

DFT study on ruthenium-catalyzed decarbonylative annulation of an alkyne with six-membered hydroxymone via C–H/C–C activation

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1. Discussion from the steady-state approximation

Since the free-energy of **INT-4** is about 9.2 kcal·mol⁻¹ above the **1a+CAT**, the formation rate of **INT-4** is much smaller than the consumption rate of **INT-4**, and thus the steady-state approximation seems not valid at the point of **INT-4**. For such case, the whole reaction of **1a+2a+CAT**→**3a** could be separated into two reaction processes of **1a+CAT**→**INT-4** and **INT-4+2a**→**3a**, within each of which the steady-state approximation should be valid.

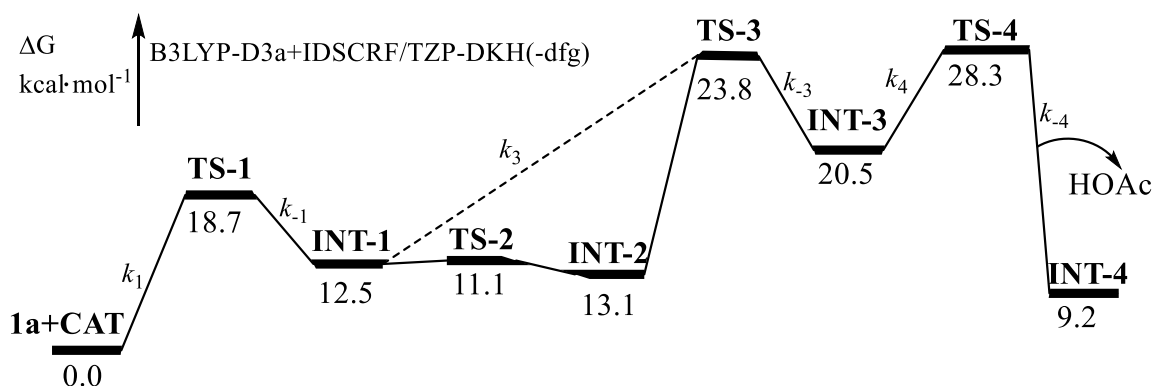


Figure S1 The free-energy profile(358.15K) for calculating the formation rate of **INT-4** from **1a+CAT**

$$\frac{d[1a][CAT]}{dt} = -k_1[1a][CAT] + k_{-1}[INT-1] \quad (1)$$

$$\frac{d[INT-1]}{dt} = k_1[1a][CAT] - k_{-1}[INT-1] - k_3[INT-1] + k_{-3}[INT-3] \quad (2)$$

$$\frac{d[INT-3]}{dt} = k_3[INT-1] - k_{-3}[INT-3] - k_4[INT-3] \quad (3)$$

$$\frac{d[INT-4]}{dt} = -\frac{d[1a][CAT]}{dt} = k_4[INT-3] \quad (4)$$

Since $k_{-4} \ll k_4$, one could ignore the term $k_{-4}[INT-4][HOAc]$ in the equations (3) and (4). According to the steady-state approximation, one can deduce:

$$[INT-3]_{SSA} = \frac{k_3}{k_{-3}+k_4} [INT-1] \quad \text{and} \quad [INT-1]_{SSA} = \frac{k_1}{k_{-1}+k_3-\frac{k_{-3}k_3}{k_{-3}k_4}} [1a][CAT]$$

Thus:

$$k^{1st} = \frac{k_1 k_3 k_4}{k_{-1} k_{-3} + k_{-1} k_4 + k_3 k_4} \quad (5)$$

Since the free energy of **TS-4** is much higher than those of **TS-3** and **TS-1**, i.e., k_3 is much smaller than others, allowing for omission of the 2nd and 3rd denominator terms in eq. (5), leading

to:

$$k^{1st} \approx \frac{k_1 k_3 k_4}{k_{-1} k_{-3}} \quad (6)$$

From transition state theory, one can obtain:

$$k^{1st} \approx \frac{k_B T}{h} e^{-\frac{(G^{TS-4} - G^{1a+CAT})}{RT}} \quad (7)$$

Substitute $k_1=2.898 \times 10^1 \text{ s}^{-1} \text{ dm}^3 \text{ mol}^{-1}$, $k_{-1}=1.229 \times 10^9 \text{ s}^{-1}$, $k_3=9.496 \times 10^5 \text{ s}^{-1}$, $k_{-3}=7.231 \times 10^{10} \text{ s}^{-1}$, $k_4=1.298 \times 10^8 \text{ s}^{-1}$ and $k_{-4}=1.652 \times 10^1 \text{ s}^{-1} \text{ dm}^3 \text{ mol}^{-1}$ into equation (5), one can deduce: $k^{1st}=4.01 \times 10^{-5} \text{ s}^{-1} \text{ dm}^3 \text{ mol}^{-1}$, almost the same as $k^{1st}=4.02 \times 10^{-5} \text{ s}^{-1} \text{ dm}^3 \text{ mol}^{-1}$ from equation (7).

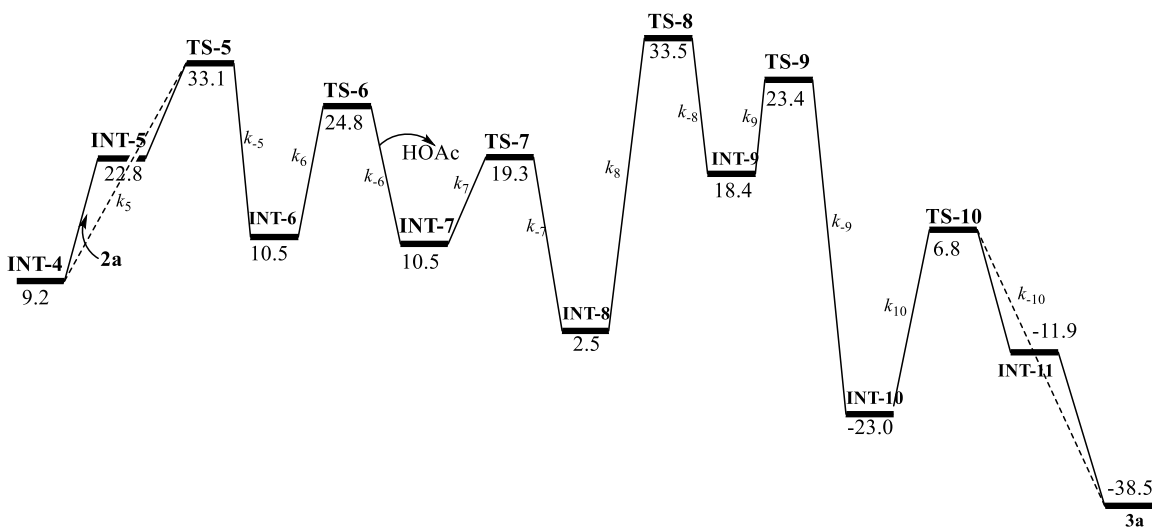


Figure S2 The free-energy profile(358.15K) for calculating the formation rate of **3a** from **INT-4**

According to steady-state approximation, the k^{sec} should be calculated as equation (8):

$$k^{sec} = \frac{k_5 k_6 k_7 k_8 k_9}{k_{-5} k_{-6} k_{-7} k_{-8} + k_{-5} k_{-6} k_{-7} k_9 + k_{-5} k_{-6} k_8 k_9 + k_{-5} k_7 k_8 k_9 + k_6 k_7 k_8 k_9} \quad (8)$$

The calculated rate k^{sec} is $7.06 \times 10^{-3} \text{ s}^{-1} \text{ dm}^3 \text{ mol}^{-1}$, which is close to that from the following equation ($k^{sec}=1.11 \times 10^{-2} \text{ s}^{-1} \text{ dm}^3 \text{ mol}^{-1}$):

$$k^{sec} \approx \frac{k_B T}{h} e^{-\frac{(G^{TS-8} - G^{INT-4})}{RT}} \quad (9)$$

The difference might originate from the contributions of both **TS-5** and **TS-8** for equation (8). Since $k^{1st}=4.02 \times 10^{-5} \text{ s}^{-1} \cdot \text{dm}^3 \cdot \text{mol}^{-1}$ is much smaller than $k^{sec}=7.06 \times 10^{-3} \text{ s}^{-1} \cdot \text{dm}^3 \cdot \text{mol}^{-1}$, **TS-4** and initial states should be the TOF-determining transition states (TDTS) and TOF-determining intermediate(TDI) if the energy span model (ESM) introduced by Kozuch and Shaik was employed(see next section).

2. Discussion from the ESM considering the concentration of intermediate INT-4

The turnover frequency (TOF) of the catalytic cycle is defined by Kozuch and Shaik(S. Kozuch, S. Shaik, *J Am Chem Soc* 2006, **128**, 3355):

$$\text{TOF} = \frac{k_B T}{h} \frac{e^{-\Delta G^r} - 1}{\sum_{ij} e^{\frac{(T_i - I_j - \delta G'_{i,j})}{RT}}} \quad (10)$$

Here ΔG^r is the energy of the global reaction. T_i and I_j are the calculated free energies of each transition state and intermediate, respectively. $\delta G'_{i,j}$ is either ΔG^r or zero, according to the position of T_i vs. I_j in the specific term of the summation, specified in eq. (11):

$$\delta G'_{i,j} = \begin{cases} \Delta G^r & \text{if } i > j \\ 0.0 & \text{if } i \leq j \end{cases} \quad (12)$$

To identify the TDI and TDTS, the energetic span model offers a quantification of the influence of each intermediate and transition state on the TOF—the so-called “degree of TOF control” (X_{TOF}) (S. Kozuch, S. Shaik, *J Am Chem Soc* 2006, **128**, 3355). The X_{TOF} was developed based on Campbell’s degree of rate control((a) C. T. Campbell, *Topics Catal* 1994, **1**, 353; (b) C. T. Campbell, *J Catal* 2001, **204**, 520; (c) C. Stegelmann, A. Andreasen, C.T. Campbell, *J Am Chem Soc* 2009, **131**, 8077; (d) C. Stegelmann, A. Andreasen, C.T. Campbell, *J Am Chem Soc* 2009, **131**, 13563; (e) J. K. Nørskov, T. Bligaard, J. Kleis, *Science* 2009, **324**, 1655) and measures how much will the TOF vary by a small change on a TS or an intermediate energy. It is calculated according to eq. (12) for transition states and eq. (13) for intermediates:

$$X_{\text{TOF},T_i} = \frac{\sum_j e^{\frac{(T_i - I_j - \delta G'_{i,j})}{RT}}}{\sum_{ij} e^{\frac{(T_i - I_j - \delta G'_{i,j})}{RT}}} \quad (12)$$

$$X_{\text{TOF},I_j} = \frac{\sum_i e^{\frac{(T_i - I_j - \delta G'_{i,j})}{RT}}}{\sum_{ij} e^{\frac{(T_i - I_j - \delta G'_{i,j})}{RT}}} \quad (13)$$

with

$$\delta G'_{i,j} = \begin{cases} \Delta G^r & \text{if } i \geq j \\ 0 & \text{if } i < j \end{cases} \quad (14)$$

If the rate constant of the formation of the last intermediate(*int*) for the reaction of first reactant is smaller than that of the consuming of the *int*, meaning that the formed *int* could react with **2a** quickly and then this int could not go back to reactants. In such case, the reaction with second reactant could start with this intermediate and the formation of *int* could be the rate-controlling step.

$$TOF = k_i[C_i] - k_{-i}[C_{i+1}] = \frac{\Delta}{M} \quad (15)$$

$$\delta G'_{i,j} = \begin{cases} \Delta G^r + \Delta G_k^{int} & \text{if } i \geq k, j < k \\ \Delta G_k^{int} & \text{if } i < k \text{ and } j \geq k \end{cases} \quad (16)$$

Herein ΔG_k^{int} is the free-energy relative to the the lowest free-energy species before the last intermediate k in the first reaction process between catalyst and first reactant. For example, if one has the following free-energy profile curve, one can assume **INT-2** is the initial state for the reaction of second reactant.

