268	1290	1299	1306	1314
		1327	1335	1335	1345	1354	1374	1386	1387	1399	1400	1403	1409
		1413	1426	1456	1466	1469	1469	1470	1471	1472	1476	1480	1484
		1486	1489	1491	1495	1499	1508	1511	1517	1519	1613	1628	1630
		1645	1710	1782	1793	2089	2130	2154	2189	2994	3015	3021	3027
		3045	3048	3049	3053	3060	3062	3068	3070	3084	3093	3101	3101
		3111	3114	3120	3121	3122	3124	3127	3134	3142	3146	3151	3166
		3166	3180	3192	3201	3215	3216						
TS3-n-Z	D3a	-128	7	19	20	25	29	31	36	38	41	43	
		47	50	54	55	63	71	72	73	79	84	85	89
		95	95	97	105	108	112	116	120	124	133	140	151
		160	167	169	174	181	193	202	215	221	229	247	251
		261	266	270	272	282	283	290	290	296	303	308	314
		314	324	336	352	362	364	379	382	406	415	426	429

		436	442	446	461	471	472	475	477	479	491	512	540
		546	556	570	574	603	612	612	627	633	648	663	669
		707	708	717	725	740	763	771	776	787	802	829	863
		871	895	899	909	919	926	936	955	956	973	1005	1013
		1017	1019	1023	1023	1026	1033	1041	1043	1045	1046	1051	1061
		1071	1079	1092	1095	1106	1119	1120	1128	1130	1145	1172	1179
		1203	1205	1218	1239	1252	1263	1269	1288	1300	1308	1312	1327
		1337	1349	1356	1362	1386	1390	1400	1401	1402	1410	1416	1427
		1468	1469	1470	1470	1472	1473	1476	1476	1485	1486	1487	1493
		1498	1510	1513	1519	1525	1612	1628	1630	1633	1667	1781	1793
		2146	2150	2186	3003	3020	3024	3031	3038	3040	3049	3052	3060
		3062	3071	3087	3092	3093	3098	3106	3108	3120	3121	3124	3126
		3136	3138	3153	3165	3165	3177	3182	3193	3200	3206	3217	
TS6-n-Z	D3a	-221	12	19	22	25	26	27	35	38	39	45	
		48	53	55	56	61	64	69	72	77	79	83	87
		91	97	101	105	107	109	121	123	124	128	130	140
		157	170	177	182	190	197	206	211	227	234	242	249
		256	259	272	277	296	303	307	311	317	323	328	343
		353	363	369	371	388	393	407	415	421	426	429	430
		438	445	454	459	467	472	478	480	485	489	526	529
		558	566	573	581	591	600	606	613	619	632	634	665
		696	708	719	733	754	762	768	775	797	799	830	867
		867	887	893	902	906	920	921	952	962	963	998	1007
		1008	1019	1021	1023	1029	1032	1036	1037	1041	1047	1048	1051
		1071	1073	1081	1093	1106	1114	1116	1126	1130	1141	1157	1166
		1200	1206	1212	1235	1247	1265	1269	1279	1301	1303	1314	1322
		1336	1355	1368	1375	1381	1392	1399	1400	1402	1404	1413	1423
		1463	1466	1467	1469	1470	1472	1480	1483	1483	1486	1488	1495
		1501	1510	1515	1518	1522	1627	1629	1635	1692	1720	1786	1797
		2096	2144	2156	2997	3020	3023	3029	3033	3048	3049	3054	3058
		3061	3086	3086	3096	3096	3098	3101	3114	3119	3121	3121	3124
		3132	3139	3144	3146	3167	3168	3184	3194	3203	3216	3218	

Table S7 The calculated total electronic energies, enthalpies, entropies and free energies in a.u. , PhO₂S with downward direction of **1a** in the toluene solvent with the temperature of 383.75 K.

Species	E _{elec} /a.u.	H/a.u.	S _g	S _l	G _g /a.u.	G _l /a.u.
CAT	-10590.41705 ^a	-10590.35690	144.5	120.8	-10590.44529	-10590.43081
1aa	-1781.23739 ^a	-1780.71188	254.5	233.2	-1780.86753	-1780.85448
2aa	-1781.33348 ^a	-1780.80459	232.0	210.3	-1780.94648	-1780.93321
3aa	-1781.28867 ^a	-1780.76154	235.3	213.7	-1780.90546	-1780.89225

COMa	-12371.65658 ^a	-12371.06873	352.2	331.0	-12371.28412	-12371.27114
TS1a	-12371.62987 ^a	-12371.04283	342.6	321.0	-12371.25233	-12371.23914
INT1a	-12371.64010 ^a	-12371.05213	343.8	322.2	-12371.26235	-12371.24917
TS2a	-12371.62431 ^a	-12371.03849	336.2	314.7	-12371.24410	-12371.23092
INT2a	-12371.70410 ^a	-12371.11483	334.1	312.7	-12371.31914	-12371.30605
TS3a	-12371.64997 ^a	-12371.06269	336.8	315.5	-12371.26868	-12371.25561
INT3a	-12371.69604 ^a	-12371.10628	332.3	310.9	-12371.30951	-12371.29639
TS4a	-12371.67428 ^a	-12371.08629	326.6	305.2	-12371.28601	-12371.27296
INT4a	-12371.71308 ^a	-12371.12233	332.0	310.6	-12371.32535	-12371.31226
TS5a	-12371.68923 ^a	-12371.10031	330.5	309.2	-12371.30244	-12371.28937
TS6a	-12371.64482 ^a	-12371.05771	336.1	314.6	-12371.26323	-12371.25012

Table S8 Coordinates of All Stationary Points **CAT+1a**(PhO₂S with downward direction of 1a), Computed at B3LYP-D3a+IDSCRF/ TZP-DKH(-d_{fg}) level in toluene solvent.

CAT				1aa			
Rh	-1.61780	-0.00000	0.09014	C	0.50270	-0.06827	-0.28295
Cl	-0.00003	-1.66443	0.87352	C	0.31242	1.21203	-0.15131
C	-2.81197	1.33788	-0.48262	C	-0.29406	-1.18091	0.35313
O	-3.52530	2.15415	-0.81982	H	-0.31772	-1.04566	1.43184
Rh	1.61781	-0.00001	0.09027	H	0.18193	-2.13745	0.14287
Cl	-0.00002	1.66421	0.87396	C	-1.75022	-1.29932	-0.12556
C	2.81192	-1.33779	-0.48285	C	-1.91320	-1.45470	-1.65265
O	3.52528	-2.15394	-0.82029	H	-2.88470	-1.91638	-1.82201
C	-2.81197	-1.33774	-0.48294	H	-1.14426	-2.15291	-1.98859
O	-3.52526	-2.15396	-0.82036	C	-1.81954	-0.21850	-2.41714
C	2.81195	1.33791	-0.48244	O	-2.41771	-0.15177	0.38748
O	3.52539	2.15409	-0.81963	O	-2.30977	-2.52559	0.38843
				C	-3.75032	0.04697	0.19968
				C	-2.51399	-2.73167	1.71620
				O	-2.20193	-1.96168	2.58706
				O	-4.49042	-0.74715	-0.31798
				C	-3.20024	-4.05218	1.92555
				H	-4.18179	-4.02883	1.44995
				H	-2.62896	-4.85285	1.45533
				H	-3.30756	-4.24222	2.98947
				C	-4.14620	1.38262	0.75923
				H	-5.20395	1.55310	0.58166
				H	-3.93713	1.40738	1.82954

	H	-3.55100	2.16888	0.29387				
	C	-1.63986	1.97654	-3.90335				
	H	-2.33097	2.75327	-3.56869				
	H	-0.62583	2.37929	-3.85719				
	H	-1.86521	1.76150	-4.94990				
	C	-1.75790	0.77511	-3.08801				
	C	0.10500	2.49144	-0.09699				
	H	-0.55693	2.91466	-0.85061				
	C	0.70242	3.47330	0.90217				
	C	1.51825	2.75151	1.97268				
	H	2.34002	2.19951	1.51559				
	H	1.94510	3.46750	2.67560				
	H	0.90486	2.04375	2.53117				
	C	1.61224	4.44177	0.11154				
	H	2.41988	3.89275	-0.37387				
	H	1.04955	4.97022	-0.66012				
	H	2.04310	5.18351	0.78592				
	C	-0.45268	4.27040	1.47733				
	H	-1.04918	4.79064	0.73113				
	C	-0.77882	4.40157	2.75614				
	H	-0.22962	3.91338	3.55050				
	H	-1.61999	5.01486	3.05313				
	S	1.84445	-0.56583	-1.39740				
	O	2.34433	0.62004	-2.09022				
	O	1.36512	-1.72551	-2.15759				
	C	3.14606	-1.15201	-0.30791				
	C	4.02441	-0.23078	0.25255				
	C	3.26899	-2.51415	-0.06379				
	C	5.04155	-0.68756	1.07897				
	H	3.92156	0.82037	0.02267				
	C	4.29233	-2.96030	0.76492				
	H	2.58973	-3.20845	-0.53726				
	C	5.17355	-2.04954	1.33633				
	H	5.73765	0.01696	1.51455				
	H	4.40444	-4.01943	0.95608				
	H	5.97156	-2.40087	1.97763				
	2aa	3aa						
	C	-0.39293	0.08081	-1.19499	C	-1.14332	-0.24604	-0.85562
	C	-0.66531	-1.21438	-0.89738	C	1.30676	-0.35876	-1.07621
	C	0.98761	0.69354	-1.22771	H	2.09384	0.16773	-0.53957

