

DFT Study on Ruthenium-Catalyzed N-methylbenzamide-directed 1,4-Addition of the *Ortho* C-H Bond to Maleimide *via* C-H/C-C Activation

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Figure S1. Proposed mechanism for the ruthenium-catalyzed amide-directed *ortho* C-H activation and C-C coupling reaction, along with $\Delta G(373\text{K}, \text{kcal mol}^{-1})$ and key geometric parameters (\AA) determined at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg)(middle, in blue) in DCE solution, and also $\Delta G(373\text{K}, \text{kcal mol}^{-1})$ determined at B3LYP+IDSCRF/TZP-DKH(-dfg) (up, in black) and B3LYP-D3+IDSCRF/TZP-DKH(-dfg)(down, in purple) for comparison. s1

Table S1. The calculated total electronic energies, enthalpies, entropies and free energies in a.u., in the DCE solvent with the temperature of 373.15K, along with some of them in DMF or CH_3CN s2-s4

Table S2 Coordinates of all stationary points **CAT+1a+2a**, computed at B3LYP-D3a+IDSCRF/ TZP-DKH(-dfg) level in DCE solvent s5-s20

Table S3 Coordinates of all stationary points **CAT+1a+2a**, computed at B3LYP+IDSCRF/ TZP-DKH(-dfg) level in DCE solvent s21-s36

Table S4 Coordinates of all stationary points **CAT+1a+2a**, computed at B3LYP-D3+IDSCRF/ TZP-DKH(-dfg) level in DCE solvent s37-s50

Table S5 Coordinates of stationary points for the reaction of **CAT+DMF+1a** and **CAT+CH₃CN+1a**, computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in DMF and CH_3CN solvent, respectively. s50-s58

Table S6 Coordinates of the first transition state for **CAT-B+1a** and **CAT-O+1a**, Computed at B3LYP-D3a+IDSCRF/ TZP-DKH(-dfg) level in DCE solvent s58-s61

Table S7 Frequencies of all stationary points for the overall catalytic cycle, computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level, and some of them computed at B3LYP+IDSCRF/TZP-DKH(-dfg) and B3LYP-D3+IDSCRF/TZP-DKH(-dfg) s61-s88

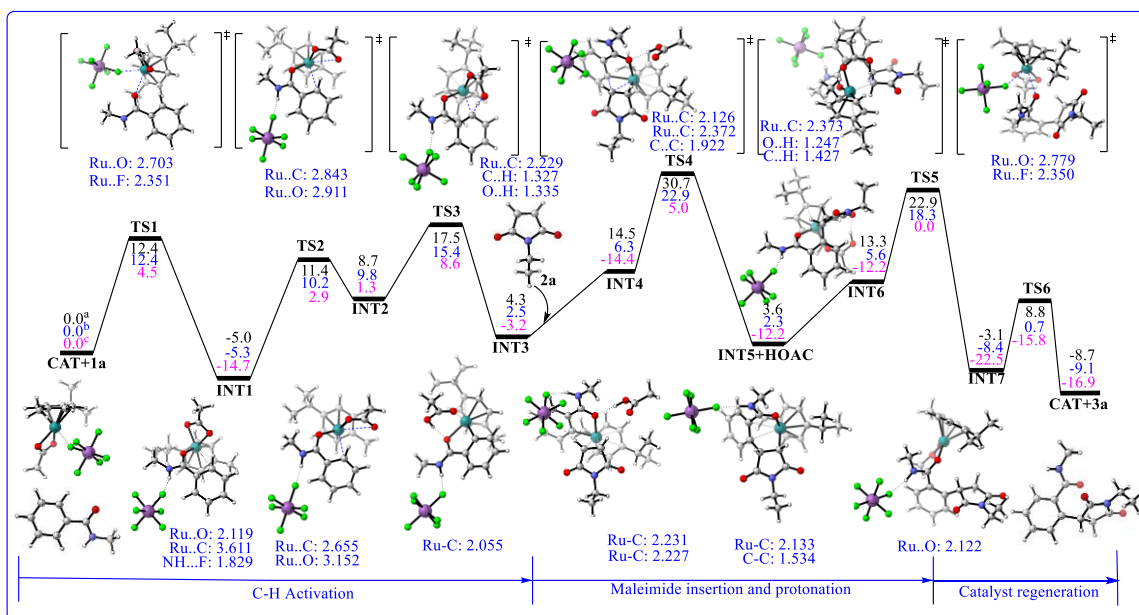


Figure S1 Proposed mechanism for the ruthenium-catalyzed amide-directed ortho C–H activation and C–C coupling reaction, along with $\Delta G(373\text{K}, \text{kcal mol}^{-1})$ and key geometric parameters (\AA) determined at B3LYP-D3a+ IDSCRF/TZP-DKH(-dfg)(middle, in blue) in DCE solution, and also $\Delta G(373\text{K}, \text{kcal mol}^{-1})$ determined at B3LYP+IDSCRF/TZP-DKH(-dfg) (up, in black) and B3LYP-D3+IDSCRF/TZP-DKH(-dfg) (down, in purple) for comparison.

Table S1 The calculated total electronic energies, enthalpies, entropies and free energies in a.u. , in the DCE solvent with the temperature of 373.15K, along with some of them in DMF or CH₃CN solvent

Species	$E_{\text{elec}}/\text{a.u.}$	$H/\text{a.u.}$	S_g	S_l	$G_g/\text{a.u.}$	$G_l/\text{a.u.}$
DCE						
1a	-440.41980 ^a	-440.24982	104.5	81.6	-440.31196	-440.29832
	-440.44477 ^b	-440.27478	104.8	81.9	-440.33710	-440.32346
	-440.45292 ^c	-440.28279	104.5	81.6	-440.34494	-440.33130
2a	-438.21638 ^a	-438.07858	97.9	74.6	-438.13682	-438.12294
	-438.23675 ^b	-438.09892	98.3	75.0	-438.15738	-438.14350
	-438.24248 ^c	-438.10452	97.8	74.5	-438.16269	-438.14881
HOAc	-229.18174 ^a	-229.11324	73.2	52.6	-229.15674	-229.14454
	-229.18972 ^b	-229.12124	73.1	52.6	-229.16469	-229.15176
	-229.18875 ^c	-229.12022	73.0	52.5	-229.16364	-229.15144
3a	-878.66473 ^a	-878.35295	160.4	138.2	-878.44831	-878.43512

	-878.71454 ^b -878.73953 ^c	-878.40249 -878.42725	155.2 156.9	132.9 134.6	-878.49476 -878.52054	-878.48154 -878.50730
Pre-CAT	-11421.81336 ^a -11421.90648	-11421.33044 -11421.42319	233.0 231.9	211.5 210.4	-11421.46897 -11421.56107	-11421.45623 -11421.54831
AgSbF₆	-12042.26473 ^a -12042.27665 ^b	-12042.23550 -12042.24742	119.2 115.7	93.7 90.3	-12042.30635 -12042.31625	-12042.29121 -12042.30111
(AgCl)₄	-22480.50894 ^a -22480.54157 ^b	-22480.48247 -22480.51509	146.3 146.0	120.5 120.3	-22480.56945 -22480.60192	-22480.55414 -22480.58661
CAT-(SbF₆)₂	-18555.23767 -18555.29858	-18554.94781 -18555.00843	233.9 231.4	212.0 209.5	-18555.08689 -18555.14605	-18555.07386 -18555.13301
Cu(OAc)₂·H₂O	-2171.04567 ^a -2171.06563 ^b	-2170.89879 -2170.91996	143.1 143.9	119.5 120.2	-2170.98390 -2171.00433	-2170.96985 -2170.99028
CuOAcSbF₆·H₂O	-8824.71737 ^a -8824.74128 ^b	-8824.60050 -8824.62439	162.3 160.9	138.8 137.4	-8824.69703 -8824.72006	-8824.68306 -8824.70610
CAT-O	-5247.95806 ^b	-5247.60751	178.3	156.3	-5247.71351	-5247.70044
CAT	-11901.58953 ^a -11901.64486 ^b -11901.67687 ^c	-11901.26920 -11901.32431 -11901.35614	204.7 203.7 205.9	182.8 181.8 183.9	-11901.39092 -11901.44542 -11901.47855	-11901.37791 -11901.43240 -11901.46551
TS1	-12342.00105 ^a -12342.08540 ^b -12342.13909 ^c	-12341.50934 -12341.59323 -12341.64634	268.6 261.7 262.5	247.3 240.3 241.1	-12341.66908 -12341.74887 -12341.80245	-12341.65639 -12341.73615 -12341.78969
INT1	-12342.03030 ^a -12342.11225 ^b -12342.17249 ^c	-12341.53659 -12341.61842 -12341.67743	269.6 266.7 261.9	248.1 245.3 240.2	-12341.69690 -12341.77699 -12341.83315	-12341.68412 -12341.76428 -12341.82030
TS2	-12342.00233 ^a -12342.08601 ^b -12342.13993 ^c	-12341.51024 -12341.59357 -12341.64673	269.8 266.8 266.1	248.6 245.5 244.6	-12341.67069 -12341.75222 -12341.80495	-12341.65804 -12341.73956 -12341.79219
INT2	-12342.00323 ^a -12342.08707 ^b -12342.14215 ^c	-12341.50958 -12341.59319 -12341.64774	270.2 268.6 268.7	248.9 247.3 247.2	-12341.67026 -12341.75289 -12341.80750	-12341.65761 -12341.74022 -12341.79475
TS3	-12341.99031 ^a -12342.07474 ^b -12342.12662 ^c	-12341.50271 -12341.58697 -12341.63825	266.1 264.0 264.8	244.8 242.8 243.5	-12341.66097 -12341.74398 -12341.79571	-12341.64829 -12341.73135 -12341.78307
INT3	-12342.01553 ^a -12342.10074 ^b -12342.15225 ^c	-12341.52215 -12341.60679 -12341.65780	265.8 265.2 263.7	244.5 243.9 242.4	-12341.68021 -12341.76448 -12341.81463	-12341.66755 -12341.75182 -12341.80196
INT3 + 2a	-12780.23191 ^a -12780.33749 ^b -12780.38900 ^c	-12779.60073 -12779.70571 -12779.76232	363.7 363.5 361.5	319.1 318.9 316.9	-12779.81703 -12779.92186 -12779.97732	-12779.79049 -12779.89532 -12779.95077
INT4	-12780.23207 ^a	-12779.59748	321.4	300.2	-12779.78860	-12779.77599

	-12780.35085 ^b	-12779.71547	313.7	292.4	-12779.90200	-12779.88934
	-12780.43094	-12779.79495	313.8	292.4	-12779.98153	-12779.96883
TS4	-12780.20775 ^a	-12779.57460	316.4	295.2	-12779.76272	-12779.75013
	-12780.32205 ^b	-12779.68849	314.5	293.3	-12779.87552	-12779.86290
	-12780.40098 ^c	-12779.76642	309.7	288.4	-12779.95057	-12779.93790
INT5	-12551.05508 ^a	-12550.49154	286.0	264.6	-12550.66159	-12550.64885
	-12551.15274 ^b	-12550.58883	282.0	260.8	-12550.75653	-12550.74389
	-12551.21945 ^c	-12550.65540	287.8	266.5	-12550.82656	-12550.81389
INT5 +HOAc	-12780.23682 ^a	-12779.60478	359.2	317.2	-12779.81833	-12779.79339
	-12780.34246 ^b	-12779.71007	355.1	313.4	-12779.92122	-12779.89565
	-12780.40820 ^c	-12779.77562	360.8	319.0	-12779.99020	-12779.96533
INT6	-12780.24061 ^a	-12779.60591	310.8	289.4	-12779.79073	-12779.77798
	-12780.35092 ^b	-12779.71604	314.5	293.3	-12779.90304	-12779.89044
	-12780.42729 ^c	-12779.79152	313.6	292.4	-12779.97801	-12779.96539
TS5	-12780.21296 ^a	-12779.58366	322.0	300.9	-12779.77513	-12779.76258
	-12780.32687 ^b	-12779.69705	312.5	291.3	-12779.88286	-12779.87026
	-12780.40433 ^c	-12779.77374	310.9	289.7	-12779.95861	-12779.94599
INT7	-12780.26348 ^a	-12779.62780	317.7	296.4	-12779.81674	-12779.80407
	-12780.37124 ^b	-12779.73559	319.2	298.1	-12779.92539	-12779.91286
	-12780.44341 ^c	-12779.80662	315.8	294.7	-12779.99440	-12779.98183
TS6	-12780.24559 ^a	-12779.61173	313.0	291.6	-12779.79786	-12779.78516
	-12780.35935 ^b	-12779.72491	312.8	291.5	-12779.91091	-12779.89827
	-12780.43575 ^c	-12779.80065	308.1	286.7	-12779.98385	-12779.97112
CAT + 3a	-12780.25426 ^a	-12779.62215	365.1	321.0	-12779.83923	-12779.81303
	-12780.35940 ^b	-12779.72680	358.9	132.9	-12779.94018	-12779.91394
	-12780.41640 ^c	-12779.78339	362.8	318.5	-12779.99909	-12779.97281
TS1-N	-12342.08236 ^b	-12341.58953	258.8	237.1	-12341.74342	-12341.73050
TS1-O	-5688.38442 ^b	-5687.86227	234.2	212.6	-5688.00154	-5687.98868
TS1-O-N	-5688.38944 ^b	-5687.86696	236.2	214.5	-5688.00740	-5687.99451
CH₃CN						
1a	-440.43790 ^b	-440.26790	104.7	81.8	-440.33019	-440.31655
2a	-438.23039 ^b	-438.09256	97.8	74.4	-438.15070	-438.13682
CAT	-11901.63560 ^b	-11901.31507	204.6	182.7	-11901.43674	-11901.42371
CH₃CN	-132.81377 ^b	-132.76256	60.9	37.0	-132.79875	-132.78454
CAT+ CH₃CN	-12034.44937 ^b	-12034.07763	265.5	219.7	-12034.23549	-12034.20825
COM1- CCN	-12034.48526 ^b	-12034.11054	233.7	212.1	-12034.24951	-12034.23664
TS1-CCN	-12474.90681 ^b	-12474.36075	295.5	274.3	-12474.53648	-12474.52385
TS1a-CCN	-12474.90852 ^b	-12474.36230	299.6	278.5	-12474.54044	-12474.52794

INT1a-CCN	-12474.92851 ^b	-12474.38085	305.5	284.4	-12474.56249	-12474.54999
TS1b-CCN	-12474.90519 ^b	-12474.35912	306.5	285.4	-12474.54136	-12474.52887
INT1	-12342.11332 ^b	-12341.61962	269.2	247.8	-12341.77968	-12341.76698
TS2	-12342.08806 ^b	-12341.59571	268.1	246.8	-12341.75514	-12341.74247
INT2	-12342.08909 ^b	-12341.59532	270.0	248.7	-12341.75589	-12341.74322
TS3	-12342.07661 ^b	-12341.58895	265.8	244.5	-12341.74699	-12341.73437
INT3	-12342.10200 ^b	-12341.60817	265.0	243.7	-12341.76577	-12341.75310
INT4	-12780.35268 ^b	-12779.71753	315.6	294.3	-12779.90520	-12779.89254
TS4	-12780.32427 ^b	-12779.69084	315.5	294.3	-12779.87846	-12779.86584
INT5	-12551.15468 ^b	-12550.59095	284.0	262.8	-12550.75986	-12550.74723
HOAc	-229.18648 ^b	-229.11809	73.1	48.7	-229.16155	-229.14705
INT5+HOAc	-12780.34116	-12779.70904	357.1	311.5	-12779.92141	-12779.89428
INT6	-12780.35290 ^b	-12779.71813	314.5	293.3	-12779.90518	-12779.89257
TS5	-12780.32873 ^b	-12779.69904	314.1	293.0	-12779.88583	-12779.87324
INT7	-12780.37442 ^b	-12779.73879	322.7	301.7	-12779.93070	-12779.91819
3a	-878.70438 ^b	-878.39237	156.3	134.0	-878.48528	-878.47206
3a+CAT	-12780.33998 ^b	-12779.70744	360.9	316.7	-12779.92202	-12779.89577
DMF^a						
1a	-440.44691 ^b	-440.27698	104.7	81.7	-440.33923	-440.32559
DMF	-248.62040 ^b	-248.50841	81.3	57.7	-248.55675	-248.54274
CAT	-11901.63565 ^b	-11901.31512	204.6	182.7	-11901.43679	-11901.42377
COM1-DMF	-12150.29145 ^b	-12149.85652	242.5	221.0	-12150.00073	-12149.98796
TS1a-DMF	-12590.72002 ^b	-12590.11246	311.5	290.5	-12590.29768	-12590.28520
INT1a-DMF	-12590.74145 ^b	-12590.13250	312.8	291.8	-12590.31853	-12590.30602
INT1	-12342.11738 ^b	-12341.62370	267.8	246.4	-12341.78293	-12341.77023

- a) Without dispersion; b) with half of the sum of solute dispersion and solvent-solute dispersion; c) only with full solute dispersion.

Table S2 Coordinates of all Stationary points for the reaction of **CAT+1a+2a**, computed at B3LYP-D3a+IDSCRF/ TZP-DKH(-dfg) level in DCE solvent

1a				2a			
C	0.24456	0.10694	-0.03917	C	1.94717	0.66478	0.25002
C	0.79385	-1.16780	-0.19525	C	1.94721	-0.66469	0.24999
C	2.17073	-1.35000	-0.14747	H	2.76151	1.34974	0.43726
C	3.01171	-0.26229	0.06059	H	2.76160	-1.34960	0.43720
C	2.47146	1.01148	0.21048	C	0.56199	1.14075	-0.06825
C	1.09717	1.19544	0.15318	O	0.16855	2.28218	-0.16047
H	0.15581	-2.02358	-0.38267	C	0.56204	-1.14073	-0.06817
H	2.58671	-2.34190	-0.27956	O	0.16867	-2.28218	-0.16048
H	4.08524	-0.40588	0.09975	N	-0.21341	-0.00001	-0.24996
H	3.12346	1.86259	0.36890	C	-1.63713	-0.00005	-0.56626
H	0.66595	2.18272	0.25647	H	-1.82696	-0.88291	-1.17684
C	-1.23051	0.37412	-0.09781	H	-1.82700	0.88275	-1.17690
O	-1.67142	1.48427	-0.39799	C	-2.51957	-0.00002	0.67648
N	-2.05104	-0.66174	0.18892	H	-2.33614	0.88639	1.28549
H	-1.66232	-1.51087	0.57132	H	-3.57102	-0.00006	0.38268
C	-3.49526	-0.50650	0.17557	H	-2.33610	-0.88639	1.28556
H	-3.83339	0.17378	0.96130				
H	-3.82281	-0.10489	-0.78343				
H	-3.95232	-1.48245	0.32867				
3a				CAT			
C	1.92677	0.17309	0.11498	Ru	1.23699	0.55452	0.20568
C	3.31709	0.30918	0.10125	C	1.54831	0.09594	2.36162
C	4.14391	-0.77037	-0.17643	C	0.96292	-1.01623	1.73017
C	3.57839	-2.00466	-0.46222	C	1.52849	-1.60382	0.56412
C	2.19652	-2.14482	-0.46232	C	2.70379	-1.08544	-0.01242
C	1.34812	-1.07834	-0.16413	C	3.29823	0.05683	0.61178
H	3.75734	1.27062	0.33699	C	2.73147	0.63323	1.76789
H	5.22006	-0.64551	-0.16778	H	0.00427	-1.37705	2.07625
H	4.20722	-2.85756	-0.68886	H	0.97364	-2.38925	0.07402
H	1.76049	-3.10851	-0.70190	H	4.15208	0.53371	0.14871
C	1.08589	1.35931	0.48085	H	3.15354	1.55072	2.15762
O	0.12475	1.26158	1.24650	C	0.90459	0.74689	3.54601
N	1.45965	2.54063	-0.05142	H	1.30705	0.31731	4.46774
H	2.14999	2.54430	-0.78930	H	1.10284	1.81861	3.56121
C	0.71299	3.75914	0.21025	H	-0.17308	0.58760	3.53475
H	0.58315	3.89512	1.28341	C	3.30840	-1.63608	-1.28174
H	1.27014	4.60305	-0.19237	H	3.78202	-0.79190	-1.79228
H	-0.27626	3.72906	-0.25304	C	4.41062	-2.64197	-0.90800
C	-0.80698	-1.61419	1.19537	H	3.98821	-3.50723	-0.39186
C	-0.13803	-1.35797	-0.16712	H	4.91139	-2.99619	-1.81062

H	-0.90724	-2.67087	1.44190	H	5.16402	-2.19267	-0.25815
H	-0.28699	-2.24778	-0.78924	C	2.28816	-2.25418	-2.23759
C	-2.17094	-0.97055	1.08197	H	2.78335	-2.52900	-3.17000
O	-3.08563	-1.03773	1.87523	H	1.84405	-3.16319	-1.82626
C	-1.03384	-0.31053	-0.81937	H	1.48503	-1.55479	-2.47518
O	-0.80844	0.32242	-1.82772	O	1.42947	1.53931	-1.68268
N	-2.21458	-0.24654	-0.09917	C	0.99547	2.62776	-1.18461
C	-3.34355	0.59335	-0.48662	O	0.82824	2.65054	0.07656
H	-2.93068	1.45188	-1.01524	C	0.66952	3.80349	-2.03841
H	-3.81010	0.94180	0.43421	H	-0.37670	3.73094	-2.34595
C	-4.35005	-0.14814	-1.35765	H	1.29072	3.80635	-2.93223
H	-4.76328	-1.00874	-0.82958	H	0.79801	4.72668	-1.47617
H	-5.17391	0.51798	-1.62075	Sb	-2.51550	-0.40093	-0.10404
H	-3.88577	-0.49590	-2.28193	F	-0.81820	0.51783	-0.50669
H	-0.27280	-1.11485	2.00278	F	-2.72458	-0.68398	-1.96010
				F	-4.13841	-1.28523	0.29917
				F	-2.15521	-0.07921	1.73381
				F	-1.51935	-2.01648	0.02210
				F	-3.36527	1.28047	-0.24931
TS1				INT1			
Ru	0.57872	0.96691	-0.06623	Ru	-3.12885	-0.03733	0.11454
C	0.70306	0.33264	-2.20658	C	-3.66570	0.99396	-1.78330
C	-0.17959	1.43926	-2.06607	C	-2.45715	0.29534	-1.96761
C	0.23544	2.61920	-1.40939	C	-2.35586	-1.09093	-1.65695
C	1.54394	2.74046	-0.85686	C	-3.45734	-1.81503	-1.16318
C	2.40542	1.61528	-0.98546	C	-4.68492	-1.10112	-0.98525
C	2.00462	0.44177	-1.67319	C	-4.78907	0.26720	-1.28014
H	-1.21039	1.33396	-2.37182	H	-1.57054	0.83567	-2.26922
H	-0.49505	3.39671	-1.23962	H	-1.38503	-1.56211	-1.72138
H	3.36519	1.62902	-0.48599	H	-5.52417	-1.60508	-0.52340
H	2.65836	-0.41775	-1.67486	H	-5.70872	0.79091	-1.05631
C	0.21808	-0.94257	-2.81866	C	-3.77391	2.46176	-2.04967
H	0.76290	-1.79961	-2.42818	H	-4.23083	2.61722	-3.03150
H	-0.84660	-1.07789	-2.63800	H	-4.40651	2.94913	-1.30732
H	0.37595	-0.89999	-3.90080	H	-2.79586	2.93827	-2.04728
C	2.03058	3.97325	-0.13198	C	-3.37947	-3.27674	-0.78520
H	2.68414	3.61939	0.67170	H	-4.19451	-3.45607	-0.07767
C	2.88041	4.81153	-1.10226	C	-3.63502	-4.13795	-2.03196
H	2.27352	5.17310	-1.93598	H	-2.83865	-4.00282	-2.76791
H	3.29096	5.67897	-0.58261	H	-3.66663	-5.19378	-1.75728
H	3.71263	4.23619	-1.51192	H	-4.58387	-3.88374	-2.50848

C	0.91891	4.81620	0.49228	C	-2.07095	-3.66152	-0.09339
H	1.36160	5.61489	1.08952	H	-2.11926	-4.70249	0.22988
H	0.29869	5.29139	-0.27171	H	-1.21201	-3.56935	-0.76158
H	0.27473	4.21990	1.13798	H	-1.89527	-3.03902	0.78490
O	-0.43107	1.85698	1.62723	O	-3.75772	-0.67081	2.07321
C	0.38033	1.33189	2.45041	C	-3.83811	0.53321	2.46860
O	1.38294	0.72859	1.96253	O	-3.66372	1.44123	1.59442
C	0.14340	1.40613	3.92227	C	-4.08789	0.86821	3.90089
H	-0.51817	0.58565	4.21065	H	-3.12469	0.96605	4.40790
H	-0.34908	2.34296	4.17831	H	-4.65107	0.07235	4.38482
H	1.08077	1.30342	4.46559	H	-4.61503	1.81718	3.98342
Sb	-3.25589	-0.53694	-0.02663	Sb	4.74061	-0.37808	-0.02812
F	-1.38372	-0.26468	0.33321	F	5.49144	1.18201	-0.81019
F	-3.55393	1.32427	0.21754	F	3.62150	0.73630	1.07962
F	-5.10217	-0.80332	-0.38906	F	3.92696	-1.90313	0.77859
F	-2.91357	-2.38344	-0.30802	F	5.80951	-1.49602	-1.13004
F	-2.90084	-0.21895	-1.87769	F	3.35619	-0.36945	-1.34422
F	-3.51892	-0.85187	1.82536	F	6.07332	-0.36371	1.32308
C	3.10536	-2.52494	0.26981	C	0.01302	1.72992	0.11057
C	3.92210	-3.40774	-0.44082	C	1.05247	1.87636	-0.81077
C	5.29987	-3.22714	-0.45869	C	1.18763	3.06823	-1.51163
C	5.87332	-2.16914	0.23800	C	0.30481	4.11833	-1.28385
C	5.06338	-1.28510	0.94490	C	-0.72535	3.97443	-0.35869
C	3.68562	-1.45512	0.95484	C	-0.88124	2.78011	0.33019
H	3.48760	-4.22418	-1.00585	H	1.74376	1.06441	-0.99447
H	5.92457	-3.91081	-1.02134	H	1.98739	3.17580	-2.23437
H	6.94838	-2.03222	0.22738	H	0.42025	5.05008	-1.82512
H	5.50827	-0.46163	1.49145	H	-1.40715	4.79581	-0.17278
H	3.04428	-0.77311	1.49545	H	-1.68112	2.66198	1.04894
C	1.61319	-2.65418	0.30757	C	-0.15046	0.47376	0.88412
O	0.88211	-1.66929	0.44685	O	-1.28096	-0.02199	1.15216
N	1.11014	-3.89818	0.16970	N	0.94391	-0.12308	1.32641
H	1.74581	-4.68225	0.21492	H	1.84104	0.33605	1.20266
C	-0.31771	-4.16969	0.20670	C	0.93175	-1.39092	2.04119
H	-0.86451	-3.27904	-0.08523	H	0.19166	-2.05421	1.59925
H	-0.54905	-4.98313	-0.48115	H	1.92166	-1.83202	1.95605
H	-0.64119	-4.45719	1.21094	H	0.68168	-1.24534	3.09417
TS2				INT2			
Ru	3.13682	-0.09655	0.06290	Ru	3.00886	-0.06632	0.05421
C	4.19189	-1.06184	-1.62430	C	4.20468	-0.92963	-1.61818
C	3.21428	-0.16481	-2.15951	C	3.19907	-0.05929	-2.14961

C	3.16512	1.17301	-1.75251	C	3.07724	1.27036	-1.72610
C	4.08398	1.67974	-0.78139	C	3.93014	1.78313	-0.70355
C	5.07508	0.78779	-0.28615	C	4.91823	0.91567	-0.16666
C	5.14351	-0.55966	-0.71084	C	5.07002	-0.41557	-0.63641
H	2.44466	-0.55012	-2.81518	H	2.47459	-0.45862	-2.84808
H	2.35209	1.79362	-2.10196	H	2.26335	1.86853	-2.10936
H	5.72920	1.12388	0.50809	H	5.52163	1.25773	0.66405
H	5.84816	-1.23418	-0.24508	H	5.77746	-1.07487	-0.15335
C	4.18698	-2.50953	-1.99802	C	4.31271	-2.35175	-2.06850
H	3.20185	-2.82808	-2.33287	H	3.37803	-2.70163	-2.50282
H	4.89258	-2.66716	-2.81946	H	5.08866	-2.42614	-2.83620
H	4.49542	-3.12825	-1.15667	H	4.58464	-2.99832	-1.23599
C	4.06757	3.10868	-0.29348	C	3.83155	3.19414	-0.17346
H	4.43272	3.08704	0.73783	H	4.08338	3.14299	0.89031
C	5.06585	3.92350	-1.13461	C	4.90031	4.05273	-0.87364
H	4.75454	3.95894	-2.18144	H	4.70279	4.12045	-1.94616
H	5.11264	4.94778	-0.76115	H	4.88721	5.06370	-0.46307
H	6.07111	3.50042	-1.09255	H	5.90276	3.64364	-0.73702
C	2.68512	3.75846	-0.29499	C	2.44857	3.82766	-0.30849
H	2.74867	4.74783	0.16030	H	2.44631	4.80048	0.18530
H	2.30074	3.89424	-1.30866	H	2.18012	3.99667	-1.35400
H	1.97170	3.16394	0.27306	H	1.68291	3.20856	0.15522
O	3.63114	-2.52745	1.58658	O	3.99085	-2.76546	1.35168
C	3.74333	-1.60353	2.40220	C	3.83892	-1.90268	2.21510
O	3.53675	-0.36350	2.09472	O	3.34980	-0.71501	1.99616
C	4.14357	-1.84921	3.83793	C	4.21789	-2.14667	3.66107
H	3.53474	-1.25061	4.51512	H	3.46503	-1.73772	4.33437
H	5.18374	-1.54433	3.97547	H	5.15969	-1.63397	3.87183
H	4.05038	-2.90556	4.07935	H	4.34904	-3.21144	3.84080
C	0.00326	-0.79882	-0.19741	C	0.08343	-0.66504	-0.17046
C	-1.05111	-0.98344	-1.08921	C	-0.84656	-0.76852	-1.19995
C	-1.16139	-2.18174	-1.78397	C	-0.84900	-1.90133	-2.00593
C	-0.23363	-3.19998	-1.58518	C	0.06148	-2.93293	-1.78670
C	0.81563	-3.02167	-0.68995	C	0.97938	-2.84130	-0.74855
C	0.93180	-1.82443	0.00259	C	0.99376	-1.70864	0.06041
H	-1.77445	-0.19794	-1.25869	H	-1.54999	0.03170	-1.38861
H	-1.98023	-2.31959	-2.47922	H	-1.56925	-1.97898	-2.81139
H	-0.33311	-4.13528	-2.12313	H	0.04278	-3.81257	-2.41882
H	1.52686	-3.81732	-0.50701	H	1.67359	-3.64657	-0.54571
H	1.69213	-1.75037	0.78188	H	1.61339	-1.69899	0.95482
C	0.21075	0.45353	0.56592	C	0.20940	0.53221	0.69747