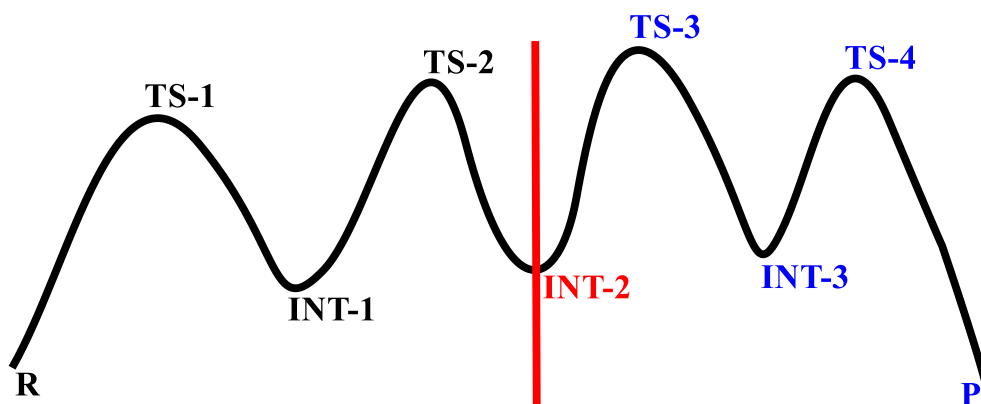


Figure S3 The supposed free-energy profile, herein the **INT-2** is last intermediate for the reaction of first reactant with catalyst.

For the stationary points within each part, the equation (14) is employed, e.g., $\mathbf{R} \rightarrow \mathbf{TS-1} \rightarrow \mathbf{INT-1} \rightarrow \mathbf{TS-2}$ and $\mathbf{INT-2} \rightarrow \mathbf{TS-3} \rightarrow \mathbf{INT-3} \rightarrow \mathbf{TS-4}$. However, for the cross terms between two parts (separated by red line in **Figure S3**) in eqs. (12) and (13), the equation (16) should be employed.

Determining TDI should be careful, since equations (12) and (13) sometime find not-real TDI. If $C_0 \rightleftharpoons C_1 \rightleftharpoons C_2 \cdots \rightleftharpoons C_{n-1} \rightleftharpoons C_n$ is met, and then any intermediate could be TDI. However, if $C_0 C_1 \rightarrow C_2$, C_1 could not be regarded as TDI even if C_1 is lower in free-energy than C_0 (see **Figure S4**), which is not the same as that from equations (13) and (14). Therefore, one should identify such

intermediates carefully, and then delete the contribution of each such intermediate for the forward direction to the following TS in equation (13).

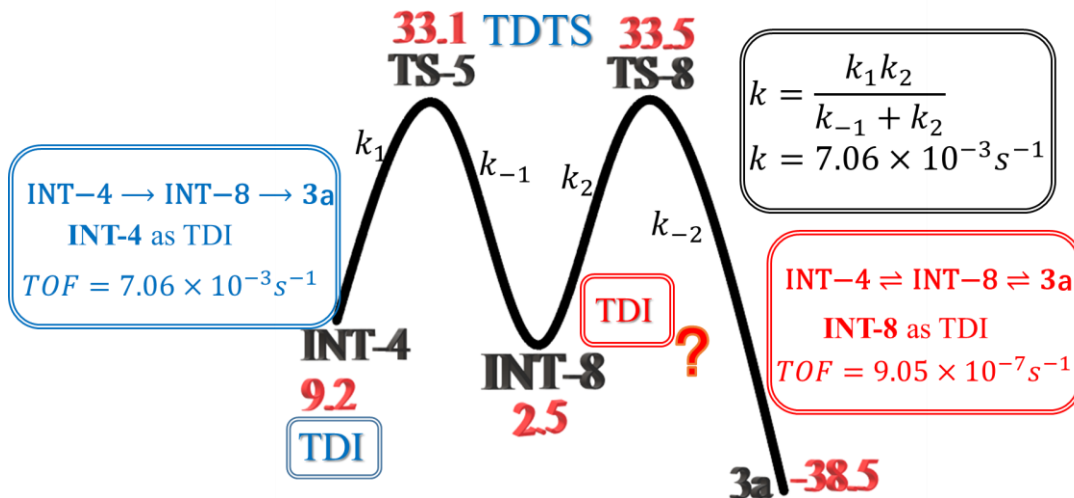


Figure S4 A simple example to illustrate that INT-8 is not a TDI for the case of $\text{INT-4} \rightarrow \text{INT-8} \rightarrow 3a$

If one can find TDTS and TDI from eqs. (12)-(16), the TOF could be shortened to

$$\text{TOF} = \frac{k_B T}{h} e^{-\delta E / RT} \quad (17)$$

$$\delta E = \begin{cases} G^{\text{TDTS}} - G^{\text{TDI}} & \text{if TDTS appears after TDI} \\ G^{\text{TDTS}} - G^{\text{TDI}} + \Delta G^r & \text{if TDTS appears before TDI} \end{cases} \quad (18)$$

Table S1 The calculated total electronic energies, enthalpies, entropies and free energies in a.u. , in the tert-butanol solvent with the temperature of 358.15K.

Species	$E_{\text{elec/a.u.}}$	$H/\text{a.u.}$	S_g	S_l	$G_g/\text{a.u.}$	$G_l/\text{a.u.}$
1a	-803.63621 ^a	-803.40382	126.5	104.0	-803.47603	-803.46318
	-803.60968 ^b	-803.37725	128.5	106.0	-803.45059	-803.43774
	-803.56427 ^c	-803.33202	127.5	105.0	-803.40481	-803.39196
2a	-539.69719 ^a	-539.48952	113.1	90.8	-539.55406	-539.54133
	-539.67412 ^b	-539.46754	108.0	85.7	-539.52918	-539.51645
	-539.63967 ^c	-539.43208	114.8	92.5	-539.49761	-539.48489

HOAc	-229.19616 ^a	-229.12816	72.4	52.6	-229.16936	-229.15816
	-229.18700 ^b	-229.11897	72.2	52.8	-229.16028	-229.14908
	-229.18205 ^c	-229.11404	72.2	52.6	-229.15523	-229.14403
CAT	-5247.98764 ^a	-5247.63932	174.2	152.3	-5247.73911	-5247.72659
	-5247.96470 ^b	-5247.61629	174.3	152.4	-5247.71579	-5247.70328
	-5247.90532 ^c	-5247.55725	176.2	154.3	-5247.65779	-5247.64530
1a+CAT	-6051.62385 ^a	-6051.04314	301.3	256.9	-6051.21514	-6051.18977
	-6051.57438 ^b	-6050.99354	302.8	258.4	-6051.16638	-6051.14102
	-6051.46959 ^c	-6050.88927	303.7	259.3	-6051.06260	-6051.03726
TS-1	-6051.60962 ^a	-6051.02745	253.7	232.3	-6051.17224	-6051.16003
	-6051.57234 ^b	-6050.99003	252.5	231.1	-6051.13417	-6051.12196
INT-1	-6051.62084 ^a	-6051.03911	250.6	229.2	-6051.18214	-6051.16991
	-6051.58362 ^b	-6051.00180	250.8	229.4	-6051.14494	-6051.13271
TS-2	-6051.62029 ^a	-6051.04173	249.9	228.5	-6051.18437	-6051.17212
	-6051.58309 ^b	-6051.00441	249.0	227.5	-6051.14652	-6051.13428
INT-2	-6051.62095 ^a	-6051.03889	259.3	227.8	-6051.18115	-6051.16892
	-6051.58377 ^b	-6051.00161	250.1	228.6	-6051.14434	-6051.13211
TS-3	-6051.59958 ^a	-6051.01755	256.6	235.2	-6051.16400	-6051.15181
	-6051.56282 ^b	-6050.98073	256.8	235.5	-6051.12729	-6051.11516
INT-3	-6051.60404 ^a	-6051.02129	258.7	237.4	-6051.16892	-6051.15676
	-6051.54963 ^b	-6050.96952	297.9	256.8	-6051.13955	-6051.11608
TS-4	-6051.58900 ^a	-6051.01190	254.0	232.7	-6051.15687	-6051.14469
	-6051.55114 ^b	-6050.97389	253.2	231.8	-6051.11839	-6051.10621
	-6051.42679 ^c	-6050.85011	257.1	236.0	-6050.99687	-6050.98481
INT-4	-5822.41337 ^a	-5821.90273	221.6	200.2	-5822.02923	-5822.01701
	-5822.37793 ^b	-5821.86717	222.6	201.2	-5821.99422	-5821.98201
INT-4+HOAc	-6051.60953 ^a	-6051.03089	294.0	252.8	-6051.19859	-6051.17517
	-6051.56493 ^b	-6050.98614	294.8	254.0	-6051.15450	-6051.13109
INT-4+2a	-6362.11056 ^a	-6361.39225	334.7	291.0	-6361.58329	-6361.55834
	-6362.05205 ^b	-6361.29925	330.6	286.9	-6361.52340	-6361.49846
INT-5	-6362.10406 ^a	-6361.38137	293.0	272.0	-6361.54858	-6361.53663
	-6362.05899 ^b	-6361.33772	289.2	268.2	-6361.50276	-6361.49081
TS-5	-6362.08667 ^a	-6361.36631	290.7	269.8	-6361.53221	-6361.52027
	-6362.04162 ^b	-6361.32115	291.2	270.3	-6361.48738	-6361.47545
	-6361.87204 ^c	-6361.15234	295.7	274.8	-6361.32110	-6361.30919
INT-6	-6362.12618 ^a	-6361.40320	289.2	268.3	-6361.56824	-6361.55631
	-6362.08156 ^b	-6361.35846	290.3	269.4	-6361.52416	-6361.51223
TS-6	-6362.10053 ^a	-6361.37985	290.2	269.2	-6361.54548	-6361.53348
	-6362.05560 ^b	-6361.33480	289.7	268.7	-6361.50014	-6361.48815
INT-7+HOAc	-6362.11490 ^a	-6361.39470	323.9	283.0	-6361.57946	-6361.55619