H	0.97896	1.68454	-0.78097	H	1.63533	-0.46524	-2.11160
H	1.32990	0.81115	-2.25739	C	1.20345	-1.76647	-0.46624
C	1.99576	-0.16432	-0.48556	C	0.00267	-2.56094	-1.00102
C	1.84957	-1.60806	-0.92772	H	-0.08111	-3.50460	-0.46713
H	2.61528	-2.20650	-0.45058	H	0.21118	-2.79406	-2.04848
H	2.05034	-1.61994	-2.00331	C	-1.20070	-1.69530	-0.88889
C	0.46168	-2.13600	-0.66191	O	1.09154	-1.55238	0.94947
O	1.71087	0.02223	0.91016	O	2.35201	-2.55082	-0.80842
O	3.34927	0.19875	-0.79002	C	1.08753	-2.58138	1.83636
C	2.38871	-0.64372	1.87829	C	3.60301	-2.22249	-0.38476
C	3.82921	1.44423	-0.52463	O	3.86532	-1.26068	0.28849
O	3.18472	2.33477	-0.03599	O	1.22439	-3.74030	1.54018
O	3.29967	-1.40652	1.67978	C	4.58925	-3.24369	-0.87538
C	5.27670	1.52880	-0.91875	H	4.32286	-4.22628	-0.48423
H	5.85532	0.80509	-0.34320	H	4.55229	-3.30397	-1.96379
H	5.39277	1.27519	-1.97300	H	5.58899	-2.97076	-0.55063
H	5.64625	2.53283	-0.73265	C	0.89120	-2.05273	3.22859
C	1.83332	-0.28350	3.22739	H	0.99495	-2.86281	3.94441
H	2.45615	-0.71424	4.00593	H	1.61562	-1.26561	3.43609
H	1.78030	0.79956	3.33519	H	-0.10429	-1.61262	3.31098
H	0.81602	-0.66983	3.31340	C	-3.54366	-2.80993	-1.17275
C	1.44564	-4.36220	-0.06925	H	-4.14967	-2.60376	-2.06005
H	1.94509	-4.60522	-1.01139	H	-3.05849	-3.77810	-1.30103
H	2.19998	-3.94024	0.59641	H	-4.24028	-2.87074	-0.33380
H	1.10055	-5.29900	0.36751	C	-2.54861	-1.73483	-0.96072
C	0.28786	-3.42193	-0.29160	C	-2.69353	-0.19977	-0.82406
C	-2.04198	-1.76227	-0.81302	H	-3.11639	0.29246	-1.70363
H	-2.72275	-1.36623	-1.54581	C	-3.43951	0.30326	0.44462
C	-2.69165	-2.09178	0.52958	C	-2.86859	-0.33577	1.71310
C	-1.95224	-1.84553	1.82535	H	-3.37737	0.05228	2.59638
H	-2.08470	-0.81127	2.15217	H	-2.97165	-1.42146	1.71120
H	-2.34766	-2.49238	2.61322	H	-1.80729	-0.10025	1.80783
H	-0.88241	-2.02965	1.74482	C	-3.32938	1.83304	0.56205
C	-4.18064	-1.83719	0.62618	H	-3.92604	2.18089	1.40721
H	-4.38933	-0.80809	0.92870	H	-2.29528	2.13017	0.71692
H	-4.67853	-2.00699	-0.32922	H	-3.68118	2.33162	-0.34091
H	-4.63535	-2.49947	1.36848	C	-4.90609	-0.01659	0.24029
C	-2.25342	-3.19666	-0.39354	H	-5.32479	0.39298	-0.67692
H	-3.05735	-3.71182	-0.90537	C	-5.70941	-0.68671	1.05643
C	-1.05583	-4.06011	-0.09866	H	-5.36398	-1.11760	1.98776
H	-1.10042	-4.45599	0.92472	H	-6.75620	-0.82533	0.81727

H	-1.08474	-4.94935	-0.73798	C	0.00475	0.42013	-1.01945
S	-1.61450	1.33543	-1.60836	S	0.13056	2.13294	-1.47159
O	-2.94834	0.77001	-1.81706	O	-1.20917	2.71737	-1.53146
C	-1.69475	2.37622	-0.14467	C	1.04099	2.94017	-0.14904
C	-2.52929	2.00547	0.90386	C	0.34839	3.52592	0.90468
H	-3.12754	1.10912	0.82590	H	-0.73162	3.51035	0.91751
C	-2.59890	2.81498	2.02894	C	1.06228	4.15551	1.91578
H	-3.25026	2.54070	2.84840	H	0.53256	4.62354	2.73516
C	-1.84191	3.98163	2.09705	C	2.45242	4.19442	1.86904
H	-1.90338	4.61253	2.97452	H	3.00490	4.68767	2.65836
C	-1.01616	4.34455	1.03928	C	3.13405	3.61260	0.80589
H	-0.43523	5.25607	1.09007	C	2.42960	2.98385	-0.21342
H	-0.31456	3.81348	-0.93096	H	2.94409	2.55139	-1.05948
C	-0.93785	3.53967	-0.09172	H	4.21443	3.65379	0.76427
O	-1.01367	2.14147	-2.67722	O	0.99395	2.17134	-2.65829
COMa				TS1a			
C	-2.10641	0.01368	1.04787	C	1.00390	1.09007	-0.84056
C	-1.75981	1.39209	-1.05844	C	1.54077	-1.41747	-1.08368
H	-2.55282	2.13245	-0.98321	H	2.36517	-1.89872	-1.60013
H	-1.66120	1.10368	-2.10411	H	0.62920	-1.70352	-1.60620
C	-0.44172	2.08386	-0.66685	C	1.47018	-2.01619	0.32887
C	0.73143	1.09647	-0.76172	C	0.09171	-1.92190	1.00630
H	0.82853	0.78818	-1.80312	H	0.09226	-2.61893	1.84277
H	0.46139	0.19670	-0.20727	H	-0.66171	-2.25941	0.29889
C	2.01120	1.58459	-0.24809	C	-0.26598	-0.61409	1.55200
O	-0.62399	2.53184	0.67981	O	2.50901	-1.39303	1.07955
O	-0.14596	3.12730	-1.59562	O	1.62587	-3.44309	0.22992
C	-0.03942	3.61556	1.25312	C	2.78861	-1.74926	2.36406
C	-0.92258	4.24480	-1.68545	C	2.79174	-4.04505	-0.12461
O	-1.95046	4.40403	-1.08124	O	3.80020	-3.45866	-0.42135
O	0.72162	4.36894	0.70414	O	2.23685	-2.63814	2.95663
C	-0.29209	5.23453	-2.61774	C	2.63087	-5.53585	-0.06469
H	0.58083	5.66311	-2.12191	H	2.45132	-5.83508	0.96924
H	0.05023	4.74716	-3.52950	H	1.76488	-5.84600	-0.64906
H	-1.00286	6.02292	-2.84791	H	3.53091	-6.01507	-0.43809
C	-0.52183	3.74755	2.66836	C	3.87314	-0.86774	2.91016
H	0.07943	4.48730	3.18920	H	4.16481	-1.21728	3.89616
H	-1.56446	4.07044	2.65550	H	4.72891	-0.86212	2.23515
H	-0.48843	2.78742	3.18060	H	3.50469	0.15781	2.97506
C	3.69544	3.19432	1.04862	C	-0.46255	1.03591	3.62957