O	1.37954	0.81375	0.88417	O	1.36239	0.90633	1.05409
N	-0.83319	1.17267	0.93515	N	-0.87345	1.17011	1.09245
H	-1.77144	0.84127	0.72260	H	-1.78768	0.81523	0.81657
C	-0.71132	2.41194	1.68906	C	-0.82907	2.34715	1.94875
H	-0.29967	3.20894	1.06821	H	-0.42758	3.20728	1.41116
H	-1.70414	2.70158	2.02454	H	-1.84396	2.57017	2.26835
H	-0.06229	2.27145	2.55283	H	-0.20530	2.15957	2.82219
Sb	-5.25546	0.15451	0.02953	Sb	-5.21640	0.06340	0.02072
F	-3.40904	0.51225	0.41265	F	-3.37443	0.42607	0.42124
F	-5.20651	1.50867	-1.30608	F	-5.15574	1.41834	-1.31364
F	-4.69490	-1.12533	-1.26411	F	-4.64743	-1.21563	-1.26835
F	-5.23844	-1.19068	1.37183	F	-5.20614	-1.28140	1.36337
F	-7.08504	-0.19979	-0.35020	F	-7.04378	-0.28977	-0.37049
F	-5.74146	1.45455	1.32961	F	-5.71357	1.36261	1.31801
TS3				INT3			
Ru	-2.97886	0.16974	-0.06253	Ru	-2.92410	0.36841	-0.09156
C	-3.33545	2.09710	-1.17273	C	-3.65911	1.98589	-1.41013
C	-3.41800	1.00270	-2.05367	C	-3.57338	0.77288	-2.13106
C	-4.31515	-0.08296	-1.82858	C	-4.33026	-0.38749	-1.77300
C	-5.14485	-0.10433	-0.69289	C	-5.07625	-0.40262	-0.59730
C	-5.02506	0.96907	0.24185	C	-5.07101	0.78870	0.20935
C	-4.14405	2.03864	0.00243	C	-4.43499	1.96669	-0.21236
H	-2.74404	0.95341	-2.89985	H	-2.92256	0.72153	-2.99430
H	-4.30190	-0.91605	-2.51505	H	-4.23543	-1.27511	-2.38156
H	-5.58810	0.94113	1.16486	H	-5.57509	0.77756	1.16679
H	-4.04212	2.81023	0.75431	H	-4.47320	2.84480	0.41829
C	-2.41227	3.24747	-1.42819	C	-2.94886	3.22349	-1.86432
H	-1.58446	2.95141	-2.07190	H	-2.08305	2.97498	-2.47792
H	-2.95580	4.05482	-1.92675	H	-3.62290	3.84075	-2.46498
H	-2.00735	3.64055	-0.49701	H	-2.61247	3.81785	-1.01538
C	-6.08879	-1.24152	-0.38276	C	-5.84425	-1.60658	-0.10241
H	-6.05719	-1.37670	0.70224	H	-5.75007	-1.60314	0.98859
C	-7.51702	-0.81824	-0.76917	C	-7.33402	-1.43070	-0.44282
H	-7.59733	-0.66294	-1.84767	H	-7.48363	-1.42844	-1.52509
H	-8.22413	-1.59971	-0.48574	H	-7.91596	-2.25182	-0.02023
H	-7.81524	0.10530	-0.26961	H	-7.73063	-0.49518	-0.04421
C	-5.70905	-2.56972	-1.03429	C	-5.31899	-2.94461	-0.61974
H	-6.38269	-3.35238	-0.68164	H	-5.85572	-3.76274	-0.13690
H	-5.80372	-2.52944	-2.12207	H	-5.47101	-3.04924	-1.69649
H	-4.68981	-2.85830	-0.77865	H	-4.25467	-3.07089	-0.41447
O	-1.78282	-0.98506	2.60017	O	-1.62111	-2.64676	0.82017

C	-2.59160	-1.82366	2.11363	C	-2.31954	-2.06501	1.77207
O	-3.22464	-1.62418	1.03629	O	-2.79869	-0.93362	1.67216
C	-2.80903	-3.12189	2.83894	C	-2.49313	-2.89435	3.00051
H	-1.87301	-3.68394	2.84171	H	-2.90300	-3.86900	2.73077
H	-3.58851	-3.70975	2.36182	H	-3.14592	-2.39076	3.70741
H	-3.07060	-2.91844	3.87811	H	-1.51535	-3.06698	3.45539
C	-0.12005	0.89890	0.37474	Sb	5.34285	-0.26183	-0.15810
C	0.95128	1.78007	0.47755	F	4.84803	-1.55468	1.14567
C	0.84233	2.89245	1.30421	F	3.64407	0.60521	0.12466
C	-0.32194	3.10940	2.03542	F	5.77252	1.04193	-1.47105
C	-1.38663	2.22106	1.93682	F	7.00524	-1.13654	-0.44103
C	-1.31945	1.10843	1.09245	F	6.08959	0.84399	1.19538
H	1.86464	1.61503	-0.07942	F	4.50447	-1.32717	-1.50314
H	1.67116	3.58526	1.38422	C	-0.16411	1.20492	0.50702
H	-0.39424	3.96840	2.69261	C	0.91724	1.93164	1.01909
H	-2.26893	2.37604	2.54716	C	0.67841	3.00365	1.86002
H	-1.75135	0.03117	1.73520	C	-0.63402	3.33413	2.19335
C	-0.13061	-0.29294	-0.49296	C	-1.70596	2.61120	1.68067
O	-1.24697	-0.83570	-0.75787	C	-1.50166	1.53660	0.81268
N	0.98604	-0.80533	-0.97621	H	1.93593	1.66030	0.77083
H	1.88085	-0.40499	-0.71043	H	1.50613	3.57511	2.26111
C	1.00239	-1.98624	-1.82551	H	-0.82303	4.16715	2.86219
H	0.36083	-1.84081	-2.69489	H	-2.70862	2.89715	1.97466
H	2.02568	-2.15255	-2.15295	H	-1.45241	-1.99633	0.08516
H	0.65135	-2.86379	-1.28009	C	-0.02236	0.03005	-0.34645
Sb	5.40876	-0.25252	-0.13963	O	-1.09944	-0.55889	-0.73206
F	3.53809	0.06921	-0.44831	N	1.14374	-0.46216	-0.71630
F	5.82873	1.05964	-1.44964	H	1.99619	-0.01815	-0.39068
F	5.38393	1.09795	1.19792	C	1.28179	-1.64649	-1.55440
F	4.92299	-1.55597	1.15819	H	0.67486	-1.54632	-2.45392
F	7.25465	-0.58257	0.17054	H	2.33030	-1.74324	-1.82121
F	5.36054	-1.58818	-1.49485	H	0.96540	-2.54389	-1.01907
INT4				TS4			
Ru	1.27241	-0.44111	-0.24864	Ru	-1.94747	-0.23170	0.68149
C	0.26722	-1.02346	-2.31038	C	-2.95374	-0.77679	2.73086
C	-0.23944	0.19550	-1.84064	C	-3.17362	0.56618	2.42371
C	0.60635	1.32023	-1.62477	C	-3.76734	0.96359	1.18437
C	1.98239	1.25094	-1.86581	C	-4.20074	0.02035	0.23813
C	2.51517	-0.04980	-2.10583	C	-3.85744	-1.33999	0.49330
C	1.68296	-1.16349	-2.33927	C	-3.22607	-1.72325	1.69522
H	-1.29538	0.30735	-1.65474	H	-2.86038	1.33423	3.11957

H	0.15008	2.24418	-1.30064	H	-3.87921	2.01934	0.98692
H	3.58633	-0.17778	-2.18495	H	-4.08653	-2.09420	-0.24833
H	2.13507	-2.11460	-2.58743	H	-2.97388	-2.76536	1.84592
C	-0.65615	-2.13493	-2.68844	C	-2.37702	-1.20696	4.04084
H	-1.53898	-2.13415	-2.05122	H	-1.89872	-0.37353	4.55399
H	-0.98140	-1.97512	-3.72104	H	-3.17384	-1.59114	4.68401
H	-0.16724	-3.10473	-2.63517	H	-1.64599	-2.00352	3.90809
C	2.87527	2.46433	-1.90783	C	-4.98628	0.38531	-0.99688
H	3.87169	2.15518	-1.58862	H	-4.74803	-0.36001	-1.75752
C	2.97572	2.92089	-3.37726	C	-6.48563	0.27171	-0.66671
H	2.00333	3.24977	-3.75097	H	-6.77608	1.00663	0.08807
H	3.67127	3.75838	-3.45286	H	-7.07790	0.45491	-1.56499
H	3.33672	2.12069	-4.02601	H	-6.74163	-0.72037	-0.28967
C	2.42454	3.60951	-1.00385	C	-4.64778	1.75880	-1.57174
H	3.15844	4.41511	-1.04700	H	-5.20042	1.91051	-2.50002
H	1.46519	4.02336	-1.32155	H	-4.92809	2.56555	-0.89087
H	2.34829	3.28546	0.03302	H	-3.58471	1.84119	-1.79784
Sb	-4.18535	0.22224	-0.42730	Sb	4.50746	0.20289	-0.49274
F	-2.77222	-1.06577	-0.37692	F	2.66056	-0.24058	-0.67494
F	-3.09065	1.33631	-1.53614	F	4.11591	1.06690	1.19120
F	-5.56200	1.53297	-0.47624	F	6.34050	0.64952	-0.26560
F	-5.24526	-0.89963	0.68783	F	4.86589	-0.61798	-2.16609
F	-4.89187	-0.62039	-1.98170	F	4.78029	-1.43819	0.42259
F	-3.43873	1.05388	1.11419	F	4.16868	1.86953	-1.34565
C	-0.49888	-2.20720	1.31798	C	0.81597	-0.06753	1.73217
C	-1.18010	-3.35321	1.73841	C	1.74285	-0.26740	2.74680
C	-0.84148	-4.58628	1.21352	C	1.86196	-1.51822	3.33880
C	0.19505	-4.67323	0.28600	C	1.04581	-2.55910	2.91212
C	0.86888	-3.53418	-0.13924	C	0.11745	-2.36602	1.89570
C	0.50899	-2.28046	0.34482	C	-0.02935	-1.11453	1.29849
H	-1.97617	-3.29010	2.47284	H	2.35600	0.55427	3.09444
H	-1.36833	-5.47719	1.53137	H	2.58538	-1.67717	4.12851
H	0.48396	-5.64070	-0.10932	H	1.13349	-3.53789	3.36925
H	1.68369	-3.64136	-0.84295	H	-0.47493	-3.20421	1.56005
C	-0.69679	-0.87396	1.87203	C	0.57193	1.23611	1.11029
O	-0.00082	0.07535	1.36582	O	-0.58995	1.44873	0.62484
N	-1.49077	-0.63460	2.89731	N	1.52493	2.14219	1.03829
H	-2.05769	-1.39658	3.24616	H	2.46343	1.84223	1.28501
C	-1.64358	0.67501	3.52171	C	1.37306	3.42791	0.37062
H	-2.14730	0.53668	4.47543	H	2.36279	3.85790	0.24314
H	-0.66440	1.11869	3.69613	H	0.90820	3.30037	-0.60677

H	-2.24152	1.32732	2.88770	H	0.76280	4.10582	0.96932
C	2.73261	-1.17269	1.23119	C	-0.21369	-1.20290	-0.61302
C	2.76179	0.23343	1.24541	C	-1.20397	-0.39498	-1.30324
H	2.26629	-1.79735	1.97524	H	0.82619	-0.90652	-0.69589
H	2.25530	0.87174	1.95464	H	-0.94082	0.57558	-1.70197
C	4.00260	-1.64673	0.60293	C	-0.47718	-2.63903	-1.05461
O	4.36238	-2.78367	0.38370	O	0.13022	-3.63881	-0.74476
C	4.09787	0.65093	0.71968	C	-1.97556	-1.29712	-2.18758
O	4.57524	1.76516	0.67502	O	-2.82515	-1.01898	-3.00866
N	4.75442	-0.50711	0.31332	N	-1.53132	-2.60316	-1.94485
C	6.07729	-0.52841	-0.30066	C	-2.07312	-3.78630	-2.60627
H	6.17471	0.38504	-0.88783	H	-3.12441	-3.58175	-2.80736
H	6.09945	-1.38058	-0.98039	H	-2.00932	-4.60933	-1.89449
C	7.19841	-0.62820	0.72639	C	-1.33334	-4.12580	-3.89440
H	7.11009	-1.54555	1.31007	H	-0.28067	-4.33108	-3.69619
H	8.16529	-0.63742	0.21977	H	-1.77482	-5.01397	-4.35022
H	7.17766	0.22339	1.40770	H	-1.40158	-3.30482	-4.60932
H	-0.32031	1.84559	1.34538	H	-1.46374	2.94604	0.20062
O	-0.46208	2.81083	1.20301	O	-2.06781	3.72419	0.14201
O	1.07828	2.97119	2.82551	O	-1.29306	3.80013	-1.96195
C	0.31432	3.50343	2.04780	C	-2.00804	4.24828	-1.09311
C	0.11414	4.98522	1.91846	C	-2.91887	5.43135	-1.25186
H	-0.90163	5.24027	2.22879	H	-2.64495	6.20717	-0.53421
H	0.83056	5.51355	2.54147	H	-2.84892	5.82128	-2.26352
H	0.22002	5.29153	0.87707	H	-3.94796	5.13928	-1.03552
INT5				INT6			
Ru	2.33107	-0.72394	0.26844	Ru	2.51139	-1.01056	0.44115
C	2.71616	-1.52383	2.36463	C	3.62876	-2.22399	2.03515
C	2.67134	-2.64011	1.50228	C	2.80779	-3.11332	1.32659
C	3.42774	-2.63278	0.31421	C	2.84130	-3.12333	-0.09148
C	4.32924	-1.57470	-0.00919	C	3.74662	-2.33486	-0.84376
C	4.42164	-0.49876	0.91693	C	4.58618	-1.45290	-0.10457
C	3.61140	-0.45427	2.06487	C	4.51461	-1.37449	1.30035
H	1.98231	-3.45055	1.69805	H	2.08348	-3.72171	1.85055
H	3.27616	-3.43372	-0.39601	H	2.10663	-3.72045	-0.61275
H	5.04508	0.34939	0.67186	H	5.24479	-0.77461	-0.63198
H	3.64096	0.41449	2.70913	H	5.13050	-0.65779	1.82554
C	1.85971	-1.46648	3.58972	C	3.55229	-2.12134	3.52685
H	0.93787	-2.03059	3.45904	H	2.56093	-2.38607	3.89311
H	2.40941	-1.90461	4.42848	H	4.27369	-2.81022	3.97605
H	1.61066	-0.44010	3.85361	H	3.80544	-1.11840	3.86972

C	5.19362	-1.57547	-1.24918	C	3.85931	-2.41667	-2.34972
H	5.33763	-0.52601	-1.51980	H	4.17545	-1.42653	-2.69496
C	6.56905	-2.17287	-0.91194	C	4.96440	-3.41575	-2.72732
H	6.47833	-3.22313	-0.62284	H	4.70149	-4.42440	-2.39868
H	7.22495	-2.11860	-1.78296	H	5.10076	-3.43764	-3.81028
H	7.05090	-1.63623	-0.09240	H	5.91982	-3.14997	-2.27083
C	4.56315	-2.29101	-2.44416	C	2.54397	-2.75998	-3.05064
H	5.18735	-2.14528	-3.32722	H	2.67127	-2.67839	-4.13130
H	4.48720	-3.36842	-2.27863	H	2.23055	-3.78495	-2.83952
H	3.56632	-1.90806	-2.66583	H	1.73961	-2.08915	-2.74694
C	-0.31754	-0.44793	0.16959	C	-0.64282	0.72373	0.15777
C	-1.12566	-1.09115	1.11635	C	-1.64434	0.99891	1.08845
C	-1.36221	-0.50587	2.34305	C	-1.75026	2.25872	1.65868
C	-0.77681	0.72232	2.64520	C	-0.85489	3.24884	1.28408
C	0.00714	1.37445	1.71292	C	0.12112	2.98448	0.32876
C	0.24485	0.82472	0.44149	C	0.25119	1.72418	-0.25267
H	-1.56664	-2.04923	0.87209	H	-2.33921	0.22341	1.38059
H	-2.00384	-0.99878	3.06255	H	-2.52817	2.46066	2.38445
H	-0.95678	1.18548	3.60795	H	-0.92318	4.24056	1.71557
H	0.40286	2.35079	1.95431	H	0.77279	3.79436	0.02898
C	-0.04858	-1.12814	-1.13155	C	-0.52817	-0.66563	-0.35302
O	1.15675	-1.34040	-1.43861	O	0.55455	-1.30283	-0.37850
N	-1.05352	-1.52181	-1.88272	N	-1.64363	-1.25114	-0.76538
H	-1.99577	-1.26929	-1.58384	H	-2.49295	-0.69688	-0.81909
C	-0.86762	-2.24440	-3.13385	C	-1.70197	-2.63870	-1.19335
H	-0.13185	-3.03645	-3.00257	H	-1.20472	-3.27965	-0.46576
H	-1.82168	-2.67782	-3.42400	H	-2.74910	-2.92245	-1.26955
H	-0.52320	-1.57423	-3.92345	H	-1.21803	-2.77543	-2.16239
C	0.94896	1.62242	-0.66390	C	1.29327	1.44128	-1.33003
C	2.33225	1.03682	-0.93673	C	2.56480	0.70754	-0.82986
H	0.30516	1.64714	-1.54778	H	0.81933	0.90698	-2.15389
H	2.48396	0.64998	-1.94205	H	3.03128	0.28940	-1.73121
C	1.22059	3.06964	-0.25755	C	1.86662	2.75531	-1.86114
O	0.40064	3.92500	0.00320	O	1.36541	3.53265	-2.63995
C	3.29732	2.12336	-0.65412	C	3.47928	1.84582	-0.49842
O	4.50881	2.12547	-0.78244	O	4.43996	1.85676	0.26399
N	2.58429	3.25033	-0.22085	N	3.08925	2.95651	-1.22936
C	3.21588	4.51886	0.12883	C	3.85718	4.19639	-1.32176
H	4.19566	4.27742	0.53918	H	4.36295	4.32534	-0.36533
H	2.60993	4.97182	0.91363	H	3.13865	5.00617	-1.44764
C	3.34511	5.45878	-1.06372	C	4.85751	4.17850	-2.47027

H	2.36523	5.69988	-1.47775	H	4.34979	4.05118	-3.42719
H	3.82053	6.38988	-0.74969	H	5.40489	5.12241	-2.49740
H	3.95713	5.01098	-1.84789	H	5.58050	3.37033	-2.34726
Sb	-5.03932	-0.03349	-0.14708	O	1.63725	0.17749	2.01577
F	-3.48195	-0.78496	-0.98377	C	2.08734	1.01465	2.79820
F	-6.12187	-1.15233	-1.23962	O	3.26288	1.59218	2.68034
F	-4.95700	-1.40745	1.16798	C	1.31821	1.45116	4.00103
F	-3.90958	1.05587	0.92440	H	0.35425	0.95303	4.03157
F	-6.58436	0.71503	0.67515	H	1.89246	1.21707	4.90019
F	-5.06113	1.30754	-1.49438	H	1.18144	2.53293	3.97362
				H	3.71585	1.41100	1.81371
				Sb	-5.66459	-0.18713	-0.15901
				F	-4.00806	0.15111	-1.08453
				F	-6.05967	1.66787	-0.26215
				F	-6.50769	-0.47550	-1.83675
				F	-5.18195	-2.03243	-0.07653
				F	-7.29702	-0.52942	0.75238
				F	-4.76959	0.08943	1.50111
TS5				INT7			
Ru	2.34508	-1.17519	0.51826	Ru	2.59989	-1.82787	0.23582
C	3.23212	-2.62737	1.96746	C	3.43045	-3.85482	0.28313
C	2.35614	-3.30754	1.08176	C	2.59123	-3.73200	-0.86730
C	2.53212	-3.20257	-0.31833	C	2.79364	-2.69557	-1.79240
C	3.56796	-2.42425	-0.89158	C	3.84000	-1.73976	-1.63278
C	4.41329	-1.72325	0.01104	C	4.66400	-1.87277	-0.49339
C	4.25787	-1.81936	1.41319	C	4.47301	-2.91540	0.45263
H	1.51582	-3.86251	1.47493	H	1.74403	-4.39482	-0.98431
H	1.78697	-3.65310	-0.95879	H	2.07584	-2.57262	-2.59056
H	5.14396	-1.02713	-0.37966	H	5.40811	-1.11210	-0.28968
H	4.88683	-1.22486	2.06109	H	5.07942	-2.94301	1.34710
C	3.02152	-2.69595	3.44507	C	3.15989	-4.90336	1.31367
H	1.96168	-2.75486	3.68858	H	2.09132	-5.09372	1.40914
H	3.51010	-3.59545	3.83119	H	3.64523	-5.83772	1.01715
H	3.45718	-1.83472	3.94950	H	3.55268	-4.61032	2.28620
C	3.79842	-2.31771	-2.38264	C	4.09199	-0.62168	-2.61995
H	4.20760	-1.31828	-2.56377	H	4.55321	0.19366	-2.05357
C	4.86517	-3.34216	-2.80229	C	5.10841	-1.10125	-3.66986
H	4.51184	-4.36154	-2.62795	H	4.70103	-1.93019	-4.25398
H	5.08769	-3.23811	-3.86574	H	5.34692	-0.28861	-4.35852
H	5.79444	-3.20533	-2.24619	H	6.03748	-1.43722	-3.20573
C	2.52811	-2.46981	-3.22029	C	2.82592	-0.08084	-3.28537

H	2.75427	-2.26272	-4.26717	H	3.07450	0.79458	-3.88696
H	2.13187	-3.48685	-3.17168	H	2.37801	-0.81619	-3.95822
H	1.74487	-1.78307	-2.89684	H	2.07730	0.20597	-2.54735
C	-0.62812	0.93225	0.31383	C	-0.28003	0.73280	1.20047
C	-1.70457	1.03534	1.19570	C	-1.22710	0.41446	2.18075
C	-1.85830	2.16087	1.98960	C	-1.41220	1.23119	3.28345
C	-0.93464	3.19222	1.89064	C	-0.65301	2.38767	3.41278
C	0.12556	3.10120	0.99630	C	0.27819	2.71491	2.43798
C	0.30016	1.97826	0.19115	C	0.48501	1.90381	1.32213
H	-2.40957	0.21918	1.27803	H	-1.80563	-0.49510	2.08709
H	-2.69435	2.22917	2.67399	H	-2.14296	0.96525	4.03716
H	-1.04081	4.08050	2.50232	H	-0.79031	3.03944	4.26743
H	0.81641	3.92959	0.92070	H	0.84759	3.63253	2.54031
C	-0.52066	-0.31357	-0.49211	C	-0.11866	-0.20286	0.05149
O	0.51789	-1.02719	-0.57035	O	1.00992	-0.53503	-0.41091
N	-1.60475	-0.68482	-1.15035	N	-1.22376	-0.65729	-0.51050
H	-2.42985	-0.09448	-1.10159	H	-2.12470	-0.32548	-0.17440
C	-1.70447	-1.93773	-1.88084	C	-1.22514	-1.61142	-1.60982
H	-1.37984	-2.76783	-1.25365	H	-0.88137	-2.59080	-1.27149
H	-2.74482	-2.08288	-2.15941	H	-2.24464	-1.69135	-1.97816
H	-1.08784	-1.91702	-2.78061	H	-0.56950	-1.26762	-2.40903
C	1.43760	1.87967	-0.81097	C	1.47544	2.35760	0.27306
C	2.63517	0.98238	-0.42631	C	2.94067	2.46382	0.73075
H	1.01379	1.52763	-1.75691	H	1.41414	1.70263	-0.59384
H	2.76045	0.21600	-1.19390	H	3.57978	1.68761	0.31354
C	2.08707	3.22485	-1.14186	C	1.15288	3.75856	-0.25508
O	1.53135	4.22992	-1.52728	O	0.08261	4.15969	-0.65069
C	3.85489	1.83740	-0.57480	C	3.40735	3.82789	0.27361
O	5.01517	1.51339	-0.41585	O	4.52706	4.28536	0.34593
N	3.45191	3.11353	-0.95627	N	2.31633	4.51179	-0.24294
C	4.38893	4.20034	-1.23392	C	2.38654	5.88433	-0.74100
H	5.23702	4.06239	-0.56443	H	3.14628	6.39519	-0.15039
H	3.88341	5.12893	-0.97064	H	1.41908	6.34257	-0.53815
C	4.84111	4.22185	-2.68875	C	2.71770	5.94908	-2.22643
H	3.99137	4.35666	-3.35933	H	1.95800	5.43673	-2.81832
H	5.53405	5.05018	-2.84721	H	2.75491	6.99095	-2.54964
H	5.35306	3.29522	-2.95206	H	3.68826	5.49480	-2.43056
O	1.33270	-0.37776	2.21762	O	1.41821	-2.12886	2.01438
C	1.78944	0.67167	2.74817	C	1.96467	-1.13055	2.58373
O	2.66558	1.39384	2.17482	O	2.84083	-0.49852	1.91332
C	1.30357	1.07307	4.10640	C	1.61772	-0.73315	3.97716

H	0.42098	0.50346	4.38424	H	0.74743	-1.28269	4.32624
H	2.10019	0.88158	4.82998	H	2.46804	-0.95240	4.62705
H	1.09139	2.14080	4.12229	H	1.43028	0.33857	4.02240
H	2.70718	0.99025	0.99572	H	3.04314	2.40765	1.81501
Sb	-5.48246	-0.18396	-0.28822	Sb	-5.45939	-0.31719	-0.47397
F	-4.02771	0.74913	-1.14974	F	-3.77621	-0.03561	0.42058
F	-6.68247	1.17530	-0.85238	F	-6.33620	0.50253	0.99983
F	-5.77177	-1.13305	-1.91279	F	-5.26003	1.37127	-1.32131
F	-4.21858	-1.50948	0.25087	F	-4.49874	-1.13855	-1.90795
F	-6.89374	-1.13837	0.55589	F	-7.11232	-0.60060	-1.36734
F	-5.13236	0.77097	1.31945	F	-5.60286	-2.01124	0.37848
TS6				HOAc			
Ru	0.84343	1.59898	0.68032	H	1.88083	0.41053	0.00000
C	2.50171	3.06192	0.73033	O	1.25192	-0.34352	0.00000
C	2.35208	2.57237	-0.58331	O	-0.23441	1.33840	0.00000
C	1.10269	2.64446	-1.26586	C	0.00000	0.15164	0.00000
C	-0.03746	3.19176	-0.65814	C	-1.03199	-0.93855	0.00000
C	0.08849	3.59466	0.70909	H	-0.90044	-1.57167	0.87940
C	1.33294	3.55768	1.38140	H	-2.02801	-0.50476	0.00000
H	3.18024	2.06858	-1.06005	H	-0.90044	-1.57167	-0.87940
H	1.02508	2.17464	-2.23387				
H	-0.79245	3.89948	1.25798				
H	1.38040	3.82859	2.42758				
C	3.80103	2.97001	1.46424				
H	4.40615	2.15260	1.08073				
H	4.35133	3.90704	1.33753				
H	3.63579	2.82040	2.53123				
C	-1.38438	3.32529	-1.33376				
H	-2.12302	2.90453	-0.64303				
C	-1.69883	4.82249	-1.50571				
H	-0.97534	5.29397	-2.17523				
H	-2.69197	4.94495	-1.94095				
H	-1.67999	5.35844	-0.55528				
C	-1.49739	2.59433	-2.66906				
H	-2.51605	2.68692	-3.04940				
H	-0.83130	3.03292	-3.41715				
H	-1.26138	1.53776	-2.56080				
Sb	3.39466	-1.30215	-0.47710				
F	4.39058	0.17596	0.19136				
F	3.06967	-0.32047	-2.08028				
F	2.36652	-2.75690	-1.13432				

F	3.64998	-2.22178	1.16128
F	4.96920	-2.05730	-1.22229
F	1.78710	-0.51399	0.26903
C	-1.20621	-2.13544	-0.02531
C	-0.42875	-3.22143	0.38491
C	-0.85979	-4.05546	1.40697
C	-2.08677	-3.81855	2.01286
C	-2.85944	-2.73759	1.60930
C	-2.42988	-1.87066	0.60539
H	0.52434	-3.39460	-0.09628
H	-0.24210	-4.88709	1.72407
H	-2.44399	-4.47224	2.79994
H	-3.81796	-2.57245	2.08866
C	-0.69304	-1.27669	-1.14488
O	-0.57308	-0.04829	-1.05196
N	-0.37297	-1.93264	-2.26834
H	-0.52160	-2.93101	-2.30644
C	0.22320	-1.26359	-3.41283
H	0.57901	-2.02174	-4.10761
H	-0.50634	-0.63161	-3.92337
H	1.06474	-0.65266	-3.09202
C	-3.30767	-0.71091	0.18609
C	-3.94803	0.11734	1.31008
H	-2.72148	-0.05093	-0.45192
H	-3.51005	1.10920	1.40493
C	-4.49689	-1.16538	-0.66003
O	-4.47273	-1.90683	-1.61724
C	-5.41272	0.22466	0.95102
O	-6.26948	0.86147	1.52579
N	-5.64429	-0.55917	-0.17041
C	-6.96022	-0.71390	-0.78635
H	-7.69446	-0.64192	0.01530
H	-6.99734	-1.71890	-1.20551
C	-7.22460	0.33354	-1.86080
H	-6.49172	0.26060	-2.66555
H	-8.21671	0.18045	-2.28947
H	-7.18675	1.33997	-1.44156
O	1.18749	0.64521	2.57533
C	-0.02771	0.28063	2.66133
O	-0.81821	0.71810	1.77186
C	-0.48859	-0.64322	3.73696

H	0.23965	-0.68126	4.54430			
H	-1.45987	-0.32508	4.11449			
H	-0.60550	-1.64226	3.31256			
H	-3.86947	-0.35716	2.28875			
Pre-CAT				AgSbF₆		
Ru	-1.84608	0.36115	-0.45981	Ag	-2.35344	-0.00000 0.00001
C	-2.60071	2.43949	-0.34519	Sb	1.09622	0.00000 0.00000
C	-3.56202	1.61898	-0.97203	F	-0.35797	1.28690 0.23265
C	-4.02539	0.42582	-0.34576	F	-0.35800	-1.28690 -0.23251
C	-3.53503	0.02268	0.91356	F	2.38306	-1.35471 -0.25112
C	-2.56564	0.86791	1.54741	F	2.38313	1.35468 0.25095
C	-2.10995	2.04561	0.93967	F	1.01388	0.34429 -1.85713
H	-3.88618	1.84716	-1.97766	F	1.01416	-0.34429 1.85711
H	-4.68106	-0.22521	-0.90389			
H	-2.08795	0.53305	2.45814			
H	-1.29621	2.59267	1.39345			
C	-2.06208	3.66006	-1.02214			
H	-2.16773	3.58993	-2.10428			
H	-2.61618	4.53984	-0.68155			
H	-1.01016	3.80614	-0.78086			
C	-3.96029	-1.25922	1.59154			
H	-3.11397	-1.57481	2.20820			
C	-5.14693	-0.96879	2.52400			
H	-6.02041	-0.64578	1.95207			
H	-5.41925	-1.86975	3.07718			
H	-4.90809	-0.18700	3.24781			
C	-4.27807	-2.39635	0.62049			
H	-4.45439	-3.31673	1.18007			
H	-5.18106	-2.19361	0.03975			
H	-3.45466	-2.56649	-0.07387			
Cl	-1.93820	-0.94415	-2.52350			
Cl	-0.47428	-1.49706	0.50025			
Ru	1.76162	-0.42501	0.15927			
C	2.55026	-2.33776	-0.67494			
C	2.81358	-1.29085	-1.57818			
C	3.47655	-0.10631	-1.14699			
C	3.91396	0.06109	0.18527			
C	3.64686	-1.01076	1.09406			
C	2.97752	-2.17615	0.68213			
H	2.42479	-1.34284	-2.58583			
H	3.56273	0.71300	-1.84561			