	-6362.06251 ^b	-6361.34214	324.9	284.4	-6361.52768	-6361.50441
INT-7	-6132.91874 ^a	-6132.26654	251.5	230.4	-6132.41010	-6132.39803
	-6132.87551 ^b	-6132.22317	252.7	231.6	-6132.36740	-6132.35533
TS-7	-6132.90257 ^a	-6132.25213	246.5	225.3	-6132.39284	-6132.38071
	-6132.85941 ^b	-6132.20888	251.0	229.7	-6132.35213	-6132.34000
INT-8	-6132.93300 ^a	-6132.28066	249.2	227.9	-6132.42289	-6132.41074
	-6132.89023 ^b	-6132.23769	247.2	225.9	-6132.37880	-6132.36664
TS-8	-6132.87921 ^a	-6132.22930	252.7	231.4	-6132.37353	-6132.36137
	-6132.83709 ^b	-6132.18705	251.8	230.5	-6132.33076	-6132.31861
TS-8a	-6132.87328 ^a	-6132.22337	246.9	225.6	-6132.36429	-6132.35211
	-6132.83064 ^b	-6132.18057	246.8	225.4	-6132.32141	-6132.30924
INT-9	-6132.90793	-6132.25586	248.4	227.0	-6132.39763	-6132.38541
	-6132.86529	-6132.21309	248.7	227.3	-6132.35504	-6132.34282
TS-9	-6132.89687 ^a	-6132.24730	249.4	228.1	-6132.38967	-6132.37748
	-6132.85371 ^b	-6132.20402	252.2	230.8	-6132.33576	-6132.34795
INT-10	-6132.97006 ^a	-6132.31729	256.4	235.1	-6132.46364	-6132.45149
	-6132.90437 ^b	-6132.25296	257.1	235.8	-6132.39022	-6132.40226
TS-10	-6132.91755 ^a	-6132.26864	258.1	237.0	-6132.41595	-6132.40388
	-6132.87448 ^b	-6132.22545	258.9	237.8	-6132.37324	-6132.36117
INT-11	-6132.94778 ^a	-6132.29653	261.6	240.5	-6132.44583	-6132.43379
	-6132.90437 ^b	-6132.25296	261.6	240.5	-6132.40226	-6132.39022
³O₂	-150.37899 ^a	-150.37134	50.3	34.7	-150.40004	-150.39112
	-150.37353 ^b	-150.36587	50.3	34.7	-150.39457	-150.38568
¹O₂(o)	-150.36265 ^a	-150.35501	48.1	32.5	-150.38246	-150.37357
	-150.35751 ^b	-150.34986	48.1	32.5	-150.37732	-150.36843
INT-11+³O₂	-6283.32677 ^a	-6282.66787	311.9	275.2	-6282.84587	-6282.82491
	-6283.27790 ^b	-6282.61883	311.9	275.2	-6282.79683	-6282.77590
SP	-6283.32463 ^a					
	-6283.27619 ^b					
3a	-1228.78439 ^a	-1228.37677	178.2	156.6	-1228.47846	-1228.46615
	-1228.74831 ^b	-1228.34059	179.4	157.9	-1228.44301	-1228.43069
³pre-CAT	-5054.55701 ^a	-5054.30617	149.0	126.3	-5054.39122	-5054.37826
	-5054.53660 ^b	-5054.28570	149.6	126.9	-5054.37105	-5054.35810
¹pre-CAT	-5054.58451 ^a	-5054.33290	141.9	119.3	-5054.41389	-5054.40097
	-5054.56415 ^b	-5054.31249	142.1	119.3	-5054.39351	-5054.38058
3a+³pre-CAT	-6283.34140 ^a	-6282.68294	327.2	282.9	-6282.86968	-6282.84441
	-6283.28491 ^b	-6282.62629	329.0	284.8	-6282.81406	-6282.78879
3a+¹pre-CAT	-6283.36890 ^a	-6282.70967	322.1	275.9	-6282.89235	-6282.86712
	-6283.31246 ^b	-6282.65308	321.5	277.2	-6282.83652	-6282.81127
¹pre-CAT+	-5283.78067 ^a	-5283.46106	214.3	171.9	-5283.58325	-5283.55913

HOAc	-5283.75115 ^b	-5283.43146	214.3	172.1	-5283.55379	-5283.52966
TS-1c	-5283.77243 ^a	-5283.45258	173.1	150.9	-5283.55139	-5283.53873
	-5283.74859 ^b	-5283.42866	174.5	152.3	-5283.52826	-5283.51560
INT-1c	-5283.79255 ^a	-5283.47001	174.5	152.3	-5283.56958	-5283.55693
	-5283.76890 ^b	-5283.44628	175.2	153.1	-5283.54629	-5283.53364
¹pre-CAT+ 2HOAc	-5512.97683 ^a	-5512.58922	286.7	224.5	-5512.75261	-5512.71729
	-5512.93815 ^b	-5512.55043	286.5	224.9	-5512.71407	-5512.67874
TS-2c	-5512.97048 ^a	-5512.57895	200.7	178.8	-5512.69353	-5512.68102
	-5512.94450 ^b	-5512.55287	202.9	180.9	-5512.66865	-5512.65614
INT-2c	-5513.00395 ^a	-5512.60969	208.8	186.9	-5512.72887	-5512.71635
	-5512.97447 ^b	-5512.58031	207.3	185.3	-5512.69861	-5512.68606
INT-3c	-5361.36702 ^a	-5361.00711	189.4	167.5	-5361.11520	-5361.10269
	-5361.34818 ^b	-5360.98845	191.8	170.0	-5361.09793	-5361.08546
H₂O₂	-151.62578 ^a	-151.59518	56.3	40.2	-151.62730	-151.61812
	-151.61873 ^b	-151.58809	56.3	40.2	-151.62023	-151.61104
INT-3c+H₂O₂	-5512.99280 ^a	-5512.60229	245.7	207.7	-5512.74250	-5512.72081
	-5512.96691 ^b	-5512.57654	248.0	210.2	-5512.71816	-5512.69650
CO	-113.35827 ^a	-113.34928	48.5	32.5	-113.37694	-113.36782
	-113.35374 ^b	-113.34474	48.5	32.5	-113.37241	-113.36329
TS-3c	-5361.32888 ^a	-5360.97099	192.9	170.0	-5361.08110	-5361.06860
	-5361.30585 ^b	-5360.94774	191.9	170.0	-5361.05728	-5361.04478
CAT+CO^g+H₂O₂	-5512.97169 ^a	-5512.58378	279.0	225.0	-5512.74335	-5512.72165
	-5512.93717	-5512.54912	279.1	225.1	-5512.70843	-5512.68673

- a) B3LYP-D3a+IDSCRF/TZP-DKH(-dfg); b) B3LYP-D3+IDSCRF/TZP-DKH(-dfg); c)
B3LYP+IDSCRF/TZP-DKH(-dfg)

Table S2 Coordinates of All Stationary Points Computed at B3LYP-D3a+IDSCRF/ TZP-DKH(-dfg) level in tert-butanol

1a				2a			
C	2.25365	0.34754	-0.00698	C	0.00000	0.00000	0.60432
C	3.65823	0.34524	-0.01067	C	0.00000	0.00000	-0.60432
C	1.57920	-0.87465	0.05979	C	0.00000	0.00000	2.02730
C	4.35186	-0.84283	0.05121	C	0.00000	1.20881	2.74100
C	2.27462	-2.08304	0.12310	C	0.00000	-1.20881	2.74100
C	3.65440	-2.05883	0.11797	C	0.00000	1.20389	4.12779
H	4.17217	1.29651	-0.06386	C	0.00000	-1.20389	4.12779
H	5.43483	-0.84287	0.04820	C	0.00000	0.00000	4.82612
H	1.72116	-3.01220	0.17479	H	0.00000	2.14519	2.19690
H	4.20291	-2.99199	0.16620	H	0.00000	-2.14519	2.19690

C	1.47500	1.57038	-0.07539	H	0.00000	2.14407	4.66688
O	1.95164	2.71304	-0.15186	H	0.00000	-2.14407	4.66688
C	0.03263	1.40473	-0.06041	H	0.00000	0.00000	5.90969
C	-0.55382	0.17413	0.01099	C	0.00000	0.00000	-2.02730
O	0.22537	-0.94573	0.07074	C	0.00000	-1.20881	-2.74100
O	-0.68313	2.54905	-0.14424	C	0.00000	1.20881	-2.74100
H	-0.01705	3.27010	-0.20174	C	0.00000	-1.20389	-4.12779
C	-1.98412	-0.14254	0.01079	C	0.00000	1.20389	-4.12779
C	-2.40583	-1.44112	-0.31475	C	0.00000	0.00000	-4.82612
C	-2.95424	0.81608	0.33877	H	0.00000	-2.14519	-2.19690
C	-3.75350	-1.76555	-0.31987	H	0.00000	2.14519	-2.19690
C	-4.30044	0.47963	0.33880	H	0.00000	-2.14407	-4.66688
C	-4.70781	-0.80759	0.00702	H	0.00000	2.14407	-4.66688
H	-1.67325	-2.19361	-0.57039	H	0.00000	0.00000	-5.90969
H	-2.65418	1.81798	0.60169				
H	-4.06004	-2.77161	-0.58108				
H	-5.03586	1.23070	0.60236				
H	-5.76080	-1.06339	0.00459				
3a				CAT			
C	-3.03348	0.14151	0.70471	C	-0.08163	-2.03700	1.32554
C	-4.20372	-0.16766	1.39912	C	-0.72834	-0.88083	1.83493
C	-3.01436	0.16267	-0.68784	C	-0.37426	-2.45468	-0.00033
C	-5.34279	-0.45261	0.66728	C	-1.61896	-0.13961	1.02348
C	-4.14693	-0.12248	-1.43833	C	-1.23693	-1.68330	-0.80313
C	-5.30522	-0.42813	-0.73555	C	-1.88167	-0.50698	-0.31509
H	-4.20710	-0.18217	2.48256	H	-0.46766	-0.50414	2.81223
H	-6.26900	-0.69686	1.17204	H	0.14408	-3.30179	-0.42729
H	-4.12300	-0.10490	-2.52046	H	-1.99160	0.79541	1.41024
H	-6.20856	-0.65531	-1.29006	H	-1.34688	-1.94175	-1.84916
C	-1.69506	0.47198	1.16718	C	0.93198	-2.76726	2.14816
O	-1.25950	0.55938	2.29439	H	1.70537	-3.20642	1.51884
O	-1.80404	0.47541	-1.21937	H	1.40328	-2.10060	2.86968
C	1.48119	0.55841	-0.12746	H	0.44321	-3.57491	2.70073
C	-0.86501	0.70848	-0.13389	C	-2.77894	0.29476	-1.22941
C	0.35871	-0.19952	-0.17613	H	-2.42604	0.10777	-2.24864
C	1.89999	3.13489	-0.15526	C	-2.71217	1.80250	-0.98328
C	1.11599	1.98955	-0.13465	C	-4.21985	-0.22482	-1.12167
C	1.26539	4.37663	-0.22592	H	-4.27769	-1.29404	-1.33509
H	1.86363	5.28016	-0.24490	H	-4.61565	-0.05870	-0.11651
C	-0.27883	2.09580	-0.18408	H	-4.86571	0.29774	-1.83000
C	-0.12121	4.47143	-0.28047	H	-3.12708	2.07254	-0.00965