H	4.54940	3.51163	0.44923	H	-1.41883	0.89267	4.13412
H	3.06193	4.06208	1.24285	H	0.33004	0.67489	4.28816
H	4.07171	2.80260	1.99361	H	-0.31739	2.09969	3.45283
C	2.89808	2.19303	0.34530	C	-0.41824	0.26212	2.39064
C	-2.08236	-0.21624	2.32488	C	0.57723	2.32762	-0.67516
H	-1.15972	-0.60579	2.74943	H	-0.04802	2.73321	-1.46608
C	-3.23866	-0.02207	3.29860	C	1.09135	3.35770	0.32860
C	-4.42060	0.67490	2.62830	C	2.06906	2.73504	1.32326
H	-5.24624	0.78742	3.33149	H	2.45933	3.49334	2.00148
H	-4.14408	1.66285	2.25857	H	1.59371	1.95050	1.90933
H	-4.77781	0.08674	1.78264	H	2.91576	2.29365	0.79989
C	-3.66400	-1.42741	3.78551	C	1.82914	4.42041	-0.53140
H	-4.47094	-1.33912	4.51488	H	2.27453	5.16611	0.12745
H	-4.00849	-2.03048	2.94472	H	2.60595	3.95387	-1.13560
H	-2.83158	-1.95114	4.25796	H	1.13906	4.93119	-1.20457
C	-2.69587	0.74664	4.48705	C	-0.07832	4.05687	0.99047
H	-1.84792	0.27151	4.97542	H	-0.89213	4.30966	0.31682
C	-3.15519	1.88903	4.98043	C	-0.16004	4.44933	2.25479
H	-3.99574	2.41555	4.54694	H	0.62290	4.25760	2.97701
H	-2.69879	2.33898	5.85308	H	-1.02579	4.99198	2.61143
Rh	3.76903	0.14256	-0.20069	Rh	-1.51974	0.93087	0.34667
Cl	2.50603	-1.02357	1.62405	Cl	-1.82699	-0.84970	-1.59716
C	4.78674	1.08794	-1.44876	C	-2.71833	1.57277	1.66383
C	5.22083	-1.11166	0.07011	C	-2.46187	1.99893	-0.89337
O	5.39019	1.67236	-2.21636	O	-3.46342	1.95335	2.43371
O	6.03756	-1.87575	0.24791	O	-3.00577	2.63921	-1.65556
Rh	1.17547	-2.56977	0.22841	Rh	-4.11689	-0.99476	-0.66224
Cl	2.45015	-1.88621	-1.71327	Cl	-3.38093	-2.01273	1.40277
C	0.19442	-3.13553	1.72408	C	-4.75965	-0.28981	-2.28136
O	-0.38598	-3.48415	2.64007	O	-5.15097	0.12003	-3.26938
C	0.22976	-3.76335	-0.88120	C	-5.84991	-1.15854	0.03238
O	-0.29518	-4.50342	-1.56196	O	-6.89573	-1.27790	0.46306
C	-2.11171	0.16899	-0.24466	C	1.72589	0.07209	-1.21216
S	-2.58402	-1.29855	-1.21100	S	3.14946	0.56828	-2.29377
O	-2.73770	-2.43000	-0.29824	O	2.92303	1.94357	-2.73708
O	-1.65150	-1.37867	-2.33958	O	3.30129	-0.50874	-3.27348
C	-4.20229	-0.89548	-1.87181	C	4.60986	0.57935	-1.25105
C	-5.32966	-1.13207	-1.09248	C	5.11472	1.80066	-0.81863
C	-4.30056	-0.36305	-3.15142	C	5.23654	-0.62095	-0.93882
C	-6.58002	-0.82039	-1.60825	C	6.27243	1.81711	-0.05151
C	-5.55830	-0.05444	-3.65651	C	6.39134	-0.59031	-0.16679

C	-6.69351	-0.27983	-2.88624	C	6.90813	0.62346	0.27522
H	-5.22527	-1.57192	-0.11060	H	4.62302	2.71839	-1.10556
H	-3.40905	-0.21847	-3.74485	H	4.83654	-1.56181	-1.28335
H	-7.46646	-1.00635	-1.01649	H	6.68399	2.76188	0.27831
H	-5.65002	0.35445	-4.65403	H	6.89062	-1.51794	0.08022
H	-7.67119	-0.04101	-3.28437	H	7.81413	0.64020	0.86721
INT1a				TS2a			
C	0.94219	1.01334	-0.83148	C	-5.57655	-3.27214	2.84246
C	0.49639	-1.46596	-0.67366	C	-6.59019	-4.45434	4.82401
H	0.94687	-2.33388	-1.14388	H	-7.14844	-4.14903	5.70115
H	-0.52001	-1.37789	-1.06175	H	-5.67661	-4.94876	5.16334
C	0.40867	-1.72921	0.83242	C	-7.41156	-5.46911	4.03058
C	-0.61049	-0.84516	1.56458	C	-6.58419	-6.10802	2.92495
H	-0.73821	-1.25878	2.56544	H	-7.21904	-6.78190	2.34820
H	-1.56541	-0.94603	1.04353	H	-5.82101	-6.72340	3.41829
C	-0.30038	0.56959	1.74332	C	-5.89860	-5.22271	1.96546
O	1.72928	-1.59226	1.35659	O	-8.55088	-4.76526	3.52385
O	-0.14489	-3.03599	1.05465	O	-7.78127	-6.57796	4.85599
C	2.01373	-1.82604	2.66660	C	-9.51401	-5.39065	2.79433
C	0.50766	-4.18103	0.71489	C	-8.61040	-6.43355	5.92831
O	1.60586	-4.22032	0.22577	O	-9.10855	-5.39220	6.26633
O	1.20650	-2.18710	3.48322	O	-9.51445	-6.56627	2.53451
C	-0.34283	-5.36918	1.05827	C	-8.81655	-7.76268	6.59399
H	-0.55998	-5.36888	2.12705	H	-9.34219	-8.43137	5.91036
H	-1.29476	-5.30675	0.52951	H	-7.85529	-8.22095	6.82748
H	0.17838	-6.28112	0.78289	H	-9.40102	-7.62808	7.49926
C	3.46821	-1.56968	2.92468	C	-10.56247	-4.40255	2.37762
H	3.69541	-1.77747	3.96602	H	-11.33167	-4.90957	1.80281
H	4.07482	-2.19541	2.27006	H	-10.99550	-3.93135	3.25996
H	3.70510	-0.53134	2.68759	H	-10.10773	-3.61013	1.78171
C	-0.10341	2.73750	3.25684	C	-5.31648	-5.89716	-0.48829
H	-1.08912	3.16640	3.44510	H	-4.45783	-6.56791	-0.56052
H	0.27118	2.31070	4.18861	H	-6.23059	-6.47202	-0.64649
H	0.56127	3.53853	2.94100	H	-5.22544	-5.15100	-1.27791
C	-0.20349	1.67945	2.25029	C	-5.32102	-5.25841	0.83578
C	1.25779	2.36560	-0.88843	C	-5.00094	-2.41580	1.87264
H	1.05527	2.84974	-1.83916	H	-4.34954	-1.66953	2.31401
C	2.34926	3.11879	-0.11234	C	-5.69516	-1.86725	0.60080