H	3.87312	-0.87854	2.14341				
H	2.71771	-2.92697	1.41614				
C	1.79279	-3.55509	-1.10109				
H	1.22533	-3.97368	-0.27145				
H	1.10044	-3.31937	-1.90797				
H	2.49470	-4.31607	-1.45495				
C	4.59664	1.31292	0.68276				
H	4.27921	1.43678	1.72149				
C	4.19487	2.57744	-0.07500				
H	4.55558	2.56718	-1.10655				
H	3.11184	2.70339	-0.08472				
H	4.63571	3.44949	0.41117				
C	6.11940	1.10894	0.66198				
H	6.62109	1.98001	1.08796				
H	6.41713	0.23195	1.24045				
H	6.48072	0.97747	-0.36122				
Cl	0.40671	1.15465	-1.21305				
Cl	1.24667	0.98893	2.10086				
(AgCl)₄				CAT-(SbF₆)₂			
Ag	1.13834	1.13834	1.13834	Ru	-0.32732	0.90057	0.40233
Cl	-1.48766	1.48766	1.48766	C	0.13587	1.80134	2.34650
Cl	1.48766	-1.48766	1.48766	C	1.15085	2.13330	1.42258
Cl	1.48766	1.48766	-1.48766	C	0.84231	2.71388	0.16287
Ag	-1.13834	-1.13834	1.13834	C	-0.49292	2.99420	-0.20747
Ag	-1.13834	1.13834	-1.13834	C	-1.51884	2.68216	0.73796
Ag	1.13834	-1.13834	-1.13834	C	-1.21435	2.09670	1.97910
Cl	-1.48766	-1.48766	-1.48766	H	2.16867	1.82937	1.61996
				H	1.64532	2.83141	-0.55099
				H	-2.55691	2.78137	0.44749
				H	-2.02463	1.76007	2.61308
				C	0.45017	1.06639	3.60843
				H	0.64093	1.79025	4.40643
				H	-0.38636	0.43945	3.91586
				H	1.33641	0.44646	3.48319
				C	-0.84244	3.49280	-1.58989
				H	-1.93169	3.45156	-1.67286
				C	-0.40125	4.95779	-1.72741
				H	0.68635	5.04708	-1.67703
				H	-0.72745	5.34869	-2.69217
				H	-0.83250	5.58398	-0.94424
				C	-0.25295	2.61012	-2.69635

	H	-0.54664	3.00339	-3.67029
	H	0.83813	2.58980	-2.66508
	H	-0.62055	1.58657	-2.61793
	Sb	-2.61745	-1.36640	-0.18235
	F	-1.63484	0.06760	-1.15143
	F	-1.15716	-1.00278	1.11711
	F	-3.36508	-2.65221	0.95576
	F	-3.90574	-1.46478	-1.53799
	F	-3.55187	0.03552	0.67170
	F	-1.50679	-2.62034	-1.02046
	Sb	2.89174	-0.96305	-0.22770
	F	0.96562	-0.49974	-0.53416
	F	3.04847	-1.25020	-2.08313
	F	4.70973	-1.33383	0.09899
	F	2.55492	-0.59859	1.60724
	F	3.23110	0.88781	-0.48729
	F	2.34337	-2.74675	0.03001
Cu(OAc)₂·H₂O				
	Cu	0.00637	-0.03791	0.00008
	O	1.69063	-0.27551	-1.08770
	C	2.34378	-0.34961	0.00050
	O	1.69059	-0.27497	1.08854
	C	3.83280	-0.49323	0.00003
	H	4.16352	-1.03062	-0.88723
	H	4.16818	-0.99870	0.90395
	H	4.27790	0.50513	-0.02003
	O	-1.68354	-0.27310	-1.08850
	C	-2.33489	-0.35864	-0.00012
	O	-1.68372	-0.27187	1.08832
	C	-3.82127	-0.53085	-0.00002
	H	-4.14456	-1.05597	-0.89715
	H	-4.28680	0.45841	0.00351
	H	-4.14359	-1.06149	0.89424
	O	0.04250	2.26496	-0.00046
	H	-0.39474	2.65997	-0.77323
	H	-0.39892	2.66037	0.76973
CuOAcSbF₆·H₂O				
	Cu	-1.59125	0.56947	-0.27584
	O	-3.42907	0.60208	0.47522
	C	-3.56940	-0.60071	0.07697
	O	-2.56899	-1.10887	-0.52821
	C	-4.81479	-1.37555	0.32120
	H	-4.66693	-1.99465	1.21027
	H	-5.01464	-2.03762	-0.52047
	H	-5.65444	-0.70609	0.49636
	Sb	1.65488	-0.21926	0.05031
	F	0.14062	0.11185	-1.20688
	F	0.24715	-0.24359	1.34726
	F	2.98929	-0.44025	1.35198
	F	2.86263	-0.08374	-1.38182
	F	1.43836	-2.06333	-0.23551
	F	1.68608	1.68686	0.26024
	O	-0.94314	2.40531	0.01946
	H	-1.38119	2.89772	0.73938
	H	0.02196	2.46724	0.16960

Table S3 Coordinates of all Stationary points for the reaction of **CAT**+**1a**+**2a**, computed at B3LYP+IDSCRF/ TZP-DKH(-dfg) level in DCE solvent

1a				2a			
C	0.24463	0.10924	-0.04174	C	-1.94984	-0.66470	0.24980
C	0.79291	-1.16629	-0.20067	C	-1.94980	0.66480	0.24984
C	2.17007	-1.35114	-0.15164	H	-2.76450	-1.35002	0.43347
C	3.01294	-0.26526	0.06296	H	-2.76440	1.35017	0.43354
C	2.47378	1.00910	0.21840	C	-0.56381	-1.14069	-0.06591
C	1.09904	1.19601	0.15808	O	-0.17275	-2.28281	-0.16312
H	0.15234	-2.02088	-0.39056	C	-0.56376	1.14071	-0.06599
H	2.58464	-2.34405	-0.28769	O	-0.17261	2.28280	-0.16312
H	4.08701	-0.41081	0.10354	N	0.21453	-0.00001	-0.23994
H	3.12711	1.85898	0.38354	C	1.63770	-0.00006	-0.56482
H	0.67088	2.18509	0.26613	H	1.82373	0.88276	-1.17657
C	-1.23225	0.37590	-0.10452	H	1.82369	-0.88294	-1.17650
O	-1.67104	1.48733	-0.41050	C	2.53170	-0.00003	0.67104
N	-2.05118	-0.65715	0.18867	H	2.35463	-0.88621	1.28227
H	-1.65996	-1.50922	0.56761	H	3.58028	-0.00007	0.36733
C	-3.49759	-0.51087	0.18703	H	2.35467	0.88621	1.28220
H	-3.83083	0.18394	0.96359				
H	-3.84131	-0.13380	-0.77793				
H	-3.94444	-1.48797	0.36772				
3a				CAT			
C	-2.11044	0.38524	0.08891	Ru	1.26352	0.55495	0.19812
C	-3.13214	1.33038	-0.04874	C	1.67864	0.15355	2.35734
C	-2.84527	2.68321	-0.16209	C	1.09022	-0.98357	1.77193
C	-1.52121	3.10400	-0.15270	C	1.62363	-1.59057	0.59942
C	-0.50177	2.17032	-0.02666	C	2.76581	-1.06421	-0.03537
C	-0.77092	0.80680	0.10353	C	3.35155	0.11271	0.53195
H	-4.16428	1.00067	-0.04113	C	2.81929	0.70470	1.69750
H	-3.65021	3.40234	-0.25357	H	0.15502	-1.35937	2.17049
H	-1.28024	4.15621	-0.24560	H	1.07620	-2.40931	0.15195
H	0.52779	2.51236	-0.03390	H	4.17628	0.59702	0.02220
C	-2.47695	-1.06078	0.28518	H	3.23535	1.64214	2.04927
O	-1.97856	-1.74449	1.18099	C	1.09020	0.81177	3.56723
N	-3.40502	-1.55236	-0.56292	H	1.56917	0.41211	4.46790
H	-3.69366	-0.98843	-1.35012	H	1.25858	1.89025	3.54811
C	-3.87369	-2.92576	-0.47535	H	0.01865	0.61813	3.63626
H	-4.18162	-3.15317	0.54495	C	3.34847	-1.64434	-1.30410
H	-4.72578	-3.04623	-1.14151	H	3.78104	-0.80494	-1.85907
H	-3.09363	-3.63496	-0.76238	C	4.49689	-2.59928	-0.92707
C	0.38241	-0.16287	0.25430	H	4.11724	-3.45914	-0.36761
C	1.12098	-0.11677	1.60547	H	4.98125	-2.96829	-1.83428

H	0.02243	-1.17874	0.08941	H	5.25308	-2.09928	-0.31655
H	0.88914	-0.96428	2.24948	C	2.32455	-2.33449	-2.20739
C	1.49312	0.03897	-0.77750	H	2.80690	-2.62631	-3.14294
O	1.36633	0.16918	-1.97494	H	1.92590	-3.24270	-1.74704
C	2.59403	-0.11101	1.25745	H	1.48812	-1.67367	-2.44775
O	3.53226	-0.17357	2.02186	O	1.35558	1.48600	-1.73028
N	2.71534	0.00402	-0.12133	C	0.94443	2.59081	-1.24799
C	4.00206	0.07791	-0.81332	O	0.82115	2.64678	0.01826
H	4.69503	0.57700	-0.13689	C	0.59989	3.74542	-2.12274
H	3.85329	0.70840	-1.68930	H	-0.45486	3.66575	-2.40710
C	4.53187	-1.29428	-1.21647	H	1.20296	3.72447	-3.03099
H	3.84258	-1.79580	-1.89723	H	0.74243	4.68387	-1.58648
H	5.49082	-1.18228	-1.72555	Sb	-2.57041	-0.40635	-0.07667
H	4.68323	-1.92789	-0.34155	F	-0.85282	0.48013	-0.41939
H	0.90017	0.79207	2.16929	F	-2.72085	-0.69946	-1.94167
				F	-4.23015	-1.25770	0.26046
				F	-2.29551	-0.07282	1.77124
				F	-1.62311	-2.04436	0.10157
				F	-3.39452	1.28734	-0.27241
TS1				INT1			
Ru	0.52155	1.03877	-0.06380	Ru	-3.16402	-0.01268	0.13695
C	0.60553	0.57109	-2.25771	C	-3.78150	0.95969	-1.77330
C	-0.40345	1.53921	-1.99623	C	-2.59331	0.23470	-1.98816
C	-0.10968	2.71633	-1.27308	C	-2.49844	-1.14464	-1.64134
C	1.20184	2.97742	-0.77795	C	-3.58470	-1.83674	-1.07519
C	2.19201	1.98233	-1.02231	C	-4.78591	-1.09067	-0.84522
C	1.90912	0.81292	-1.77296	C	-4.88575	0.26891	-1.18311
H	-1.42631	1.32102	-2.26777	H	-1.71520	0.74682	-2.35674
H	-0.92468	3.37773	-1.01627	H	-1.53988	-1.63397	-1.74317
H	3.16962	2.09334	-0.57121	H	-5.60795	-1.56436	-0.32389
H	2.66742	0.04908	-1.86901	H	-5.78455	0.81489	-0.92944
C	0.25966	-0.70699	-2.95509	C	-3.88594	2.41726	-2.09989
H	0.93523	-1.50936	-2.66552	H	-4.37799	2.53383	-3.07003
H	-0.76603	-1.00069	-2.73915	H	-4.48506	2.94536	-1.35775
H	0.34940	-0.55623	-4.03542	H	-2.90368	2.88256	-2.15755
C	1.57140	4.22673	-0.00863	C	-3.53707	-3.29957	-0.68774
H	2.30912	3.92161	0.74040	H	-4.20898	-3.41372	0.16870
C	2.25854	5.21366	-0.97127	C	-4.10377	-4.14102	-1.84634
H	1.56805	5.54054	-1.75258	H	-3.46481	-4.06628	-2.72951
H	2.58881	6.09684	-0.42176	H	-4.15567	-5.19092	-1.55307
H	3.13101	4.76891	-1.45331	H	-5.10844	-3.81858	-2.12635

C	0.40238	4.89390	0.71898	C	-2.15436	-3.79838	-0.26555
H	0.77774	5.71856	1.32687	H	-2.22948	-4.83053	0.07965
H	-0.32225	5.31475	0.01776	H	-1.44279	-3.78618	-1.09421
H	-0.11709	4.19486	1.37488	H	-1.74653	-3.20023	0.55054
O	-0.49004	1.65737	1.74724	O	-3.71001	-0.56999	2.14609
C	0.43959	1.19414	2.47695	C	-3.77674	0.64883	2.49482
O	1.47717	0.77116	1.88214	O	-3.62575	1.52023	1.57950
C	0.30600	1.13219	3.96328	C	-3.99021	1.04361	3.91883
H	-0.16463	0.18343	4.23231	H	-3.01527	1.15913	4.39884
H	-0.33021	1.94018	4.32018	H	-4.54347	0.27008	4.44812
H	1.28587	1.17630	4.43504	H	-4.51323	1.99667	3.97494
Sb	-3.22775	-0.76523	-0.01426	Sb	4.81461	-0.42176	-0.03107
F	-1.35286	-0.45269	0.30343	F	5.57460	1.13984	-0.80324
F	-3.55966	1.09384	0.22024	F	3.68336	0.69103	1.06607
F	-5.07406	-1.06969	-0.34936	F	3.99482	-1.94971	0.76530
F	-2.84735	-2.60813	-0.28104	F	5.89384	-1.53684	-1.12685
F	-2.91846	-0.45561	-1.87586	F	3.44335	-0.40902	-1.36164
F	-3.46798	-1.07291	1.84338	F	6.13566	-0.40939	1.33328
C	3.36642	-2.40235	0.17057	C	0.05994	1.76086	0.04219
C	4.19514	-3.29546	-0.51386	C	1.10493	1.87959	-0.87827
C	5.57024	-3.09315	-0.54500	C	1.26992	3.06479	-1.58507
C	6.13040	-2.00463	0.11522	C	0.41195	4.13712	-1.36419
C	5.30911	-1.11118	0.79726	C	-0.62296	4.02218	-0.43997
C	3.93335	-1.30153	0.81726	C	-0.80852	2.83467	0.25484
H	3.77062	-4.13787	-1.04761	H	1.77985	1.05169	-1.05509
H	6.20304	-3.78443	-1.08878	H	2.07440	3.14976	-2.30549
H	7.20297	-1.85134	0.09547	H	0.55092	5.06328	-1.90923
H	5.74272	-0.26387	1.31558	H	-1.28492	4.86051	-0.25846
H	3.28536	-0.61172	1.34049	H	-1.60984	2.74161	0.97624
C	1.87492	-2.56146	0.22156	C	-0.12808	0.51461	0.83178
O	1.12070	-1.58578	0.27222	O	-1.26348	0.02915	1.09347
N	1.40870	-3.82813	0.20480	N	0.95927	-0.07924	1.30092
H	2.07350	-4.58292	0.29991	H	1.86066	0.37018	1.17423
C	-0.00721	-4.15390	0.26726	C	0.93788	-1.32623	2.05245
H	-0.59052	-3.28804	-0.02942	H	0.18847	-1.99535	1.63552
H	-0.22126	-4.98451	-0.40598	H	1.92247	-1.78160	1.97500
H	-0.30259	-4.43941	1.28031	H	0.69695	-1.14794	3.10256
TS2				INT2			
Ru	3.16182	-0.10310	0.04015	Ru	3.05344	-0.08447	0.04040
C	4.23414	-1.11305	-1.61502	C	4.28174	-1.00077	-1.58871
C	3.32876	-0.16232	-2.18245	C	3.33190	-0.09410	-2.16178

C	3.33348	1.17373	-1.76367	C	3.24530	1.23994	-1.74377
C	4.23774	1.62597	-0.75205	C	4.07974	1.72590	-0.69188
C	5.16164	0.67760	-0.22722	C	5.01031	0.81973	-0.11615
C	5.17533	-0.66735	-0.65882	C	5.12889	-0.51800	-0.57451
H	2.57009	-0.50077	-2.87581	H	2.62443	-0.46570	-2.89231
H	2.56897	1.83953	-2.13902	H	2.47000	1.86772	-2.15922
H	5.80204	0.97297	0.59440	H	5.59510	1.14111	0.73629
H	5.82540	-1.38110	-0.17266	H	5.79442	-1.20054	-0.06538
C	4.17472	-2.55543	-2.01032	C	4.35856	-2.42590	-2.04096
H	3.18199	-2.83106	-2.36200	H	3.41881	-2.75491	-2.48122
H	4.88230	-2.72666	-2.82758	H	5.13583	-2.51396	-2.80612
H	4.45193	-3.20126	-1.17845	H	4.61641	-3.08289	-1.21183
C	4.28166	3.05334	-0.25346	C	4.03237	3.14875	-0.17912
H	4.58168	3.00353	0.79786	H	4.24532	3.09762	0.89315
C	5.38127	3.81045	-1.02291	C	5.16931	3.94619	-0.84793
H	5.13924	3.87631	-2.08641	H	5.01562	4.01439	-1.92754
H	5.46959	4.82586	-0.63324	H	5.19180	4.96019	-0.44542
H	6.35343	3.32419	-0.92452	H	6.14438	3.48932	-0.67074
C	2.94557	3.79317	-0.33121	C	2.68796	3.85185	-0.36526
H	3.04583	4.77227	0.13932	H	2.72136	4.82978	0.11714
H	2.63389	3.96283	-1.36462	H	2.45946	4.02070	-1.42027
H	2.15849	3.24479	0.18521	H	1.87645	3.27944	0.08172
O	3.63168	-2.52415	1.67663	O	4.01567	-2.73117	1.51643
C	3.66971	-1.56684	2.45766	C	3.76894	-1.84044	2.32699
O	3.43857	-0.34441	2.09369	O	3.26979	-0.67531	2.01960
C	4.00302	-1.74230	3.92214	C	4.01987	-2.01773	3.81138
H	3.37118	-1.10715	4.54215	H	3.14711	-1.70707	4.38619
H	5.03948	-1.43910	4.08883	H	4.85293	-1.37975	4.11480
H	3.89174	-2.78499	4.21079	H	4.26389	-3.05455	4.03050
C	-0.03320	-0.83500	-0.22377	C	0.04183	-0.68514	-0.23685
C	-1.10824	-1.05956	-1.08257	C	-0.93760	-0.83364	-1.21446
C	-1.25013	-2.29632	-1.70019	C	-0.98513	-2.00325	-1.96516
C	-0.33343	-3.31486	-1.45614	C	-0.07170	-3.02981	-1.73794
C	0.73826	-3.09626	-0.59643	C	0.90072	-2.89078	-0.75485
C	0.88637	-1.85953	0.01739	C	0.96105	-1.71890	-0.00673
H	-1.82569	-0.27622	-1.28543	H	-1.64897	-0.04123	-1.40639
H	-2.08539	-2.46355	-2.36888	H	-1.74550	-2.11425	-2.72854
H	-0.45747	-4.28046	-1.93153	H	-0.12651	-3.94107	-2.32110
H	1.44243	-3.89005	-0.38026	H	1.59662	-3.69376	-0.54696
H	1.66945	-1.74440	0.76821	H	1.62219	-1.67330	0.85916
C	0.19582	0.45865	0.46407	C	0.19685	0.54127	0.58512

O	1.36923	0.83727	0.73962	O	1.35550	0.92042	0.91695
N	-0.84052	1.20093	0.81440	N	-0.87489	1.20415	0.97699
H	-1.78401	0.86217	0.64138	H	-1.79813	0.84811	0.73650
C	-0.70151	2.47788	1.50113	C	-0.80480	2.40556	1.79852
H	-0.24622	3.22443	0.84892	H	-0.37180	3.23624	1.23961
H	-1.69423	2.81568	1.78799	H	-1.81623	2.66808	2.09831
H	-0.08328	2.36971	2.39209	H	-0.19714	2.22772	2.68546
Sb	-5.31429	0.19853	0.02836	Sb	-5.27951	0.10544	0.02791
F	-3.45915	0.54454	0.38721	F	-3.42967	0.46677	0.40066
F	-5.26982	1.55008	-1.31092	F	-5.23509	1.45787	-1.31048
F	-4.77745	-1.09002	-1.26783	F	-4.72892	-1.17846	-1.26566
F	-5.29137	-1.14359	1.37456	F	-5.25420	-1.23727	1.37344
F	-7.14961	-0.14550	-0.33350	F	-7.11163	-0.24778	-0.34168
F	-5.78064	1.50402	1.33084	F	-5.76097	1.40744	1.32870
TS3				INT3			
Ru	-2.98530	0.17440	-0.06964	Ru	-2.93124	0.36053	-0.08944
C	-3.40366	2.10226	-1.18268	C	-3.71716	1.97364	-1.40050
C	-3.47485	1.00288	-2.05839	C	-3.61362	0.76338	-2.12372
C	-4.34713	-0.10026	-1.81864	C	-4.35511	-0.40889	-1.76722
C	-5.16510	-0.13489	-0.67450	C	-5.09888	-0.44110	-0.59135
C	-5.04314	0.93711	0.26273	C	-5.08363	0.74069	0.23162
C	-4.18575	2.02384	0.01000	C	-4.47252	1.93298	-0.18975
H	-2.81744	0.96802	-2.91840	H	-2.97483	0.72691	-2.99676
H	-4.33018	-0.93180	-2.50732	H	-4.25855	-1.28905	-2.38666
H	-5.59165	0.89972	1.19428	H	-5.57664	0.71730	1.19483
H	-4.08907	2.79845	0.75972	H	-4.52073	2.80725	0.44576
C	-2.53011	3.28557	-1.47035	C	-3.05482	3.23327	-1.87147
H	-1.72080	3.02260	-2.15095	H	-2.20467	3.01345	-2.51712
H	-3.12328	4.07419	-1.94176	H	-3.76743	3.83250	-2.44536
H	-2.10044	3.69230	-0.55573	H	-2.70725	3.83573	-1.03258
C	-6.10182	-1.28039	-0.36098	C	-5.88561	-1.64491	-0.11699
H	-6.04104	-1.43747	0.72001	H	-5.73109	-1.70741	0.96578
C	-7.54269	-0.84884	-0.69639	C	-7.38689	-1.39384	-0.35473
H	-7.65672	-0.67119	-1.76835	H	-7.60245	-1.32406	-1.42357
H	-8.24010	-1.63707	-0.40787	H	-7.97410	-2.21637	0.05751
H	-7.82688	0.06328	-0.16866	H	-7.72258	-0.46996	0.11943
C	-5.74558	-2.59849	-1.04879	C	-5.45076	-2.97363	-0.73632
H	-6.41205	-3.38516	-0.69159	H	-6.00416	-3.79276	-0.27468
H	-5.87016	-2.53793	-2.13265	H	-5.65726	-3.00662	-1.80866
H	-4.72077	-2.89744	-0.82816	H	-4.38592	-3.16351	-0.58950
O	-1.79877	-0.94410	2.62293	O	-1.60302	-2.64525	0.88419

C	-2.58685	-1.79990	2.13358	C	-2.27003	-2.02673	1.83726
O	-3.19621	-1.62578	1.03734	O	-2.76404	-0.90567	1.70408
C	-2.81222	-3.08498	2.88222	C	-2.38012	-2.79860	3.11082
H	-1.86032	-3.60941	2.98163	H	-2.74449	-3.80561	2.90341
H	-3.53088	-3.71686	2.36740	H	-3.04144	-2.28902	3.80533
H	-3.16602	-2.85734	3.88886	H	-1.38554	-2.89597	3.55190
C	-0.10908	0.89948	0.36422	Sb	5.36805	-0.26047	-0.16070
C	0.97373	1.76588	0.47981	F	4.87292	-1.55099	1.14663
C	0.87864	2.87235	1.31650	F	3.65835	0.59224	0.09933
C	-0.28650	3.10156	2.04267	F	5.79797	1.04227	-1.47584
C	-1.36353	2.22889	1.93107	F	7.04053	-1.12210	-0.42451
C	-1.30874	1.11837	1.08081	F	6.09073	0.86029	1.19460
H	1.88724	1.59395	-0.07500	F	4.55264	-1.34131	-1.50846
H	1.71833	3.55056	1.40682	C	-0.16275	1.20401	0.48104
H	-0.35030	3.95618	2.70616	C	0.92303	1.92657	0.99101
H	-2.24494	2.39160	2.54086	C	0.69218	2.99839	1.83503
H	-1.75460	0.05758	1.73158	C	-0.61798	3.33394	2.17284
C	-0.12981	-0.28250	-0.51901	C	-1.69470	2.61585	1.66199
O	-1.25044	-0.81256	-0.79019	C	-1.49852	1.54045	0.79174
N	0.98208	-0.79719	-1.01414	H	1.94019	1.65077	0.74072
H	1.88124	-0.41085	-0.74238	H	1.52400	3.56465	2.23469
C	0.98639	-1.96254	-1.88695	H	-0.80193	4.16630	2.84366
H	0.33884	-1.79724	-2.74814	H	-2.69488	2.90607	1.96052
H	2.00620	-2.12697	-2.22582	H	-1.46606	-2.02558	0.11991
H	0.63607	-2.84932	-1.35619	C	-0.02773	0.02719	-0.37390
Sb	5.43526	-0.25547	-0.13640	O	-1.10666	-0.56712	-0.74194
F	3.56025	0.03391	-0.45527	N	1.13748	-0.45650	-0.76269
F	5.83727	1.05833	-1.45148	H	1.99088	-0.01180	-0.44093
F	5.38872	1.10195	1.19458	C	1.27620	-1.63469	-1.61096
F	4.96041	-1.55788	1.16749	H	0.67313	-1.52640	-2.51220
F	7.28471	-0.55838	0.18156	H	2.32576	-1.73088	-1.87532
F	5.41422	-1.59788	-1.48588	H	0.95745	-2.53677	-1.08515
INT4				TS4			
Ru	-1.31163	-0.41957	0.27755	Ru	-1.97953	-0.23423	0.66715
C	-0.26315	-1.02018	2.32514	C	-3.07737	-0.72423	2.69925
C	0.26092	0.18319	1.83236	C	-3.28411	0.60838	2.34146
C	-0.56269	1.33021	1.64103	C	-3.82878	0.96805	1.06770
C	-1.93194	1.29733	1.92392	C	-4.22930	-0.00358	0.13561
C	-2.49067	0.00783	2.17323	C	-3.88373	-1.35360	0.44185
C	-1.68067	-1.12577	2.38924	C	-3.29836	-1.70041	1.67850
H	1.31715	0.26924	1.62693	H	-3.00700	1.39817	3.02843

H	-0.09061	2.24500	1.31071	H	-3.94076	2.01789	0.83924
H	-3.56274	-0.09405	2.28411	H	-4.08376	-2.13169	-0.28382
H	-2.14995	-2.06399	2.65610	H	-3.05353	-2.73795	1.86926
C	0.64172	-2.14720	2.70818	C	-2.58206	-1.11654	4.05577
H	1.53176	-2.16055	2.08072	H	-2.17631	-0.25984	4.59256
H	0.95854	-1.99286	3.74440	H	-3.41066	-1.52323	4.64250
H	0.13944	-3.11033	2.65171	H	-1.81471	-1.88787	3.99145
C	-2.79299	2.53472	2.01349	C	-4.98574	0.31513	-1.13321
H	-3.80602	2.25200	1.72198	H	-4.67906	-0.42119	-1.87865
C	-2.83892	2.96897	3.49445	C	-6.49129	0.12084	-0.86389
H	-1.84891	3.27047	3.84419	H	-6.85463	0.84294	-0.12860
H	-3.51314	3.82010	3.60314	H	-7.05293	0.26623	-1.78834
H	-3.19932	2.16676	4.14083	H	-6.70957	-0.88174	-0.49109
C	-2.34763	3.68769	1.11495	C	-4.70192	1.70208	-1.70937
H	-3.06294	4.50708	1.19661	H	-5.22699	1.81465	-2.65893
H	-1.36990	4.07815	1.40560	H	-5.05094	2.49900	-1.04849
H	-2.31083	3.38126	0.06977	H	-3.63695	1.84281	-1.89808
Sb	4.31711	0.17299	0.41488	Sb	4.54055	0.18478	-0.48887
F	2.93000	-1.14242	0.40255	F	2.69400	-0.27094	-0.66553
F	3.21222	1.28247	1.51817	F	4.12082	1.06867	1.17783
F	5.67208	1.50982	0.43461	F	6.37052	0.64199	-0.25528
F	5.39212	-0.94392	-0.69229	F	4.90474	-0.65838	-2.15094
F	5.06215	-0.63145	1.97362	F	4.81990	-1.44485	0.44749
F	3.54696	0.97179	-1.13448	F	4.20621	1.83656	-1.37274
C	0.36749	-2.22275	-1.36009	C	0.76193	-0.03167	1.79217
C	0.99101	-3.38577	-1.82568	C	1.66939	-0.20272	2.83100
C	0.63859	-4.61510	-1.30032	C	1.78062	-1.43709	3.45880
C	-0.35240	-4.68141	-0.32235	C	0.97485	-2.49119	3.04402
C	-0.97138	-3.52725	0.14527	C	0.06567	-2.32698	2.00439
C	-0.60278	-2.27793	-0.34671	C	-0.07364	-1.09171	1.36979
H	1.75016	-3.33981	-2.59972	H	2.27319	0.63006	3.16973
H	1.11967	-5.51760	-1.65571	H	2.48861	-1.57249	4.26653
H	-0.65013	-5.64377	0.07880	H	1.05568	-3.45747	3.52793
H	-1.75298	-3.62062	0.88817	H	-0.51525	-3.17757	1.67898
C	0.59045	-0.88787	-1.90682	C	0.53140	1.25695	1.13120
O	-0.07403	0.07627	-1.38532	O	-0.61895	1.45968	0.61590
N	1.39221	-0.66666	-2.93197	N	1.49245	2.15812	1.06339
H	1.91891	-1.44995	-3.29867	H	2.42525	1.85364	1.32471
C	1.60801	0.63980	-3.54403	C	1.36398	3.44572	0.39270
H	2.15024	0.48906	-4.47429	H	2.35954	3.86787	0.28532
H	0.65210	1.11339	-3.76454	H	0.91829	3.32560	-0.59446

H	2.19759	1.27389	-2.88329	H	0.74875	4.12850	0.98069
C	-2.80986	-1.11588	-1.19889	C	-0.20042	-1.23615	-0.55396
C	-2.85060	0.28817	-1.15960	C	-1.16760	-0.44879	-1.29537
H	-2.34413	-1.70583	-1.97154	H	0.84139	-0.93914	-0.61135
H	-2.36582	0.95516	-1.85839	H	-0.89605	0.51512	-1.70578
C	-4.08252	-1.62484	-0.60093	C	-0.44195	-2.68444	-0.97272
O	-4.44121	-2.77361	-0.44981	O	0.15458	-3.67477	-0.61445
C	-4.18878	0.67329	-0.60700	C	-1.89688	-1.37421	-2.19486
O	-4.66809	1.78402	-0.50850	O	-2.71115	-1.11475	-3.05723
N	-4.84284	-0.50520	-0.26034	N	-1.45499	-2.67299	-1.91131
C	-6.17943	-0.56688	0.32719	C	-1.96557	-3.87445	-2.56890
H	-6.29513	0.31719	0.95442	H	-3.00612	-3.67576	-2.82417
H	-6.20429	-1.44839	0.96796	H	-1.93572	-4.67904	-1.83415
C	-7.28450	-0.63054	-0.72216	C	-1.16750	-4.24997	-3.81307
H	-7.18024	-1.51919	-1.34612	H	-0.12519	-4.45071	-3.56278
H	-8.25741	-0.67249	-0.22904	H	-1.59019	-5.15069	-4.26191
H	-7.26524	0.25134	-1.36386	H	-1.20228	-3.45061	-4.55426
H	0.22252	1.90736	-1.44393	H	-1.49788	3.00613	0.10828
O	0.42133	2.86810	-1.35861	O	-2.08782	3.79414	0.07469
O	-1.22533	3.04158	-2.87164	O	-1.21069	4.01618	-1.97948
C	-0.37513	3.56566	-2.18316	C	-1.95652	4.41289	-1.11212
C	-0.07733	5.03687	-2.15356	C	-2.82936	5.63130	-1.21491
H	0.91788	5.21082	-2.56897	H	-2.55487	6.34708	-0.43764
H	-0.81597	5.57790	-2.73839	H	-2.71529	6.08752	-2.19423
H	-0.06667	5.40110	-1.12557	H	-3.87281	5.35760	-1.04966
INT5				INT6			
Ru	2.39368	-0.73482	0.25201	Ru	2.58572	-1.05033	0.44404
C	2.91648	-1.62573	2.30512	C	3.67773	-2.41334	1.96447
C	2.86716	-2.69478	1.38769	C	2.74833	-3.20022	1.27390
C	3.56538	-2.60041	0.16623	C	2.71453	-3.17214	-0.14654
C	4.41639	-1.49827	-0.14413	C	3.65744	-2.45532	-0.92256
C	4.50202	-0.45862	0.82512	C	4.59347	-1.65655	-0.20226
C	3.74418	-0.50145	2.00905	C	4.58849	-1.60947	1.20540
H	2.22412	-3.54398	1.57634	H	2.00044	-3.76237	1.81651
H	3.41230	-3.37439	-0.57331	H	1.91056	-3.69431	-0.64547
H	5.08335	0.42370	0.59675	H	5.28813	-1.02658	-0.74357
H	3.76787	0.33811	2.69138	H	5.28477	-0.95989	1.71809
C	2.14575	-1.67687	3.58833	C	3.70114	-2.37224	3.46234
H	1.24701	-2.28446	3.49470	H	2.72499	-2.61136	3.88304
H	2.77745	-2.12729	4.36033	H	4.41887	-3.11012	3.83291
H	1.86777	-0.68074	3.92883	H	4.02121	-1.39796	3.83235