H	-0.59290	5.44481	-0.34198	H	-3.29865	2.32497	-1.74101
C	-0.91162	3.31802	-0.25807	H	-1.68496	2.16545	-1.03102
H	-1.99219	3.39017	-0.30497	Ru	0.29913	-0.34845	-0.02989
H	2.98033	3.07388	-0.12596	O	1.36907	-0.09046	-1.90212
C	0.24357	-1.66376	-0.09849	C	2.48360	-0.21819	-1.30744
C	-0.59852	-2.37399	-0.96302	O	2.46324	-0.52975	-0.07646
C	0.96437	-2.37903	0.86647	C	3.77330	0.02174	-2.02532
C	-0.70594	-3.75614	-0.87086	H	4.02323	1.08255	-1.94603
C	0.85372	-3.75897	0.95750	H	3.67326	-0.22700	-3.08059
C	0.01897	-4.45413	0.08803	H	4.57666	-0.55490	-1.57017
H	-1.15341	-1.84281	-1.72384	O	0.78591	1.66176	0.08527
H	1.60547	-1.84309	1.55403	C	0.55589	2.44647	1.09194
H	-1.35611	-4.28935	-1.55481	O	0.06397	2.11858	2.17105
H	1.41580	-4.29337	1.71470	C	0.95166	3.88787	0.82019
H	-0.06731	-5.53204	0.15977	H	0.28968	4.30680	0.05887
C	2.87489	0.08070	-0.11089	H	1.96792	3.93649	0.42741
C	3.32537	-0.84039	-1.06159	H	0.87396	4.48103	1.72884
C	3.77533	0.54740	0.85212				
C	4.63951	-1.28718	-1.04570				
C	5.08765	0.09166	0.87301				
C	5.52455	-0.82545	-0.07654				
H	2.63964	-1.20078	-1.81811				
H	3.43949	1.25421	1.60137				
H	4.97465	-1.99672	-1.79337				
H	5.76994	0.45422	1.63313				
H	6.54973	-1.17653	-0.06336				
HOAc				O ₂			
H	1.88166	0.41195	0.00000	O	0.00000	0.00000	0.60436
O	1.25230	-0.34235	0.00000	O	0.00000	0.00000	-0.60436
O	-0.23584	1.33814	0.00000				
C	0.00000	0.15154	0.00000				
C	-1.03122	-0.93938	0.00000				
H	-0.89921	-1.57240	0.87943				
H	-2.02765	-0.50644	0.00000				
H	-0.89921	-1.57240	-0.87943				

H₂O₂				CO			
O	0.00000	0.72622	-0.06695	C	0.00000	0.00000	-0.64304
O	0.00000	-0.72622	-0.06695	O	0.00000	0.00000	0.48228
H	-0.74614	-0.91923	0.53561				
H	0.74614	0.91923	0.53561				
TS-1				INT-1			
C	-3.76999	-0.43819	-0.87373	C	-3.63776	-0.46080	-0.86006
C	-4.74875	-1.44211	-0.93937	C	-4.71682	-1.35627	-0.89862
C	-3.98818	0.65276	-0.02996	C	-3.87752	0.84891	-0.44460
C	-5.89535	-1.35182	-0.18163	C	-5.98139	-0.94621	-0.53401
C	-5.14454	0.75221	0.74491	C	-5.15120	1.27647	-0.07203
C	-6.08943	-0.25038	0.66530	C	-6.19624	0.37535	-0.11878
H	-4.57107	-2.28486	-1.59509	H	-4.52341	-2.37235	-1.21776
H	-6.64739	-2.12943	-0.23493	H	-6.81054	-1.64233	-0.56642
H	-5.27713	1.61054	1.39152	H	-5.29586	2.30208	0.24377
H	-6.98997	-0.18251	1.26408	H	-7.19035	0.69652	0.16871
C	-2.53188	-0.51577	-1.64240	C	-2.27686	-0.88628	-1.20632
O	-2.23350	-1.46447	-2.37623	O	-2.00533	-2.02381	-1.58832
C	-1.63296	0.61590	-1.47698	C	-1.26883	0.15239	-1.04753
C	-1.92757	1.64202	-0.63118	C	-1.60708	1.42277	-0.70626
O	-3.09258	1.66655	0.07448	O	-2.88078	1.77518	-0.39553
O	-0.47290	0.60798	-2.17340	O	0.05232	-0.15171	-1.20603
H	-0.20586	-0.32524	-2.30736	H	0.27338	-0.98638	-1.83264
C	-1.06096	2.78310	-0.32277	C	-0.67168	2.55025	-0.59011
C	-1.02916	3.28879	0.98298	C	-0.66996	3.34054	0.56162
C	-0.24373	3.36689	-1.29779	C	0.20716	2.84979	-1.63348
C	-0.18260	4.33850	1.30815	C	0.21237	4.40706	0.67141
C	0.59334	4.42435	-0.96775	C	1.07692	3.92636	-1.52547
C	0.63283	4.90915	0.33548	C	1.08646	4.70289	-0.37049
H	-1.65077	2.83615	1.74355	H	-1.33921	3.09487	1.37508
H	-0.26707	2.99434	-2.31114	H	0.19973	2.24164	-2.52849
H	-0.15631	4.71052	2.32563	H	0.22012	5.00782	1.57322
H	1.21566	4.87253	-1.73317	H	1.74873	4.15939	-2.34292
H	1.29256	5.72979	0.59155	H	1.77118	5.53830	-0.28372
C	2.34370	-0.46453	2.47898	C	2.15502	-0.50444	2.55089

C	3.40555	-1.03849	1.74016	C	2.97154	-1.34302	1.76576
C	1.66063	0.63783	1.89080	C	1.81043	0.78041	2.02757
C	3.78806	-0.54329	0.46387	C	3.44355	-0.92456	0.48558
C	2.00054	1.10387	0.61401	C	2.25337	1.16572	0.75661
C	3.06519	0.50845	-0.13356	C	3.08652	0.32334	-0.04893
H	3.89130	-1.92812	2.12156	H	3.18332	-2.34804	2.10430
H	0.77674	1.02256	2.37241	H	1.10858	1.40123	2.56049
H	4.56064	-1.06007	-0.08435	H	3.99015	-1.63510	-0.11615
H	1.39523	1.86805	0.15172	H	1.89486	2.09421	0.34094
C	1.92527	-1.01141	3.80851	C	1.61804	-0.96239	3.86932
H	0.84767	-0.91744	3.93487	H	0.62274	-0.55625	4.03880
H	2.20406	-2.06089	3.90541	H	1.57619	-2.04993	3.91959
H	2.41480	-0.45686	4.61445	H	2.27274	-0.61003	4.67191
C	3.33822	1.02064	-1.52807	C	3.50953	0.80413	-1.41811
H	2.35976	1.23431	-1.96758	H	2.62707	1.27164	-1.86268
C	4.05451	0.02142	-2.43319	C	3.97414	-0.30798	-2.35479
C	4.11579	2.34263	-1.43234	C	4.58743	1.88763	-1.26467
H	3.58398	3.07865	-0.82739	H	4.24441	2.71201	-0.63705
H	5.10024	2.18145	-0.98580	H	5.49216	1.47213	-0.81354
H	4.26126	2.76504	-2.42837	H	4.85292	2.29551	-2.24182
H	5.07343	-0.17680	-2.09184	H	4.89454	-0.77743	-1.99836
H	4.12527	0.42776	-3.44351	H	4.18668	0.11031	-3.34021
H	3.51351	-0.92345	-2.48629	H	3.20905	-1.07551	-2.47381
Ru	1.64447	-1.06575	0.47164	Ru	1.24473	-0.78640	0.56194
O	1.79077	-3.11842	-0.24044	O	1.11258	-2.73308	-0.29908
C	1.25247	-2.81160	-1.34554	C	1.04269	-2.97555	-1.54383
O	1.03333	-1.57846	-1.56498	O	0.87467	-2.10677	-2.43867
C	0.89719	-3.85691	-2.35205	C	1.15395	-4.41996	-1.96158
H	0.28693	-4.62607	-1.87759	H	0.15488	-4.77919	-2.21926
H	1.80842	-4.33619	-2.71595	H	1.55732	-5.03754	-1.16251
H	0.35689	-3.41600	-3.18598	H	1.77291	-4.50004	-2.85508
O	-0.26872	-1.76991	0.85123	O	-0.60852	-1.35578	1.32509
C	-1.18916	-1.30159	1.63439	C	-1.39168	-0.65266	2.08002
O	-1.14337	-0.24656	2.26677	O	-1.18397	0.49521	2.47640
C	-2.39365	-2.21933	1.75445	C	-2.65531	-1.38989	2.48903
H	-2.18521	-2.95466	2.53672	H	-2.46044	-1.91497	3.42823
H	-2.57383	-2.75982	0.82773	H	-2.94595	-2.12739	1.74378
H	-3.27674	-1.65239	2.04129	H	-3.46440	-0.68143	2.65844