C	2.95595	2.29225	1.01988	C	-7.10005	-2.43680	0.39069
H	3.78634	2.83056	1.47710	H	-7.59450	-1.90905	-0.42544
H	2.22826	2.06072	1.79412	H	-7.08733	-3.49744	0.15435
H	3.34402	1.34932	0.63894	H	-7.70327	-2.30119	1.28808
C	3.45495	3.47587	-1.14144	C	-5.80816	-0.33137	0.78647
H	4.25931	4.00542	-0.63026	H	-6.28256	0.10343	-0.09379
H	3.84532	2.58253	-1.62097	H	-6.38579	-0.08423	1.67316
H	3.06330	4.12948	-1.92276	H	-4.82113	0.12071	0.89771
C	1.77573	4.44205	0.34972	C	-4.79802	-2.05894	-0.60234
H	1.17330	4.94852	-0.39996	H	-3.78664	-1.68885	-0.45961
C	2.00272	5.05623	1.50352	C	-5.13883	-2.53124	-1.79394
H	2.61757	4.62264	2.28201	H	-6.13618	-2.88971	-2.01384
H	1.58562	6.03490	1.70287	H	-4.42013	-2.56733	-2.60256
Rh	-0.73750	2.04077	-0.02519	Rh	-3.84567	-4.21493	1.90818
Cl	-2.56606	-0.65563	-2.32328	Cl	-3.33324	-5.76915	5.54740
C	-1.54278	3.86465	0.62713	C	-2.53537	-3.98847	0.39352
C	-1.38849	2.35129	-1.80298	C	-2.56080	-3.47824	3.26734
O	-1.93403	4.88554	0.90484	O	-1.79104	-3.89169	-0.45091
O	-1.78723	2.61181	-2.82677	O	-1.78461	-3.05150	3.96495
Rh	-3.94101	-0.91136	-0.37099	Rh	-3.57971	-7.71652	4.16011
Cl	-3.21830	1.26157	0.51668	Cl	-2.68548	-6.52137	2.20630
C	-4.50900	-2.55057	-1.08619	C	-4.19801	-8.61877	5.68445
O	-4.85103	-3.53606	-1.53925	O	-4.56633	-9.14946	6.62054
C	-5.05115	-1.09901	1.13660	C	-3.73613	-9.25472	3.08754
O	-5.73305	-1.20016	2.04342	O	-3.81632	-10.18408	2.43419
C	1.27244	-0.23823	-1.05481	C	-6.24186	-3.26415	3.98593
S	2.70665	-0.54521	-2.15165	S	-6.74780	-1.66327	4.70065
O	3.12163	0.73947	-2.71862	O	-6.12844	-0.59287	3.91867
O	2.28436	-1.63168	-3.03776	O	-6.45638	-1.78986	6.12900
C	4.07796	-1.16577	-1.17070	C	-8.52548	-1.50716	4.52857
C	5.08680	-0.29065	-0.78366	C	-9.04167	-0.75634	3.47784
C	4.14600	-2.52400	-0.88475	C	-9.35204	-2.08018	5.48834
C	6.18314	-0.78719	-0.09038	C	-10.41582	-0.57725	3.38946
C	5.24744	-3.00851	-0.19045	C	-10.72490	-1.89610	5.38698
C	6.26363	-2.14440	0.20452	C	-11.25510	-1.14520	4.34296
H	5.02856	0.75362	-1.05112	H	-8.37652	-0.29470	2.76326
H	3.35920	-3.19240	-1.19755	H	-8.93383	-2.65107	6.30310
H	6.98049	-0.11725	0.20349	H	-10.82908	0.01782	2.58589
H	5.31273	-4.06493	0.03312	H	-11.37750	-2.33343	6.13066
H	7.12467	-2.53046	0.73483	H	-12.32503	-0.99565	4.27597

INT2a				TS3a			
C	1.67841	-0.15737	-0.62710	C	8.33727	0.83590	-9.73641
C	0.72134	0.40846	0.14175	C	7.00256	0.69459	-9.57421
C	2.27549	-1.49765	-0.27197	C	9.11246	-0.09611	-10.63377
H	3.29199	-1.58443	-0.64464	H	10.14795	-0.17801	-10.31750
H	1.69094	-2.31011	-0.71010	H	9.10718	0.27326	-11.66213
C	2.30310	-1.69906	1.23952	C	8.50063	-1.49450	-10.63024
C	0.90473	-1.55820	1.82130	C	7.03033	-1.44629	-11.02313
H	0.97070	-1.50088	2.90628	H	6.57410	-2.41063	-10.80919
H	0.37988	-2.48593	1.58567	H	7.00740	-1.31926	-12.10779
C	0.15201	-0.37978	1.24073	C	6.28596	-0.30658	-10.36215
O	3.20990	-0.70614	1.74603	O	8.69571	-1.99045	-9.29464
O	2.72510	-3.02672	1.58102	O	9.12539	-2.33920	-11.60565
C	3.57225	-0.66701	3.05445	C	8.40233	-3.27217	-8.95349
C	3.97754	-3.47575	1.29765	C	10.43660	-2.69240	-11.51654
O	4.81917	-2.83492	0.72386	O	11.18975	-2.30981	-10.65945
O	3.16953	-1.42474	3.89881	O	7.93337	-4.08983	-9.70208
C	4.15174	-4.87024	1.82767	C	10.78547	-3.64098	-12.62726
H	4.13326	-4.84162	2.91847	H	10.24255	-4.57613	-12.48078
H	3.32906	-5.50689	1.50294	H	10.47720	-3.23138	-13.58901
H	5.10104	-5.27358	1.48742	H	11.85464	-3.83138	-12.62224
C	4.55544	0.44687	3.27718	C	8.76354	-3.51034	-7.51461
H	4.83156	0.48495	4.32679	H	8.54963	-4.54197	-7.25135
H	5.44003	0.27854	2.66187	H	9.82086	-3.29243	-7.36123
H	4.11906	1.39796	2.96924	H	8.19454	-2.83646	-6.87260
C	-1.95553	-0.88986	2.51511	C	4.07109	-0.85664	-11.42200
H	-2.63721	-1.56626	1.98909	H	3.59219	-0.22950	-12.17822
H	-1.33756	-1.48712	3.18829	H	4.59243	-1.66787	-11.93376
H	-2.58558	-0.23490	3.11858	H	3.26717	-1.29718	-10.82500
C	-1.13232	-0.12409	1.53608	C	4.98101	-0.04794	-10.55791
C	0.06330	1.74924	-0.03125	C	6.09721	1.48378	-8.69152
H	0.05417	2.05337	-1.07171	H	6.43951	2.49541	-8.52229
C	0.69213	2.90547	0.79879	C	5.68042	0.82010	-7.35129
C	0.89601	2.59122	2.28214	C	5.59366	-0.70785	-7.37831
H	1.55909	1.73517	2.39763	H	6.55549	-1.13256	-7.66136
H	1.36380	3.44148	2.77993	H	5.34298	-1.07268	-6.38098
H	-0.02636	2.36068	2.80851	H	4.85105	-1.07920	-8.08012
C	2.09512	3.20203	0.20682	C	6.70502	1.21788	-6.26899
H	2.74374	2.33160	0.30352	H	7.66723	0.74990	-6.47322
H	2.02904	3.47045	-0.84533	H	6.84997	2.29634	-6.22811
H	2.54653	4.03068	0.75333	H	6.35448	0.87133	-5.29451

C	-0.12323	4.15539	0.55406	C	4.35381	1.45298	-6.98255
H	-0.33248	4.34150	-0.49686	H	4.40718	2.51239	-6.75145
C	-0.53765	5.04350	1.44821	C	3.17870	0.83360	-6.86306
H	-0.36059	4.92868	2.50984	H	3.06371	-0.22755	-7.03646
H	-1.07876	5.92931	1.14109	H	2.29273	1.38166	-6.56965
Rh	-1.99905	1.28323	0.29508	Rh	4.29745	1.71098	-9.77774
Cl	-1.89462	-0.31915	-1.62355	Cl	5.63173	2.80301	-11.46259
C	-2.26865	2.32851	1.84743	C	2.06558	0.91408	-9.67419
C	-2.76764	2.65938	-1.07155	C	3.73065	3.59896	-9.17603
O	-2.59729	2.85872	2.79392	O	0.97429	0.66755	-9.55205
O	-3.20950	3.38470	-1.81034	O	3.46263	4.66377	-8.91418
Rh	-3.83176	-1.55206	-0.76862	Rh	4.16325	2.69065	-13.42764
Cl	-4.46447	0.44573	0.48963	Cl	2.20870	2.78900	-12.00941
C	-3.34954	-3.06550	-1.77613	C	5.67594	2.61703	-14.54373
O	-3.06407	-3.97493	-2.39417	O	6.58938	2.57331	-15.22078
C	-5.35154	-2.44848	-0.11948	C	3.01602	2.67901	-14.91561
O	-6.27940	-2.97317	0.27386	O	2.31020	2.68552	-15.80631
S	2.14791	0.37253	-2.27452	S	9.31439	2.22396	-9.16666
O	1.57188	1.68087	-2.59579	O	8.52947	3.08576	-8.27897
O	1.84170	-0.77625	-3.13365	O	9.91491	2.78940	-10.37864
C	3.93847	0.54864	-2.28728	C	10.66101	1.53482	-8.19678
C	4.51152	1.78870	-2.02817	C	10.51167	1.40222	-6.82084
C	4.72149	-0.55221	-2.61827	C	11.84952	1.19073	-8.83130
C	5.89280	1.91992	-2.08393	C	11.56642	0.89651	-6.07279
C	6.10233	-0.41081	-2.66669	C	12.89639	0.68080	-8.07413
C	6.68703	0.82142	-2.39679	C	12.75373	0.53020	-6.69935
H	3.88557	2.64096	-1.81419	H	9.59584	1.71923	-6.34485
H	4.25138	-1.49497	-2.85775	H	11.95672	1.34295	-9.89554
H	6.34702	2.88359	-1.89426	H	11.46592	0.79975	-4.99971
H	6.71897	-1.26195	-2.92280	H	13.82459	0.40888	-8.55863
H	7.76315	0.92907	-2.44198	H	13.57422	0.13812	-6.11246
INT3a				TS4a			
C	-1.90192	0.20296	-0.85274	C	-10.44370	-2.28351	-5.50804
C	-0.99663	-0.27728	0.02807	C	-9.23097	-2.15614	-6.09461
C	-2.58606	1.53247	-0.65130	C	-11.73755	-2.48811	-6.25706
H	-3.54476	1.56580	-1.15875	H	-12.55227	-1.95014	-5.77999
H	-1.97334	2.34294	-1.05201	H	-12.00450	-3.54790	-6.26343
C	-2.81342	1.79560	0.83167	C	-11.62532	-2.01938	-7.69991
C	-1.49790	1.71908	1.59240	C	-10.37202	-2.60002	-8.33416