C	5.24359	-1.41841	-1.41021	C	3.72477	-2.53352	-2.43404
H	5.32538	-0.35541	-1.65302	H	4.05307	-1.54976	-2.78696
C	6.66030	-1.95079	-1.12903	C	4.80305	-3.55276	-2.84359
H	6.63529	-3.01205	-0.86867	H	4.53221	-4.55777	-2.51046
H	7.28479	-1.83629	-2.01700	H	4.90860	-3.57336	-3.92991
H	7.13840	-1.41176	-0.30894	H	5.77553	-3.30504	-2.41400
C	4.61940	-2.13078	-2.61241	C	2.38736	-2.85112	-3.10671
H	5.21091	-1.92374	-3.50564	H	2.49387	-2.77215	-4.18970
H	4.60442	-3.21555	-2.48115	H	2.05834	-3.86986	-2.88855
H	3.59820	-1.79448	-2.79706	H	1.60113	-2.16392	-2.79064
C	-0.25926	-0.50949	0.28013	C	-0.45938	0.96644	0.29747
C	-1.00276	-1.20699	1.24285	C	-1.39167	1.35453	1.26106
C	-1.20261	-0.66435	2.49635	C	-1.39465	2.64584	1.76759
C	-0.65224	0.57905	2.80563	C	-0.46620	3.55944	1.29183
C	0.06753	1.28305	1.85842	C	0.44695	3.18183	0.31283
C	0.27581	0.77186	0.56513	C	0.47940	1.88513	-0.20159
H	-1.42263	-2.17278	0.99001	H	-2.10834	0.63167	1.63028
H	-1.79027	-1.20100	3.23083	H	-2.11804	2.93236	2.52081
H	-0.80941	1.01183	3.78627	H	-0.45588	4.57590	1.66682
H	0.43573	2.26819	2.10812	H	1.12995	3.93346	-0.06007
C	-0.04138	-1.13734	-1.05766	C	-0.47958	-0.44761	-0.16290
O	1.15211	-1.33145	-1.41788	O	0.54789	-1.16646	-0.23640
N	-1.07355	-1.50290	-1.78755	N	-1.66017	-0.96084	-0.48557
H	-2.00794	-1.25346	-1.46126	H	-2.48467	-0.36920	-0.46839
C	-0.93167	-2.16681	-3.07801	C	-1.84605	-2.35290	-0.86600
H	-0.19991	-2.97010	-3.00697	H	-1.41104	-3.01555	-0.11750
H	-1.89815	-2.57838	-3.35832	H	-2.91494	-2.54000	-0.93849
H	-0.60523	-1.46266	-3.84528	H	-1.37679	-2.56367	-1.82850
C	0.91148	1.61532	-0.54808	C	1.46078	1.48740	-1.30347
C	2.29477	1.06900	-0.89866	C	2.69337	0.66603	-0.83470
H	0.22816	1.64516	-1.40219	H	0.91626	0.97111	-2.09510
H	2.40392	0.71559	-1.92234	H	3.09001	0.20995	-1.75124
C	1.16516	3.06210	-0.12569	C	2.12128	2.73265	-1.90165
O	0.33568	3.88803	0.19447	O	1.65507	3.51838	-2.69424
C	3.24403	2.18010	-0.64424	C	3.70597	1.73827	-0.56598
O	4.44734	2.21730	-0.83126	O	4.69260	1.69413	0.16159
N	2.52365	3.28301	-0.16182	N	3.38199	2.85295	-1.32467
C	3.13945	4.56468	0.17629	C	4.25531	4.01367	-1.50272
H	4.13757	4.34259	0.55201	H	4.77009	4.17128	-0.55528
H	2.54987	4.99751	0.98436	H	3.60809	4.86913	-1.69357
C	3.20986	5.51938	-1.01132	C	5.25497	3.82779	-2.63927

H	2.21261	5.74474	-1.39139	H	4.74290	3.67821	-3.59074
H	3.67538	6.45685	-0.70162	H	5.88169	4.71707	-2.72592
H	3.80599	5.09390	-1.81959	H	5.90538	2.97175	-2.45315
Sb	-5.14686	-0.03846	-0.17125	O	1.92079	0.20198	2.07719
F	-3.54982	-0.78632	-0.93922	C	2.47773	0.99153	2.84176
F	-6.18702	-1.17059	-1.29125	O	3.68260	1.48478	2.65672
F	-5.10592	-1.40229	1.15595	C	1.81548	1.46836	4.09427
F	-4.05514	1.06663	0.92602	H	0.84840	0.99007	4.21551
F	-6.71895	0.71086	0.59746	H	2.45670	1.25062	4.95050
F	-5.13312	1.29074	-1.53112	H	1.69274	2.55174	4.04693
				H	4.06049	1.28899	1.75676
				Sb	-6.05760	-0.16317	-0.17204
				F	-4.18324	0.16152	-0.43717
				F	-6.31651	1.69245	0.14530
				F	-6.34541	0.11331	-2.03031
				F	-5.73423	-2.01395	-0.49581
				F	-7.90847	-0.50588	0.09939
				F	-5.71253	-0.43427	1.68107
TS5				INT7			
Ru	2.41804	-1.20481	0.49231	Ru	2.64945	-1.71630	-0.14784
C	3.30147	-2.78854	1.81981	C	3.81268	-3.58185	-0.41880
C	2.42981	-3.38265	0.87404	C	3.11243	-3.23463	-1.61112
C	2.61743	-3.16200	-0.51403	C	3.31257	-1.99260	-2.26532
C	3.65983	-2.34652	-1.01347	C	4.13530	-1.00654	-1.69693
C	4.49132	-1.71338	-0.04500	C	4.75849	-1.31827	-0.44870
C	4.32657	-1.92852	1.34150	C	4.64445	-2.59466	0.15404
H	1.58771	-3.97067	1.21208	H	2.38609	-3.92866	-2.01663
H	1.87962	-3.56173	-1.19579	H	2.71867	-1.77198	-3.14074
H	5.22728	-0.98879	-0.36979	H	5.31684	-0.54632	0.06798
H	4.95283	-1.39323	2.04181	H	5.09114	-2.76999	1.12015
C	3.09465	-3.00267	3.28533	C	3.60957	-4.91214	0.23647
H	2.03835	-3.12259	3.52177	H	2.63292	-5.32930	-0.00938
H	3.61519	-3.91765	3.58395	H	4.37134	-5.60886	-0.12593
H	3.50136	-2.18008	3.87172	H	3.70486	-4.82911	1.31720
C	3.92234	-2.13501	-2.49102	C	4.34530	0.36005	-2.31304
H	4.30550	-1.11458	-2.59770	H	4.43341	1.06643	-1.48097
C	5.03526	-3.09615	-2.94737	C	5.68986	0.36444	-3.06540
H	4.71341	-4.13595	-2.85041	H	5.66681	-0.33301	-3.90588
H	5.27977	-2.91346	-3.99519	H	5.89054	1.36264	-3.45796
H	5.94575	-2.96635	-2.35962	H	6.51939	0.08468	-2.41359
C	2.68155	-2.27033	-3.37685	C	3.20362	0.82636	-3.21823

H	2.93425	-1.99544	-4.40178	H	3.37983	1.85816	-3.52524
H	2.31120	-3.29789	-3.40062	H	3.14028	0.22610	-4.12885
H	1.86962	-1.62244	-3.04254	H	2.23930	0.78122	-2.70974
C	-0.59415	0.95246	0.41091	C	-0.31496	0.51163	1.26409
C	-1.65335	1.07794	1.31357	C	-1.21784	-0.03318	2.18541
C	-1.79766	2.22144	2.08374	C	-1.45628	0.58287	3.40217
C	-0.88012	3.25327	1.94337	C	-0.80054	1.76924	3.70757
C	0.16567	3.13974	1.03510	C	0.08548	2.32068	2.79434
C	0.33325	1.99803	0.25304	C	0.35255	1.70980	1.56762
H	-2.35835	0.26476	1.42698	H	-1.71722	-0.96495	1.95543
H	-2.62167	2.30305	2.78136	H	-2.15122	0.14044	4.10510
H	-0.97822	4.15642	2.53396	H	-0.98306	2.26936	4.65107
H	0.85206	3.96875	0.92955	H	0.57215	3.25889	3.03884
C	-0.50712	-0.31098	-0.37487	C	-0.11219	-0.22441	-0.01705
O	0.54043	-1.00359	-0.50576	O	1.02963	-0.40412	-0.54641
N	-1.62021	-0.72391	-0.96098	N	-1.19163	-0.66884	-0.63080
H	-2.45214	-0.14273	-0.91201	H	-2.10668	-0.47072	-0.23107
C	-1.72153	-1.98729	-1.67634	C	-1.15921	-1.41631	-1.88114
H	-1.33169	-2.80029	-1.06449	H	-0.80459	-2.43635	-1.71730
H	-2.77144	-2.16889	-1.88957	H	-2.17137	-1.44292	-2.27733
H	-1.16115	-1.95439	-2.61211	H	-0.49561	-0.92681	-2.59249
C	1.46141	1.89038	-0.76340	C	1.29836	2.40294	0.60859
C	2.67624	1.01434	-0.37538	C	2.71184	2.69173	1.14745
H	1.02977	1.51901	-1.69802	H	1.37249	1.82376	-0.31054
H	2.82598	0.26686	-1.15744	H	3.48321	2.05840	0.70992
C	2.09172	3.24083	-1.11855	C	0.78558	3.78111	0.17326
O	1.52097	4.22433	-1.53727	O	-0.32131	4.05015	-0.23194
C	3.87909	1.89981	-0.50240	C	2.98646	4.14191	0.80509
O	5.04348	1.60543	-0.31645	O	4.02276	4.74859	0.96481
N	3.45518	3.16435	-0.90386	N	1.82634	4.69297	0.28147
C	4.37315	4.27576	-1.15617	C	1.70901	6.09555	-0.12115
H	5.19695	4.16710	-0.45176	H	2.35612	6.66880	0.54180
H	3.83111	5.19119	-0.92111	H	0.67536	6.38828	0.05965
C	4.88715	4.30405	-2.59171	C	2.08978	6.32096	-1.58040
H	4.06466	4.41143	-3.30004	H	1.44213	5.74956	-2.24682
H	5.56144	5.15223	-2.72300	H	1.98270	7.37855	-1.82767
H	5.43806	3.39275	-2.82826	H	3.12551	6.03213	-1.76393
O	1.46558	-0.49454	2.26481	O	1.74455	-1.92876	1.62038
C	1.90049	0.55332	2.81829	C	2.18674	-2.51990	2.71706
O	2.71784	1.33615	2.23876	O	3.33341	-2.89944	2.88700
C	1.45630	0.88664	4.21083	C	1.11959	-2.66197	3.77745

H	0.67017	0.21259	4.53982	H	0.73447	-1.67692	4.04501
H	2.31518	0.80181	4.88075	H	0.28004	-3.23911	3.38595
H	1.11184	1.91967	4.24734	H	1.52727	-3.15210	4.65809
H	2.74686	0.98300	1.04912	H	2.77931	2.57713	2.23077
Sb	-5.64822	-0.18636	-0.31264	Sb	-5.46462	-0.39548	-0.53728
F	-4.08867	0.64921	-1.08455	F	-3.77677	-0.47046	0.39263
F	-6.70834	1.27646	-0.90263	F	-6.32612	-0.04263	1.11933
F	-5.94341	-1.08055	-1.96614	F	-5.19511	1.46369	-0.81721
F	-4.50815	-1.61423	0.24546	F	-4.52096	-0.76745	-2.15699
F	-7.16313	-1.04035	0.45481	F	-7.11846	-0.32099	-1.47037
F	-5.29957	0.71206	1.32830	F	-5.67588	-2.26303	-0.24787
TS6				HOAc			
Ru	0.87037	1.67800	0.65894	O	-0.23227	1.33856	0.00000
C	2.57466	3.09626	0.57159	C	0.00000	0.15127	0.00000
C	2.33954	2.56841	-0.71372	O	1.25219	-0.34437	0.00000
C	1.05770	2.65682	-1.33295	H	1.87998	0.41031	0.00000
C	-0.03364	3.25823	-0.68598	C	-1.03385	-0.93775	0.00000
C	0.17598	3.69941	0.65937	H	-0.90349	-1.57108	0.87925
C	1.45460	3.64425	1.26652	H	-2.02924	-0.50286	0.00000
H	3.12567	2.02445	-1.21845	H	-0.90349	-1.57108	-0.87925
H	0.91810	2.16265	-2.28231				
H	-0.66487	4.05202	1.24224				
H	1.56522	3.94961	2.29866				
C	3.91205	2.99077	1.23568				
H	4.46738	2.13403	0.85966				
H	4.48676	3.89889	1.03120				
H	3.80529	2.89946	2.31668				
C	-1.40925	3.41506	-1.30012				
H	-2.12826	3.08320	-0.54335				
C	-1.66448	4.91252	-1.56117				
H	-0.96484	5.30101	-2.30509				
H	-2.67701	5.05231	-1.94340				
H	-1.56214	5.51036	-0.65391				
C	-1.63202	2.59675	-2.57126				
H	-2.66834	2.70342	-2.89591				
H	-0.99796	2.95118	-3.38828				
H	-1.42784	1.54009	-2.40361				
Sb	3.46323	-1.37259	-0.46121				
F	4.60048	0.04815	0.10730				
F	3.14771	-0.44072	-2.09577				
F	2.30254	-2.77151	-1.01134				

F	3.73467	-2.25293	1.19994
F	4.95345	-2.26434	-1.23746
F	1.95261	-0.44866	0.31732
C	-1.30002	-2.21136	0.01797
C	-0.54768	-3.31264	0.43611
C	-0.99629	-4.12951	1.46491
C	-2.21656	-3.85908	2.07149
C	-2.96852	-2.76767	1.65543
C	-2.52310	-1.91993	0.64002
H	0.40201	-3.50908	-0.04414
H	-0.39744	-4.97263	1.78785
H	-2.58647	-4.49596	2.86634
H	-3.92467	-2.58027	2.13190
C	-0.74817	-1.36205	-1.09549
O	-0.52446	-0.15184	-0.96930
N	-0.50932	-2.01246	-2.24422
H	-0.74582	-2.99381	-2.30233
C	0.12158	-1.37180	-3.38809
H	0.37650	-2.14053	-4.11485
H	-0.55180	-0.65241	-3.85834
H	1.03022	-0.85754	-3.07756
C	-3.38612	-0.75649	0.19420
C	-4.00667	0.11974	1.29510
H	-2.79598	-0.12364	-0.46840
H	-3.53669	1.09867	1.37284
C	-4.59092	-1.20878	-0.63548
O	-4.58925	-1.99138	-1.56058
C	-5.46481	0.26702	0.92064
O	-6.30175	0.95136	1.47017
N	-5.71844	-0.54456	-0.17688
C	-7.04041	-0.68730	-0.78749
H	-7.77089	-0.55162	0.00919
H	-7.11048	-1.71097	-1.15386
C	-7.27680	0.31024	-1.91651
H	-6.55017	0.17395	-2.71866
H	-8.27470	0.16293	-2.33338
H	-7.20810	1.33646	-1.55297
O	1.23378	0.78210	2.57923
C	0.01013	0.45905	2.70727
O	-0.78480	0.86823	1.80801
C	-0.46156	-0.37257	3.85340

H	0.33719	-0.51304	4.57786			
H	-1.31819	0.10746	4.32796			
H	-0.79130	-1.34345	3.47924			
H	-3.95372	-0.33776	2.28408			
Pre-CAT				AgSbF₆		
Ru	-1.86711	-0.34097	0.46992	Ag	2.36018	0.00000 0.00002
C	-2.54429	-2.45476	0.33452	Sb	-1.09922	-0.00000 -0.00000
C	-3.51670	-1.68378	1.01027	F	0.35767	1.28659 -0.22029
C	-4.05017	-0.50268	0.41955	F	0.35773	-1.28667 0.21932
C	-3.62391	-0.05648	-0.84950	F	-2.38554	-1.35735 0.23912
C	-2.63085	-0.84432	-1.51951	F	-2.38562	1.35745 -0.23810
C	-2.10893	-2.01762	-0.95384	F	-1.01973	0.32618 1.86000
H	-3.80579	-1.94796	2.01787	F	-1.02100	-0.32617 -1.86013
H	-4.71613	0.10825	1.01012			
H	-2.19759	-0.47458	-2.43942			
H	-1.29167	-2.52383	-1.44704			
C	-1.94784	-3.67509	0.96503			
H	-2.01807	-3.63378	2.05151			
H	-2.49180	-4.56031	0.62194			
H	-0.90166	-3.78824	0.68460			
C	-4.14071	1.20368	-1.51143			
H	-3.29210	1.63592	-2.05056			
C	-5.21581	0.82993	-2.54788			
H	-6.09154	0.39425	-2.06026			
H	-5.53951	1.72090	-3.08939			
H	-4.84163	0.10959	-3.27799			
C	-4.65896	2.26030	-0.53449			
H	-4.90140	3.17374	-1.08029			
H	-5.57181	1.93313	-0.03047			
H	-3.91439	2.50210	0.22504			
Cl	-1.99897	1.06059	2.47798			
Cl	-0.46025	1.47017	-0.55701			
Ru	1.79318	0.42142	-0.17795			
C	2.59659	2.38350	0.54632			
C	2.85429	1.38920	1.50894			
C	3.51192	0.17790	1.14817			
C	3.95837	-0.06592	-0.16990			
C	3.68472	0.94774	-1.14165			
C	3.01479	2.13613	-0.80073			
H	2.47226	1.50516	2.51401			
H	3.59928	-0.59785	1.89534			

H	3.91186	0.75388	-2.18129		
H	2.75678	2.84252	-1.57828		
C	1.86646	3.64093	0.90228		
H	1.26322	3.99546	0.06776		
H	1.21428	3.48843	1.76098		
H	2.59175	4.42069	1.15373		
C	4.67112	-1.33226	-0.59111		
H	4.34905	-1.53214	-1.61680		
C	4.31916	-2.56047	0.24970		
H	4.67912	-2.47015	1.27759		
H	3.24217	-2.73048	0.27114		
H	4.79348	-3.44408	-0.18080		
C	6.18962	-1.08265	-0.60429		
H	6.71046	-1.96326	-0.98514		
H	6.45471	-0.23440	-1.23859		
H	6.56105	-0.88026	0.40362		
Cl	0.40025	-1.06837	1.27863		
Cl	1.28576	-1.08016	-2.06480		
(AgCl)₄				CAT-(SbF₆)₂	
Ag	1.14332	1.14332	1.14332	Ru	-0.35645 0.92321 0.41953
Cl	-1.48998	1.48998	1.48998	C	0.17454 1.91776 2.31072
Cl	1.48998	-1.48998	1.48998	C	1.12538 2.24601 1.31896
Cl	1.48998	1.48998	-1.48998	C	0.73275 2.76871 0.05642
Ag	-1.14332	-1.14332	1.14332	C	-0.63028 2.99454 -0.25011
Ag	-1.14332	1.14332	-1.14332	C	-1.59340 2.67849 0.75865
Ag	1.14332	-1.14332	-1.14332	C	-1.20250 2.15035 2.00203
Cl	-1.48998	-1.48998	-1.48998	H	2.16317 1.98425 1.47152
				H	1.49374 2.89209 -0.70183
				H	-2.64845 2.73739 0.52310
				H	-1.96656 1.81038 2.69027
				C	0.58535 1.26604 3.59293
				H	0.80069 2.04179 4.33384
				H	-0.21104 0.63571 3.98746
				H	1.48228 0.66481 3.45143
				C	-1.07980 3.45052 -1.62012
				H	-2.16511 3.32217 -1.65085
				C	-0.76995 4.94954 -1.77961
				H	0.30722 5.13123 -1.78077
				H	-1.17347 5.30516 -2.72868
				H	-1.21623 5.54193 -0.97878
				C	-0.47799 2.61565 -2.75764

	H	-0.87645	2.96324	-3.71152
	H	0.60889	2.70673	-2.80328
	H	-0.73291	1.56134	-2.64625
	Sb	-2.56253	-1.46606	-0.14595
	F	-1.62565	-0.00447	-1.12171
	F	-1.18917	-0.95711	1.19677
	F	-3.27076	-2.75645	1.01393
	F	-3.77541	-1.70355	-1.55475
	F	-3.63436	-0.10853	0.61100
	F	-1.33986	-2.68386	-0.87540
	Sb	2.92715	-0.90966	-0.24638
	F	0.97654	-0.48716	-0.46306
	F	3.00108	-1.20086	-2.10739
	F	4.76386	-1.24522	0.00825
	F	2.65731	-0.53411	1.59738
	F	3.22571	0.94502	-0.53253
	F	2.43716	-2.70636	0.03870
Cu(OAc)₂·H₂O				
	Cu	-0.00694	-0.05234	-0.00008
	O	-1.69154	-0.27741	1.08783
	C	-2.34554	-0.34336	-0.00043
	O	-1.69152	-0.27727	-1.08857
	C	-3.83711	-0.46635	0.00013
	H	-4.17540	-0.99984	0.88677
	H	-4.17994	-0.96589	-0.90416
	H	-4.26800	0.53809	0.02145
	O	1.68300	-0.27754	1.08865
	C	2.33530	-0.35488	0.00017
	O	1.68316	-0.27697	-1.08839
	C	3.82474	-0.50492	0.00012
	H	4.15611	-1.02466	0.89732
	H	4.27536	0.49110	-0.00389
	H	4.15518	-1.03100	-0.89377
	O	-0.03755	2.26166	-0.00022
	H	0.40071	2.65363	0.77323
	H	0.40848	2.65381	-0.76912
CuOAcSbF₆·H₂O				
	Cu	1.63160	0.55096	0.28234
	O	3.46434	0.61112	-0.47155
	C	3.62333	-0.59171	-0.07965
	O	2.63494	-1.11512	0.53175
	C	4.87634	-1.34983	-0.34085
	H	4.72480	-1.96996	-1.22849
	H	5.09642	-2.01014	0.49698
	H	5.70452	-0.66921	-0.52667
	Sb	-1.68534	-0.21448	-0.05165
	F	-0.11327	0.06396	1.15499
	F	-0.33641	-0.27194	-1.40047
	F	-3.07931	-0.38380	-1.29880
	F	-2.82329	-0.04565	1.43473
	F	-1.51703	-2.06627	0.22376
	F	-1.66684	1.69561	-0.24608
	O	0.96800	2.38149	-0.02012
	H	1.39816	2.87343	-0.74477
	H	0.00094	2.43866	-0.16130

Table S4 Coordinates of all Stationary points for the reaction of **CAT+1a+2a**, computed at B3LYP-D3+IDSCRF/ TZP-DKH(-dft) level in DCE solvent

1a				2a			
C	0.24399	0.10885	-0.04261	C	1.94287	0.66477	0.25422
C	0.79099	-1.16608	-0.20013	C	1.94276	-0.66501	0.25429
C	2.16716	-1.35003	-0.14934	H	2.75590	1.34947	0.44429
C	3.00847	-0.26364	0.06392	H	2.75568	-1.34981	0.44440
C	2.46956	1.01039	0.21595	C	0.55916	1.14068	-0.07134
C	1.09588	1.19615	0.15498	O	0.16411	2.28141	-0.16403
H	0.15125	-2.01902	-0.39181	C	0.55905	-1.14072	-0.07152
H	2.58235	-2.34140	-0.28325	O	0.16380	-2.28139	-0.16403
H	4.08118	-0.40846	0.10563	N	-0.21315	0.00003	-0.26022
H	3.12197	1.85959	0.37900	C	-1.63727	0.00013	-0.56755
H	0.66411	2.18250	0.25979	H	-1.83211	-0.88315	-1.17489
C	-1.22941	0.37534	-0.10276	H	-1.83202	0.88353	-1.17474
O	-1.67196	1.48426	-0.40461	C	-2.50172	0.00007	0.68699
N	-2.04618	-0.66188	0.18729	H	-2.30497	0.88605	1.29199
H	-1.65300	-1.50630	0.57487	H	-3.55781	0.00014	0.41251
C	-3.48984	-0.50888	0.18399	H	-2.30506	-0.88603	1.29184
H	-3.82555	0.15196	0.98697				
H	-3.81909	-0.08378	-0.76370				
H	-3.94514	-1.48860	0.31435				
3a				CAT			
C	1.90326	0.21368	0.13414	Ru	1.24533	0.53512	0.20866
C	3.28469	0.41267	0.14922	C	1.53316	0.12316	2.36738
C	4.16186	-0.62235	-0.14343	C	0.93035	-0.99448	1.76391
C	3.65561	-1.87155	-0.47365	C	1.48501	-1.61411	0.61053
C	2.28152	-2.07222	-0.50236	C	2.66668	-1.12533	0.02148
C	1.38552	-1.05146	-0.18941	C	3.29351	0.00608	0.63240
H	3.67495	1.38730	0.41517	C	2.73469	0.61855	1.77299
H	5.23075	-0.45169	-0.11359	H	-0.03731	-1.32456	2.11264
H	4.32511	-2.68850	-0.71318	H	0.91104	-2.39106	0.13010
H	1.89000	-3.04542	-0.77561	H	4.15510	0.45642	0.15874
C	1.00350	1.35072	0.50831	H	3.17260	1.53563	2.14402
O	0.05611	1.20329	1.28298	C	0.88485	0.82983	3.51543
N	1.30795	2.54618	-0.03378	H	1.26422	0.43083	4.45973
H	1.98765	2.57851	-0.78053	H	1.10265	1.89727	3.48859
C	0.48570	3.71680	0.21525	H	-0.19476	0.68894	3.48800
H	0.35381	3.85858	1.28708	C	3.21330	-1.68858	-1.26654
H	0.98299	4.58904	-0.20383	H	3.85101	-0.91259	-1.69881
H	-0.50216	3.61203	-0.24000	C	4.08727	-2.91104	-0.95285
C	-0.74812	-1.69955	1.13374	H	3.48604	-3.71417	-0.52080
C	-0.08674	-1.38269	-0.21863	H	4.54698	-3.28568	-1.86850

H	-0.84837	-2.76596	1.33116	H	4.88325	-2.66442	-0.24801
H	-0.20386	-2.25327	-0.87236	C	2.11984	-2.01784	-2.28461
C	-2.11092	-1.04949	1.05910	H	2.57662	-2.32218	-3.22698
O	-3.01302	-1.13479	1.86461	H	1.48591	-2.84026	-1.94823
C	-1.00115	-0.33200	-0.83565	H	1.48609	-1.15065	-2.47356
O	-0.78903	0.33108	-1.82761	O	1.48492	1.50140	-1.68301
N	-2.17182	-0.29561	-0.10162	C	1.04039	2.59498	-1.20594
C	-3.30131	0.55900	-0.44548	O	0.84601	2.63182	0.05078
H	-2.89145	1.44221	-0.93398	C	0.73037	3.75847	-2.08057
H	-3.76601	0.86082	0.49198	H	-0.31639	3.69069	-2.38682
C	-4.30310	-0.14939	-1.34785	H	1.35266	3.73741	-2.97289
H	-4.70764	-1.03496	-0.85596	H	0.86767	4.68963	-1.53434
H	-5.13184	0.52044	-1.58284	Sb	-2.47357	-0.37910	-0.09690
H	-3.83368	-0.45402	-2.28427	F	-0.77456	0.50052	-0.56335
H	-0.20759	-1.23877	1.95894	F	-2.72610	-0.69471	-1.94160
				F	-4.09798	-1.23114	0.36161
				F	-2.06871	-0.02273	1.72624
				F	-1.50060	-2.00684	0.04525
				F	-3.29873	1.31305	-0.25551
TS1				INT1			
Ru	0.64138	0.89496	-0.07219	Ru	-2.58682	-0.45893	-0.09037
C	0.72570	0.11884	-2.15930	C	-3.03375	0.21737	-2.13638
C	0.04321	1.36535	-2.11951	C	-1.63754	0.31472	-1.93098
C	0.63635	2.49366	-1.50885	C	-0.89805	-0.79573	-1.45665
C	1.92595	2.41857	-0.90436	C	-1.51221	-2.04231	-1.20899
C	2.58720	1.16202	-0.94478	C	-2.91462	-2.13431	-1.44245
C	2.01293	0.03900	-1.58746	C	-3.66802	-1.03598	-1.90139
H	-0.98213	1.41613	-2.45550	H	-1.14941	1.27122	-2.03810
H	0.04668	3.39241	-1.40618	H	0.13526	-0.65117	-1.17465
H	3.51495	1.03932	-0.40301	H	-3.43215	-3.04354	-1.16524
H	2.51086	-0.91506	-1.52319	H	-4.74093	-1.12234	-1.99659
C	0.05264	-1.09820	-2.70634	C	-3.83862	1.41508	-2.52603
H	0.43511	-2.00121	-2.23513	H	-3.93376	1.44982	-3.61478
H	-1.02363	-1.04388	-2.56014	H	-4.83976	1.36769	-2.09924
H	0.24907	-1.16135	-3.78049	H	-3.35575	2.33294	-2.19582
C	2.58690	3.58078	-0.20732	C	-0.73141	-3.21854	-0.66975
H	3.14756	3.15577	0.63092	H	-1.45500	-4.01833	-0.49076
C	3.59044	4.22829	-1.17420	C	0.27532	-3.70163	-1.72153
H	3.07373	4.65140	-2.03877	H	1.04259	-2.94420	-1.89617
H	4.12567	5.03504	-0.67111	H	0.77279	-4.60863	-1.37463
H	4.32390	3.50584	-1.53613	H	-0.21294	-3.92251	-2.67241

C	1.60882	4.61331	0.34894	C	-0.03886	-2.89769	0.65692
H	2.15493	5.35186	0.93693	H	0.47483	-3.78439	1.03147
H	1.09628	5.15164	-0.45155	H	0.70209	-2.10836	0.53489
H	0.85851	4.14824	0.98732	H	-0.76612	-2.57659	1.40223
O	-0.31646	2.04403	1.49249	O	-3.63504	-1.29984	1.58920
C	0.35418	1.45582	2.39628	C	-4.23364	-0.20009	1.80411
O	1.28675	0.68921	2.01006	O	-4.06030	0.73009	0.95474
C	0.03327	1.64059	3.84120	C	-5.07281	0.00448	3.02021
H	-0.75877	0.93796	4.11099	H	-4.43948	0.41020	3.81285
H	-0.33353	2.64988	4.01996	H	-5.48580	-0.94272	3.36119
H	0.90707	1.43261	4.45513	H	-5.86696	0.72044	2.81698
Sb	-3.27037	-0.27078	-0.05410	Sb	3.74601	-0.12054	-0.02192
F	-1.40093	-0.05291	0.34740	F	3.77871	1.23744	-1.35451
F	-3.52026	1.59244	0.21303	F	3.30641	1.21492	1.28575
F	-5.11532	-0.49001	-0.45124	F	3.61314	-1.43903	1.34405
F	-2.96662	-2.11752	-0.36071	F	4.18541	-1.44700	-1.30994
F	-2.87291	0.07081	-1.89135	F	1.90112	-0.39015	-0.42077
F	-3.56681	-0.60415	1.78875	F	5.58811	0.14598	0.35622
C	2.78645	-2.64425	0.38978	C	-0.37492	2.13657	0.52518
C	3.56864	-3.46389	-0.42563	C	0.75453	2.50374	-0.20473
C	4.94555	-3.28380	-0.48159	C	0.68347	3.56575	-1.09692
C	5.54972	-2.29234	0.28335	C	-0.50302	4.27505	-1.24524
C	4.77268	-1.47554	1.10049	C	-1.62619	3.91819	-0.50288
C	3.39621	-1.64309	1.14741	C	-1.56872	2.84402	0.37171
H	3.10428	-4.22170	-1.04516	H	1.66766	1.93873	-0.11357
H	5.54459	-3.91295	-1.12830	H	1.55592	3.83050	-1.68061
H	6.62317	-2.15378	0.24010	H	-0.55470	5.10422	-1.94019
H	5.24146	-0.70302	1.69810	H	-2.54883	4.47476	-0.61230
H	2.77709	-1.00079	1.75687	H	-2.44302	2.54326	0.93233
C	1.29478	-2.74685	0.43738	C	-0.36628	0.97063	1.44277
O	0.58914	-1.75583	0.64182	O	-1.35366	0.18638	1.51337
N	0.76489	-3.96724	0.21997	N	0.69134	0.79177	2.21285
H	1.38295	-4.76647	0.21711	H	1.46441	1.43695	2.11426
C	-0.66927	-4.20257	0.24884	C	0.89546	-0.35316	3.08677
H	-1.18957	-3.29652	-0.04575	H	0.00202	-0.96805	3.07516
H	-0.91405	-5.00838	-0.44225	H	1.75005	-0.93230	2.73684
H	-1.00658	-4.48206	1.25050	H	1.08617	-0.00874	4.10320
TS2				INT2			
Ru	2.87586	-0.13767	0.05353	Ru	2.72533	-0.10185	0.04581
C	3.69196	-0.99332	-1.81347	C	3.70429	-0.96192	-1.76892
C	2.56766	-0.16603	-2.13727	C	2.65505	-0.06735	-2.14322