TS-2				INT-2			
C	-3.61342	-0.43227	-0.85693	C	-3.59012	-0.45464	-0.86895
C	-4.69598	-1.32441	-0.88779	C	-4.66657	-1.35482	-0.90314
C	-3.85029	0.88241	-0.45579	C	-3.84059	0.86111	-0.47844
C	-5.96009	-0.90733	-0.53004	C	-5.93675	-0.94602	-0.55821
C	-5.12435	1.31767	-0.09128	C	-5.12200	1.28808	-0.12719
C	-6.17212	0.41963	-0.13010	C	-6.16246	0.38207	-0.16838
H	-4.50477	-2.34441	-1.19552	H	-4.46503	-2.37519	-1.20302
H	-6.79106	-1.60162	-0.55598	H	-6.76197	-1.64711	-0.58620
H	-5.26648	2.34709	0.21322	H	-5.27473	2.31842	0.16908
H	-7.16583	0.74690	0.15196	H	-7.16095	0.70337	0.10355
C	-2.25339	-0.86629	-1.19715	C	-2.22469	-0.87846	-1.19711
O	-1.99382	-2.00928	-1.57397	O	-1.95835	-2.02042	-1.57745
C	-1.23210	0.16417	-1.03883	C	-1.20062	0.15244	-1.02780
C	-1.57504	1.43964	-0.71119	C	-1.56559	1.42982	-0.71745
O	-2.85127	1.80383	-0.41310	O	-2.85082	1.78905	-0.43582
O	0.07633	-0.14987	-1.19599	O	0.09349	-0.16486	-1.18424
H	0.35553	-1.07047	-1.89351	H	0.45081	-1.27857	-1.98853
C	-0.63609	2.56376	-0.59202	C	-0.64085	2.56567	-0.60426
C	-0.64101	3.36079	0.55516	C	-0.66015	3.37890	0.53147
C	0.25715	2.85263	-1.62629	C	0.25646	2.85092	-1.63625
C	0.24841	4.42106	0.67047	C	0.21847	4.44930	0.63835
C	1.13425	3.92272	-1.51357	C	1.12271	3.93070	-1.53296
C	1.13725	4.70483	-0.36218	C	1.11151	4.72813	-0.39201
H	-1.32241	3.12572	1.36183	H	-1.34464	3.14858	1.33698
H	0.25589	2.23893	-2.51736	H	0.26727	2.22387	-2.51779
H	0.25017	5.02625	1.56939	H	0.20861	5.06641	1.52914
H	1.81740	4.14640	-2.32428	H	1.80901	4.14982	-2.34232
H	1.82776	5.53504	-0.27137	H	1.79365	5.56593	-0.30779
C	2.12432	-0.54429	2.56540	C	2.11789	-0.49376	2.57281
C	2.94030	-1.38168	1.78130	C	2.93742	-1.33685	1.80212
C	1.78789	0.74474	2.04548	C	1.76719	0.78170	2.02739
C	3.42003	-0.95750	0.50551	C	3.40571	-0.93243	0.51519
C	2.24728	1.14044	0.78272	C	2.22668	1.16451	0.75980
C	3.08120	0.29912	-0.02183	C	3.06304	0.31518	-0.03229
H	3.14563	-2.38985	2.11462	H	3.15308	-2.33723	2.15221
H	1.08394	1.36491	2.57636	H	1.05788	1.40464	2.54784
H	3.96570	-1.66789	-0.09754	H	3.95408	-1.65008	-0.07704
H	1.89876	2.07510	0.37262	H	1.87305	2.09114	0.33720
C	1.57485	-1.00652	3.87729	C	1.57624	-0.93354	3.89579
H	0.57924	-0.59828	4.03966	H	0.57329	-0.53914	4.04735

H	1.52940	-2.09416	3.92228	H	1.54975	-2.02043	3.96732
H	2.22310	-0.65949	4.68740	H	2.21684	-0.55532	4.69799
C	3.52239	0.78825	-1.38209	C	3.49561	0.78297	-1.40293
H	2.64846	1.26724	-1.83082	H	2.61081	1.23057	-1.86253
C	3.98694	-0.31923	-2.32423	C	3.98669	-0.33458	-2.31946
C	4.60874	1.86011	-1.20868	C	4.55767	1.88245	-1.25569
H	4.26634	2.68215	-0.57776	H	4.19632	2.71164	-0.64524
H	5.50487	1.43263	-0.75159	H	5.46289	1.48656	-0.78810
H	4.88825	2.27394	-2.17944	H	4.82869	2.27886	-2.23612
H	4.89935	-0.80056	-1.96331	H	4.90792	-0.78858	-1.94571
H	4.21220	0.10532	-3.30405	H	4.20507	0.07248	-3.30813
H	3.21755	-1.07988	-2.45833	H	3.23587	-1.11581	-2.43974
Ru	1.22279	-0.79718	0.56193	Ru	1.20823	-0.77535	0.56950
O	1.08320	-2.74026	-0.34541	O	1.08133	-2.76394	-0.29853
C	0.99935	-2.95647	-1.58192	C	1.03493	-3.03703	-1.51052
O	0.81288	-2.05150	-2.45840	O	0.83297	-2.16080	-2.44083
C	1.11336	-4.37322	-2.06752	C	1.21593	-4.44835	-1.97401
H	1.73775	-4.41109	-2.96017	H	0.24639	-4.83103	-2.30118
H	0.11594	-4.71940	-2.34827	H	1.59873	-5.07286	-1.17140
H	1.51331	-5.02409	-1.29409	H	1.88577	-4.47485	-2.83378
O	-0.63224	-1.37128	1.31595	O	-0.64274	-1.34866	1.33387
C	-1.41687	-0.67451	2.07475	C	-1.43114	-0.65249	2.08853
O	-1.20838	0.46898	2.48348	O	-1.22568	0.49162	2.49719
C	-2.68340	-1.41277	2.47333	C	-2.69838	-1.39176	2.48371
H	-2.95787	-2.16293	1.73481	H	-2.52871	-1.87910	3.44781
H	-3.49866	-0.70552	2.61676	H	-2.95916	-2.15652	1.75539
H	-2.50294	-1.92008	3.42509	H	-3.51948	-0.68656	2.60250
TS-3				INT-3			
C	-3.66543	1.28877	-0.47894	C	3.85310	1.08927	0.14649
C	-4.62963	2.26956	-0.19334	C	4.92268	1.95138	-0.15215
C	-4.10057	0.00404	-0.80688	C	4.14485	-0.22402	0.52389
C	-5.97268	1.96616	-0.24106	C	6.22457	1.51098	-0.06866
C	-5.45883	-0.31505	-0.85763	C	5.46231	-0.68104	0.60986
C	-6.38572	0.66751	-0.57500	C	6.49227	0.18736	0.31424
H	-4.28449	3.26374	0.06001	H	4.68905	2.96620	-0.44750
H	-6.71195	2.72721	-0.02323	H	7.04343	2.18200	-0.29750
H	-5.75787	-1.32289	-1.11734	H	5.64874	-1.70495	0.90920
H	-7.44235	0.43025	-0.61230	H	7.51700	-0.15877	0.37982
C	-2.23350	1.57782	-0.43766	C	2.46422	1.53356	0.04176
O	-1.77973	2.67936	-0.11332	O	2.14703	2.66844	-0.31762
C	-1.34512	0.46420	-0.79033	C	1.44524	0.51821	0.36401

C	-1.87610	-0.77292	-1.07070	C	1.85167	-0.72717	0.77919
O	-3.22646	-0.99251	-1.08434	O	3.16804	-1.10824	0.82985
O	-0.04576	0.71381	-0.83112	O	0.19293	0.86543	0.17121
H	0.41524	2.47183	-0.98121	C	0.94138	-1.79787	1.16252
C	-1.12224	-2.01687	-1.24439	C	1.23150	-3.14017	0.90358
C	-1.73769	-3.24351	-0.95405	C	-0.25331	-1.47516	1.84465
C	0.22917	-2.02707	-1.63051	C	0.33455	-4.13233	1.27987
C	-1.02137	-4.43013	-1.01813	C	-1.14804	-2.48969	2.20884
C	0.93813	-3.22077	-1.69590	C	-0.86357	-3.81615	1.91929
C	0.32138	-4.42541	-1.38216	H	2.15369	-3.40544	0.40325
H	-2.77821	-3.26406	-0.66249	H	0.57105	-5.16877	1.06707
H	-1.51627	-5.36427	-0.77887	H	-2.04527	-2.22496	2.75524
H	1.97701	-3.18447	-1.99234	H	-1.55240	-4.60175	2.20481
H	0.87835	-5.35372	-1.42800	C	-3.51830	-0.70997	-0.81501
C	3.05373	-0.91512	1.64791	C	-2.77512	0.24763	-1.56873
C	2.57357	0.37145	2.00654	C	-2.93821	-1.97243	-0.60281
C	2.09039	-1.93639	1.50734	C	-1.52752	-0.08696	-2.13756
C	1.19755	0.59694	2.26103	C	-1.66297	-2.28554	-1.15660
C	0.71778	-1.73345	1.85118	C	-0.95306	-1.37645	-1.97058
C	0.25520	-0.48073	2.27343	H	-3.13859	1.26005	-1.66507
H	3.23667	1.22405	1.96132	H	-3.42947	-2.68670	0.04278
H	2.38855	-2.89136	1.09629	H	-0.97083	0.70588	-2.61272
H	0.86326	1.61054	2.42720	H	-1.20480	-3.23208	-0.90354
H	0.02556	-2.54818	1.70005	C	-4.80353	-0.31557	-0.16383
C	4.48979	-1.13786	1.29123	H	-5.13568	-1.07244	0.54533
H	4.58346	-1.90149	0.52099	H	-4.67609	0.62806	0.36656
H	4.94556	-0.21823	0.92578	H	-5.57881	-0.18532	-0.92337
H	5.04617	-1.46313	2.17475	C	0.35948	-1.78526	-2.59913
C	-1.17170	-0.19228	2.67779	H	0.89744	-2.37369	-1.85092
H	-1.48301	0.69774	2.12293	C	1.23978	-0.60733	-3.01278
C	-1.19471	0.16050	4.17555	C	0.07672	-2.69924	-3.80212
C	-2.15388	-1.32243	2.38698	H	-0.50004	-3.57945	-3.51242
H	-2.13799	-1.62368	1.34258	H	-0.48602	-2.16315	-4.57046
H	-1.93704	-2.20195	2.99855	H	1.01477	-3.03854	-4.24571
H	-3.16706	-0.99793	2.62743	H	0.80644	-0.06396	-3.85590
H	-0.86789	-0.69097	4.77732	H	2.21750	-0.97282	-3.33004
H	-2.20990	0.42108	4.47945	H	1.38706	0.09542	-2.19515
H	-0.54677	1.00769	4.40472	Ru	-1.45251	-0.44969	0.02023
Ru	1.40045	-0.25244	0.31657	O	-2.38978	0.76344	1.44714
O	1.73793	3.33011	0.77550	C	-1.96331	1.40181	2.48971
C	1.76768	3.68915	-0.38591	O	-0.88207	1.23655	3.05587