H	-1.70557	1.73864	2.65960	H	-10.31438	-2.29210	-9.37187
H	-0.95922	2.63956	1.35686	H	-10.48119	-3.68862	-8.32017
C	-0.65398	0.52195	1.20372	C	-9.13934	-2.22180	-7.55915
O	-3.75853	0.79697	1.24855	O	-11.59117	-0.58252	-7.63400
O	-3.30604	3.12051	1.06861	O	-12.71071	-2.47938	-8.50817
C	-4.27731	0.77139	2.50156	C	-11.47235	0.18505	-8.74827
C	-4.51009	3.53792	0.58933	C	-13.99919	-2.11360	-8.24808
O	-5.25407	2.86136	-0.07113	O	-14.33251	-1.40763	-7.33385
O	-3.98671	1.54185	3.38034	O	-11.37948	-0.24300	-9.86970
C	-4.76637	4.95316	1.02217	C	-14.91549	-2.70810	-9.27800
H	-4.78751	5.00289	2.11154	H	-14.65823	-2.31583	-10.26286
H	-3.95789	5.60063	0.68139	H	-14.78786	-3.79015	-9.31497
H	-5.71415	5.29261	0.61504	H	-15.94456	-2.45919	-9.03658
C	-5.26418	-0.35606	2.61799	C	-11.48404	1.63894	-8.36875
H	-5.77052	-0.30109	3.57722	H	-11.42071	2.25014	-9.26410
H	-5.98350	-0.30808	1.80074	H	-12.39704	1.86861	-7.81881
H	-4.73784	-1.30844	2.53398	H	-10.64332	1.85744	-7.70823
C	1.09041	1.01091	2.94696	C	-7.72559	-2.28079	-9.64732
H	1.96612	1.56788	2.60030	H	-7.74600	-3.34516	-9.89819
H	0.38667	1.73017	3.36862	H	-8.49906	-1.78227	-10.23546
H	1.42860	0.35889	3.75510	H	-6.76199	-1.89246	-9.96935
C	0.50733	0.23313	1.81594	C	-7.93993	-2.11844	-8.17669
C	-0.22450	-1.55404	-0.08136	C	-7.91183	-2.08546	-5.38149
H	-0.00523	-1.81368	-1.10654	H	-7.89853	-2.71205	-4.50159
C	-0.73255	-2.79192	0.70600	C	-7.25660	-0.69221	-5.10246
C	-1.98054	-2.54718	1.55644	C	-8.23009	0.49224	-5.11708
H	-2.82910	-2.30511	0.91721	H	-8.87947	0.43921	-4.24518
H	-2.22362	-3.44549	2.12710	H	-7.67212	1.43006	-5.07216
H	-1.84851	-1.72254	2.25426	H	-8.86267	0.50919	-6.00422
C	-0.96800	-3.97908	-0.23208	C	-6.52144	-0.69874	-3.76038
H	-1.78378	-3.77221	-0.92018	H	-7.23309	-0.81911	-2.94637
H	-0.08071	-4.18513	-0.83389	H	-5.79329	-1.50692	-3.69450
H	-1.20564	-4.87640	0.34463	H	-5.98663	0.24322	-3.62103
C	0.48763	-3.09531	1.56879	C	-6.26051	-0.66069	-6.25312
H	1.08148	-3.95534	1.28204	H	-5.21115	-0.47535	-6.05989
C	0.83887	-2.43972	2.71739	C	-6.74873	-0.48217	-7.56360
H	0.17008	-1.74721	3.20364	H	-7.67066	0.05087	-7.72424
H	1.66836	-2.80973	3.30429	H	-6.03517	-0.38023	-8.36939
Rh	1.63898	-1.23946	0.90576	Rh	-6.44874	-2.72716	-6.76378
Cl	2.18212	0.51768	-0.74948	Cl	-7.43146	-5.09668	-6.99926
C	3.34448	-0.90583	2.07671	C	-4.93602	-3.00722	-8.18789

C	2.62208	-2.58969	-0.33584	C	-5.31336	-3.45341	-5.30231
O	4.15536	-0.73107	2.83882	O	-4.14540	-2.94627	-8.98956
O	3.01865	-3.33722	-1.07831	O	-4.70273	-3.89567	-4.46305
Rh	4.55863	1.19825	-0.87247	Rh	-6.01425	-6.73718	-8.16699
Cl	5.37106	-0.99998	-0.31844	Cl	-3.98425	-5.81802	-7.24637
C	3.97494	2.93089	-1.31635	C	-7.57693	-7.48538	-8.89218
O	3.62812	3.98096	-1.58727	O	-8.52605	-7.93982	-9.32967
C	6.35508	1.71201	-1.02828	C	-4.93492	-8.01646	-9.01037
O	7.44937	2.00369	-1.12569	O	-4.26666	-8.79119	-9.50765
S	-2.37951	-0.57519	-2.38892	S	-10.66127	-2.40238	-3.72906
O	-1.70355	-1.86442	-2.55882	O	-9.50679	-1.82386	-3.03522
C	-4.13489	-0.91357	-2.18934	C	-12.08018	-1.35933	-3.36183
C	-4.53409	-2.08272	-1.55081	C	-11.94800	0.02332	-3.41999
H	-3.79552	-2.78725	-1.19740	H	-11.00871	0.47057	-3.71221
C	-5.88891	-2.34454	-1.40356	C	-13.03548	0.81782	-3.08561
H	-6.21062	-3.25536	-0.91567	H	-12.94621	1.89547	-3.12397
C	-6.83015	-1.44412	-1.89496	C	-14.23419	0.22944	-2.69191
H	-7.88606	-1.65289	-1.78111	H	-15.07816	0.85302	-2.42701
C	-6.41939	-0.28448	-2.54165	C	-14.35131	-1.15429	-2.63509
H	-7.15136	0.40961	-2.93220	H	-15.28287	-1.60914	-2.32552
H	-4.72813	0.87439	-3.20953	H	-13.33607	-3.03781	-2.93561
C	-5.06486	-0.01315	-2.69342	C	-13.27078	-1.95987	-2.97586
O	-2.25427	0.44758	-3.43108	O	-11.05480	-3.78362	-3.43630
INT4a				TS5a			
C	-2.15728	-0.41496	-0.61710	C	-1.78227	0.62838	-0.33930
C	-1.09134	-0.76220	0.13064	C	-1.06295	-0.44265	-0.71041
C	-2.63834	0.98896	-0.86515	C	-2.33657	0.86226	1.03938
H	-3.71330	1.07464	-0.72730	H	-3.38072	1.16379	0.99844
H	-2.42037	1.25486	-1.90252	H	-1.77720	1.67872	1.50163
C	-1.94433	1.99670	0.03762	C	-2.21188	-0.36317	1.93711
C	-0.45836	1.66033	0.16550	C	-0.85399	-1.03424	1.73232
H	0.02971	2.46244	0.70012	H	-0.74401	-1.83529	2.45126
H	-0.04923	1.61278	-0.84535	H	-0.09235	-0.27825	1.93037
C	-0.31366	0.31528	0.83126	C	-0.74833	-1.50006	0.30296
O	-2.63693	1.91036	1.29706	O	-3.30378	-1.22260	1.56140
O	-1.97935	3.31865	-0.49526	O	-2.25870	-0.02118	3.32045
C	-2.32819	2.71879	2.34530	C	-3.54154	-2.39897	2.20123
C	-3.16158	3.95832	-0.73539	C	-3.34976	0.59447	3.86263
O	-4.24382	3.47649	-0.53155	O	-4.33586	0.89022	3.24176
O	-1.44299	3.53402	2.33960	O	-2.87562	-2.83063	3.10546