C	2.48726	1.16199	-1.70689	C	2.61504	1.26650	-1.70395
C	3.51085	1.71977	-0.88418	C	3.59092	1.74373	-0.78893
C	4.63527	0.90305	-0.57646	C	4.61489	0.84811	-0.37254
C	4.73677	-0.42837	-1.05980	C	4.68163	-0.47678	-0.88092
H	1.72040	-0.60828	-2.64324	H	1.83338	-0.44743	-2.73521
H	1.58382	1.71939	-1.90193	H	1.77329	1.88373	-1.97727
H	5.38651	1.27837	0.10500	H	5.32066	1.16495	0.38238
H	5.55380	-1.05369	-0.72886	H	5.41872	-1.16049	-0.48512
C	3.72404	-2.43096	-2.22117	C	3.71925	-2.37386	-2.25820
H	2.71728	-2.81769	-2.36463	H	2.71539	-2.69880	-2.52735
H	4.26466	-2.52663	-3.16682	H	4.34853	-2.44512	-3.14940
H	4.22527	-3.03327	-1.46614	H	4.10851	-3.03505	-1.48773
C	3.45186	3.12312	-0.33404	C	3.56309	3.13802	-0.21422
H	3.84333	3.07231	0.68648	H	3.84613	3.04583	0.83848
C	4.39148	4.01340	-1.16413	C	4.63848	3.97677	-0.92564
H	4.05138	4.07099	-2.20059	H	4.41064	4.07296	-1.98954
H	4.40202	5.02412	-0.75397	H	4.67208	4.97774	-0.49351
H	5.41405	3.63347	-1.16153	H	5.62850	3.52947	-0.82788
C	2.04585	3.71564	-0.28190	C	2.20005	3.82186	-0.28936
H	2.07571	4.68146	0.22322	H	2.24171	4.77494	0.23872
H	1.64388	3.88492	-1.28313	H	1.91371	4.03430	-1.32166
H	1.36043	3.06988	0.26315	H	1.42197	3.21495	0.17024
O	3.38486	-2.71030	1.10953	O	3.85340	-2.96442	0.90865
C	3.80354	-1.94676	1.99073	C	3.75745	-2.20793	1.87215
O	3.71607	-0.66226	1.89274	O	3.27762	-0.99891	1.82916
C	4.46493	-2.46032	3.24574	C	4.19449	-2.62735	3.26128
H	4.12017	-1.90422	4.11680	H	3.39504	-2.44349	3.97964
H	5.54393	-2.31087	3.16543	H	5.05220	-2.02607	3.56907
H	4.26371	-3.52164	3.36961	H	4.46847	-3.67948	3.26793
C	-0.09249	-0.43200	0.15107	C	0.01730	-0.33355	0.16106
C	-0.98781	-0.22855	-0.89226	C	-0.77106	-0.19063	-0.97845
C	-1.18271	-1.23624	-1.82749	C	-0.85775	-1.23938	-1.88026
C	-0.49421	-2.44197	-1.72209	C	-0.16235	-2.42946	-1.66039
C	0.39167	-2.65062	-0.67187	C	0.60195	-2.58821	-0.51607
C	0.59789	-1.64584	0.26599	C	0.69854	-1.54423	0.40781
H	-1.51673	0.70859	-0.99045	H	-1.29587	0.73654	-1.16412
H	-1.88100	-1.07760	-2.63850	H	-1.47286	-1.12963	-2.76331
H	-0.65777	-3.22194	-2.45532	H	-0.23803	-3.23686	-2.37789
H	0.92211	-3.58841	-0.57047	H	1.12345	-3.51488	-0.31752
H	1.24305	-1.83121	1.11731	H	1.17667	-1.70010	1.36453
C	0.25740	0.62398	1.13013	C	0.26416	0.77887	1.11662

O	1.47771	0.80425	1.40577	O	1.46798	0.99488	1.43543
N	-0.70244	1.33766	1.68438	N	-0.74367	1.49427	1.56713
H	-1.66542	1.07846	1.47386	H	-1.68447	1.21327	1.28861
C	-0.46477	2.39679	2.65257	C	-0.59409	2.61583	2.48224
H	-1.16153	3.21199	2.46448	H	0.45299	2.89977	2.53421
H	-0.61318	2.02834	3.66918	H	-1.18618	3.45590	2.12129
H	0.55611	2.75503	2.55421	H	-0.93955	2.33924	3.47929
Sb	-4.74182	0.00298	-0.01500	Sb	-4.78136	-0.03323	-0.03714
F	-3.23521	0.61548	1.00788	F	-3.18871	0.70734	0.74237
F	-3.91776	0.72018	-1.57956	F	-4.71291	1.33117	-1.36228
F	-3.86114	-1.65524	-0.29491	F	-3.70451	-1.14121	-1.14278
F	-5.51518	-0.68464	1.57840	F	-4.76791	-1.36981	1.31365
F	-6.22723	-0.58881	-1.04772	F	-6.35660	-0.76842	-0.81135
F	-5.58036	1.68036	0.29284	F	-5.81875	1.10130	1.08100
TS3				INT3			
Ru	-2.94627	0.15833	-0.05949	Ru	-2.90737	0.37009	-0.09923
C	-3.06880	2.07883	-1.20421	C	-3.63020	1.99018	-1.40623
C	-3.19532	0.98353	-2.07933	C	-3.55467	0.78049	-2.13349
C	-4.18816	-0.02205	-1.89412	C	-4.30850	-0.38001	-1.77172
C	-5.07437	0.04078	-0.80352	C	-5.04307	-0.39550	-0.58846
C	-4.92952	1.12224	0.11744	C	-5.04595	0.79820	0.21318
C	-3.95216	2.11271	-0.08399	C	-4.40812	1.97399	-0.20967
H	-2.47498	0.86172	-2.87803	H	-2.90159	0.72796	-2.99427
H	-4.20034	-0.86843	-2.56309	H	-4.21032	-1.27047	-2.37432
H	-5.54460	1.15376	1.00581	H	-5.54450	0.78473	1.17277
H	-3.82496	2.88287	0.66475	H	-4.43658	2.85014	0.42316
C	-2.01920	3.12644	-1.40290	C	-2.89588	3.21841	-1.84415
H	-1.19352	2.74129	-1.99998	H	-2.02674	2.95617	-2.44669
H	-2.44438	3.98689	-1.92544	H	-3.55055	3.85244	-2.44758
H	-1.62581	3.47057	-0.44781	H	-2.55819	3.79664	-0.98494
C	-6.10607	-1.02120	-0.51950	C	-5.77429	-1.60991	-0.07170
H	-6.12492	-1.14349	0.56704	H	-5.66290	-1.59199	1.01715
C	-7.48147	-0.50153	-0.96860	C	-7.27079	-1.47456	-0.39276
H	-7.50363	-0.35647	-2.05095	H	-7.43219	-1.48489	-1.47295
H	-8.25529	-1.22438	-0.70616	H	-7.82684	-2.30555	0.04414
H	-7.72819	0.44894	-0.49275	H	-7.68229	-0.54457	0.00286
C	-5.79303	-2.37951	-1.14109	C	-5.21669	-2.93597	-0.58310
H	-6.53432	-3.10886	-0.81209	H	-5.71782	-3.76491	-0.08174
H	-5.83585	-2.34335	-2.23193	H	-5.38358	-3.05612	-1.65558
H	-4.80864	-2.73352	-0.83687	H	-4.14542	-3.02229	-0.39501
O	-1.89175	-1.09855	2.61304	O	-1.59787	-2.63304	0.78351

C	-2.77506	-1.85421	2.11842	C	-2.29909	-2.06301	1.73899
O	-3.38088	-1.59235	1.04002	O	-2.78194	-0.93228	1.65067
C	-3.11860	-3.12631	2.83866	C	-2.47589	-2.90300	2.95851
H	-2.25703	-3.79549	2.79490	H	-2.90261	-3.86731	2.67826
H	-3.97912	-3.60937	2.38398	H	-3.11802	-2.39781	3.67351
H	-3.31297	-2.90984	3.88916	H	-1.49821	-3.09565	3.40441
C	-0.10794	0.78779	0.48742	Sb	5.29153	-0.26311	-0.14954
C	0.97189	1.65404	0.61722	F	4.75444	-1.58083	1.11245
C	0.85947	2.76069	1.45058	F	3.60954	0.62858	0.14127
C	-0.31592	2.98793	2.16126	F	5.75440	1.06916	-1.42174
C	-1.39108	2.11706	2.03156	F	6.93974	-1.16067	-0.44127
C	-1.31849	1.01312	1.17875	F	6.04679	0.78464	1.24474
H	1.89326	1.48143	0.07842	F	4.44791	-1.27102	-1.53431
H	1.69518	3.44166	1.55136	C	-0.15381	1.20611	0.49606
H	-0.38939	3.84297	2.82249	C	0.92627	1.93515	1.00547
H	-2.28889	2.28099	2.61542	C	0.68555	3.00521	1.84805
H	-1.79038	-0.07387	1.78426	C	-0.62708	3.33104	2.18581
C	-0.11873	-0.40664	-0.37646	C	-1.69768	2.60490	1.67585
O	-1.23590	-0.94937	-0.64048	C	-1.49040	1.53344	0.80639
N	0.99708	-0.92405	-0.85282	H	1.94411	1.66635	0.75481
H	1.88966	-0.50395	-0.61275	H	1.51224	3.57869	2.24691
C	1.01305	-2.10362	-1.70295	H	-0.81674	4.16274	2.85518
H	0.35772	-1.96262	-2.56248	H	-2.70110	2.88532	1.97081
H	2.03375	-2.26006	-2.04271	H	-1.42825	-1.97410	0.05427
H	0.67630	-2.98338	-1.15260	C	-0.01259	0.03470	-0.35968
Sb	5.35793	-0.23360	-0.16228	O	-1.09030	-0.55123	-0.74986
F	3.49437	0.11867	-0.47314	N	1.15066	-0.46119	-0.72867
F	5.79344	1.07029	-1.47464	H	2.00402	-0.02052	-0.40127
F	5.34660	1.11958	1.17274	C	1.27934	-1.64524	-1.56790
F	4.84632	-1.52807	1.13487	H	0.65931	-1.54438	-2.45788
F	7.19772	-0.58784	0.15179	H	2.32415	-1.74035	-1.84688
F	5.28802	-1.57032	-1.51460	H	0.96908	-2.54124	-1.02695
INT4				TS4			
Ru	1.23760	-0.41985	-0.25568	Ru	-1.92168	-0.27649	0.73962
C	0.30109	-1.01258	-2.33347	C	-2.76872	-1.15366	2.72366
C	-0.24704	0.18804	-1.86585	C	-3.05076	0.21028	2.63590
C	0.56195	1.33159	-1.61797	C	-3.72844	0.76509	1.50559
C	1.94436	1.29762	-1.82224	C	-4.18981	-0.04578	0.45465
C	2.51613	0.01559	-2.06906	C	-3.80097	-1.41589	0.48591
C	1.72006	-1.11661	-2.33326	C	-3.08299	-1.94715	1.57736
H	-1.30506	0.26937	-1.69115	H	-2.71051	0.87830	3.41612

H	0.07458	2.23720	-1.28895	H	-3.88238	1.83347	1.47233
H	3.59132	-0.08218	-2.11897	H	-4.04781	-2.05698	-0.34952
H	2.20118	-2.05465	-2.57361	H	-2.78586	-2.98718	1.55202
C	-0.58768	-2.14526	-2.72702	C	-2.07610	-1.74428	3.90777
H	-1.47204	-2.17209	-2.09266	H	-1.58651	-0.97256	4.50003
H	-0.91219	-1.98528	-3.75916	H	-2.80323	-2.25525	4.54413
H	-0.07267	-3.10092	-2.67590	H	-1.33053	-2.47610	3.59992
C	2.80361	2.53191	-1.81068	C	-5.05041	0.47512	-0.66612
H	3.81207	2.23269	-1.52410	H	-4.92318	-0.20487	-1.50924
C	2.86318	3.07010	-3.25300	C	-6.51814	0.41040	-0.21083
H	1.87456	3.39181	-3.58742	H	-6.69521	1.09132	0.62490
H	3.53564	3.92801	-3.29616	H	-7.17428	0.70100	-1.03260
H	3.22930	2.31381	-3.94937	H	-6.79514	-0.59636	0.10695
C	2.33425	3.60716	-0.83498	C	-4.67188	1.87494	-1.13967
H	3.03762	4.44000	-0.84652	H	-5.32023	2.16697	-1.96669
H	1.35387	4.00075	-1.10942	H	-4.79071	2.61810	-0.34933
H	2.29397	3.22015	0.18138	H	-3.64381	1.89566	-1.49645
Sb	-4.06508	0.23055	-0.41935	Sb	4.45836	0.21682	-0.47161
F	-2.65497	-1.05864	-0.39812	F	2.59877	-0.11604	-0.69845
F	-2.99963	1.36854	-1.53213	F	4.10885	1.09084	1.21898
F	-5.45088	1.53252	-0.43416	F	6.30912	0.56340	-0.22169
F	-5.10054	-0.90615	0.70424	F	4.79737	-0.61805	-2.14266
F	-4.78740	-0.60161	-1.97194	F	4.62474	-1.43647	0.44465
F	-3.30006	1.05484	1.11388	F	4.21504	1.90385	-1.31415
C	-0.52397	-2.23710	1.24969	C	0.88708	-0.23848	1.64920
C	-1.19647	-3.39892	1.63478	C	1.87523	-0.58935	2.55769
C	-0.82700	-4.61642	1.09406	C	2.04877	-1.92128	2.90908
C	0.23265	-4.67068	0.19013	C	1.21992	-2.88971	2.35589
C	0.89702	-3.51420	-0.20012	C	0.22973	-2.54419	1.44475
C	0.50192	-2.27754	0.29528	C	0.03408	-1.21267	1.08316
H	-2.00951	-3.35822	2.35138	H	2.50024	0.17300	3.00294
H	-1.34729	-5.52062	1.38180	H	2.82437	-2.19925	3.61036
H	0.54573	-5.62585	-0.21498	H	1.34713	-3.93049	2.62775
H	1.73007	-3.59182	-0.88523	H	-0.36905	-3.32437	1.00071
C	-0.74301	-0.91967	1.82832	C	0.59442	1.14412	1.27342
O	-0.06522	0.04936	1.33679	O	-0.59601	1.41158	0.89898
N	-1.52524	-0.71050	2.86747	N	1.52929	2.06907	1.30014
H	-2.07750	-1.48556	3.21042	H	2.48631	1.75158	1.42848
C	-1.64821	0.57812	3.54040	C	1.31590	3.43984	0.85966
H	-2.11878	0.41136	4.50581	H	2.26480	3.96458	0.92594
H	-0.65942	1.00926	3.68939	H	0.96262	3.46071	-0.17195

H	-2.25904	1.25532	2.94731	H	0.58555	3.93898	1.49631
C	2.64807	-1.13676	1.26272	C	-0.25681	-0.98058	-0.78551
C	2.68489	0.26982	1.26265	C	-1.28402	-0.07401	-1.27382
H	2.16504	-1.75218	2.00293	H	0.77807	-0.67178	-0.87539
H	2.16761	0.92022	1.95244	H	-1.05280	0.95575	-1.50826
C	3.91016	-1.62585	0.63495	C	-0.55605	-2.32540	-1.43645
O	4.25828	-2.76651	0.41574	O	0.06911	-3.35751	-1.34105
C	4.02459	0.67207	0.73940	C	-2.11461	-0.82385	-2.23873
O	4.51480	1.78037	0.68997	O	-3.00759	-0.42296	-2.95587
N	4.66822	-0.49342	0.33520	N	-1.67374	-2.15367	-2.22486
C	5.98115	-0.52590	-0.29502	C	-2.26733	-3.21567	-3.02747
H	6.07253	0.37882	-0.89641	H	-3.32939	-2.98934	-3.11575
H	5.99270	-1.38853	-0.96113	H	-2.15356	-4.14288	-2.46665
C	7.10988	-0.61182	0.72409	C	-1.62042	-3.32799	-4.40196
H	7.02092	-1.52000	1.32141	H	-0.55636	-3.54801	-4.31033
H	8.07358	-0.63002	0.21262	H	-2.09041	-4.13284	-4.96928
H	7.09127	0.24988	1.39209	H	-1.73959	-2.39875	-4.95990
H	-0.45051	1.75961	1.29650	H	-1.44124	2.85917	0.49487
O	-0.57743	2.73062	1.17037	O	-2.02280	3.64062	0.32548
O	0.99941	2.83328	2.76197	O	-1.19921	3.39635	-1.74457
C	0.22917	3.39180	2.00772	C	-1.91710	3.98614	-0.96490
C	0.05743	4.87905	1.90898	C	-2.77994	5.16265	-1.31482
H	-0.93485	5.14968	2.27627	H	-2.52262	6.01251	-0.68057
H	0.81643	5.38137	2.50183	H	-2.64672	5.42296	-2.36088
H	0.11595	5.19735	0.86801	H	-3.82614	4.91850	-1.12336
INT5				INT6			
Ru	2.27665	-0.69496	0.22761	Ru	2.52101	-0.98353	0.43306
C	2.82178	-1.57593	2.26146	C	3.69659	-2.10755	2.02823
C	3.02723	-2.58317	1.30041	C	2.96113	-3.05838	1.30389
C	3.76289	-2.29217	0.13170	C	3.01114	-3.05089	-0.11332
C	4.40834	-1.03757	-0.06943	C	3.85917	-2.18324	-0.84575
C	4.25020	-0.05769	0.94995	C	4.62916	-1.25537	-0.08886
C	3.44145	-0.30324	2.07219	C	4.53488	-1.19477	1.31459
H	2.53407	-3.53955	1.40397	H	2.27553	-3.72006	1.81382
H	3.79004	-3.03098	-0.65628	H	2.32696	-3.69191	-0.65029
H	4.67043	0.92593	0.79776	H	5.23591	-0.52224	-0.60380
H	3.26036	0.48873	2.78622	H	5.08071	-0.43362	1.85336
C	1.98696	-1.83010	3.47451	C	3.57346	-2.00312	3.51573
H	1.22023	-2.57833	3.28311	H	2.60069	-2.35381	3.85752
H	2.63310	-2.20098	4.27555	H	4.34345	-2.61690	3.99080
H	1.50887	-0.91815	3.82506	H	3.72150	-0.97688	3.85106

C	5.23787	-0.73200	-1.29146	C	3.97120	-2.21832	-2.35057
H	5.18524	0.35011	-1.42895	H	4.28006	-1.21568	-2.66360
C	6.69956	-1.11727	-1.02348	C	5.08101	-3.19719	-2.75828
H	6.79424	-2.19428	-0.86381	H	4.82186	-4.21616	-2.46082
H	7.32222	-0.84609	-1.87775	H	5.21996	-3.18441	-3.84062
H	7.09187	-0.60760	-0.14170	H	6.03198	-2.93931	-2.28884
C	4.71233	-1.39684	-2.56339	C	2.65400	-2.54283	-3.05486
H	5.27230	-1.03218	-3.42546	H	2.78023	-2.44600	-4.13396
H	4.83393	-2.48206	-2.53429	H	2.33348	-3.56758	-2.85625
H	3.65607	-1.17752	-2.72164	H	1.85602	-1.87195	-2.73672
C	-0.36162	-0.91101	0.11258	C	-0.68595	0.54445	0.16426
C	-0.98172	-1.81052	0.98708	C	-1.67358	0.73621	1.12628
C	-1.26553	-1.43121	2.28296	C	-1.84001	1.97439	1.72651
C	-0.92032	-0.15446	2.72079	C	-1.01637	3.02494	1.35134
C	-0.32533	0.74618	1.86030	C	-0.05219	2.84116	0.36559
C	-0.04326	0.40289	0.52896	C	0.13272	1.60379	-0.24646
H	-1.23350	-2.80223	0.63364	H	-2.30563	-0.08854	1.42119
H	-1.75850	-2.12356	2.95314	H	-2.60957	2.11119	2.47491
H	-1.14201	0.14653	3.73684	H	-1.13117	4.00024	1.80820
H	-0.11698	1.74785	2.20684	H	0.54485	3.69267	0.06883
C	0.01541	-1.38258	-1.25327	C	-0.50200	-0.82136	-0.38246
O	1.24636	-1.45347	-1.51695	O	0.60950	-1.40645	-0.41680
N	-0.91882	-1.74735	-2.10175	N	-1.58654	-1.44305	-0.81867
H	-1.88098	-1.53600	-1.83902	H	-2.45222	-0.91389	-0.86299
C	-0.61669	-2.25728	-3.43143	C	-1.57351	-2.81271	-1.30062
H	0.14455	-3.03316	-3.36736	H	-1.04914	-3.45465	-0.59348
H	-1.52725	-2.67476	-3.85321	H	-2.60390	-3.14521	-1.39912
H	-0.24946	-1.46035	-4.08016	H	-1.07347	-2.88505	-2.26820
C	0.47080	1.42177	-0.49017	C	1.17463	1.39089	-1.33404
C	1.90744	1.08518	-0.88944	C	2.47996	0.73478	-0.82297
H	-0.22066	1.45288	-1.33743	H	0.73337	0.83166	-2.15848
H	2.04869	0.77860	-1.92221	H	2.98725	0.35720	-1.71922
C	0.55562	2.83618	0.07508	C	1.66879	2.74058	-1.84750
O	-0.35682	3.51282	0.50063	O	1.13460	3.48964	-2.63146
C	2.70627	2.28883	-0.58655	C	3.30907	1.92505	-0.45940
O	3.88254	2.50733	-0.81876	O	4.25012	1.99026	0.32408
N	1.87244	3.23237	0.02670	N	2.85879	3.01603	-1.18257
C	2.32735	4.55259	0.44587	C	3.54770	4.30109	-1.24390
H	3.36018	4.44088	0.77266	H	3.98833	4.47069	-0.26218
H	1.71728	4.84476	1.29984	H	2.78701	5.06013	-1.42250
C	2.22064	5.57836	-0.67561	C	4.61097	4.32781	-2.33352

H	1.18647	5.68348	-1.00547	H	4.16425	4.15582	-3.31343
H	2.56875	6.55110	-0.32474	H	5.10473	5.30056	-2.34745
H	2.83283	5.28187	-1.52802	H	5.36826	3.56298	-2.15492
Sb	-4.64474	-0.02193	-0.15782	O	1.51598	0.08845	1.99807
F	-3.26620	-0.88251	-1.18432	C	1.86649	0.96991	2.78166
F	-5.91234	-0.60554	-1.45034	O	2.98523	1.65326	2.68492
F	-4.87161	-1.65201	0.80052	C	1.03296	1.33448	3.96433
F	-3.33633	0.54396	1.08862	H	0.09387	0.79136	3.93938
F	-6.02086	0.81244	0.86053	H	1.58386	1.09185	4.87584
F	-4.35614	1.57024	-1.15998	H	0.84794	2.40840	3.96609
				H	3.48314	1.49673	1.83914
				Sb	-5.51688	-0.20200	-0.17141
				F	-3.84886	0.11407	-1.07985
				F	-5.91366	1.64656	-0.34708
				F	-6.32483	-0.55321	-1.85560
				F	-5.00892	-2.03625	-0.01713
				F	-7.16855	-0.53200	0.70861
				F	-4.68083	0.13136	1.50692
TS5				INT7			
Ru	2.32988	-1.17018	0.49070	Ru	-2.11877	-1.96102	-0.28531
C	3.21450	-2.62433	1.92442	C	-2.78951	-4.04364	-0.30501
C	2.43128	-3.31926	0.96814	C	-2.11978	-3.78403	0.93121
C	2.66986	-3.14102	-0.41622	C	-2.50743	-2.71551	1.75276
C	3.67837	-2.27395	-0.89919	C	-3.59128	-1.85863	1.39337
C	4.44319	-1.57325	0.07478	C	-4.25713	-2.12558	0.18046
C	4.22444	-1.74083	1.45977	C	-3.86406	-3.20162	-0.66357
H	1.60412	-3.93317	1.29422	H	-1.24422	-4.36387	1.19193
H	1.98114	-3.59589	-1.11348	H	-1.90918	-2.49036	2.62310
H	5.14072	-0.81261	-0.24857	H	-5.02690	-1.44450	-0.16037
H	4.77840	-1.13683	2.16399	H	-4.33858	-3.32274	-1.62710
C	2.91765	-2.74955	3.38255	C	-2.30458	-5.12108	-1.22050
H	1.85043	-2.88081	3.55324	H	-1.21819	-5.19767	-1.18907
H	3.43976	-3.62429	3.77964	H	-2.72347	-6.08204	-0.91083
H	3.26026	-1.87359	3.93091	H	-2.61250	-4.92881	-2.24719
C	3.94317	-2.05210	-2.36893	C	-4.02382	-0.69711	2.25532
H	4.32164	-1.02908	-2.46338	H	-4.45700	0.04848	1.58281
C	5.05184	-3.00734	-2.83316	C	-5.13672	-1.17182	3.20255
H	4.72717	-4.04622	-2.73793	H	-4.76334	-1.94198	3.88144
H	5.29513	-2.82158	-3.88037	H	-5.49559	-0.33513	3.80373
H	5.96092	-2.87974	-2.24316	H	-5.98247	-1.58420	2.65030
C	2.69512	-2.17896	-3.24254	C	-2.88085	-0.04239	3.03176

H	2.93324	-1.88557	-4.26535	H	-3.23786	0.87456	3.50208
H	2.33161	-3.20823	-3.27691	H	-2.51633	-0.69286	3.82984
H	1.88383	-1.54602	-2.88102	H	-2.04189	0.20125	2.38125
C	-0.69152	0.76209	0.29804	C	0.32033	1.16376	-1.06777
C	-1.76620	0.76846	1.18500	C	1.37678	1.11961	-1.98377
C	-1.96918	1.84676	2.03049	C	1.48415	2.05943	-2.99424
C	-1.09649	2.92485	1.97829	C	0.53000	3.06271	-3.09803
C	-0.03911	2.92916	1.07595	C	-0.51549	3.12035	-2.18689
C	0.18125	1.85519	0.21930	C	-0.64423	2.18324	-1.16506
H	-2.42727	-0.08533	1.22990	H	2.10589	0.32485	-1.92652
H	-2.80510	1.84184	2.71705	H	2.30344	2.00244	-3.69932
H	-1.23965	3.77485	2.63410	H	0.59904	3.80412	-3.88444
H	0.61430	3.78949	1.03834	H	-1.24248	3.91920	-2.26931
C	-0.52482	-0.43511	-0.56444	C	0.20707	0.07191	-0.06971
O	0.53874	-1.10965	-0.65026	O	-0.92605	-0.31897	0.34289
N	-1.58271	-0.80495	-1.26054	N	1.30863	-0.48614	0.38878
H	-2.41541	-0.22701	-1.19892	H	2.21292	-0.11004	0.11680
C	-1.64218	-2.02873	-2.04069	C	1.28804	-1.64360	1.26814
H	-1.23109	-2.85804	-1.46634	H	0.88768	-2.50993	0.73792
H	-2.68501	-2.22853	-2.27320	H	2.30863	-1.83926	1.58275
H	-1.07522	-1.93183	-2.96793	H	0.66134	-1.44505	2.13717
C	1.31711	1.84600	-0.78503	C	-1.81288	2.28941	-0.21972
C	2.54492	0.98224	-0.42939	C	-3.12589	1.68011	-0.73326
H	0.90968	1.51621	-1.74528	H	-1.55649	1.81850	0.72870
H	2.71116	0.25729	-1.22600	H	-3.31204	0.67796	-0.36123
C	1.91071	3.22882	-1.04577	C	-2.19946	3.71647	0.16194
O	1.31866	4.22396	-1.40020	O	-1.46267	4.62106	0.48055
C	3.72798	1.89551	-0.51076	C	-4.20106	2.64125	-0.29019
O	4.89822	1.61445	-0.34460	O	-5.40117	2.47164	-0.31940
N	3.27436	3.16958	-0.82898	N	-3.58430	3.80147	0.15284
C	4.16744	4.30688	-1.03085	C	-4.31628	4.97786	0.61388
H	4.99281	4.18735	-0.33070	H	-5.24611	5.01308	0.04829
H	3.60531	5.20036	-0.76319	H	-3.71327	5.84685	0.35418
C	4.67430	4.38834	-2.46486	C	-4.58868	4.92971	2.11171
H	3.84379	4.50118	-3.16273	H	-3.65479	4.88765	2.67367
H	5.33478	5.24941	-2.57707	H	-5.13265	5.82399	2.41917
H	5.23483	3.49051	-2.72786	H	-5.19147	4.05735	2.36734
O	1.24470	-0.44259	2.17366	O	-0.50173	-2.27195	-1.67993
C	1.66386	0.61347	2.72108	C	-1.02560	-1.46687	-2.51714
O	2.54228	1.35401	2.17588	O	-2.13390	-0.94204	-2.18670
C	1.12954	0.99118	4.06671	C	-0.38255	-1.16367	-3.82641

H	0.13796	0.56954	4.20882	H	0.66368	-1.45886	-3.81571
H	1.79745	0.58124	4.82895	H	-0.90237	-1.72213	-4.60848
H	1.10808	2.07268	4.17506	H	-0.47597	-0.10195	-4.04714
H	2.61122	0.94967	0.98946	H	-3.14297	1.62150	-1.82281
Sb	-5.35020	-0.17990	-0.29989	Sb	5.42963	0.10880	0.59832
F	-3.90259	0.75576	-1.16899	F	3.80856	0.47221	-0.37745
F	-6.55243	1.17204	-0.87676	F	6.29707	1.47983	-0.39091
F	-5.61758	-1.14113	-1.92149	F	4.88777	1.37812	1.90525
F	-4.08891	-1.50228	0.25512	F	4.47451	-1.24759	1.54638
F	-6.76349	-1.13812	0.53539	F	7.01907	-0.26703	1.56885
F	-5.02056	0.77872	1.30831	F	5.90519	-1.16901	-0.72598
TS6				HOAc			
Ru	0.60099	1.52618	0.76530	H	1.87932	0.40963	0.00000
C	1.97776	3.24277	0.78191	O	1.25139	-0.34473	0.00000
C	1.84243	2.77156	-0.54002	O	-0.23289	1.33858	0.00000
C	0.56247	2.64372	-1.15338	C	0.00000	0.15162	0.00000
C	-0.61824	2.96599	-0.46773	C	-1.03276	-0.93767	0.00000
C	-0.48541	3.35344	0.90293	H	-0.90130	-1.57055	0.87927
C	0.78115	3.51945	1.50773	H	-2.02818	-0.50307	0.00000
H	2.71418	2.42474	-1.07344	H	-0.90130	-1.57055	-0.87927
H	0.50945	2.18624	-2.12830				
H	-1.37222	3.47979	1.50839				
H	0.84110	3.76334	2.55923				
C	3.30837	3.33349	1.45513				
H	4.01724	2.64568	1.00251				
H	3.69088	4.35370	1.36420				
H	3.21806	3.09903	2.51562				
C	-2.00580	2.86344	-1.06070				
H	-2.58799	2.22700	-0.38583				
C	-2.64669	4.26165	-1.05992				
H	-2.08453	4.94073	-1.70498				
H	-3.66728	4.20013	-1.44029				
H	-2.68535	4.69711	-0.06073				
C	-2.05105	2.25666	-2.45948				
H	-3.08827	2.18720	-2.79039				
H	-1.52102	2.88788	-3.17745				
H	-1.61608	1.26064	-2.46852				
Sb	3.37071	-0.89186	-0.62133				
F	4.14811	0.63353	0.20394				
F	2.84569	0.20683	-2.09024				
F	2.57542	-2.41102	-1.43133				

F	3.79549	-1.94115	0.90099
F	5.02440	-1.28744	-1.46404
F	1.68445	-0.44456	0.22816
C	-0.90695	-2.32323	0.01034
C	0.00225	-3.33988	0.29972
C	-0.25039	-4.24577	1.32139
C	-1.42936	-4.14530	2.04574
C	-2.33035	-3.12293	1.76901
C	-2.07779	-2.18514	0.77333
H	0.91755	-3.40462	-0.27251
H	0.46919	-5.02279	1.54678
H	-1.64779	-4.85306	2.83605
H	-3.23833	-3.05946	2.35429
C	-0.59594	-1.38500	-1.11485
O	-0.68278	-0.15414	-1.00718
N	-0.20692	-1.96001	-2.25720
H	-0.19101	-2.96741	-2.31347
C	0.22316	-1.18213	-3.40445
H	0.75403	-1.84030	-4.08869
H	-0.62913	-0.73914	-3.92400
H	0.89692	-0.39216	-3.08096
C	-3.03333	-1.05256	0.49268
C	-3.92758	-0.52569	1.61637
H	-2.42590	-0.22144	0.13343
H	-3.49834	0.33057	2.13170
C	-3.99906	-1.32029	-0.65203
O	-3.78118	-1.91346	-1.68458
C	-5.22104	-0.15020	0.92817
O	-6.14413	0.49150	1.38225
N	-5.20110	-0.69587	-0.34660
C	-6.30218	-0.57623	-1.29633
H	-7.21605	-0.48454	-0.71168
H	-6.33907	-1.50582	-1.86303
C	-6.12100	0.61937	-2.22288
H	-5.20369	0.52040	-2.80469
H	-6.96007	0.68510	-2.91704
H	-6.07551	1.54766	-1.65150
O	1.25264	0.59601	2.59470
C	0.13265	0.01276	2.73870
O	-0.79077	0.34842	1.93590
C	-0.06898	-1.04548	3.76670

H	0.64068	-0.92389	4.58226	
H	-1.09237	-1.02442	4.13642	
H	0.09734	-2.01559	3.29373	
H	-4.16722	-1.27745	2.36985	

Table S5 Coordinates of stationary points for the reaction of **CAT+DMF+1a** and **CAT+CH₃CN+1a**, computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in DMF and CH₃CN solvent, respectively.