O	0.94353	3.23830	-1.32473	C	-2.94857	2.44228	2.99137
C	2.75289	4.68962	-0.92759	H	-2.88294	3.31389	2.33623
H	3.51625	4.15076	-1.49371	H	-2.70044	2.74495	4.00698
H	3.22836	5.22903	-0.11199	H	-3.97058	2.06658	2.94636
H	2.26543	5.38537	-1.61077	H	-0.37062	-0.47918	2.26802
O	2.65160	0.82204	-0.96173	H	-0.29432	2.47754	0.05724
C	3.32938	0.11898	-1.80401	O	-0.79926	3.33861	0.14408
O	3.25646	-1.11122	-1.89535	O	-1.17585	3.09606	-2.05666
C	4.25202	0.93214	-2.68780	C	-1.30995	3.71728	-1.01730
H	5.02012	1.40786	-2.07464	C	-2.09641	4.99713	-0.90628
H	3.69071	1.72647	-3.18143	H	-1.49457	5.76945	-0.42520
H	4.72680	0.29597	-3.43141	H	-2.41386	5.32903	-1.89141
H	0.71613	-1.11607	-1.94994	H	-2.97351	4.82993	-0.27726
TS-4				INT-4			
C	3.75513	1.39485	-0.44850	C	-3.73118	-0.20198	-1.14277
C	4.73013	2.28762	-0.92678	C	-4.85295	0.03994	-1.95144
C	4.17340	0.19065	0.11847	C	-3.91744	-0.29628	0.23736
C	6.06877	1.97781	-0.83464	C	-6.10555	0.18070	-1.39336
C	5.52987	-0.13308	0.21614	C	-5.18059	-0.15437	0.81423
C	6.46694	0.76042	-0.25963	C	-6.26705	0.08226	-0.00398
H	4.39546	3.21906	-1.36525	H	-4.70127	0.10971	-3.02095
H	6.81613	2.66993	-1.20299	H	-6.96619	0.36619	-2.02441
H	5.81853	-1.07557	0.66454	H	-5.28399	-0.23308	1.88933
H	7.52045	0.51765	-0.18654	H	-7.25156	0.19284	0.43498
C	2.32987	1.68970	-0.53920	C	-2.38909	-0.35877	-1.71267
O	1.89297	2.73516	-1.02744	O	-2.17180	-0.28971	-2.92778
C	1.41638	0.65556	-0.01645	C	-1.33313	-0.60724	-0.73780
C	1.93275	-0.48889	0.55005	C	-1.61109	-0.67393	0.60107
O	3.29046	-0.70794	0.60046	O	-2.88001	-0.51942	1.08252
O	0.14116	0.93943	-0.14115	O	-0.09379	-0.79568	-1.20580
C	1.18123	-1.58088	1.16592	C	-0.61922	-0.90063	1.64965
C	1.85544	-2.75587	1.53987	C	-1.06121	-1.41478	2.88206
C	-0.20855	-1.46854	1.42621	C	0.74660	-0.59133	1.45290
C	1.18725	-3.79087	2.17424	C	-0.17466	-1.65205	3.91620
C	-0.83755	-2.51578	2.11792	C	1.61426	-0.84364	2.52308
C	-0.16528	-3.67099	2.48255	C	1.17407	-1.36564	3.73302
H	2.90974	-2.85804	1.33097	H	-2.11071	-1.64335	3.01344
H	1.72948	-4.68971	2.44509	H	-0.53142	-2.05943	4.85484
H	-1.88289	-2.40788	2.38603	H	2.67090	-0.63335	2.40840
H	-0.68160	-4.46634	3.00730	H	1.88334	-1.54553	4.53405
C	-3.34951	-0.09413	-1.26056	C	3.22743	1.15850	-1.55643

C	-2.23608	0.09265	-2.09385	C	2.00318	1.63835	-2.01076
C	-3.43439	-1.30931	-0.51012	C	3.48855	1.21563	-0.14369
C	-1.22645	-0.90926	-2.19739	C	1.03289	2.13875	-1.08571
C	-2.44220	-2.29211	-0.63062	C	2.58174	1.80935	0.74536
C	-1.31443	-2.12441	-1.49553	C	1.31457	2.29166	0.28916
H	-2.09263	1.04664	-2.57987	H	1.73535	1.53774	-3.05434
H	-4.24248	-1.44955	0.19591	H	4.40004	0.77781	0.24181
H	-0.34798	-0.68784	-2.78511	H	0.05703	2.40359	-1.46541
H	-2.50186	-3.17745	-0.01269	H	2.81176	1.83377	1.80244
C	-4.37337	0.98052	-1.08084	C	4.22387	0.52017	-2.47344
H	-4.67300	1.05281	-0.03535	H	4.60508	-0.40618	-2.04124
H	-3.98317	1.94345	-1.40445	H	3.77960	0.29624	-3.44270
H	-5.26219	0.74443	-1.67360	H	5.07613	1.18735	-2.63132
C	-0.29690	-3.23511	-1.61019	C	0.37177	2.94720	1.27195
H	-0.11737	-3.60121	-0.59606	H	0.44795	2.37753	2.20292
C	1.03878	-2.79015	-2.19871	C	-1.09040	2.94151	0.83313
C	-0.89502	-4.39035	-2.42886	C	0.85156	4.38048	1.54994
H	-1.82607	-4.75619	-1.99202	H	1.88138	4.39771	1.91166
H	-1.10461	-4.07081	-3.45276	H	0.80253	4.98645	0.64158
H	-0.19244	-5.22487	-2.47182	H	0.21997	4.85191	2.30567
H	0.94168	-2.52435	-3.25437	H	-1.25086	3.58240	-0.03733
H	1.75938	-3.60658	-2.13269	H	-1.71883	3.32526	1.63846
H	1.45091	-1.93392	-1.66587	H	-1.43104	1.93743	0.58583
Ru	-1.45639	-0.40007	-0.05656	Ru	1.55154	0.16191	-0.28783
O	-2.28763	0.98031	1.32975	O	2.57590	-1.75964	-0.40296
C	-1.69342	1.29863	2.39391	C	2.10951	-2.86700	-0.71317
O	-0.63905	0.71750	2.79302	O	0.88286	-3.05502	-1.08967
C	-2.25119	2.41884	3.22295	C	2.96583	-4.09477	-0.67314
H	-1.59670	3.28470	3.10451	H	3.97638	-3.84634	-0.36118
H	-2.25463	2.14129	4.27677	H	2.98083	-4.56086	-1.65984
H	-3.25309	2.68184	2.89279	H	2.52833	-4.81498	0.02088
H	-0.49147	-0.27311	1.98859	H	0.38270	-2.12178	-1.13794
H	-0.31961	2.59302	-0.06271				
O	-0.75059	3.42966	0.27303				
O	-1.87181	3.37151	-1.67135				
C	-1.66322	3.87106	-0.58175				
C	-2.41740	5.05739	-0.04354				
H	-1.72247	5.82835	0.29205				
H	-3.08305	5.45623	-0.80441				
H	-3.00106	4.74619	0.82570				

INT-5				TS-5			
C	-4.12970	-0.76377	0.85304	C	1.61708	3.58649	-0.71973
C	-5.25000	-1.60405	0.95399	C	2.02363	4.86813	-0.31360
C	-4.31467	0.60973	1.02424	C	2.38365	2.92249	-1.68000
C	-6.49838	-1.08424	1.22158	C	3.14791	5.45460	-0.85267
C	-5.57441	1.14784	1.29330	C	3.52417	3.50760	-2.23408
C	-6.65818	0.29838	1.39196	C	3.89908	4.76901	-1.81882
H	-5.09907	-2.66766	0.82060	H	1.42487	5.37682	0.43088
H	-7.35657	-1.74025	1.30243	H	3.45325	6.44398	-0.53451
H	-5.67738	2.21868	1.41760	H	4.09177	2.96070	-2.97678
H	-7.63948	0.70740	1.60164	H	4.78249	5.23029	-2.24424
C	-2.79134	-1.29385	0.57056	C	0.41775	2.95231	-0.16536
O	-2.58481	-2.49252	0.34805	O	-0.30756	3.50840	0.66195
C	-1.72796	-0.29461	0.55178	C	0.13359	1.60445	-0.67465
C	-2.01786	1.03678	0.67242	C	0.95775	1.04445	-1.61147
O	-3.28577	1.48625	0.91342	O	2.06204	1.67928	-2.11190
O	-0.47264	-0.70729	0.40362	O	-0.95834	0.99409	-0.24902
C	-1.04886	2.11382	0.48160	C	0.74018	-0.26668	-2.20274
C	-1.36772	3.38466	0.99515	C	1.02450	-0.44076	-3.56633
C	0.12907	1.93337	-0.28057	C	0.26948	-1.36046	-1.43623
C	-0.56491	4.48213	0.74816	C	0.83782	-1.66183	-4.18746
C	0.90523	3.06991	-0.52641	C	0.14787	-2.60271	-2.08601
C	0.57046	4.32472	-0.03726	C	0.39581	-2.75130	-3.43656
H	-2.26273	3.49926	1.59216	H	1.38201	0.40722	-4.13642
H	-0.82703	5.45093	1.15686	H	1.04809	-1.77112	-5.24460
H	1.81227	2.97766	-1.10793	H	-0.12581	-3.47541	-1.50885
H	1.20611	5.17528	-0.25755	H	0.26842	-3.72068	-3.90456
C	2.02519	-0.22471	-2.94578	C	-1.60179	-2.40283	1.97936
C	1.26426	-1.42499	-2.81755	C	-2.33472	-1.19175	2.14628
C	1.33700	0.99409	-3.11889	C	-1.75293	-3.10512	0.75961
C	-0.12149	-1.37331	-2.72152	C	-3.08549	-0.67876	1.08648
C	-0.07758	1.02045	-3.11195	C	-2.58244	-2.60745	-0.27653
C	-0.83604	-0.13829	-2.87537	C	-3.22872	-1.37207	-0.15856
H	1.77698	-2.36701	-2.67682	H	-2.25205	-0.62967	3.06640
H	1.89266	1.91259	-3.24768	H	-1.21396	-4.03193	0.61167
H	-0.67625	-2.27841	-2.50835	H	-3.52045	0.30447	1.20140
H	-0.57348	1.97609	-3.20138	H	-2.62484	-3.15239	-1.20770
C	3.52077	-0.27559	-2.95599	C	-0.75855	-2.94398	3.09229
H	3.94729	0.70195	-2.73540	H	-0.07044	-3.70547	2.72904
H	3.89316	-0.99288	-2.22599	H	-0.18529	-2.15038	3.57153
H	3.87480	-0.58590	-3.94309	H	-1.39699	-3.40335	3.85204