C	-2.89461	5.33544	-1.26774	C	-3.12722	0.82755	5.32784
H	-2.34398	5.91275	-0.52378	H	-2.91928	-0.12063	5.82425
H	-2.27122	5.27636	-2.16015	H	-2.25651	1.46863	5.47122
H	-3.83556	5.82581	-1.49837	H	-4.00758	1.29364	5.76016
C	-3.25702	2.44392	3.49268	C	-4.74818	-3.06631	1.60606
H	-2.97998	3.06003	4.34299	H	-4.96053	-3.98567	2.14333
H	-4.28198	2.66258	3.19098	H	-5.60469	-2.39383	1.65420
H	-3.21634	1.38779	3.76157	H	-4.56315	-3.28489	0.55291
C	1.13734	1.35846	2.60217	C	-0.47051	-3.94007	0.97037
H	1.53144	2.04710	1.86154	H	-0.12655	-3.61167	1.94546
H	0.46601	1.92349	3.25435	H	-1.45078	-4.40861	1.10488
H	1.96652	1.01159	3.21539	H	0.20586	-4.71244	0.60569
C	0.40323	0.18343	2.00186	C	-0.59610	-2.83924	-0.04419
C	-0.39761	-2.07014	0.10756	C	-0.24997	-0.57716	-1.95166
H	-0.50010	-2.60374	-0.82453	H	0.38234	0.26728	-2.19307
C	-0.42887	-2.95370	1.36729	C	-0.73366	-1.36131	-3.15180
C	-1.78086	-2.94580	2.09722	C	-2.23296	-1.45259	-3.39577
H	-2.51589	-3.48192	1.49722	H	-2.57033	-0.54082	-3.88538
H	-1.69377	-3.45007	3.06281	H	-2.45669	-2.29639	-4.05250
H	-2.16179	-1.93899	2.26871	H	-2.80635	-1.57109	-2.47699
C	-0.09664	-4.40743	1.02687	C	0.00721	-0.95568	-4.41938
H	-0.84443	-4.81440	0.34613	H	-0.31895	0.03283	-4.74189
H	0.87976	-4.51990	0.55924	H	1.08654	-0.92070	-4.25994
H	-0.09723	-5.01196	1.93574	H	-0.19267	-1.66892	-5.22121
C	0.71485	-2.28356	2.12104	C	-0.07312	-2.48670	-2.43119
H	1.42008	-2.95427	2.60063	H	0.75203	-2.96728	-2.93543
C	0.37853	-1.04949	2.91750	C	-0.84802	-3.33493	-1.45872
H	-0.58466	-1.11441	3.43288	H	-1.92051	-3.36331	-1.67296
H	1.13210	-0.89900	3.68765	H	-0.47950	-4.35708	-1.53063
Rh	1.53909	-1.27598	0.45483	Rh	1.28409	-1.64966	-0.70462
Cl	1.85831	-0.06303	-1.84283	Cl	1.82470	0.86739	0.36253
C	3.34214	-0.70642	1.37292	C	2.40217	-2.50400	0.70146
C	2.37776	-2.80914	-0.36302	C	2.81922	-1.56899	-1.91013
O	4.19343	-0.65750	2.11709	O	2.93548	-3.05254	1.53308
O	2.89090	-3.67288	-0.87819	O	3.64545	-1.53671	-2.68127
Rh	3.91062	0.93329	-0.93419	Rh	4.15596	1.57531	0.66784
Cl	5.14930	-1.08966	-1.35403	Cl	5.01750	-0.65647	0.31669
C	3.00219	2.56015	-0.68729	C	3.52284	3.32066	0.94690
O	2.45744	3.55308	-0.56007	O	3.14033	4.38011	1.11960
C	5.54288	1.66006	-0.35118	C	5.93438	2.10738	0.90955
O	6.54291	2.08512	-0.01819	O	7.02151	2.41338	1.05616

S	-3.09340	-1.62217	-1.57413	S	-2.02471	2.03863	-1.43437
O	-2.74774	-2.98260	-1.15600	O	-1.60609	1.67405	-2.78968
C	-4.79780	-1.33421	-1.08666	C	-3.80387	2.28212	-1.45164
C	-5.25311	-1.84421	0.12425	C	-4.60064	1.46788	-2.24889
H	-4.58212	-2.39177	0.77092	H	-4.15388	0.69046	-2.85107
C	-6.58332	-1.65652	0.47340	C	-5.97135	1.68508	-2.27303
H	-6.95541	-2.05438	1.40826	H	-6.60315	1.06295	-2.89312
C	-7.43967	-0.97028	-0.38352	C	-6.52930	2.70719	-1.51024
H	-8.47722	-0.83110	-0.10881	H	-7.59818	2.87511	-1.53519
C	-6.97065	-0.46803	-1.59189	C	-5.72015	3.51719	-0.72170
H	-7.63931	0.06048	-2.25814	H	-6.15539	4.31485	-0.13462
H	-5.25606	-0.27564	-2.89009	H	-3.69755	3.93182	-0.09080
C	-5.63991	-0.64696	-1.95075	C	-4.34684	3.30703	-0.68704
O	-2.96784	-1.23980	-2.98284	O	-1.43404	3.20179	-0.77280
TS6a							
C	-2.07665	5.43425	-6.94632				
C	-4.18544	4.25042	-6.49082				
H	-5.23127	4.54378	-6.52982				
H	-4.05746	3.61040	-5.61523				
C	-3.89178	3.41731	-7.74726				
C	-2.40654	3.06439	-7.88298				
H	-2.21555	2.63509	-8.86456				
H	-2.18919	2.28480	-7.14631				
C	-1.56033	4.25478	-7.57954				
O	-4.34617	4.22848	-8.84308				
O	-4.56912	2.15917	-7.69211				
C	-4.39287	3.75094	-10.11754				
C	-5.93005	2.07249	-7.68757				
O	-6.67063	3.02020	-7.69865				
O	-4.02539	2.65391	-10.44678				
C	-6.34678	0.63091	-7.68298				
H	-5.98503	0.14601	-8.59074				
H	-5.89672	0.11434	-6.83482				
H	-7.42943	0.56467	-7.63149				
C	-4.98312	4.78839	-11.02825				
H	-4.98531	4.41835	-12.04910				
H	-6.00158	5.01245	-10.70864				
H	-4.40989	5.71381	-10.96490				
C	0.67786	3.75106	-8.68036				
H	1.36542	3.11160	-8.12461				

H	0.09477	3.12831	-9.36520
H	1.27415	4.44017	-9.28034
C	-0.24507	4.49281	-7.76611
C	-0.94236	6.39444	-7.17127
H	-0.65112	6.98268	-6.30328
C	-0.96322	7.28999	-8.42353
C	-1.34495	6.56554	-9.71477
H	-1.46035	7.29010	-10.52151
H	-0.59743	5.83623	-10.01955
H	-2.29644	6.04922	-9.59356
C	-2.03028	8.38852	-8.16966
H	-2.00166	9.10187	-8.99358
H	-3.02516	7.94676	-8.12950
H	-1.84949	8.91962	-7.23712
C	0.36806	7.99988	-8.52164
H	0.68302	8.48763	-7.60251
C	1.12438	8.12283	-9.60355
H	0.86462	7.66977	-10.55120
H	2.04888	8.68418	-9.57209
Rh	1.02314	5.31291	-6.12640
Cl	-0.49514	4.54318	-4.31425
C	2.36138	5.93078	-7.30147
C	2.29569	5.53193	-4.67135
O	3.26326	6.23917	-7.92178
O	3.02113	5.62632	-3.80902
Rh	-0.31669	2.10127	-4.60313
Cl	1.91475	2.31338	-5.50095
C	-2.03332	1.90382	-3.86487
O	-3.07278	1.78219	-3.41576
C	-0.11640	0.24426	-4.78696
O	0.03091	-0.87786	-4.89344
C	-3.28934	5.46012	-6.37823
S	-3.80070	6.70970	-5.20395
O	-2.75412	7.72975	-5.12667
C	-5.28820	7.47879	-5.84531
C	-5.20277	8.71835	-6.46923
H	-4.24576	9.20833	-6.56529
C	-6.36566	9.32355	-6.92804
H	-6.31310	10.29367	-7.40426
C	-7.59339	8.69060	-6.76437
H	-8.49705	9.16675	-7.12223

C	-7.66735	7.45581	-6.12792
C	-6.51308	6.84504	-5.65657
H	-6.56328	5.90513	-5.12634
H	-8.62473	6.97277	-5.98619
O	-4.19062	5.95675	-4.01029

Table S9 Frequencies of all stationary points for the overall catalytic cycle, PhO₂S with downward direction of **1a** computed at and some of them computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dftg).