1a(DMF solvent)				DMF(DMF solvent)			
C	0.24436	0.10679	-0.03528	C	0.85754	-0.64089	-0.00000
C	0.79387	-1.16652	-0.20255	O	1.95362	-0.09056	-0.00001
C	2.17098	-1.34830	-0.15843	H	0.76043	-1.73932	-0.00000
C	3.01197	-0.26220	0.05817	N	-0.33785	-0.02004	0.00000
C	2.47146	1.00998	0.22086	C	-0.43357	1.42906	-0.00000
C	1.09699	1.19383	0.16640	H	-0.97124	1.77336	0.88731
H	0.15581	-2.02148	-0.39457	H	0.57003	1.84581	-0.00001
H	2.58703	-2.33905	-0.29961	H	-0.97126	1.77334	-0.88732
H	4.08574	-0.40575	0.09467	C	-1.58122	-0.76890	0.00000
H	3.12329	1.85987	0.38730	H	-2.17390	-0.52978	-0.88706
H	0.66671	2.18043	0.28043	H	-1.36686	-1.83700	0.00004
C	-1.23078	0.37362	-0.09218	H	-2.17392	-0.52972	0.88702
O	-1.67121	1.48592	-0.39128				
N	-2.05134	-0.65961	0.19565				
H	-1.66304	-1.51649	0.56332				
C	-3.49583	-0.50698	0.17718				
H	-3.83635	0.17772	0.95793				
H	-3.82316	-0.11320	-0.78535				
H	-3.95092	-1.48272	0.33682				
CAT(DMF solvent)				COM1-DMF(DMF solvent)			
Ru	1.24111	0.54965	0.20503	Ru	-2.30740	-0.21948	-0.08822
C	1.56611	0.11138	2.36236	C	-3.12879	-0.88006	-2.04146
C	0.97766	-1.00703	1.74463	C	-1.75096	-0.60645	-2.18307
C	1.53661	-1.60450	0.58045	C	-0.78032	-1.20051	-1.34052
C	2.70706	-1.08906	-0.00890	C	-1.16590	-2.10448	-0.31736
C	3.30586	0.05788	0.60295	C	-2.55034	-2.40573	-0.17561
C	2.74606	0.64353	1.75761	C	-3.50381	-1.79267	-1.01261
H	0.02137	-1.36543	2.10016	H	-1.43746	0.15796	-2.88369
H	0.98043	-2.39561	0.10080	H	0.25430	-0.90059	-1.42090
H	4.15562	0.53182	0.12956	H	-2.89343	-3.03960	0.62780
H	3.16968	1.56481	2.13637	H	-4.55575	-1.95338	-0.81078

C	0.92997	0.77432	3.54453	C	-4.15936	-0.21418	-2.90048
H	1.34185	0.35676	4.46727	H	-5.09036	-0.06660	-2.35277
H	1.12563	1.84648	3.54493	H	-3.80738	0.75302	-3.25854
H	-0.14713	0.61125	3.54421	H	-4.37882	-0.83808	-3.77151
C	3.29994	-1.64660	-1.28089	C	-0.10672	-2.68413	0.58886
H	3.78217	-0.80779	-1.79177	H	0.65019	-1.91016	0.70703
C	4.39109	-2.66661	-0.91245	C	-0.60940	-3.07643	1.97713
H	3.95938	-3.52648	-0.39525	H	-1.30313	-3.91999	1.93790
H	4.88352	-3.02575	-1.81743	H	0.23833	-3.38492	2.59112
H	5.15154	-2.22635	-0.26497	H	-1.10253	-2.24067	2.47401
C	2.26788	-2.25028	-2.23415	C	0.55322	-3.87675	-0.12235
H	2.75627	-2.53034	-3.16829	H	1.36631	-4.26300	0.49344
H	1.81329	-3.15340	-1.82164	H	-0.16605	-4.68292	-0.28759
H	1.47342	-1.53954	-2.46713	H	0.97409	-3.58686	-1.08606
O	1.42553	1.51992	-1.69205	O	-1.90435	0.17063	1.99389
C	1.00087	2.61476	-1.20031	C	-3.06598	0.66472	2.14995
O	0.82939	2.64508	0.06021	O	-3.86132	0.59544	1.16103
C	0.69237	3.79028	-2.06097	C	-3.46514	1.32401	3.42784
H	-0.35184	3.72676	-2.37693	H	-3.21379	2.38592	3.36716
H	1.32074	3.78319	-2.94954	H	-2.92001	0.89058	4.26455
H	0.82601	4.71417	-1.50155	H	-4.53917	1.23516	3.58200
Sb	-2.51963	-0.39707	-0.09916	Sb	3.31909	-0.04342	-0.00322
F	-0.81924	0.50642	-0.50269	F	1.46005	0.19677	0.39017
F	-2.72988	-0.68174	-1.95638	F	3.13473	-1.90499	0.33715
F	-4.15387	-1.26575	0.29806	F	5.16224	-0.26993	-0.40864
F	-2.16719	-0.07094	1.73871	F	3.44625	1.83080	-0.34754
F	-1.54228	-2.02201	0.03526	F	2.84957	-0.34324	-1.82924
F	-3.35841	1.29104	-0.25153	F	3.72333	0.25944	1.83001
				C	-0.67884	2.30023	-0.23911
				O	-1.85308	1.85240	-0.24200
				N	-0.39659	3.58497	-0.35082
				C	-1.43840	4.59614	-0.47777
				H	-2.41097	4.11447	-0.47347
				H	-1.37131	5.29786	0.35587
				H	-1.30332	5.14574	-1.41122
				H	0.17925	1.63519	-0.13625
				C	0.98655	4.04943	-0.33998
				H	1.19591	4.59602	-1.26150
				H	1.14396	4.72016	0.50705
				H	1.66859	3.20544	-0.26358

TS1a-DMF(DMF solvent)				INT1(DMF solvent)			
Ru	3.26239	-0.23906	-0.19597	Ru	-3.14336	-0.04035	0.12254
C	2.66796	-1.80634	-1.71445	C	-3.72252	1.00544	-1.75563
C	3.29775	-0.73330	-2.36092	C	-2.51176	0.31829	-1.96779
C	4.55531	-0.24429	-1.91088	C	-2.39534	-1.07006	-1.67414
C	5.23545	-0.84645	-0.81741	C	-3.48249	-1.80757	-1.16857
C	4.60061	-1.95742	-0.17762	C	-4.71127	-1.10455	-0.95983
C	3.33289	-2.39347	-0.58902	C	-4.83092	0.26591	-1.23872
H	2.77487	-0.20049	-3.14427	H	-1.63484	0.86782	-2.28126
H	4.95439	0.65031	-2.36589	H	-1.42222	-1.53323	-1.76226
H	5.04415	-2.37969	0.71463	H	-5.53850	-1.61949	-0.48794
H	2.81843	-3.14578	-0.00679	H	-5.75066	0.78018	-0.99344
C	1.32781	-2.30211	-2.15131	C	-3.84687	2.47438	-2.00774
H	1.46783	-3.11111	-2.87518	H	-4.31693	2.63282	-2.98293
H	0.75758	-2.69590	-1.31344	H	-4.47569	2.94996	-1.25464
H	0.75059	-1.51385	-2.63240	H	-2.87314	2.95969	-2.01396
C	6.56507	-0.35008	-0.30438	C	-3.38572	-3.27324	-0.81052
H	6.56813	-0.54190	0.77198	H	-4.20002	-3.47411	-0.10793
C	7.68933	-1.18086	-0.94448	C	-3.62559	-4.12060	-2.06973
H	7.71761	-1.02932	-2.02637	H	-2.82990	-3.96296	-2.80198
H	8.65485	-0.87806	-0.53507	H	-3.64184	-5.18060	-1.80982
H	7.56116	-2.24831	-0.75452	H	-4.57731	-3.87387	-2.54443
C	6.79169	1.14662	-0.51343	C	-2.07311	-3.64843	-0.12077
H	7.71491	1.44737	-0.01539	H	-2.10705	-4.69407	0.18924
H	6.89867	1.39823	-1.57119	H	-1.21438	-3.53454	-0.78597
H	5.97282	1.73199	-0.09524	H	-1.90799	-3.03393	0.76522
O	4.09156	0.59249	1.59703	O	-3.74760	-0.68413	2.08780
C	3.35611	0.08134	2.51689	C	-3.82347	0.51799	2.49049
O	2.41972	-0.68065	2.21719	O	-3.65285	1.43071	1.62079
C	3.68274	0.42362	3.94665	C	-4.06546	0.84618	3.92575
H	2.79716	0.32346	4.57141	H	-3.09977	0.96610	4.42332
H	4.09175	1.42999	4.02369	H	-4.60715	0.03870	4.41483
H	4.44006	-0.27546	4.31047	H	-4.61225	1.78363	4.01403
C	2.29047	2.54014	0.32864	Sb	4.76335	-0.37124	-0.02722
O	2.87675	1.84337	-0.52635	F	5.51686	1.19162	-0.80355
H	1.90317	2.10353	1.24936	F	3.63831	0.73692	1.07694
N	2.08541	3.84076	0.19091	F	3.95800	-1.90297	0.77351
C	2.53158	4.56826	-0.99055	F	5.84402	-1.48316	-1.12584
H	3.00433	3.87663	-1.68055	F	3.38916	-0.36582	-1.35134
H	1.67566	5.04310	-1.47424	F	6.09362	-0.35421	1.32867
H	3.24449	5.34212	-0.69920	C	0.00874	1.71794	0.09508

C	1.40620	4.61075	1.22345	C	1.04706	1.86636	-0.82736
H	0.50717	5.07631	0.81424	C	1.18005	3.05864	-1.52796
H	1.12617	3.95779	2.04804	C	0.29550	4.10721	-1.29946
H	2.06616	5.39503	1.59951	C	-0.73350	3.96146	-0.37339
Sb	-5.77061	0.30649	-0.15692	C	-0.88664	2.76681	0.31572
F	-4.10159	0.58484	0.75164	H	1.73775	1.05437	-1.01332
F	-4.82118	-0.52614	-1.58995	H	1.97743	3.16755	-2.25340
F	-7.42308	0.03944	-1.06173	H	0.40787	5.03886	-1.84186
F	-6.66361	1.14353	1.30069	H	-1.41704	4.78160	-0.18744
F	-5.94786	-1.38120	0.70077	H	-1.68510	2.64768	1.03593
F	-5.55112	1.99371	-1.01116	C	-0.15132	0.46066	0.86750
C	-0.99838	-1.52572	0.42242	O	-1.27802	-0.04198	1.13426
C	-2.20718	-2.03114	-0.06445	N	0.94669	-0.13158	1.30981
C	-2.61602	-3.31258	0.28387	H	1.83977	0.33472	1.19056
C	-1.82690	-4.09621	1.11873	C	0.93898	-1.40009	2.02298
C	-0.62278	-3.59517	1.60476	H	0.21565	-2.07297	1.56766
C	-0.20468	-2.31840	1.25375	H	1.93545	-1.82901	1.95369
H	-2.82528	-1.44803	-0.73400	H	0.66970	-1.25990	3.07198
H	-3.55007	-3.70040	-0.10486				
H	-2.14877	-5.09535	1.38952				
H	-0.00797	-4.20217	2.25957				
H	0.72740	-1.91637	1.62436				
C	-0.50932	-0.16136	0.05226				
O	0.69693	0.11800	-0.02361				
N	-1.45899	0.75112	-0.21217				
H	-2.41934	0.54842	0.03396				
C	-1.14639	2.10874	-0.60958				
H	-0.83153	2.71765	0.24217				
H	-0.34721	2.10695	-1.34927				
H	-2.03796	2.55734	-1.04434				
1a(CH₃CN solvent)				CH₃CN (CH₃CN solvent)			
C	0.24432	0.10783	-0.04124	C	0.00000	0.00000	0.27994
C	0.79307	-1.16669	-0.20180	N	0.00000	0.00000	1.42990
C	2.16992	-1.34935	-0.15286	C	0.00000	0.00000	-1.17459
C	3.01089	-0.26278	0.06267	H	0.00000	1.02517	-1.54712
C	2.47077	1.01051	0.21929	H	-0.88782	-0.51258	-1.54712
C	1.09649	1.19529	0.15931	H	0.88782	-0.51258	-1.54712
H	0.15414	-2.02088	-0.39269				
H	2.58566	-2.34044	-0.28942				
H	4.08403	-0.40686	0.10322				
H	3.12252	1.86002	0.38532				

H	0.66599	2.18204	0.26825				
C	-1.23056	0.37371	-0.10296				
O	-1.67164	1.48253	-0.41422				
N	-2.04914	-0.65784	0.19560				
H	-1.65778	-1.50742	0.57630				
C	-3.49389	-0.50822	0.18412				
H	-3.83285	0.17086	0.97026				
H	-3.82443	-0.10874	-0.77457				
H	-3.94629	-1.48575	0.33876				
CAT(CH₃CN solvent)				COMI-CCN(CH₃CN solvent)			
Ru	1.24105	0.54966	0.20506	Ru	2.33545	0.04711	0.16477
C	1.56578	0.11123	2.36240	C	2.99512	-1.14057	1.91710
C	0.97738	-1.00712	1.74453	C	1.61094	-0.89607	2.03385
C	1.53644	-1.60453	0.58036	C	0.72496	-1.22570	0.97350
C	2.70695	-1.08906	-0.00884	C	1.18322	-1.81957	-0.22166
C	3.30573	0.05781	0.60317	C	2.58366	-2.08777	-0.31793
C	2.74582	0.64339	1.75780	C	3.47002	-1.76474	0.72202
H	0.02104	-1.36551	2.09990	H	1.23190	-0.36906	2.89936
H	0.98026	-2.39555	0.10057	H	-0.31277	-0.93139	1.04653
H	4.15556	0.53176	0.12991	H	2.99736	-2.46568	-1.24237
H	3.16941	1.56464	2.13668	H	4.53213	-1.91732	0.58413
C	0.92948	0.77413	3.54450	C	3.95567	-0.71917	2.98300
H	1.34116	0.35650	4.46730	H	4.87434	-0.32518	2.54803
H	1.12519	1.84628	3.54499	H	3.51822	0.03766	3.63266
H	-0.14763	0.61114	3.54397	H	4.21999	-1.58552	3.59620
C	3.29993	-1.64648	-1.28085	C	0.20458	-2.12016	-1.33415
H	3.78211	-0.80760	-1.79165	H	-0.55451	-1.33950	-1.28719
C	4.39114	-2.66643	-0.91244	C	0.82523	-2.08756	-2.73047
H	3.95948	-3.52639	-0.39533	H	1.52821	-2.90969	-2.88625
H	4.88364	-3.02547	-1.81743	H	0.03767	-2.19216	-3.47830
H	5.15153	-2.22618	-0.26490	H	1.34663	-1.14766	-2.91789
C	2.26794	-2.25015	-2.23419	C	-0.48222	-3.46669	-1.06043
H	2.75640	-2.53013	-3.16832	H	-1.23224	-3.66152	-1.82853
H	1.81338	-3.15332	-1.82176	H	0.24093	-4.28638	-1.07403
H	1.47346	-1.53944	-2.46717	H	-0.98690	-3.46823	-0.09318
O	1.42572	1.52001	-1.69192	O	2.99734	0.81199	-1.73290
C	1.00093	2.61481	-1.20017	C	3.83676	1.58064	-1.16484
O	0.82942	2.64508	0.06034	O	3.93856	1.48747	0.09896
C	0.69232	3.79031	-2.06082	C	4.63201	2.57491	-1.94231
H	-0.35189	3.72667	-2.37675	H	4.05964	3.50366	-2.00963
H	1.32067	3.78327	-2.94940	H	4.81185	2.21104	-2.95244

H	0.82587	4.71420	-1.50139	H	5.57258	2.78767	-1.43746
Sb	-2.51955	-0.39707	-0.09925	Sb	-3.34427	0.15142	0.08271
F	-0.81913	0.50647	-0.50287	F	-1.67008	0.50089	-0.76561
F	-2.72986	-0.68173	-1.95644	F	-3.43618	-1.54357	-0.77514
F	-4.15368	-1.26583	0.29813	F	-5.00119	-0.17002	0.95792
F	-2.16688	-0.07101	1.73862	F	-3.20943	1.84797	0.95392
F	-1.54206	-2.02196	0.03510	F	-2.40810	-0.65280	1.54657
F	-3.35833	1.29103	-0.25148	F	-4.24204	0.96575	-1.38535
				C	0.32634	2.54780	0.20154
				N	1.10434	1.70902	0.17368
				C	-0.67177	3.59318	0.23582
				H	-0.74980	4.05483	-0.74978
				H	-1.63200	3.15321	0.51036
				H	-0.38648	4.35176	0.96633
TS1-CCN(CH₃CN solvent)				TS1a-CCN(CH₃CN solvent)			
Ru	3.15467	-0.11176	0.25470	Ru	-3.36952	-0.05813	-0.12915
C	4.44074	-0.32738	2.01789	C	-3.06528	1.44921	-1.80007
C	3.38168	-1.25810	2.10012	C	-3.62784	0.27954	-2.32466
C	3.11526	-2.16928	1.04289	C	-4.78421	-0.30186	-1.73102
C	3.88445	-2.17124	-0.13941	C	-5.43799	0.30425	-0.62360
C	4.92840	-1.20624	-0.24702	C	-4.88059	1.52346	-0.12182
C	5.20589	-0.30826	0.81670	C	-3.70365	2.05159	-0.66433
H	2.69578	-1.20459	2.93323	H	-3.12052	-0.24878	-3.12087
H	2.24144	-2.80375	1.10434	H	-5.12450	-1.26042	-2.09512
H	5.47402	-1.09587	-1.17179	H	-5.29478	1.96469	0.77546
H	5.94967	0.46348	0.67378	H	-3.23029	2.89379	-0.17866
C	4.67491	0.68296	3.09523	C	-1.81333	2.03503	-2.36544
H	5.08321	1.60565	2.68389	H	-2.08063	2.81630	-3.08394
H	3.74892	0.91133	3.62151	H	-1.20242	2.48541	-1.58667
H	5.39258	0.28710	3.81943	H	-1.22415	1.28027	-2.88309
C	3.55097	-3.13200	-1.25662	C	-6.66321	-0.28446	0.03128
H	2.48677	-3.36227	-1.15814	H	-6.61141	-0.00021	1.08573
C	3.78832	-2.57046	-2.65922	C	-7.91736	0.35978	-0.58158
H	4.85235	-2.42642	-2.86135	H	-8.00846	0.10443	-1.64020
H	3.41309	-3.27790	-3.40056	H	-8.80980	-0.00191	-0.06792
H	3.27956	-1.61754	-2.80189	H	-7.89525	1.44790	-0.49563
C	4.34313	-4.43201	-1.03745	C	-6.73080	-1.80996	-0.03608
H	4.07379	-5.16428	-1.80077	H	-7.58505	-2.16123	0.54472
H	5.41815	-4.24915	-1.10901	H	-6.86663	-2.16811	-1.05914
H	4.13679	-4.86896	-0.05877	H	-5.83031	-2.26378	0.37821
O	3.02856	0.78780	-1.81933	O	-3.93592	-0.71186	1.82054

C	3.24825	1.93985	-1.34858	C	-3.13897	-0.07174	2.59994
O	3.46803	2.03662	-0.10270	O	-2.32371	0.74353	2.14002
C	3.22338	3.15180	-2.22707	C	-3.22756	-0.37334	4.07318
H	2.18778	3.47781	-2.34242	H	-2.82767	0.45651	4.65258
H	3.61822	2.91050	-3.21306	H	-2.63088	-1.26355	4.28636
H	3.79035	3.96494	-1.77814	H	-4.25531	-0.58199	4.36737
Sb	-5.01751	-0.59697	0.08110	Sb	5.67422	-0.47095	-0.05321
F	-5.20654	0.25126	-1.61054	F	3.98225	-0.69080	0.82785
F	-3.33366	0.28707	0.31095	F	4.77545	0.34575	-1.52691
F	-4.76696	-1.43753	1.77038	F	7.34776	-0.25189	-0.93159
F	-6.68149	-1.48718	-0.14889	F	6.52454	-1.29380	1.43729
F	-5.87425	0.87814	0.92269	F	5.86795	1.23039	0.77410
F	-4.09686	-2.04392	-0.76157	F	5.43811	-2.17261	-0.87314
C	0.01501	-1.17842	-1.40696	C	0.89145	1.55866	0.13576
N	0.95504	-0.79174	-0.87405	C	2.13246	1.95812	-0.36605
C	-1.17964	-1.65906	-2.07550	C	2.55699	3.27207	-0.20727
H	-1.43657	-0.98615	-2.89493	C	1.75185	4.19215	0.45486
H	-0.99774	-2.65534	-2.48133	C	0.51680	3.79509	0.95952
H	-2.01826	-1.70608	-1.37955	C	0.08281	2.48636	0.79570
C	-0.08170	2.42608	0.35203	H	2.76807	1.26320	-0.89852
C	-1.16426	2.49992	-0.52891	H	3.51675	3.57634	-0.60763
C	-1.39593	3.66348	-1.25087	H	2.08560	5.21597	0.57858
C	-0.56245	4.76519	-1.08694	H	-0.10934	4.50849	1.48298
C	0.51169	4.69777	-0.20504	H	-0.86882	2.16129	1.19185
C	0.75976	3.52904	0.50145	C	0.38407	0.16275	-0.04236
H	-1.82872	1.65594	-0.65760	O	-0.81940	-0.08923	-0.19502
H	-2.22972	3.71019	-1.94122	N	1.31001	-0.80905	-0.04831
H	-0.75040	5.67490	-1.64541	H	2.26821	-0.59462	0.19551
H	1.16077	5.55542	-0.07298	C	0.96238	-2.20358	-0.23323
H	1.60306	3.45794	1.17297	H	0.37076	-2.58173	0.60432
C	0.20899	1.20286	1.15417	H	0.38648	-2.33394	-1.15043
O	1.37181	0.89811	1.49747	H	1.88246	-2.78009	-0.30461
N	-0.83217	0.46030	1.52919	C	-2.54822	-3.18676	-0.32018
H	-1.76338	0.70764	1.22362	N	-2.81310	-2.07773	-0.22991
C	-0.68206	-0.77957	2.26914	C	-2.20002	-4.58885	-0.42604
H	-0.06666	-1.48984	1.71565	H	-1.53543	-4.74201	-1.27789
H	-0.21410	-0.59849	3.23780	H	-3.10429	-5.18261	-0.56814
H	-1.67107	-1.20533	2.42311	H	-1.69775	-4.91369	0.48644

TS1b-CCN(CH₃CN solvent)				INT1(CH₃CN solvent)			
Ru	3.00104	-0.08696	-0.14166	Ru	-3.13779	-0.03405	0.11778
C	2.59038	-1.18293	-2.02214	C	-3.68331	1.00713	-1.77278
C	3.39354	-0.06007	-2.33119	C	-2.48341	0.29728	-1.96986
C	4.59356	0.17487	-1.62495	C	-2.39293	-1.09075	-1.66435
C	5.06658	-0.70474	-0.61559	C	-3.49698	-1.80503	-1.16223
C	4.25656	-1.83255	-0.32183	C	-4.71539	-1.07953	-0.96931
C	3.03806	-2.07151	-1.00296	C	-4.80852	0.29055	-1.25929
H	3.03645	0.67876	-3.03478	H	-1.59451	0.82928	-2.27986
H	5.10659	1.11057	-1.79204	H	-1.42749	-1.57157	-1.74072
H	4.52067	-2.46996	0.51208	H	-5.55545	-1.57665	-0.50126
H	2.41366	-2.90022	-0.70187	H	-5.72078	0.82270	-1.02471
C	1.28807	-1.40555	-2.72159	C	-3.77992	2.47620	-2.03627
H	1.47510	-1.94826	-3.65302	H	-4.24630	2.63648	-3.01284
H	0.60458	-1.99796	-2.11761	H	-4.39995	2.96891	-1.28691
H	0.81155	-0.45928	-2.97701	H	-2.79729	2.94308	-2.04479
C	6.35184	-0.47767	0.14764	C	-3.42978	-3.26947	-0.79279
H	6.17565	-0.84126	1.16462	H	-4.25171	-3.44957	-0.09354
C	7.46302	-1.33572	-0.47972	C	-3.67957	-4.12065	-2.04768
H	7.66433	-1.01914	-1.50625	H	-2.87670	-3.98411	-2.77627
H	8.38589	-1.23023	0.09355	H	-3.71859	-5.17813	-1.78039
H	7.19450	-2.39375	-0.49810	H	-4.62336	-3.85796	-2.52944
C	6.77041	0.98936	0.23649	C	-2.12855	-3.66567	-0.09316
H	7.64485	1.07863	0.88327	H	-2.18400	-4.70895	0.22140
H	7.05093	1.38859	-0.74142	H	-1.26398	-3.57099	-0.75373
H	5.97084	1.60097	0.65383	H	-1.95707	-3.05041	0.79114
O	3.78698	1.43440	1.90239	O	-3.75327	-0.66841	2.08258
C	3.24984	0.51386	2.53461	C	-3.82771	0.53558	2.47995
O	2.78747	-0.52096	1.92386	O	-3.65039	1.44422	1.60735
C	3.08951	0.54553	4.03298	C	-4.07555	0.87015	3.91276
H	3.35920	-0.41844	4.46507	H	-3.11178	0.98002	4.41626
H	2.04096	0.73205	4.27578	H	-4.62919	0.06979	4.40010
H	3.70019	1.33473	4.46574	H	-4.61238	1.81374	3.99519
Sb	-5.52852	0.31175	-0.03666	Sb	4.75954	-0.38088	-0.02862
F	-3.84304	0.54913	0.85578	F	5.51391	1.18111	-0.80581
F	-4.61471	-0.50452	-1.50045	F	3.63716	0.72936	1.07638
F	-7.19623	0.08048	-0.92172	F	3.95198	-1.91128	0.77260
F	-6.38911	1.13353	1.44740	F	5.83837	-1.49411	-1.12768
F	-5.70851	-1.38686	0.79726	F	3.38444	-0.37431	-1.35198
F	-5.29446	2.01192	-0.85923	F	6.09039	-0.36536	1.32671
C	-0.60998	-1.29149	0.30185	C	0.01666	1.72123	0.10300

C	-1.76007	-1.75044	-0.34688	C	1.05448	1.86800	-0.82023
C	-2.10790	-3.09266	-0.27339	C	1.19225	3.06216	-1.51665
C	-1.32024	-3.97996	0.45229	C	0.31335	4.11437	-1.28261
C	-0.18296	-3.52140	1.11015	C	-0.71504	3.97018	-0.35556
C	0.17854	-2.18311	1.03195	C	-0.87331	2.77352	0.32892
H	-2.37829	-1.07728	-0.92556	H	1.74098	1.05334	-1.00985
H	-2.99372	-3.44435	-0.78832	H	1.98916	3.16976	-2.24266
H	-1.59467	-5.02694	0.50908	H	0.42954	5.04742	-1.82154
H	0.42368	-4.20899	1.68774	H	-1.39462	4.79259	-0.16587
H	1.05475	-1.81739	1.54938	H	-1.67197	2.65497	1.04891
C	-0.21517	0.13956	0.22153	C	-0.14846	0.46244	0.87171
O	0.97406	0.53629	0.16143	O	-1.27745	-0.03561	1.13727
N	-1.19152	1.04046	0.21793	N	0.94695	-0.13537	1.31258
H	-2.14535	0.74275	0.39304	H	1.84193	0.32757	1.19406
C	-0.93245	2.46569	0.10208	C	0.93406	-1.40499	2.02365
H	-0.39559	2.84073	0.97544	H	0.20558	-2.07285	1.56904
H	-0.33087	2.67034	-0.78310	H	1.92795	-1.83929	1.95102
H	-1.88818	2.97815	0.01924	H	0.66826	-1.26497	3.07351
C	2.87759	3.65616	-0.71394				
N	2.90302	2.52058	-0.55095				
C	2.84425	5.09651	-0.90322				
H	3.79248	5.43881	-1.31980				
H	2.67816	5.59159	0.05455				
H	2.03854	5.36518	-1.58762				

Table S5 Coordinates of the first transition state for **CAT+1a** and **CAT-O+1a**, Computed at B3LYP-D3a+IDSCRF/ TZP-DKH(-dfg) in DCE solvent

TS1				TS1-N			
Ru	0.57872	0.96691	-0.06623	Ru	-0.29181	-1.68216	-0.00432
C	0.70306	0.33264	-2.20658	C	-0.92010	-3.04048	1.68346
C	-0.17959	1.43926	-2.06607	C	-1.70782	-1.87531	1.70369
C	0.23544	2.61920	-1.40939	C	-2.41857	-1.41820	0.56087
C	1.54394	2.74046	-0.85686	C	-2.36120	-2.13053	-0.65506
C	2.40542	1.61528	-0.98546	C	-1.52403	-3.28594	-0.70414
C	2.00462	0.44177	-1.67319	C	-0.79979	-3.71532	0.43437
H	-1.21039	1.33396	-2.37182	H	-1.72472	-1.26470	2.59627
H	-0.49505	3.39671	-1.23962	H	-2.92804	-0.46930	0.62006
H	3.36519	1.62902	-0.48599	H	-1.37630	-3.79530	-1.64715
H	2.65836	-0.41775	-1.67486	H	-0.10917	-4.54309	0.33949
C	0.21808	-0.94257	-2.81866	C	-0.18738	-3.54702	2.88664
H	0.76290	-1.79961	-2.42818	H	-0.64580	-4.48415	3.21420