C	-2.34750	-0.16235	-2.88940	C	-4.05357	-0.75298	-1.26325
H	-2.65539	-0.81535	-2.06945	H	-3.84758	0.31957	-1.23111
C	-2.83446	-0.80200	-4.20038	C	-5.55000	-0.95377	-0.98362
C	-2.99466	1.20590	-2.68732	C	-3.67740	-1.25131	-2.65787
H	-2.60784	1.71488	-1.80600	H	-2.60771	-1.14303	-2.84331
H	-2.83506	1.85334	-3.55337	H	-3.94634	-2.30108	-2.80012
H	-4.07223	1.08765	-2.56535	H	-4.21547	-0.67609	-3.41329
H	-2.53401	-0.19727	-5.05977	H	-5.81013	-2.01515	-1.01373
H	-3.92372	-0.87386	-4.20036	H	-6.15079	-0.43668	-1.73471
H	-2.43054	-1.80678	-4.33539	H	-5.83021	-0.56651	-0.00197
Ru	0.67137	0.11094	-1.15467	Ru	-0.98426	-1.04834	0.30814
C	2.21820	-0.90667	0.06929	C	0.88012	-0.60335	1.12777
C	2.41493	0.29351	0.31915	C	1.27759	-1.45188	0.24206
C	2.46146	-2.32155	0.16577	C	1.36712	0.18337	2.23006
C	1.41224	-3.24529	0.24810	C	0.50403	0.98188	2.99013
C	3.78556	-2.78247	0.18993	C	2.73752	0.18308	2.54850
C	1.68933	-4.59984	0.35583	C	0.98780	1.73576	4.05064
C	4.05163	-4.14098	0.29287	C	3.21503	0.94079	3.60486
C	3.00531	-5.05397	0.37425	C	2.34177	1.71627	4.36583
H	0.39340	-2.88271	0.24991	H	-0.54092	1.02764	2.71795
H	4.59876	-2.06952	0.12879	H	3.41985	-0.41633	1.95934
H	0.87135	-5.30705	0.42872	H	0.30567	2.35130	4.62551
H	5.07881	-4.48651	0.30911	H	4.27350	0.92857	3.83896
H	3.21434	-6.11434	0.45399	H	2.71843	2.30740	5.19235
C	3.02846	1.42492	0.95449	C	2.30166	-2.48571	0.11321
C	4.19444	1.98277	0.41709	C	2.61525	-3.26450	1.23516
C	2.46960	1.98866	2.10733	C	3.04514	-2.66705	-1.05830
C	4.79481	3.07519	1.02786	C	3.63495	-4.20479	1.18363
C	3.07699	3.07783	2.71342	C	4.07023	-3.60144	-1.10386
C	4.23693	3.62771	2.17597	C	4.36443	-4.37845	0.01234
H	4.62981	1.55200	-0.47547	H	2.05806	-3.11837	2.15013
H	1.56719	1.55930	2.51697	H	2.82675	-2.06405	-1.92756
H	5.69973	3.49621	0.60534	H	3.86047	-4.80197	2.05956
H	2.63846	3.50592	3.60725	H	4.64435	-3.72268	-2.01509
H	4.70522	4.48214	2.65049	H	5.16133	-5.11175	-0.02916
H	0.16878	-0.78960	1.90709	H	-2.23179	1.98623	-0.28327
O	0.55566	-0.67491	2.83093	O	-2.99987	2.58466	-0.56184
O	-0.39731	-2.65522	3.30481	O	-3.62568	2.51217	1.59378
C	0.28332	-1.70321	3.62901	C	-3.75884	2.94656	0.46397
C	0.92505	-1.55035	4.98377	C	-4.81405	3.94768	0.07485
H	0.61129	-0.61057	5.44158	H	-5.50394	4.10634	0.89977

H	0.65154	-2.38481	5.62426	H	-4.33404	4.89381	-0.18523
H	2.01036	-1.51006	4.87218	H	-5.35438	3.60408	-0.80832
INT-6				TS-6			
C	2.10013	3.43408	0.10072	C	2.36675	-3.16351	0.33255
C	2.63972	4.59932	0.67243	C	3.12845	-4.23050	-0.17125
C	2.77385	2.85333	-0.97662	C	3.00278	-2.22000	1.14991
C	3.80083	5.15273	0.18012	C	4.46677	-4.35112	0.13435
C	3.95364	3.40479	-1.48218	C	4.35851	-2.33129	1.45773
C	4.45921	4.54988	-0.90275	C	5.08139	-3.39438	0.95350
H	2.11350	5.04446	1.50709	H	2.63060	-4.94941	-0.80943
H	4.20831	6.05195	0.62581	H	5.04467	-5.17867	-0.25843
H	4.44685	2.92375	-2.31772	H	4.81746	-1.58104	2.08908
H	5.37320	4.98493	-1.28940	H	6.13405	-3.48506	1.19449
C	0.86501	2.83548	0.61505	C	0.95628	-3.00513	-0.03340
O	0.25740	3.29288	1.58480	O	0.34991	-3.79801	-0.75837
C	0.39838	1.64794	-0.11351	C	0.32695	-1.78726	0.48827
C	1.15067	1.15313	-1.13403	C	1.04996	-0.90051	1.30682
O	2.31637	1.72666	-1.57357	O	2.33649	-1.17478	1.70961
O	-0.74388	1.08417	0.23796	O	-0.84004	-1.42267	0.08102
C	0.83212	-0.05759	-1.92934	C	0.25864	-0.11115	2.28179
C	0.57386	0.12005	-3.31715	C	-0.21018	-0.66203	3.46871
C	1.17809	-1.35835	-1.46512	C	-0.13052	1.18147	1.88948
C	0.66844	-0.92453	-4.20020	C	-1.06190	0.07153	4.28524
C	1.30020	-2.40612	-2.40674	C	-1.02303	1.89928	2.70578
C	1.06357	-2.19514	-3.74209	C	-1.47651	1.34559	3.88908
H	0.32760	1.11437	-3.67021	H	0.08835	-1.66490	3.75142
H	0.47023	-0.76578	-5.25337	H	-1.41189	-0.34783	5.22067
H	1.60873	-3.38158	-2.05133	H	-1.35738	2.88171	2.39868
H	1.17938	-3.00934	-4.44833	H	-2.16304	1.90596	4.51311
C	-2.13189	-2.76902	-0.99724	C	-1.20951	1.31540	-2.71200
C	-2.73093	-2.11352	0.11393	C	-1.92002	0.10670	-2.53086
C	-2.09574	-2.04675	-2.21259	C	-1.52185	2.39633	-1.84216
C	-3.23922	-0.80783	-0.01101	C	-2.93115	0.01065	-1.54392
C	-2.73313	-0.78436	-2.37759	C	-2.58102	2.30670	-0.89965
C	-3.28594	-0.13190	-1.27977	C	-3.32080	1.12295	-0.75274
H	-2.73157	-2.58429	1.08660	H	-1.67463	-0.76364	-3.12482
H	-1.57198	-2.47409	-3.05585	H	-0.97252	3.32244	-1.92202
H	-3.58976	-0.30386	0.87757	H	-3.39159	-0.95426	-1.39160
H	-2.67445	-0.29516	-3.33922	H	-2.78552	3.15289	-0.25628

C	-1.56107	-4.14903	-0.88806	C	-0.19696	1.47756	-3.80326
H	-0.80336	-4.31868	-1.65131	H	0.65492	2.07448	-3.47906
H	-1.10816	-4.31380	0.08926	H	0.17012	0.51450	-4.15249
H	-2.34800	-4.89622	-1.02426	H	-0.65901	1.99128	-4.65151
C	-3.88919	1.24931	-1.37490	C	-4.42799	1.02112	0.27223
H	-3.88036	1.66400	-0.36682	H	-4.38629	1.93665	0.86953
C	-5.35098	1.14209	-1.83491	C	-4.25358	-0.16599	1.22375
C	-3.08788	2.20138	-2.26417	C	-5.79227	0.97303	-0.43011
H	-2.05476	2.27645	-1.92323	H	-5.93512	1.83644	-1.08291
H	-3.08734	1.88094	-3.30850	H	-5.88430	0.07036	-1.03909
H	-3.53209	3.19798	-2.23071	H	-6.59884	0.96552	0.30608
H	-5.41048	0.74562	-2.85159	H	-4.31800	-1.11614	0.69242
H	-5.82271	2.12679	-1.82716	H	-5.04171	-0.15664	1.97967
H	-5.92857	0.48433	-1.18217	H	-3.28915	-0.12783	1.73053
Ru	-1.13738	-0.79264	-0.67156	Ru	-1.03383	0.69305	-0.54632
C	0.33135	-1.38599	0.68985	C	0.99132	0.67879	-0.19077
C	1.45023	-1.59959	-0.01426	C	0.54646	1.68791	0.68354
C	0.17960	-1.41333	2.14467	C	2.20391	0.55612	-0.97408
C	-0.50561	-2.43956	2.80438	C	3.42219	1.08650	-0.51705
C	0.72787	-0.38083	2.91563	C	2.22012	-0.23884	-2.12898
C	-0.63331	-2.43888	4.18712	C	4.60024	0.85771	-1.21108
C	0.59565	-0.37850	4.29767	C	3.39801	-0.46402	-2.82413
C	-0.08654	-1.40584	4.94112	C	4.59340	0.08668	-2.37025
H	-0.91952	-3.25968	2.23195	H	3.43572	1.67866	0.38849
H	1.25813	0.42095	2.41990	H	1.29504	-0.69366	-2.45823
H	-1.16026	-3.24937	4.67797	H	5.53033	1.27738	-0.84506
H	1.02537	0.43233	4.87505	H	3.38868	-1.08068	-3.71547
H	-0.19090	-1.40211	6.01974	H	5.51560	-0.09279	-2.91036
C	2.79485	-2.01929	0.41929	C	1.02034	3.09284	0.62080
C	3.00843	-2.77323	1.58197	C	1.34378	3.68847	-0.60494
C	3.91222	-1.66998	-0.35183	C	1.23793	3.84237	1.78269
C	4.28937	-3.14801	1.96166	C	1.83974	4.98087	-0.67190
C	5.19391	-2.04488	0.03026	C	1.73664	5.13838	1.71944
C	5.39012	-2.78549	1.19040	C	2.03370	5.71840	0.49263
H	2.16406	-3.07259	2.18588	H	1.21889	3.11975	-1.51381
H	3.77548	-1.08900	-1.25592	H	1.03647	3.40374	2.75017
H	4.42951	-3.73452	2.86271	H	2.07808	5.41418	-1.63646
H	6.04208	-1.75638	-0.58023	H	1.89937	5.69281	2.63668
H	6.38892	-3.08154	1.48901	H	2.41893	6.72999	0.44271
H	-1.86705	1.93898	1.18621	H	-1.97677	-2.66388	0.18691
O	-2.60888	2.52596	1.52276	O	-2.59311	-3.37904	0.51851