Species	Frequencies(cm ⁻¹)												
CAT	35	41	52	89	90	93	96	101	117	143	243	277	
	283	300	415	416	432	434	459	466	467	468	469	470	
	610	613	2096	2098	2152	2168							
1aa	14	21	32	39	40	43	52	52	57	62	67	74	
	79	81	91	109	113	128	134	160	167	173	184	199	
	201	229	249	270	271	283	288	297	302	306	313	332	
	344	361	375	394	398	405	415	421	435	459	465	476	
	509	527	543	571	589	597	603	610	632	663	684	696	
	707	725	755	766	774	776	798	854	861	863	877	894	
	934	943	951	953	955	969	987	1004	1017	1019	1023	1026	
	1029	1042	1045	1050	1056	1061	1064	1066	1069	1080	1103	1110	1128
	1160	1172	1176	1187	1200	1204	1213	1225	1254	1283	1285	1298	1326
	1334	1347	1348	1351	1383	1400	1400	1401	1414	1417	1436	1456	1459
	1468	1469	1469	1473	1477	1479	1480	1485	1489	1492	1504	1515	1516
	1627	1630	1701	1784	1795	2035	2357	3032	3038	3049	3060	3061	3067
	3087	3091	3092	3104	3112	3114	3115	3116	3116	3120	3120	3124	3141
	3152	3164	3167	3183	3193	3202	3214	3216	3230				
2aa	21	30	40	45	46	54	63	72	80	87	96	99	
	108	116	117	147	165	178	183	186	208	211	226	236	
	246	256	276	289	299	304	307	344	356	368	373	410	
	416	418	434	447	456	473	493	513	530	542	554	568	
	595	602	612	633	636	664	684	710	718	742	753	764	
	775	795	799	807	864	880	905	917	922	932	952	955	
	975	979	995	1003	1016	1019	1021	1022	1025	1030	1042	1047	1053
	1061	1068	1069	1076	1086	1097	1103	1125	1133	1149	1158	1169	1174
	1187	1201	1218	1221	1236	1255	1259	1274	1298	1312	1319	1334	1339
	1351	1352	1379	1390	1400	1402	1405	1410	1417	1429	1448	1466	1469
	1469	1471	1471	1472	1482	1484	1485	1492	1494	1504	1505	1510	1517
	1609	1628	1630	1672	1780	1792	2990	3024	3025	3031	3032	3037	3059

	3060 3066 3077 3079 3086 3103 3113 3119 3120 3124 3135 3149 3163 3164 3178 3180 3192 3201 3216 3220 3236
3aa	27 29 37 44 55 56 64 71 80 82 86 100 116 120 138 155 156 167 181 188 199 201 211 227 238 248 264 281 283 299 303 308 320 333 338 353 380 392 416 426 438 449 470 484 495 522 538 543 574 593 602 609 622 633 642 669 703 709 715 733 760 773 789 799 821 862 864 882 899 917 936 951 953 954 956 984 1003 1018 1021 1021 1023 1027 1033 1043 1048 1049 1052 1057 1070 1072 1075 1083 1104 1108 1130 1134 1161 1179 1187 1195 1203 1210 1216 1224 1252 1257 1270 1278 1298 1316 1326 1334 1347 1352 1358 1379 1400 1400 1405 1412 1421 1456 1466 1467 1468 1472 1473 1474 1479 1480 1484 1486 1491 1504 1510 1517 1627 1629 1662 1701 1742 1783 1793 3028 3042 3049 3054 3058 3060 3060 3065 3077 3104 3108 3110 3114 3118 3121 3121 3122 3131 3146 3146 3165 3167 3180 3193 3202 3221 3222 3222
COMa	13 18 22 26 30 35 39 42 44 45 51 53 58 60 62 63 73 73 79 81 87 91 94 96 101 103 108 112 120 125 128 140 141 144 146 163 179 180 188 195 208 218 243 256 259 260 266 273 294 298 298 301 305 309 315 328 348 361 372 382 396 401 405 408 416 424 432 443 445 448 467 468 469 471 474 481 483 494 507 523 555 580 588 592 596 604 610 616 633 659 676 697 709 716 744 759 775 781 795 836 857 868 870 894 935 948 953 956 956 974 997 1008 1023 1023 1029 1031 1033 1038 1038 1047 1053 1064 1066 1067 1068 1082 1104 1125 1130 1132 1161 1170 1189 1203 1205 1213 1219 1251 1281 1288 1295 1315 1335 1349 1352 1375 1385 1398 1400 1402 1408 1418 1437 1451 1458 1466 1467 1471 1471 1472 1474 1481 1486 1487 1490 1504 1514 1516 1627 1629 1702 1784 1791 2029 2083 2093 2150 2159 2184 3038 3043 3048 3062 3062 3067 3092 3106 3107 3110 3112 3114 3116 3116 3120 3125 3126 3127 3141 3150 3166 3167 3184 3195 3203 3214 3218 3228
TS1a	-64 14 21 23 28 29 38 44 46 49 51 56 61 65 69 73 80 83 84 90 92 93 97 101 105 107 111 117 121 122 127 135 138 155 158 167 181 186 188 194 208 214 221 246 253 261 270 281 285 286 304 305 309 320 322 336 349 356 377 382 385 395 403 406 415 420 431 443 448 456 461

	467 468 474 476 480 482 504 513 517 547 555 589 594 602 609 611 620 632 658 685 699 708 724 741 755 771 779 796 848 865 878 891 913 928 933 954 956 961 973 981 998 1004 1019 1021 1025 1032 1039 1041 1044 1047 1067 1068 1069 1073 1079 1108 1111 1126 1139 1156 1174 1187 1207 1208 1220 1222 1252 1282 1289 1302 1324 1335 1348 1351 1358 1397 1402 1403 1405 1411 1415 1427 1455 1459 1466 1466 1470 1471 1476 1482 1484 1486 1494 1495 1510 1513 1519 1627 1629 1700 1784 1795 1961 2074 2092 2137 2153 2214 3044 3044 3058 3060 3061 3093 3097 3106 3111 3118 3120 3124 3129 3130 3133 3134 3138 3140 3152 3156 3165 3167 3181 3192 3201 3225 3229 3241
INT1a	13 19 24 27 37 38 44 45 52 56 60 63 66 69 71 72 81 83 85 92 93 97 100 105 113 121 122 132 133 140 142 157 169 174 177 183 187 194 198 204 213 225 237 245 251 256 266 273 280 280 285 301 308 311 313 329 340 346 357 363 374 395 398 404 410 417 419 427 428 448 458 463 473 474 477 479 494 497 524 540 545 555 563 602 611 612 620 627 632 662 689 706 707 727 748 753 773 786 801 851 862 879 898 927 934 945 955 956 960 981 1001 1005 1008 1020 1024 1026 1030 1038 1043 1047 1049 1060 1065 1070 1073 1080 1107 1109 1125 1137 1160 1179 1185 1194 1205 1224 1230 1252 1269 1282 1306 1329 1335 1345 1355 1356 1382 1394 1402 1402 1404 1408 1423 1455 1461 1466 1466 1470 1471 1472 1483 1484 1486 1497 1503 1508 1515 1519 1627 1628 1698 1785 1793 1812 2074 2140 2149 2177 2204 3043 3045 3046 3060 3061 3062 3063 3103 3105 3105 3120 3122 3122 3124 3129 3133 3147 3147 3157 3157 3169 3170 3181 3194 3203 3225 3228 3243
TS2a	-251 15 19 23 29 41 43 48 50 52 56 59 65 67 70 75 77 85 86 87 88 95 98 101 104 111 125 130 132 136 158 159 165 174 177 178 185 194 202 207 218 235 241 249 269 275 278 280 287 305 308 311 311 321 328 335 343 358 364 377 389 395 402 411 418 425 431 438 447 457 467 472 475 477 479 485 489 503 521 534 547 564 582 603 609 612 621 623 631 662 692 702 710 729 748 759 775 804 823 855 856 897 906 922 934 949 952 955 959 976 999 1012 1014 1022 1023 1026 1029 1043 1047 1048 1051 1062 1069 1069 1071 1079 1093 1107 1124 1129 1156 1167 1188 1198 1204 1222 1225 1251 1260 1286 1294 1321 1333 1335 1344 1353