H	-0.84660	-1.07789	-2.63800	H	0.85919	-3.75380	2.65875
H	0.37595	-0.89999	-3.90080	H	-0.23948	-2.84367	3.71455
C	2.03058	3.97325	-0.13198	C	-3.09472	-1.69814	-1.90102
H	2.68414	3.61939	0.67170	H	-2.56442	-2.14814	-2.74527
C	2.88041	4.81153	-1.10226	C	-4.51201	-2.29580	-1.85590
H	2.27352	5.17310	-1.93598	H	-5.08710	-1.86874	-1.03102
H	3.29096	5.67897	-0.58261	H	-5.03591	-2.07117	-2.78647
H	3.71263	4.23619	-1.51192	H	-4.49186	-3.38037	-1.73151
C	0.91891	4.81620	0.49228	C	-3.12758	-0.18700	-2.11591
H	1.36160	5.61489	1.08952	H	-3.64769	0.03346	-3.04969
H	0.29869	5.29139	-0.27171	H	-3.65892	0.33331	-1.31789
H	0.27473	4.21990	1.13798	H	-2.12442	0.22819	-2.18404
O	-0.43107	1.85698	1.62723	O	0.44501	-1.09568	-1.93314
C	0.38033	1.33189	2.45041	C	1.58149	-1.61966	-1.70738
O	1.38294	0.72859	1.96253	O	1.72678	-2.18567	-0.57736
C	0.14340	1.40613	3.92227	C	2.67089	-1.60068	-2.72089
H	-0.51817	0.58565	4.21065	H	2.40759	-0.94924	-3.55039
H	-0.34908	2.34296	4.17831	H	2.82129	-2.61722	-3.09206
H	1.08077	1.30342	4.46559	H	3.60127	-1.27158	-2.26163
Sb	-3.25589	-0.53694	-0.02663	F	-0.42625	0.85403	-0.19617
F	-1.38372	-0.26468	0.33321	C	3.51797	0.27013	0.27814
F	-3.55393	1.32427	0.21754	C	2.94280	1.25859	-0.52454
F	-5.10217	-0.80332	-0.38906	C	3.66321	1.81753	-1.57341
F	-2.91357	-2.38344	-0.30802	C	4.96199	1.39720	-1.83379
F	-2.90084	-0.21895	-1.87769	C	5.54206	0.41214	-1.03868
F	-3.51892	-0.85187	1.82536	C	4.82486	-0.14588	0.00873
C	3.10536	-2.52494	0.26981	H	1.94188	1.62528	-0.35182
C	3.92210	-3.40774	-0.44082	H	3.20491	2.58604	-2.18366
C	5.29987	-3.22714	-0.45869	H	5.52185	1.83610	-2.65136
C	5.87332	-2.16914	0.23800	H	6.55502	0.08115	-1.23534
C	5.06338	-1.28510	0.94490	H	5.26527	-0.90914	0.63598
C	3.68562	-1.45512	0.95484	C	2.82950	-0.35507	1.45094
H	3.48760	-4.22418	-1.00585	O	3.41544	-1.12299	2.20122
H	5.92457	-3.91081	-1.02134	N	1.50599	-0.02764	1.67789
H	6.94838	-2.03222	0.22738	H	1.16503	0.79361	1.20345
H	5.50827	-0.46163	1.49145	C	1.02527	-0.12775	3.05616
H	3.04428	-0.77311	1.49545	H	1.10427	-1.15242	3.40182
C	1.61319	-2.65418	0.30757	H	1.61261	0.50622	3.72506
O	0.88211	-1.66929	0.44685	H	-0.00854	0.20340	3.08436
N	1.11014	-3.89818	0.16970	Sb	-1.17617	2.59224	0.23396
H	1.74581	-4.68225	0.21492	F	-1.89002	4.27853	0.72207

C	-0.31771	-4.16969	0.20670	F	-1.99552	2.67966	-1.46913
H	-0.86451	-3.27904	-0.08523	F	-0.30193	2.42204	1.92120
H	-0.54905	-4.98313	-0.48115	F	0.39721	3.38581	-0.47825
H	-0.64119	-4.45719	1.21094	F	-2.70285	1.69741	0.94682
TS1-O				TS1-O-N			
Ru	-1.00085	0.08888	-0.32430	Ru	-0.96670	0.41062	-0.05250
C	-1.75647	-1.26017	-1.96630	C	-1.82471	1.63075	-1.71105
C	-2.07295	-1.82594	-0.72261	C	-1.81600	2.33024	-0.46336
C	-2.71449	-1.05074	0.28207	C	-0.60664	2.53639	0.25339
C	-3.10887	0.29336	0.03870	C	0.62244	2.00624	-0.20077
C	-2.83149	0.84017	-1.25387	C	0.57333	1.23908	-1.39055
C	-2.14070	0.09579	-2.21694	C	-0.61116	1.07744	-2.15536
H	-1.71827	-2.81236	-0.46993	H	-2.74833	2.67364	-0.03978
H	-2.82498	-1.48068	1.26393	H	-0.66401	3.01359	1.22123
H	-3.03737	1.88612	-1.43849	H	1.46686	0.72112	-1.70815
H	-1.82302	0.57472	-3.13268	H	-0.59221	0.44791	-3.03450
C	-0.99841	-2.02076	-3.00806	C	-3.10216	1.41959	-2.45832
H	-0.56980	-2.93275	-2.59923	H	-3.93733	1.32032	-1.76799
H	-1.67619	-2.28917	-3.82408	H	-3.28770	2.28304	-3.10430
H	-0.19068	-1.41614	-3.41859	H	-3.04779	0.53207	-3.08787
C	-3.78553	1.14806	1.08403	C	1.93351	2.18874	0.52966
H	-3.50704	2.18209	0.86199	H	2.53526	1.30440	0.31224
C	-5.30965	1.01811	0.93592	C	2.66843	3.41050	-0.04390
H	-5.63430	-0.00445	1.14490	H	2.10384	4.32782	0.14254
H	-5.81468	1.68325	1.63920	H	3.64791	3.51493	0.42660
H	-5.63976	1.27797	-0.07199	H	2.81856	3.31884	-1.12135
C	-3.33545	0.84479	2.51335	C	1.78925	2.29269	2.04762
H	-3.77505	1.57247	3.19800	H	2.77850	2.30540	2.50771
H	-3.65951	-0.14552	2.84144	H	1.28237	3.21393	2.34550
H	-2.25016	0.90195	2.60166	H	1.23235	1.44893	2.45526
O	-0.57030	2.02611	0.48337	O	-1.11488	0.15159	2.00204
C	0.18566	2.56081	-0.40399	C	-0.79028	-1.00580	2.46089
O	0.43511	1.98169	-1.47549	O	-0.23268	-1.88877	1.79268
C	0.78509	3.90734	-0.08091	C	-1.14467	-1.24537	3.91013
H	0.14971	4.47103	0.60056	H	-1.01313	-0.33703	4.49693
H	0.95703	4.47257	-0.99568	H	-0.54420	-2.05452	4.32060
H	1.75026	3.74711	0.40532	H	-2.19881	-1.52744	3.96967
O	0.18519	-0.36761	1.32678	O	-2.49634	-0.95476	-0.08996
C	0.15893	-1.44768	2.03857	C	-3.73632	-0.73163	0.22606
O	-0.56354	-2.42917	1.85373	O	-4.21339	0.36087	0.52386
C	1.12573	-1.41300	3.21101	C	-4.58413	-1.99018	0.20824

H	1.35814	-2.42424	3.54023	H	-4.44382	-2.53129	-0.72834
H	0.65063	-0.88134	4.03978	H	-5.63469	-1.74176	0.34127
H	2.03658	-0.87524	2.95297	H	-4.26515	-2.65192	1.01637
C	3.35998	-0.16661	-0.21475	C	2.81761	-1.42927	-0.65022
C	4.24609	-0.31932	0.85510	C	2.81998	-1.49443	0.74528
C	5.16878	0.67562	1.15179	C	3.89737	-0.99373	1.46675
C	5.21868	1.83222	0.38059	C	4.97651	-0.41521	0.80785
C	4.33382	1.99346	-0.68083	C	4.98064	-0.34654	-0.58208
C	3.40488	1.00378	-0.97212	C	3.91208	-0.85781	-1.30476
H	4.21086	-1.20317	1.48102	H	1.99062	-1.93195	1.28280
H	5.84490	0.54998	1.98930	H	3.89202	-1.05547	2.54850
H	5.94094	2.60695	0.61086	H	5.81260	-0.02221	1.37456
H	4.36492	2.89546	-1.28081	H	5.81929	0.10106	-1.10238
H	2.68966	1.13159	-1.77104	H	3.90915	-0.82329	-2.38640
C	2.34383	-1.20099	-0.58929	C	1.70147	-1.95899	-1.50557
O	1.34488	-0.92399	-1.26168	O	1.87367	-2.15567	-2.70991
N	2.57865	-2.46215	-0.17317	N	0.49916	-2.17947	-0.91825
H	3.47090	-2.68642	0.24089	H	0.38631	-2.11216	0.09306
C	1.67210	-3.55255	-0.49011	C	-0.53847	-2.89969	-1.64148
H	2.04832	-4.46056	-0.02221	H	-0.75133	-2.40920	-2.59080
H	0.67908	-3.33827	-0.09845	H	-0.22906	-3.92659	-1.85370
H	1.60788	-3.70952	-1.56919	H	-1.43671	-2.89711	-1.03193

Table S7 Frequencies of all stationary points for the overall catalytic cycle, computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level, and some of them computed at B3LYP+IDSCRF/TZP-DKH(-dfg) and B3LYP-D3+IDSCRF/TZP-DKH(-dfg)

Species	Frequencies(cm ⁻¹)
1a	56 85 111 150 220 300 352 411 415 454 515 635 684 709 724 818 841 863 952 999 1011 1016 1023 1052 1103 1142 1171 1178 1180 1201 1302 1331 1355 1442 1467 1478 1493 1523 1552 1616 1640 1670 3011 3069 3111 3144 3151 3159 3167 3178 3529
1a D3a	42 74 107 152 219 299 353 410 415 455 514 636 687 709 724 818 843 863 953 999 1015 1018 1026 1055 1106 1147 1174 1182 1183 1205 1305 1335 1358 1450 1477 1482 1504 1528 1559 1620 1644 1680 3033 3092 3133 3160 3167 3175 3184 3194 3573
1a D3	48 73 107 151 220 300 355 411 415 457 515 637 688 709 723 818 844 863 953 999

		1016 1019 1028 1056 1106 1147 1177 1182 1183 1205 1307 1337 1359 1450 1477 1483 1505 1528 1561 1621 1645 1681 3035 3096 3136 3164 3172 3180 3189 3199 3576
2a		52 111 147 201 295 302 346 435 570 607 642 703 718 779 791 848 955 978 986 1056 1104 1116 1142 1230 1329 1373 1385 1413 1426 1478 1492 1501 1645 1727 1807 3040 3070 3101 3107 3124 3217 3236
2a	D3a	46 106 143 201 295 301 346 435 570 609 642 705 721 780 791 847 957 978 986 1058 1105 1117 1144 1232 1329 1373 1387 1414 1428 1479 1492 1501 1646 1729 1810 3039 3069 3100 3107 3124 3214 3234
2a	D3	55 107 145 203 298 303 349 436 571 612 641 708 725 781 790 846 958 977 987 1058 1106 1118 1146 1233 1329 1373 1388 1414 1429 1480 1493 1501 1645 1730 1813 3042 3075 3104 3111 3129 3220 3240
3a		23 29 50 54 70 76 101 113 121 150 175 190 209 243 287 310 320 348 360 401 446 476 499 554 559 583 601 636 647 684 695 739 774 778 808 815 820 853 900 948 973 979 994 1011 1016 1053 1066 1076 1115 1120 1137 1147 1178 1182 1186 1190 1217 1243 1255 1290 1300 1313 1323 1364 1378 1380 1409 1421 1449 1461 1475 1478 1481 1493 1501 1503 1524 1555 1615 1640 1674 1721 1805 3037 3042 3066 3076 3084 3098 3105 3109 3116 3130 3137 3155 3168 3178 3189 3555
3a	D3a	47 49 56 61 84 88 107 119 146 166 178 209 233 242 271 306 313 354 388 401 443 484 504 524 571 581 606 639 659 681 698 736 775 778 800 818 828 858 903 951 970 981 998 1013 1021 1059 1071 1082 1117 1134 1141 1147 1181 1188 1190 1195 1224 1247 1268 1298 1307 1309 1331 1376 1383 1384 1409 1424 1446 1451 1475 1479 1482 1492 1501 1503 1525 1561 1616 1642 1678 1720 1806 3018 3036 3039 3074 3080 3098 3101 3106 3126 3128 3136 3157 3168 3176 3187 3555
3a	D3	34 39 45 62 79 82 102 118 145 168 177 213 232 243 272 307 314 354 389 399 446 484 503 526 572 582 607 638 660 682 700 738 775 779 801 820 830 860 901 953 971 980 999 1012 1023 1061 1072 1082 1119 1135 1143

	1147 1183 1189 1190 1195 1226 1249 1268 1297 1306 1312 1334 1375 1381 1385 1409 1427 1447 1451 1475 1478 1484 1492 1501 1503 1526 1561 1618 1644 1680 1722 1809 3027 3036 3041 3077 3085 3101 3104 3110 3131 3131 3140 3162 3172 3181 3192 3557
AcOH	66 433 544 588 650 868 1003 1069 1197 1345 1409 1467 1473 1767 3053 3110 3160 3498
AcOH D3a	62 432 544 588 650 869 1004 1069 1198 1345 1409 1467 1473 1770 3052 3109 3160 3504
AcOH D3	64 433 543 589 651 870 1004 1069 1199 1346 1409 1468 1473 1771 3054 3112 3162 3510
CAT-O	29 35 45 57 61 62 63 95 105 117 130 174 187 196 214 216 234 244 260 269 285 297 328 353 391 401 426 446 451 488 523 528 577 625 626 646 672 674 690 694 815 892 904 915 935 938 962 969 978 983 1007 1016 1022 1033 1054 1062 1069 1080 1107 1134 1166 1178 1221 1235 1307 1330 1339 1356 1384 1389 1402 1415 1417 1422 1425 1448 1465 1466 1471 1477 1485 1486 1492 1496 1498 1504 1510 1525 1535 1565 1645 3019 3028 3035 3036 3046 3050 3090 3096 3098 3099 3103 3108 3113 3127 3139 3145 3176 3193 3222 3236
CAT-O D3a	30 38 42 50 63 68 80 89 115 119 132 174 186 196 215 218 233 245 266 267 287 299 330 353 392 404 435 446 452 488 524 527 583 624 626 648 673 676 691 696 817 895 903 915 936 939 963 971 978 984 1010 1017 1022 1033 1056 1062 1069 1081 1111 1135 1169 1180 1225 1239 1309 1333 1343 1358 1384 1390 1401 1416 1419 1424 1425 1448 1465 1467 1474 1476 1485 1486 1492 1500 1500 1503 1512 1525 1535 1567 1648 3019 3026 3035 3036 3045 3049 3089 3095 3097 3098 3102 3109 3112 3127 3137 3144 3176 3193 3222 3237
pre-CAT	19 31 32 43 49 55 70 85 92 94 111 117 128 138 145 150 159 160 177 179 194 214 225 231 235 238 241 242 250 254 263 269 273 281 308 310 350 352 368 371 393 394 409 416 443 443 450 450 522 526 567 569 643 645 664 666 692 692 814 815

	893 894 904 914 932 933 939 941 971 972 979 982 990 991 1007 1009 1015 1020 1055 1055 1079 1081 1107 1108 1136 1136 1164 1166 1181 1185 1221 1221 1236 1238 1308 1311 1335 1340 1359 1360 1401 1402 1416 1416 1417 1418 1421 1424 1425 1425 1469 1470 1485 1487 1488 1489 1491 1492 1496 1497 1503 1504 1511 1511 1527 1533 1564 1565 3026 3027 3028 3032 3035 3035 3035 3041 3089 3089 3095 3095 3099 3099 3101 3104 3112 3112 3134 3136 3186 3189 3193 3195 3197 3207 3208 3218
Pre-CAT D3a	18 21 41 51 58 64 70 73 83 99 107 110 131 143 153 161 169 176 180 186 197 201 211 228 244 247 252 252 255 257 261 263 269 273 277 302 335 339 348 358 407 418 428 440 453 459 468 486 515 541 563 570 572 593 598 602 603 610 615 648 681 696 820 893 946 954 974 983 1001 1017 1026 1035 1060 1077 1114 1133 1176 1189 1221 1235 1306 1342 1359 1407 1418 1421 1428 1432 1473 1486 1489 1491 1494 1502 1510 1531 1567 3033 3037 3039 3045 3099 3104 3104 3109 3120 3140 3182 3192 3208 3219
AgSbF₆	6 106 110 156 178 183 243 250 251 261 280 320 449 485 556 579 596 598
AgSbF₆ D3a	31 106 111 155 178 184 242 250 251 261 281 320 450 485 556 579 596 597
CAT-(SbF₆)₂	17 26 28 49 53 55 62 69 77 92 101 105 131 143 151 163 164 174 183 186 194 198 209 227 240 245 248 250 252 257 258 261 267 270 275 304 330 335 347 356 405 414 424 435 452 453 463 485 513 538 561 567 570 592 596 598 602 606 615 648 680 694 818 889 942 952 972 975 1000 1015 1024 1028 1058 1077 1110 1133 1173 1189 1219 1232 1305 1339 1359 1404 1418 1421 1426 1429 1473 1486 1489 1490 1494 1500 1509 1529 1566 3033 3038 3039 3045 3099 3105 3106 3109 3122 3140 3179 3191 3202 3211
CAT-(SbF₆)₂ D3a	18 21 41 51 58 64 70 73 83 99 107 110 131 143 153 161 169 176 180 186 197 201 211 228 244 247 252 252 255 257 261 263 269 273 277 302 335 339 348 358 407 418 428 440 453 459 468 486 515 541 563 570 572 593 598 602 603 610 615 648

	681 696 820 893 946 954 974 983 1001 1017 1026 1035 1060 1077 1114 1133 1176 1189 1221 1235 1306 1342 1359 1407 1418 1421 1428 1432 1473 1486 1489 1491 1494 1502 1510 1531 1567 3033 3037 3039 3045 3099 3104 3104 3109 3120 3140 3182 3192 3208 3219
$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$	12 26 41 45 72 75 88 114 140 182 190 194 258 302 344 390 430 455 480 619 624 690 703 953 960 1023 1025 1071 1072 1385 1386 1441 1444 1463 1465 1496 1501 1518 1524 1600 3049 3049 3114 3115 3149 3149 3659 3729
$\text{Cu}(\text{OAc})_2 \cdot \text{H}_2\text{O}$ D3a	12 22 38 44 70 76 87 115 140 180 191 198 258 300 346 389 434 455 480 619 624 690 703 954 960 1024 1025 1071 1072 1385 1386 1441 1443 1463 1465 1497 1502 1518 1524 1600 3047 3048 3113 3113 3148 3148 3655 3725
$\text{CuOAcSbF}_6 \cdot \text{H}_2\text{O}$	18 24 50 60 67 90 98 117 147 163 177 182 191 245 252 255 262 274 278 283 334 362 423 444 484 495 552 563 593 596 605 621 712 757 961 1019 1071 1389 1424 1462 1496 1512 1599 3050 3116 3154 3558 3635
$\text{CuOAcSbF}_6 \cdot \text{H}_2\text{O}$ D3a	21 26 57 64 71 95 108 120 149 166 177 183 194 248 250 255 262 273 279 280 335 361 427 443 485 497 551 563 595 597 607 621 713 758 962 1020 1072 1389 1424 1462 1496 1513 1599 3048 3115 3152 3564 3633
CAT	24 35 40 45 47 48 66 67 98 109 117 146 157 163 177 179 189 203 210 230 248 252 256 261 262 268 271 296 300 306 327 354 401 406 413 447 453 487 498 510 531 562 570 583 586 592 623 645 673 697 698 819 891 929 939 948 966 970 983 1006 1009 1015 1025 1057 1064 1076 1105 1133 1163 1181 1218 1233 1311 1329 1356 1376 1393 1408 1412 1415 1421 1421 1449 1466 1471 1475 1480 1488 1492 1497 1499 1503 1536 1564 3003 3003 3008 3010 3013 3067 3071 3076 3077 3079 3082 3099 3114 3150 3162 3163 3189
CAT D3a	28 40 44 48 55 58 66 76 96 111 122 149 160 175 182 184 192 205 214 232 248 251 256 263 265 270 275 301 305 317 334 359 407 411 416 450 459 487 499 511

		533 565 572 585 591 598 624 650 676 699 702 822 896 930 945 949 969 974 984 1005 1015 1019 1028 1063 1070 1082 1111 1140 1169 1187 1224 1239 1313 1337 1364 1387 1404 1417 1423 1427 1430 1438 1464 1478 1487 1489 1492 1500 1505 1506 1512 1516 1542 1570 3028 3032 3037 3039 3051 3096 3100 3100 3103 3108 3114 3130 3148 3180 3192 3205 3228
CAT	D3	16 27 41 50 52 57 63 76 100 111 122 147 160 173 181 185 193 200 214 234 238 250 255 258 263 266 269 294 309 320 335 352 408 414 418 451 463 491 499 511 537 566 574 585 591 599 623 650 684 700 702 823 897 929 942 947 969 976 984 1006 1015 1019 1026 1065 1070 1081 1115 1137 1173 1187 1225 1239 1312 1341 1362 1386 1402 1417 1423 1425 1431 1438 1464 1479 1487 1490 1492 1498 1502 1507 1511 1517 1543 1570 3032 3036 3040 3042 3052 3098 3103 3104 3107 3114 3117 3133 3152 3187 3198 3216 3232
TS1		-70 11 17 26 40 47 48 53 54 55 61 66 70 76 85 93 99 110 113 128 145 149 161 170 173 177 181 190 214 228 234 253 256 257 262 264 267 269 278 279 293 313 315 352 357 393 401 411 419 425 443 449 482 487 503 520 526 537 561 573 580 582 587 627 635 650 669 682 690 696 716 730 815 818 840 874 891 920 940 943 963 969 971 992 1003 1008 1011 1014 1021 1022 1025 1032 1054 1057 1071 1078 1104 1107 1137 1141 1161 1170 1183 1183 1185 1206 1222 1236 1304 1305 1330 1332 1361 1364 1386 1403 1414 1418 1420 1426 1442 1446 1466 1473 1481 1487 1489 1491 1493 1502 1506 1507 1507 1512 1520 1530 1537 1562 1575 1618 1642 1671 3024 3031 3034 3035 3037 3051 3092 3093 3098 3104 3109 3115 3116 3148 3148 3162 3168 3176 3177 3183 3187 3203 3207 3212 3215 3558
TS1	D3a	-68 21 25 35 46 49 53 54 62 62 71 74 77 80 100 103 110 114 131 137 154 158 165 172 175 183 185 198 216 231 235 253 256 259 264 267 268 270 280 283 295 318 324 355 359 399 407 418 421 427 447 450 482 494 506 516 528 533 566 575 584 585 590 627 636 650 670 685 690 698

		715	729	817	821	844	873	898	924	940	947
		964	971	974	986	1003	1011	1012	1019	1023	1025
		1032	1056	1061	1072	1081	1107	1109	1138	1142	1166
		1184	1185	1187	1207	1225	1239	1307	1308	1332	1335
		1363	1365	1386	1403	1415	1423	1424	1428	1447	1448
		1466	1477	1482	1487	1488	1492	1495	1503	1508	1509
		1510	1514	1523	1531	1539	1563	1576	1619	1644	1670
		3023	3030	3031	3036	3037	3051	3092	3093	3097	3102
		3111	3113	3122	3147	3150	3160	3167	3175	3181	3185
		3186	3206	3214	3216	3217	3556				
TS1	D3	-57	12	24	36	45	50	51	54	61	62
		69	72	76	84	98	104	106	117	134	134
		156	160	164	171	174	183	187	202	219	229
		244	254	258	260	262	266	269	280	281	284
		296	321	323	356	363	400	410	419	419	431
		447	453	482	500	508	518	530	535	568	577
		587	588	592	626	637	651	673	687	690	700
		714	729	818	822	847	872	901	929	947	949
		961	972	976	989	1000	1009	1015	1019	1022	1024
		1026	1028	1056	1062	1072	1082	1110	1112	1142	1144
		1171	1175	1184	1186	1188	1208	1230	1245	1310	1311
		1337	1339	1365	1366	1386	1405	1417	1424	1426	1430
		1447	1453	1466	1478	1483	1486	1491	1492	1499	1504
		1508	1511	1512	1516	1532	1539	1565	1575	1620	1646
		1673	3027	3032	3032	3041	3041	3052	3096	3099	3100
		3106	3116	3116	3127	3150	3158	3165	3172	3176	3180
		3190	3197	3207	3218	3221	3234	3557			
INT1		10	17	35	39	45	46	52	54	58	63
		65	67	77	78	92	95	114	124	141	149
		166	169	171	177	180	185	196	202	226	236
		246	260	261	262	265	269	271	273	283	294
		296	327	352	355	368	393	397	412	418	430
		448	455	488	494	503	528	544	563	574	577
		578	585	626	633	647	674	690	694	695	711
		718	752	810	817	872	876	893	914	931	941
		965	969	971	974	989	1009	1013	1017	1020	1022
		1023	1026	1055	1056	1070	1080	1108	1115	1137	1146
		1166	1180	1182	1186	1201	1215	1220	1234	1310	1328
		1334	1361	1366	1376	1387	1404	1417	1421	1426	1428
		1443	1447	1465	1474	1481	1486	1487	1488	1492	1497
		1499	1501	1504	1511	1526	1535	1541	1568	1586	1613
		1632	1643	3026	3031	3037	3039	3047	3051	3095	3100
		3100	3100	3104	3111	3115	3118	3138	3149	3158	3166
		3177	3180	3187	3194	3197	3202	3202	3207	3494	

INT1 D3a	14	17	39	42	46	49	55	59	62	65		
	68	70	81	83	98	103	115	128	137	147		
	166	169	171	174	181	188	196	200	227	232		
	245	257	260	262	265	270	272	273	286	289		
	299	329	349	359	373	396	398	416	420	438		
	448	457	490	493	504	534	546	565	575	578		
	580	586	626	635	649	680	692	694	696	712		
	720	754	812	819	875	878	895	920	937	941		
	965	971	973	979	991	1012	1014	1020	1020	1022	1025	
	1028	1056	1057	1069	1079	1114	1116	1135	1148	1169	1182	1182
	1186	1204	1216	1223	1237	1308	1332	1337	1361	1370	1378	
	1386	1402	1418	1421	1425	1430	1443	1449	1465	1475	1483	
	1486	1487	1490	1491	1497	1500	1502	1502	1510	1526	1537	
	1542	1570	1586	1618	1635	1646	3027	3031	3036	3038	3048	
	3050	3093	3099	3099	3102	3111	3113	3120	3140	3147	3163	
	3164	3176	3181	3185	3194	3196	3204	3206	3208	3486		
	INT1 D3	21	32	38	42	49	50	57	61	63	66	
		78	84	87	94	98	107	117	123	141	145	
		166	171	175	177	183	188	193	208	236	242	
		248	257	260	264	265	273	276	280	285	288	
304		332	351	358	382	398	407	418	434	449		
451		454	492	492	510	545	548	561	578	582		
583		589	626	636	647	651	687	695	695	697		
711		738	812	823	868	875	902	924	939	951		
964		967	972	990	1012	1012	1018	1021	1026	1029	1035	
1055		1056	1070	1080	1096	1115	1125	1136	1156	1172	1181	1185
1196		1200	1211	1227	1240	1329	1335	1345	1357	1366	1371	
1386		1408	1418	1424	1425	1434	1443	1444	1466	1476	1484	
1486		1489	1496	1498	1500	1503	1504	1507	1520	1527	1536	
1540		1576	1586	1625	1645	1649	3032	3036	3041	3046	3051	
3057		3099	3103	3106	3109	3116	3118	3132	3138	3150	3169	
3177		3181	3184	3191	3201	3205	3220	3229	3265	3553		
TS2		-73	12	15	20	36	40	47	51	52	58	
		62	68	72	74	82	89	95	101	104	134	
		151	161	163	175	177	179	183	190	210	225	
		230	244	253	258	259	263	267	270	279	283	
	283	312	351	357	365	387	403	426	429	437		
	447	450	504	505	506	527	535	573	577	578		
	578	588	623	634	648	668	684	693	695	709		
	734	808	809	856	871	879	894	910	930	937		
	944	961	973	990	1001	1001	1012	1018	1019	1023	1027	

		1029 1049 1052 1066 1078 1106 1113 1139 1144 1173 1178 1182 1185 1196 1205 1226 1236 1306 1333 1335 1348 1354 1360 1386 1399 1405 1415 1419 1428 1434 1450 1463 1472 1477 1480 1483 1487 1492 1493 1499 1500 1510 1511 1520 1527 1571 1593 1620 1628 1636 1644 3027 3032 3036 3041 3048 3051 3083 3095 3100 3106 3107 3109 3110 3127 3143 3146 3151 3173 3181 3186 3188 3193 3203 3206 3207 3452
TS2	D3a	-84 20 24 26 32 41 42 51 57 58 60 65 69 74 86 91 99 103 112 135 151 159 163 177 178 181 185 193 214 227 234 245 256 258 258 264 267 271 280 283 284 315 353 359 369 389 404 426 431 442 449 453 505 506 507 529 537 575 578 579 579 590 624 636 650 669 685 696 697 710 736 808 813 870 873 881 898 916 936 940 945 963 976 994 1001 1002 1014 1018 1022 1026 1028 1029 1050 1054 1066 1079 1108 1114 1141 1145 1175 1179 1182 1187 1196 1207 1229 1239 1308 1333 1334 1351 1358 1361 1391 1403 1405 1415 1419 1430 1435 1451 1463 1473 1476 1481 1484 1488 1492 1493 1500 1502 1511 1513 1523 1528 1574 1595 1618 1631 1638 1650 3027 3031 3036 3042 3048 3051 3076 3094 3099 3105 3107 3107 3111 3133 3144 3144 3150 3171 3183 3185 3188 3192 3203 3206 3208 3445
TS2	D3	-100 14 23 25 33 35 45 48 50 57 60 63 77 82 90 106 111 123 129 138 151 156 166 167 173 184 188 196 217 231 234 253 256 257 261 262 265 271 273 281 288 321 359 361 368 374 406 423 432 447 455 457 500 504 507 526 559 565 574 581 584 588 626 637 650 670 688 697 702 721 740 808 817 860 874 897 897 926 941 943 948 955 976 996 1004 1008 1020 1022 1023 1026 1029 1030 1050 1059 1068 1083 1106 1110 1139 1145 1172 1174 1183 1190 1198 1206 1229 1240 1311 1328 1337 1358 1362 1365 1394 1403 1407 1415 1419 1426 1433 1445 1463 1473 1477 1480 1484 1489 1493 1496 1501 1503 1509 1516 1524 1529 1573 1601 1615 1627 1639 1668 3029 3035 3043 3047 3051 3051 3099 3105 3109 3110 3116 3117 3143 3147 3151 3160 3169 3177 3191 3194 3198 3199 3203 3214 3222 3425
INT2		20 23 29 33 41 47 50 53 57 60 63 67 70 79 89 95 100 111 132 137