	1362 1387 1396 1402 1403 1404 1420 1452 1453 1465 1469 1470 1472 1473 1481 1484 1485 1493 1502 1506 1514 1518 1627 1628 1698 1735 1783 1792 1916 2076 2141 2146 2179 2973 3036 3044 3047 3055 3059 3063 3096 3101 3104 3110 3112 3119 3124 3132 3139 3146 3150 3153 3167 3167 3178 3182 3193 3203 3223 3227 3235
INT2a	14 18 29 32 37 38 47 50 54 57 61 64 67 70 71 78 80 86 92 93 94 96 101 108 112 122 123 131 139 142 151 165 173 177 189 196 208 216 225 242 246 256 263 270 273 276 279 285 294 302 306 313 322 325 334 349 367 383 397 409 416 421 422 431 440 444 452 463 468 472 473 475 495 502 514 523 534 547 565 569 586 605 613 614 627 634 656 662 693 702 709 716 739 769 773 780 802 830 862 886 903 914 930 933 953 955 958 979 1003 1017 1019 1021 1022 1025 1029 1041 1044 1047 1050 1057 1065 1068 1074 1079 1089 1107 1108 1123 1126 1140 1163 1172 1189 1205 1206 1220 1252 1254 1272 1293 1301 1310 1331 1335 1343 1353 1375 1386 1400 1401 1403 1405 1424 1456 1467 1467 1469 1470 1473 1475 1479 1484 1485 1491 1495 1509 1513 1520 1607 1628 1630 1644 1701 1782 1792 2090 2130 2155 2191 3015 3048 3054 3059 3060 3061 3062 3070 3099 3112 3117 3119 3120 3121 3122 3140 3145 3145 3147 3149 3163 3167 3184 3195 3203 3219 3226 3239
TS3a	-162 18 21 23 25 29 32 41 46 52 54 56 60 66 67 72 77 85 87 89 92 94 99 101 103 110 113 120 140 147 152 157 162 169 175 178 188 196 212 220 234 240 249 257 263 268 271 281 283 291 295 302 307 307 311 328 336 351 358 376 382 405 416 425 430 437 442 443 458 463 470 473 474 478 498 504 529 543 549 566 586 607 611 612 628 633 645 660 694 704 709 716 738 767 773 778 801 827 862 874 900 913 928 945 955 957 968 973 1001 1016 1018 1020 1023 1025 1030 1033 1044 1046 1051 1059 1068 1072 1075 1079 1094 1102 1106 1122 1126 1147 1172 1179 1188 1202 1204 1219 1253 1257 1275 1290 1302 1311 1331 1335 1347 1351 1367 1389 1400 1401 1403 1403 1422 1454 1470 1470 1471 1472 1472 1476 1479 1483 1485 1490 1493 1505 1516 1518 1607 1628 1630 1633 1670 1782 1792 2083 2147 2156 2189 3016 3040 3049 3054 3058 3060 3061 3064 3088 3109 3118 3120 3121 3121 3132 3137 3139 3148 3154 3165 3167 3182 3183 3194 3202 3217 3226 3237

INT3a	10	16	23	28	32	39	46	52	54	57	60		
	64	69	72	76	86	88	89	92	95	102	109	115	
	120	124	127	133	136	145	155	170	178	181	195	211	
	220	226	232	238	241	245	260	269	270	279	281	288	
	291	294	305	306	315	317	328	343	351	360	376	385	
	394	407	416	418	426	432	437	442	450	466	473	473	
	475	478	496	498	521	532	540	557	568	594	604	612	
	615	629	634	661	667	704	711	718	739	768	770	778	
	801	802	828	861	878	903	914	932	950	956	960	976	
	1003	1009	1014	1019	1020	1021	1025	1036	1041	1046	1046	1054	1060
	1070	1071	1072	1081	1098	1103	1105	1123	1128	1149	1178	1187	1202
	1203	1219	1221	1252	1255	1275	1296	1302	1307	1313	1334	1344	1352
	1363	1393	1401	1402	1404	1408	1417	1446	1468	1470	1473	1476	1479
	1480	1483	1484	1487	1492	1494	1497	1515	1518	1581	1616	1628	1630
	1640	1781	1792	2078	2145	2172	2194	3023	3036	3048	3055	3061	3061
	3064	3073	3095	3098	3113	3121	3121	3128	3130	3146	3156	3162	3166
	3168	3170	3183	3188	3194	3203	3218	3220	3258				
	TS4a	-293	16	23	25	32	38	41	46	48	50	53	
		58	64	67	71	76	77	89	94	96	100	107	112
		117	124	126	131	138	158	161	168	180	183	191	199
204		211	218	222	226	246	253	259	267	273	279	284	
289		306	307	309	315	340	343	355	357	361	373	382	
412		413	420	423	430	443	446	452	470	476	478	480	
482		487	497	508	519	522	551	566	579	605	609	612	
614		618	633	658	668	706	712	716	736	770	773	788	
803		826	850	862	878	900	908	917	931	953	958	961	
966		1002	1012	1020	1022	1024	1025	1027	1034	1043	1046	1053	1061
1072		1074	1077	1083	1089	1105	1107	1121	1124	1148	1169	1187	1198
1201		1210	1218	1226	1243	1251	1273	1292	1303	1309	1332	1335	1344
1353		1392	1393	1403	1403	1408	1412	1431	1469	1469	1470	1472	1474
1480		1484	1485	1489	1494	1495	1503	1511	1519	1528	1595	1609	1628
1631		1783	1795	2071	2140	2156	2181	3029	3042	3045	3048	3054	3058
3063		3082	3105	3111	3117	3124	3128	3131	3138	3144	3165	3167	3167
3168		3176	3179	3182	3194	3203	3215	3218	3261				
INT4a		15	19	21	30	31	32	40	43	50	52	54	60
		63	70	71	76	81	93	96	102	102	104	108	111
		113	116	123	132	139	145	155	172	179	185	192	202
	206	209	219	243	253	255	270	273	278	291	294	309	
	311	325	332	345	348	365	369	374	388	397	398	416	

	429 431 440 450 452 453 469 473 479 484 488 494 502 508 526 537 543 555 578 593 601 608 610 626 632 669 685 703 710 715 734 751 772 785 800 808 864 865 892 910 918 944 946 955 959 962 977 994 1005 1017 1019 1021 1024 1026 1029 1040 1047 1048 1060 1066 1069 1082 1087 1092 1105 1114 1125 1129 1161 1180 1189 1196 1203 1216 1219 1227 1249 1254 1278 1279 1294 1307 1322 1336 1340 1355 1356 1384 1393 1399 1401 1401 1424 1426 1466 1468 1470 1471 1475 1482 1483 1486 1487 1496 1498 1504 1515 1518 1525 1571 1628 1630 1638 1786 1797 2074 2123 2143 2170 3027 3038 3048 3049 3058 3059 3060 3070 3103 3105 3109 3116 3118 3120 3120 3132 3133 3140 3156 3166 3168 3184 3194 3204 3206 3210 3215 3219
TS5a	-242 19 21 25 28 29 35 39 41 45 49 57 60 61 66 69 76 79 82 94 97 104 108 113 118 122 123 128 136 142 148 156 170 175 185 195 206 211 218 232 244 251 256 271 274 280 299 303 308 317 330 338 344 350 362 374 384 390 400 414 416 428 431 442 446 449 449 463 476 477 479 481 494 504 522 529 539 548 572 584 591 602 609 613 620 632 668 686 706 716 730 753 768 778 799 801 855 862 881 910 915 920 940 949 955 957 971 977 1005 1007 1018 1023 1026 1026 1030 1035 1047 1048 1060 1069 1072 1081 1091 1104 1104 1124 1127 1141 1166 1188 1188 1195 1202 1209 1219 1249 1254 1280 1284 1291 1301 1305 1312 1336 1340 1352 1357 1388 1390 1401 1401 1408 1426 1428 1467 1467 1468 1470 1473 1477 1483 1485 1485 1490 1499 1504 1506 1516 1522 1552 1628 1630 1655 1787 1797 2067 2135 2135 2166 3030 3036 3039 3045 3061 3061 3062 3070 3097 3101 3101 3107 3119 3120 3120 3130 3130 3160 3169 3169 3171 3182 3190 3191 3195 3204 3221 3224
TS6a	-234 14 22 26 28 32 34 43 46 48 50 54 58 60 70 71 73 79 81 84 92 96 100 103 107 110 122 123 126 128 130 142 158 171 174 193 194 200 204 211 236 240 251 252 274 278 287 293 303 306 311 317 325 327 339 352 364 382 390 400 413 417 427 428 431 439 447 451 455 470 474 477 480 482 492 501 525 546 560 578 580 597 600 607 613 616 632 654 671 700 708 715 735 765 771 785 798 828 861 876 891 904 921 934 951 956 961 967 1002 1007 1017 1018 1019 1025 1031 1032 1038 1043 1047 1049

	1064 1069 1072 1077 1081 1097 1107 1119 1126 1141 1158 1162 1188
	1204 1208 1212 1248 1253 1273 1284 1297 1316 1330 1335 1354 1359
	1376 1389 1396 1400 1401 1402 1422 1458 1463 1467 1467 1469 1470
	1471 1482 1483 1484 1485 1497 1510 1514 1518 1627 1628 1633 1686
	1704 1786 1795 2078 2097 2145 2158 3019 3032 3047 3058 3060 3061
	3067 3087 3100 3101 3114 3120 3120 3120 3121 3130 3135 3136 3138
	3155 3167 3167 3183 3195 3203 3221 3231 3233