		151	163	175	177	179	183	185	196	219	227		
		236	251	255	258	259	263	271	278	279	281		
		283	313	351	355	367	383	396	425	430	445		
		449	453	504	505	518	530	544	573	575	578		
		578	589	620	635	646	670	676	694	697	713		
		742	808	813	867	876	888	894	916	929	941		
		945	965	974	991	1001	1003	1012	1021	1022	1025	1028	
		1040	1049	1057	1064	1078	1106	1109	1139	1144	1173	1178	1184
		1189	1196	1205	1224	1239	1311	1321	1334	1335	1356	1363	
		1391	1392	1404	1415	1418	1427	1430	1451	1464	1475	1476	
		1479	1484	1490	1492	1494	1498	1502	1510	1514	1527	1527	
		1573	1597	1624	1634	1646	1652	3028	3033	3037	3043	3048	
		3052	3096	3101	3105	3106	3107	3107	3111	3130	3144	3145	
		3152	3175	3182	3184	3186	3195	3201	3208	3209	3435		
INT2	D3a	21	24	26	33	48	50	51	58	60	60		
		68	70	72	77	93	98	103	122	133	139		
		155	163	174	178	179	183	188	196	218	230		
		239	251	257	258	258	264	272	273	280	282		
		284	312	353	357	367	381	397	421	430	447		
		448	454	506	507	518	530	548	575	576	579		
		579	591	620	637	648	671	679	695	700	715		
		742	808	815	866	882	894	896	918	931	943		
		949	957	976	994	1002	1006	1011	1022	1024	1027	1029	
		1039	1048	1057	1065	1079	1105	1107	1140	1145	1174	1178	1183
		1190	1196	1206	1227	1242	1312	1327	1334	1338	1357	1364	
		1393	1397	1403	1414	1418	1426	1430	1451	1464	1477	1477	
		1479	1484	1489	1492	1496	1499	1503	1510	1514	1527	1528	
		1574	1601	1624	1635	1647	1659	3028	3032	3038	3043	3046	
		3052	3095	3100	3106	3107	3109	3112	3128	3135	3143	3147	
		3151	3173	3182	3184	3186	3197	3200	3206	3210	3424		
INT2	D3	14	19	23	34	42	45	48	54	62	66		
		70	75	79	88	97	108	116	126	135	141		
		159	162	167	171	179	184	189	206	220	232		
		242	254	259	263	264	264	272	280	281	284		
		286	324	358	360	362	381	398	418	431	448		
		451	454	506	509	522	526	556	572	573	579		
		584	591	623	634	647	673	677	689	707	720		
		739	801	819	856	859	898	918	933	936	942		
		946	953	977	993	1004	1006	1015	1017	1024	1027	1030	
		1031	1051	1063	1066	1083	1106	1107	1139	1147	1171	1172	1186
		1188	1199	1206	1228	1241	1310	1330	1332	1334	1364	1365	

		1392 1397 1402 1413 1417 1423 1427 1444 1465 1475 1476 1477 1487 1490 1493 1500 1501 1506 1510 1515 1524 1525 1572 1601 1618 1632 1655 1681 3031 3036 3042 3046 3050 3054 3100 3105 3108 3110 3111 3115 3134 3145 3155 3163 3179 3193 3194 3197 3198 3205 3209 3210 3224 3402
TS3		-1127 11 25 30 32 36 41 47 54 55 57 63 72 80 91 97 117 130 144 152 158 161 169 172 176 185 200 210 217 234 235 242 255 258 261 263 268 270 273 275 288 308 322 349 353 370 392 406 416 443 448 460 475 499 505 523 531 550 568 569 578 578 587 638 645 658 672 688 700 706 721 762 779 817 818 869 893 903 913 940 942 954 974 983 986 995 1006 1021 1026 1029 1034 1044 1060 1064 1071 1079 1105 1135 1139 1145 1163 1179 1184 1187 1196 1212 1220 1239 1312 1314 1323 1326 1362 1373 1385 1395 1402 1413 1415 1421 1425 1446 1451 1472 1476 1478 1481 1486 1489 1491 1493 1500 1501 1502 1506 1513 1539 1571 1574 1603 1610 1631 1640 3030 3032 3039 3039 3048 3054 3094 3099 3101 3104 3105 3113 3117 3132 3150 3157 3162 3175 3178 3183 3186 3196 3200 3217 3477
INT3		17 25 28 35 42 42 45 50 54 61 63 66 85 97 116 121 125 150 159 160 166 171 172 183 187 196 203 211 218 239 245 250 256 256 259 262 263 271 274 275 282 322 337 363 375 392 410 420 438 443 459 475 499 502 513 516 530 536 566 571 573 574 580 611 639 642 668 671 695 704 723 760 815 816 852 873 892 894 908 911 934 939 971 972 984 1011 1015 1021 1024 1034 1046 1054 1069 1070 1081 1084 1103 1136 1142 1156 1156 1180 1181 1187 1194 1217 1235 1277 1300 1314 1320 1329 1358 1360 1390 1400 1410 1412 1425 1427 1436 1453 1466 1469 1471 1472 1476 1486 1490 1493 1498 1503 1505 1509 1511 1541 1547 1573 1596 1618 1625 1690 3011 3030 3034 3035 3054 3057 3093 3098 3098 3101 3103 3111 3127 3145 3146 3151 3156 3166 3174 3177 3188 3192 3205 3234 3247 3541
TS3	D3a	-1131 18 24 33 35 42 48 54 55 57 61 66 77 82 95 100 119 132 147 151 161 164 171 173 176 186 202 209 216 235 237 245 256 258 263 264 269 272 275 276

		290	310	325	352	356	372	396	407	416	446
		449	463	476	500	506	525	534	553	570	570
		579	579	588	637	647	660	673	691	701	707
		721	762	776	817	820	871	896	904	912	940
		941	955	975	984	986	996	1008	1024	1026	1030
		1045	1061	1065	1071	1081	1108	1136	1140	1146	1165
		1188	1198	1213	1224	1242	1313	1316	1324	1327	1364
		1386	1392	1402	1416	1418	1423	1425	1447	1451	1474
		1480	1481	1489	1490	1491	1493	1499	1502	1503	1507
		1541	1572	1575	1604	1610	1633	1643	3030	3033	3038
		3047	3053	3093	3098	3101	3103	3104	3112	3121	3133
		3156	3160	3173	3179	3183	3184	3196	3200	3219	3475
TS3	D3	-1136	15	22	28	33	35	46	48	54	57
		61	66	79	84	95	102	123	136	151	159
		163	170	171	174	177	189	204	210	218	233
		239	247	256	258	263	268	270	272	274	276
		291	314	329	356	365	374	401	412	418	449
		452	467	480	501	507	526	533	558	571	575
		580	581	589	635	648	662	676	692	703	707
		715	734	772	818	821	871	900	909	924	943
		945	957	976	991	992	1005	1012	1027	1028	1031
		1046	1065	1066	1071	1084	1110	1138	1142	1146	1168
		1189	1199	1220	1228	1245	1314	1320	1330	1331	1365
		1385	1392	1403	1418	1420	1425	1428	1447	1452	1474
		1481	1483	1489	1490	1493	1494	1500	1503	1505	1508
		1541	1574	1575	1606	1611	1634	1646	3033	3036	3043
		3049	3055	3097	3102	3106	3106	3107	3116	3123	3137
		3158	3165	3178	3184	3189	3190	3202	3214	3223	3477
INT4		10	14	19	22	29	33	38	43	47	51
		54	60	62	66	70	70	75	82	92	93
		99	113	125	126	140	149	158	161	167	168
		172	174	175	182	187	198	200	204	225	240
		249	255	259	259	263	265	267	271	275	283
		298	299	323	334	340	361	368	382	408	424
		438	441	444	446	456	457	499	503	510	523
		531	539	566	568	576	582	591	597	606	609
		622	638	663	695	701	706	710	715	717	753
		774	781	785	812	821	856	877	888	892	897
		910	917	944	948	957	973	973	979	993	1013
		1015	1015	1019	1034	1038	1043	1068	1070	1070	1072
		1101	1105	1130	1138	1140	1147	1151	1168	1185	1188
		1194	1199								

		1219 1233 1239 1240 1285 1317 1318 1324 1334 1366 1370 1371 1373 1375 1393 1404 1406 1415 1416 1417 1422 1426 1429 1443 1465 1469 1473 1474 1475 1486 1486 1488 1491 1491 1492 1500 1504 1506 1513 1514 1547 1563 1579 1603 1625 1631 1714 1754 1787 3031 3036 3040 3042 3052 3060 3064 3068 3098 3102 3103 3106 3107 3109 3110 3121 3125 3132 3149 3150 3151 3160 3161 3179 3183 3190 3194 3205 3207 3222 3241 3442 3523
INT4	D3a	25 26 35 37 39 44 50 54 57 58 63 65 72 73 78 79 84 90 103 104 108 121 133 134 145 154 161 166 168 173 175 178 180 190 194 204 207 210 229 244 253 259 260 261 266 270 274 275 279 289 303 304 329 341 345 366 373 388 412 425 442 444 448 453 459 466 501 506 512 523 533 546 569 572 580 585 591 599 610 614 625 643 666 697 704 709 711 718 723 755 775 784 787 812 825 861 881 888 896 907 913 928 947 951 962 972 976 982 997 1014 1016 1017 1018 1018 1037 1042 1045 1070 1070 1073 1077 1083 1105 1108 1136 1141 1144 1148 1152 1172 1187 1190 1199 1201 1222 1237 1242 1250 1289 1321 1323 1328 1336 1368 1373 1375 1378 1380 1396 1405 1408 1416 1417 1422 1424 1427 1432 1444 1467 1471 1473 1476 1477 1487 1488 1488 1492 1492 1494 1502 1506 1508 1516 1520 1549 1566 1582 1605 1628 1636 1722 1758 1794 3030 3037 3041 3043 3052 3063 3066 3067 3097 3101 3102 3106 3108 3110 3110 3123 3128 3137 3149 3151 3153 3159 3161 3181 3189 3191 3202 3209 3217 3227 3254 3414 3539
INT4	D3	17 20 26 36 38 48 51 53 56 59 62 66 69 75 81 85 90 95 101 110 117 126 137 139 149 156 165 168 169 173 175 182 182 195 198 204 210 212 232 244 255 259 262 265 267 269 272 276 281 289 304 309 332 344 345 370 376 391 411 427 443 446 449 459 462 473 502 509 512 523 536 551 569 573 581 589 591 599 612 616 625 644 670 698 705 712 712 720 726 754 774 784 788 812 825 866 885 888 898 910 912 935 949 952 964 971 977 984 998 1014 1016 1018 1019 1020 1032 1044 1048 1068 1070 1073 1077 1083

		1105 1110 1138 1141 1143 1148 1154 1175 1188 1192 1198 1203 1224 1237 1243 1258 1290 1321 1322 1331 1337 1369 1375 1375 1382 1382 1398 1405 1408 1417 1418 1426 1426 1428 1432 1445 1467 1472 1474 1477 1478 1485 1487 1490 1492 1492 1494 1502 1506 1508 1516 1524 1551 1567 1583 1607 1631 1641 1724 1754 1798 3033 3042 3043 3047 3054 3067 3067 3073 3101 3103 3106 3110 3112 3113 3114 3126 3136 3141 3155 3155 3156 3162 3166 3186 3194 3199 3209 3210 3219 3232 3280 3379 3541
TS4		-295 21 24 29 34 38 40 43 47 52 56 58 60 63 67 69 74 79 88 97 100 105 112 123 127 134 140 157 159 164 169 172 178 185 190 197 211 218 227 231 246 248 257 259 260 270 273 274 277 286 307 310 317 344 351 363 372 382 407 420 436 443 444 447 459 468 483 505 508 527 553 559 574 577 581 585 598 607 609 634 647 653 682 685 694 696 703 710 719 748 781 786 795 808 821 849 870 883 892 892 914 942 945 946 958 974 976 984 992 997 1003 1003 1014 1017 1018 1034 1059 1069 1070 1072 1077 1098 1105 1121 1130 1135 1139 1147 1165 1185 1187 1191 1199 1219 1224 1236 1238 1245 1294 1313 1322 1333 1336 1348 1365 1369 1373 1374 1381 1399 1405 1411 1416 1417 1421 1422 1428 1450 1467 1470 1474 1476 1477 1484 1485 1488 1488 1492 1493 1501 1502 1505 1510 1512 1552 1567 1574 1602 1618 1638 1719 1765 1791 3029 3037 3038 3043 3050 3052 3063 3071 3094 3098 3100 3104 3105 3109 3110 3114 3114 3128 3129 3152 3155 3160 3170 3175 3179 3181 3182 3187 3194 3207 3215 3444 3486
TS4	D3a	-305 21 25 31 32 35 42 47 49 51 56 61 65 66 69 71 77 79 90 97 105 109 114 125 131 134 142 157 160 165 169 174 182 187 191 198 212 219 229 233 246 249 256 259 262 271 272 275 278 289 310 314 321 348 353 367 374 386 408 423 436 444 447 449 463 469 484 507 509 530 556 560 574 579 582 587 599 608 613 635 646 655 683 686 697 698 711 718 720 748 780 787 796 808 823 860 878 890 897 902 919 945 946 949 960 975 975 984 994 998

		1004 1005 1015 1017 1022 1034 1059 1069 1070 1073 1077 1097 1107 1123 1132 1136 1141 1148 1168 1185 1188 1192 1202 1221 1224 1239 1245 1246 1296 1314 1322 1334 1337 1349 1365 1375 1376 1378 1383 1402 1406 1412 1416 1421 1422 1423 1431 1450 1467 1472 1474 1476 1476 1486 1487 1488 1488 1492 1493 1502 1502 1506 1511 1514 1553 1569 1575 1604 1621 1644 1722 1764 1796 3028 3038 3039 3042 3049 3052 3067 3070 3093 3100 3100 3103 3104 3109 3109 3113 3121 3127 3132 3155 3156 3159 3168 3178 3181 3181 3182 3190 3194 3209 3219 3399 3476
TS4	D3	-308 22 25 32 36 40 48 51 57 58 60 61 67 70 72 79 83 88 97 105 112 120 127 132 135 142 155 158 163 167 172 179 189 192 193 197 213 221 228 230 242 250 256 262 263 270 274 282 284 295 310 319 324 351 356 371 377 392 413 425 433 445 451 452 466 470 484 512 516 536 559 562 576 584 585 592 600 611 615 638 649 659 685 693 699 702 715 720 746 754 786 789 797 808 825 866 883 889 903 915 932 947 953 955 973 977 982 988 994 997 1007 1010 1016 1018 1026 1034 1060 1070 1073 1078 1079 1100 1112 1126 1136 1138 1145 1148 1174 1185 1190 1193 1206 1221 1223 1241 1246 1258 1300 1312 1324 1339 1341 1359 1365 1374 1383 1385 1385 1404 1408 1411 1419 1423 1426 1430 1435 1451 1468 1474 1474 1477 1480 1487 1488 1489 1490 1493 1493 1502 1502 1509 1511 1515 1552 1574 1576 1606 1624 1651 1724 1759 1799 3031 3042 3045 3047 3052 3055 3072 3073 3097 3103 3105 3107 3108 3112 3113 3114 3130 3135 3141 3156 3162 3162 3174 3184 3188 3188 3189 3196 3200 3214 3215 3353 3456
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TS5	-1319 2 16 18 22 33 42 45 47 50 52 54 56 61 63 75 78 87 91 104 106 113 129 138 146 151 154 154 165 169 176 179 183 189 200 204 209 219 230 244 251 254 257 258 260 263 271 272 276 282 310 316 320 347 354 366 376 382 398 423 425 433 441 447 469 488 492 503 528 551 561 566 571 576 579 580 581 601 637 642 651 662 675 686 694 697 718 723 745 749 775 784 803 816 818 842 881 894 901 919 942 943 947 952 971 983 997 1005 1008 1015 1017 1022 1023 1031 1041 1048 1053 1071 1072 1079 1085 1108 1114 1128 1139 1145 1148 1169 1181 1189 1193 1199 1202 1220

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INT7		11 14 20 22 27 27 32 33 42 44 46 49 53 54 59 68 73 82 90 94 100 114 126 132 138 144 149 151 160 162 165 166 175 184 198 203 211 221 235 246 252 254 256 259 265 267 274 280 282 285 310 317 331 341 350 356 372 394 404 413 432 444 448 450 488 501 504 526 543 550 561 563 572 573 582 583 586 602 618 637 644 647 670 674 686 694 699 736 766 779 804 811 818 820 824 869 893 896 917 929 940 943 947 972 973 978 979 995 998 1011 1014 1020 1022 1029 1052 1059 1066 1067 1081 1084 1105 1115 1124 1137 1138 1146 1169 1179 1186 1187 1195 1199 1222 1226 1238 1246 1255 1261 1303 1306 1315 1323 1335 1362 1363 1373 1379 1380 1393 1402 1410 1413 1418 1421 1422 1427 1442 1463 1464 1473 1476 1476 1481 1489 1492 1493 1493 1494 1499 1501 1504 1512 1518 1528 1530 1560 1569 1613 1625 1644 1687 1725 1809 3020 3032 3036 3038 3042 3043 3052 3070 3077 3097 3100 3101 3101 3106 3106 3110 3110 3110 3113 3114 3131 3142 3149 3156 3157 3172 3176 3179 3188 3200 3208 3230 3446
INT7	D3a	10 17 21 29 32 36 41 44 50 53 57 59 62 70 72 80 89 94 103 113 114 121 128 135 142 145 152 162 168 172 177 178 186 196 204 215 225 234 242 249 256 258 260 264 272 276 277 282 288 301 315 322 332 338 353 355 371 385 411 413 427 446 451 455 492 493 500 505 530 553 562 565 572 578 582 582 586 604 627 635 647 648 677 686 692 694 697 736 769 780 796 813 816 820 825 870 897 900 921 940 946 951 966 973 973 978 984 996 997 1012 1013

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TS6	-56 16 21 23 26 33 37 42 46 51 53 54 60 63 68 76 79 83 86 89 95 105 111 116 123 136 149 150 163 172 177 182 185 197 201 207 213 216 226 250 254 257 259 260 263 275 277 282 286 293 297 312 315 330 348 357 363 388 395 410 429 448 449 459 484 487 489 504 505 518 542 556 572 574 576 577 582 585 602 632 637 645 648 668 686 691 694 697 748 770 779 804 817 822 833 856 894 909 935 945

		946	951	967	973	975	981	989	994	997	1015	1017
		1020	1024	1028	1056	1064	1067	1071	1077	1083	1102	1115
		1122	1136	1138	1154	1164	1178	1181	1185	1190	1194	1218
		1234	1241	1251	1300	1305	1311	1317	1320	1327	1356	1373
		1377	1380	1388	1398	1409	1410	1420	1421	1423	1425	1442
		1453	1464	1471	1473	1475	1481	1483	1491	1492	1492	1497
		1501	1501	1504	1505	1509	1520	1527	1529	1540	1561	1563
		1616	1640	1657	1713	1800	3015	3031	3035	3037	3042	3043
		3054	3076	3077	3091	3092	3098	3101	3104	3105	3109	3110
		3113	3124	3127	3130	3142	3147	3149	3157	3170	3180	3183
		3191	3202	3204	3224	3542						
TS6	D3a	-51	22	26	27	28	32	40	49	50	51	
		56	59	63	65	70	80	83	88	94	96	
		102	112	115	122	129	140	147	152	161	177	
		181	186	188	200	204	211	214	216	226	251	
		256	259	261	263	266	277	281	287	291	297	
		301	311	320	334	351	360	367	393	404	413	
		431	449	452	460	483	487	496	506	511	517	
		543	559	572	577	579	579	582	588	604	629	
		638	646	652	669	689	694	697	699	745	771	
		781	807	819	824	836	858	898	911	935	947	
		949	951	970	974	977	986	992	996	1002	1018	1019
		1021	1027	1028	1060	1066	1071	1071	1080	1086	1104	1118
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		1501	1501	1506	1508	1508	1524	1529	1532	1540	1564	1568
		1619	1642	1659	1721	1805	3016	3030	3034	3037	3041	3044
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		3118	3126	3129	3137	3147	3148	3157	3158	3170	3183	3183
		3194	3210	3213	3232	3560						
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		181	187	196	206	212	213	219	224	229	251	
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		304	313	320	341	356	361	370	395	410	417	
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		529	561	573	575	576	584	588	589	610	629	
		643	649	654	663	693	696	701	702	738	762	

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TS1-O-N	-73 14 32 35 41 46 50 53 53 59 63 67 73 92 95 110 127 130 147 148 161 172 177 179 183 209 228 238 241 245 264 277 285 317 324 352 359 379 392 416 421 441 445 447 494 517 525 530 573 618 621 635 636 659 669 680 684 691 701 719 773 821 825 850 869 895 922 929 939 945 947 963 972 974 996 1006 1009 1011 1019 1023 1030 1031 1033 1054 1058 1062 1066 1080 1106 1107 1134 1149 1160 1168 1180 1182 1183 1211 1220 1238 1305 1310 1324 1334 1339 1359 1361 1368 1389 1401 1403 1408 1413 1419 1428 1456 1464 1466 1475 1476 1476 1480 1485 1489 1492 1498 1502 1507 1510 1512 1530 1531 1563 1566 1616 1623 1642 1653 1671 3027 3033 3033 3036 3046 3048 3048 3090 3096 3099 3100 3103 3104 3107 3115 3141 3141 3143 3163 3168 3174 3184 3186 3197 3200 3201 3202 3215 3359
DMF D3a DMF solvent	121 171 242 321 346 401 660 870 1027 1077 1103 1129 1176 1272 1420 1436 1441 1470 1476 1495 1501 1538 1704 2967 3020 3026 3069 3074 3121 3152
1a D3a DMF solvent	43 75 109 152 222 300 354 411 415 456 515 636 687 709 724 818 844 863 953 1000 1015 1019 1026 1054 1106 1147 1175 1181 1183 1204 1308 1335 1358 1449 1477 1481 1504 1528 1562 1619 1644 1673 3033 3091 3133 3158 3165 3173 3182 3192 3556
CAT D3a DMF solvent	28 41 41 44 49 52 67 72 99 111 121 149 159 174 180 183 192 204 213 232 247 251 255 262 264 267 273 299 305 315 332 357 406 411 415 450 458 489 499 510 533 564 572 584 588 596 623 649 677 699 702 822 896 930 945 948 968 973 985 1005 1014 1018 1027 1063 1070 1082 1111 1139 1170 1187 1224 1239 1313 1338 1364 1386 1404 1417 1423 1427 1429 1436 1463 1478 1487 1488 1492 1499 1505 1505 1511 1514 1542 1569 3030 3033 3039 3040 3052 3098 3102 3103 3105 3110 3116 3131 3151 3181 3192 3201 3225
COM1-DMF D3a DMF solvent	11 16 31 41 48 51 54 60 64 69 73 76 87 102 105 115 153 160 164 168 174 182 183 188 202 211 227 240 247 252

	258 259 261 267 269 273 285 291 306 333 355 386 392 399 415 416 428 445 453 495 500 502 528 568 569 570 574 585 625 647 674 694 700 705 817 877 898 921 944 949 966 976 988 1002 1008 1021 1023 1062 1070 1070 1075 1081 1110 1134 1136 1140 1174 1181 1186 1229 1245 1267 1310 1344 1369 1386 1403 1419 1422 1423 1425 1429 1442 1449 1457 1465 1474 1482 1485 1487 1489 1491 1496 1500 1501 1503 1509 1511 1522 1528 1539 1571 1677 3031 3034 3035 3037 3043 3049 3087 3092 3093 3096 3098 3109 3113 3115 3119 3124 3132 3147 3154 3170 3175 3176 3218 3223
TS1a-DMF D3a DMF solvent	-105 17 17 26 29 33 37 39 45 50 52 56 60 64 65 72 76 79 88 94 108 114 119 125 134 143 146 155 163 166 171 171 176 178 182 189 214 225 238 241 256 258 259 260 262 268 270 271 275 276 311 317 353 359 375 390 396 409 416 419 424 426 445 457 481 496 503 527 531 564 569 573 577 583 627 636 649 673 677 682 697 698 701 721 739 817 820 855 877 882 896 926 940 942 954 974 978 984 997 1010 1020 1021 1024 1025 1027 1031 1035 1057 1060 1067 1075 1077 1112 1114 1129 1133 1140 1148 1169 1178 1180 1184 1185 1197 1213 1227 1240 1269 1311 1327 1333 1343 1363 1373 1378 1402 1405 1417 1419 1424 1426 1433 1446 1448 1454 1465 1468 1473 1477 1480 1483 1484 1487 1490 1492 1495 1497 1498 1505 1507 1511 1532 1536 1537 1572 1596 1600 1618 1646 1655 1674 3027 3031 3033 3036 3036 3042 3042 3047 3091 3092 3096 3097 3098 3100 3106 3109 3114 3120 3136 3136 3142 3149 3159 3170 3170 3180 3181 3184 3197 3203 3212 3224 3542
INT1 D3a DMF solvent	10 17 37 43 48 51 55 59 61 62 67 68 81 82 95 105 115 127 139 146 165 169 171 172 180 187 196 200 227 232 244 257 259 261 264 268 270 271 283 287 298 329 349 358 371 394 398 415 420 437 448 457 491 493 504 535 545 563 574 576 580 585 626 635 648 681 692 694 695 706 713 746 811 819 874 876 895 920 937 941 965 969 973 981 992 1012 1013 1020 1021 1023 1024 1028 1056 1056 1069 1079 1115 1115 1135 1148 1170 1182 1183

	1186 1204 1214 1223 1237 1309 1331 1338 1361 1368 1376 1386 1402 1418 1420 1424 1430 1441 1449 1465 1475 1483 1485 1488 1489 1491 1497 1499 1501 1501 1510 1524 1536 1541 1570 1587 1616 1634 1645 3027 3030 3036 3037 3047 3049 3093 3098 3099 3101 3111 3112 3119 3140 3146 3162 3162 3173 3178 3182 3191 3193 3203 3203 3208 3501
1a D3a CH ₃ CN solvent	44 72 108 150 220 299 354 411 415 459 516 636 686 709 724 818 843 863 953 1000 1015 1018 1026 1054 1105 1147 1175 1181 1183 1204 1308 1334 1358 1449 1477 1481 1504 1527 1562 1618 1643 1673 3035 3094 3136 3162 3169 3177 3186 3196 3559
CH ₃ CN D3a CH ₃ CN solvent	386 386 925 1058 1058 1407 1464 1464 2354 3050 3121 3121
CAT D3a CH ₃ CN solvent	29 41 41 44 49 52 67 72 99 111 121 149 159 174 180 183 192 204 213 232 247 251 255 262 264 267 273 299 305 315 332 357 406 411 415 450 458 489 499 510 533 564 572 584 588 596 623 649 677 699 702 822 896 930 945 948 968 973 985 1005 1014 1018 1027 1063 1070 1082 1111 1139 1170 1187 1224 1239 1313 1338 1364 1386 1404 1417 1423 1427 1429 1436 1463 1478 1487 1488 1492 1499 1505 1505 1512 1514 1542 1569 3030 3033 3039 3040 3052 3098 3102 3103 3105 3110 3116 3131 3151 3181 3192 3201 3225
COM1-CCN D3a CH ₃ CN solvent	16 28 35 39 44 54 57 60 61 69 89 95 115 119 143 151 166 172 174 179 189 200 215 230 239 247 256 256 260 264 267 272 275 284 292 312 328 356 376 403 429 436 444 450 462 497 500 502 524 565 569 574 577 582 629 647 667 695 696 818 898 918 937 944 962 967 975 995 1011 1021 1023 1043 1056 1061 1063 1071 1080 1113 1141 1175 1192 1227 1249 1319 1350 1369 1388 1404 1408 1417 1422 1424 1432 1441 1456 1465 1469 1475 1485 1486 1492 1500 1502 1506 1510 1523 1540 1573 2398 3028 3032 3037 3044 3049 3082 3091 3100 3106 3107 3109 3113 3119 3125 3131 3148 3186 3191 3205 3221
TS1-CCN D3a CH ₃ CN solvent	-99 13 23 30 31 35 37 42 47 51 56 62 63 65 78 83 89 97 100 110 117 128 139 144 151 157 164 165 168 169

	173	178	188	200	207	225	235	239	253	256
	258	259	267	268	270	270	274	311	318	353
	360	390	403	409	420	423	425	430	446	456
	472	500	504	526	535	569	570	574	576	586
	602	630	636	651	673	683	687	696	713	737
	822	824	855	867	897	928	934	944	955	958
	965	972	973	1002	1006	1012	1020	1023	1025	1028
	1053	1057	1060	1060	1072	1076	1110	1110	1135	1146
	1184	1185	1196	1210	1227	1242	1309	1330	1334	1348
	1369	1386	1402	1412	1413	1420	1426	1430	1447	1448
	1468	1472	1479	1481	1485	1488	1489	1491	1500	1502
	1510	1513	1528	1533	1547	1561	1595	1598	1636	1645
	3029	3036	3037	3043	3046	3049	3054	3092	3097	3100
	3102	3116	3117	3124	3128	3131	3143	3143	3161	3173
	3187	3188	3206	3207	3216	3216	3562			
TS1a-CCN	-112	9	21	26	36	38	38	41	43	47
D3a	51	55	58	59	63	67	74	77	86	91
CH ₃ CN solvent	108	120	125	126	149	150	156	167	170	175
	178	181	212	216	234	236	238	247	257	259
	261	264	267	270	270	274	276	300	315	352
	357	363	391	411	422	425	443	450	456	466
	487	496	503	530	531	564	571	577	577	584
	625	635	650	659	676	685	686	698	719	736
	817	818	853	879	895	925	942	944	953	956
	973	973	987	1003	1013	1019	1020	1026	1027	1029
	1053	1054	1057	1058	1068	1077	1111	1112	1140	1156
	1183	1186	1196	1211	1227	1241	1309	1326	1335	1342
	1371	1375	1402	1405	1418	1418	1421	1425	1433	1450
	1456	1465	1472	1478	1479	1482	1487	1489	1491	1496
	1508	1512	1534	1535	1576	1586	1607	1618	1645	1660
	3029	3031	3034	3036	3042	3047	3048	3086	3093	3098
	3109	3110	3115	3120	3121	3135	3142	3150	3160	3171
	3181	3188	3198	3207	3210	3221	3545			
TS1b-CCN	-142	12	13	16	20	24	26	32	36	41
D3a	48	49	51	54	63	68	74	78	87	95
CH ₃ CN solvent	100	118	120	123	143	152	156	162	165	170
	170	178	185	195	220	230	243	251	256	258
	260	263	263	270	275	277	282	317	350	355
	362	385	397	400	407	418	422	433	440	451
	490	496	504	526	540	564	571	577	578	585
	626	635	646	667	682	690	696	701	715	736

	811 818 873 876 897 917 931 938 942 951 970 975 985 1001 1013 1014 1021 1024 1026 1026 1029 1054 1056 1057 1058 1068 1082 1110 1113 1139 1148 1173 1182 1185 1187 1205 1211 1226 1240 1313 1330 1337 1360 1368 1369 1373 1402 1407 1415 1418 1421 1424 1425 1451 1462 1462 1463 1476 1477 1479 1483 1489 1493 1494 1501 1505 1510 1517 1527 1533 1566 1600 1608 1619 1634 1645 2373 3025 3028 3036 3038 3046 3048 3049 3090 3095 3100 3102 3105 3107 3121 3121 3124 3142 3145 3146 3163 3174 3181 3184 3198 3204 3205 3208 3215 3498
INT1 D3a CH ₃ CN solvent	6 15 36 42 47 49 56 57 60 63 67 68 81 82 95 106 116 127 138 146 165 169 171 172 180 187 196 200 227 233 245 258 259 261 264 268 270 271 283 288 298 328 348 358 371 395 398 416 420 437 448 457 491 493 504 535 546 563 573 576 580 585 626 635 648 681 692 694 696 707 714 746 811 819 874 876 895 920 937 941 965 970 973 980 992 1011 1013 1020 1020 1022 1024 1028 1056 1057 1069 1079 1114 1115 1134 1148 1169 1182 1183 1186 1204 1214 1223 1237 1308 1331 1338 1360 1369 1376 1386 1402 1418 1420 1424 1430 1441 1449 1465 1475 1483 1485 1487 1489 1491 1497 1499 1501 1502 1510 1524 1536 1542 1570 1587 1616 1634 1645 3027 3031 3036 3038 3047 3049 3094 3099 3099 3102 3110 3113 3119 3140 3147 3162 3164 3175 3179 3184 3192 3194 3203 3204 3208 3500