O	-3.17642	0.82684	2.88138	C	-3.46118	-3.75173	-0.41527
C	-3.33171	1.96633	2.48357	O	-3.53506	-3.23460	-1.51422
C	-4.38741	2.90072	3.01376	C	-4.34811	-4.87676	0.04487
H	-4.98608	2.39968	3.76986	H	-5.07274	-5.12234	-0.72690
H	-3.91382	3.78586	3.44287	H	-4.86276	-4.59250	0.96442
H	-5.02693	3.24077	2.19703	H	-3.73887	-5.75373	0.27263
INT-7				TS-7			
C	4.06354	-1.16549	-0.33430	C	3.45295	-1.66239	0.04370
C	5.33885	-1.70835	-0.54802	C	4.54956	-2.18256	-0.66734
C	3.95736	0.16243	0.11610	C	3.59385	-0.43660	0.72133
C	6.47757	-0.95988	-0.33223	C	5.74947	-1.51170	-0.70129
C	5.10854	0.92591	0.31624	C	4.81616	0.23761	0.69095
C	6.35421	0.36579	0.09658	C	5.87654	-0.29641	-0.01276
H	5.39858	-2.73139	-0.89729	H	4.41809	-3.12452	-1.18475
H	7.45716	-1.39084	-0.49712	H	6.58956	-1.91460	-1.25275
H	5.00234	1.94876	0.65479	H	4.90291	1.17960	1.21580
H	7.24188	0.96407	0.26661	H	6.81926	0.23808	-0.03621
C	2.86093	-1.94834	-0.64596	C	2.19422	-2.38588	0.08573
O	2.88793	-3.05719	-1.18584	O	1.99848	-3.49594	-0.38095
C	1.60864	-1.26355	-0.32339	C	1.04601	-1.63703	0.75348
C	1.57633	0.01290	0.44953	C	1.24618	-0.22753	1.25515
O	2.77905	0.78639	0.35917	O	2.61976	0.12526	1.46999
O	0.48630	-1.74130	-0.62877	O	-0.07283	-2.13558	0.81721
C	1.28619	-0.40347	1.87058	C	0.48141	-0.01004	2.52574
C	2.12629	-1.10343	2.72529	C	0.80076	-0.50812	3.77550
C	-0.00915	-0.01115	2.23938	C	-0.64726	0.78174	2.28902
C	1.68610	-1.39466	4.00961	C	-0.02190	-0.19220	4.85309
C	-0.43942	-0.31920	3.53859	C	-1.45908	1.10112	3.38281
C	0.40684	-0.99937	4.40294	C	-1.14037	0.61217	4.64579
H	3.12000	-1.39613	2.40948	H	1.68855	-1.11410	3.91713
H	2.33488	-1.91427	4.70409	H	0.21325	-0.55617	5.84587
H	-1.41078	-0.01797	3.89664	H	-2.32296	1.73857	3.27226
H	0.06634	-1.21767	5.40889	H	-1.77277	0.87430	5.48673
C	-2.59085	0.47624	-2.05018	C	-1.71283	0.14457	-2.44376
C	-1.96448	-0.63548	-2.66262	C	-1.23270	-1.18999	-2.59115
C	-3.26672	0.24944	-0.83421	C	-2.80574	0.36306	-1.55897
C	-2.09055	-1.92784	-2.09430	C	-1.80216	-2.22201	-1.83827
C	-3.38566	-1.04421	-0.26760	C	-3.43636	-0.70165	-0.86687
C	-2.82783	-2.16686	-0.90955	C	-2.90494	-1.99412	-0.95570
H	-1.40674	-0.51149	-3.58173	H	-0.41479	-1.40519	-3.26679
H	-3.69361	1.09109	-0.30980	H	-3.17899	1.36908	-1.43294

H	-1.55822	-2.74398	-2.56143	H	-1.36151	-3.20714	-1.88854
H	-3.90785	-1.16741	0.67197	H	-4.27808	-0.50414	-0.21578
C	-2.57566	1.83886	-2.67104	C	-1.20049	1.26745	-3.29407
H	-2.53720	2.61609	-1.90872	H	-1.24743	2.21563	-2.75995
H	-1.72683	1.96648	-3.33893	H	-0.17276	1.10003	-3.60816
H	-3.49075	1.98389	-3.25322	H	-1.81884	1.35667	-4.19288
C	-2.99588	-3.54780	-0.31900	C	-3.56100	-3.12228	-0.18561
H	-3.13726	-3.40570	0.75706	H	-3.99119	-2.67217	0.71456
C	-1.77899	-4.45322	-0.51662	C	-2.60360	-4.23036	0.25381
C	-4.26562	-4.20341	-0.88414	C	-4.71219	-3.70491	-1.02095
H	-5.14865	-3.58815	-0.70167	H	-5.44068	-2.93754	-1.28884
H	-4.17458	-4.35313	-1.96302	H	-4.33140	-4.14681	-1.94548
H	-4.42854	-5.17891	-0.42085	H	-5.23067	-4.48780	-0.46271
H	-1.64747	-4.72805	-1.56577	H	-2.22545	-4.79562	-0.60157
H	-1.91383	-5.37997	0.04431	H	-3.13141	-4.93731	0.89723
H	-0.86309	-3.97040	-0.17541	H	-1.75049	-3.83177	0.79940
Ru	-1.16829	-0.57995	-0.54701	Ru	-1.17523	-0.51688	-0.40286
C	0.30450	0.86215	0.04061	C	0.49667	0.66966	0.18521
C	-0.63296	0.77938	1.15636	C	-0.70479	1.19210	0.86342
C	0.66780	2.03340	-0.81481	C	1.46340	1.36848	-0.71098
C	1.10278	3.23442	-0.24528	C	2.11978	2.52513	-0.27281
C	0.75678	1.89734	-2.19940	C	1.87009	0.80838	-1.92092
C	1.55340	4.28231	-1.03691	C	3.11219	3.12144	-1.03753
C	1.21368	2.93979	-2.99808	C	2.86869	1.39679	-2.68974
C	1.60435	4.14154	-2.42032	C	3.48915	2.56034	-2.25424
H	1.09793	3.34254	0.83256	H	1.85152	2.95333	0.68539
H	0.46233	0.95784	-2.64839	H	1.39927	-0.10648	-2.25378
H	1.87488	5.20766	-0.57243	H	3.60055	4.02053	-0.67901
H	1.26630	2.81070	-4.07326	H	3.16370	0.94111	-3.62805
H	1.95649	4.95789	-3.04013	H	4.26620	3.02295	-2.85153
C	-1.77716	1.68473	1.46066	C	-1.49821	2.39575	0.48639
C	-1.88610	2.99274	0.97558	C	-1.01510	3.44590	-0.30151
C	-2.84611	1.20997	2.24006	C	-2.83516	2.48939	0.91194
C	-2.99083	3.78728	1.26736	C	-1.81524	4.53754	-0.62959
C	-3.94379	2.00179	2.53892	C	-3.62981	3.58034	0.59743
C	-4.02457	3.30497	2.05743	C	-3.12367	4.62131	-0.17630
H	-1.11234	3.40387	0.35176	H	-0.00606	3.42035	-0.67525
H	-2.84855	0.18111	2.56769	H	-3.27469	1.66438	1.45487
H	-3.03576	4.79506	0.86977	H	-1.40166	5.32990	-1.24374
H	-4.74976	1.59148	3.13689	H	-4.65722	3.60935	0.94310
H	-4.88291	3.92566	2.28537	H	-3.74353	5.47357	-0.42846

INT-8				TS-8			
C	2.95136	-1.75513	0.22649	C	2.74981	-1.92206	0.22619
C	3.84017	-2.50850	-0.54836	C	3.74197	-2.40591	-0.63333
C	3.39060	-0.53710	0.76473	C	3.02279	-0.79933	1.01216
C	5.13043	-2.07250	-0.78133	C	4.97554	-1.78470	-0.69759
C	4.69750	-0.10468	0.55253	C	4.27065	-0.19353	0.98223
C	5.55709	-0.86718	-0.21845	C	5.24055	-0.68704	0.12413
H	3.48743	-3.44896	-0.95309	H	3.52603	-3.28246	-1.23129
H	5.80697	-2.66118	-1.38842	H	5.73822	-2.15549	-1.37117
H	5.01154	0.83733	0.98362	H	4.45424	0.66976	1.60757
H	6.56881	-0.51800	-0.38975	H	6.21081	-0.20616	0.08636
C	1.59911	-2.26969	0.52444	C	1.48481	-2.64371	0.41126
O	1.29608	-3.45021	0.37417	O	1.32757	-3.80855	0.08475
C	0.66721	-1.26172	1.07317	C	0.32337	-1.89571	1.07745
C	1.20028	0.13876	1.42784	C	0.76995	-0.11225	1.46143
O	2.60883	0.25331	1.55262	O	2.09217	-0.33036	1.90455
O	-0.49955	-1.55631	1.56766	O	-0.40738	-2.45305	1.86353
C	0.49095	0.65398	2.64175	C	-0.15604	0.25372	2.57100
C	0.83358	0.51070	3.96944	C	-0.13442	-0.11747	3.89420
C	-0.68287	1.29727	2.23479	C	-1.15489	1.07535	2.03142
C	-0.01677	1.04624	4.93859	C	-1.15324	0.35153	4.73343
C	-1.53073	1.81906	3.20628	C	-2.15896	1.54079	2.86853
C	-1.18614	1.69158	4.55285	C	-2.14887	1.16820	4.21896
H	1.75063	0.00691	4.25177	H	0.65330	-0.75345	4.27910
H	0.23769	0.96544	5.98877	H	-1.16066	0.07722	5.78145
H	-2.43390	2.34919	2.94124	H	-2.92952	2.20801	2.51034
H	-1.83900	2.11454	5.30799	H	-2.93036	1.53788	4.87324
C	-1.18628	-0.41858	-2.62166	C	-0.22131	-1.12872	-2.74345
C	-0.64158	-1.68454	-2.31814	C	-0.36397	-2.32999	-2.03989
C	-2.33884	-0.02073	-1.91078	C	-1.22728	-0.15159	-2.53541
C	-1.30565	-2.56049	-1.42108	C	-1.50117	-2.59423	-1.22849
C	-3.01806	-0.89692	-1.03249	C	-2.36980	-0.43614	-1.74510
C	-2.52992	-2.20173	-0.81248	C	-2.56688	-1.69231	-1.11930
H	0.27322	-2.01111	-2.79630	H	0.41182	-3.07982	-2.10059
H	-2.72331	0.97850	-2.05516	H	-1.13504	0.82355	-2.99575
H	-0.84285	-3.50503	-1.18120	H	-1.52076	-3.52466	-0.67950
H	-3.91351	-0.56185	-0.52693	H	-3.11450	0.33756	-1.61853
C	-0.60106	0.47846	-3.66937	C	0.90682	-0.90802	-3.70358
H	-0.58627	1.51631	-3.33914	H	1.10726	0.15357	-3.84512
H	0.41091	0.18357	-3.93647	H	1.81939	-1.39848	-3.36352
H	-1.21707	0.42375	-4.57184	H	0.64973	-1.32656	-4.68131

C	-3.29207	-3.13533	0.09988	C	-3.85861	-1.98433	-0.39208
H	-3.71225	-2.51260	0.89585	H	-4.20879	-1.02887	0.01207
C	-2.42978	-4.21810	0.74523	C	-3.70261	-2.95868	0.77465
C	-4.46008	-3.75632	-0.68407	C	-4.91419	-2.48590	-1.39065
H	-5.11773	-2.99299	-1.10395	H	-5.06453	-1.77486	-2.20542
H	-4.08708	-4.37242	-1.50610	H	-4.60738	-3.43975	-1.82746
H	-5.05536	-4.39406	-0.02749	H	-5.87294	-2.63569	-0.88933
H	-2.09049	-4.94947	0.00730	H	-3.44040	-3.96107	0.42696
H	-3.01842	-4.75900	1.48869	H	-4.64726	-3.04188	1.31549
H	-1.55525	-3.78740	1.23122	H	-2.93003	-2.62811	1.46880
Ru	-0.85854	-0.66640	-0.30111	Ru	-0.57285	-0.56577	-0.44682
C	0.54829	0.92081	0.25175	C	0.55875	0.90854	0.36593
C	-0.72118	1.37522	0.74505	C	-0.82933	1.33543	0.59585
C	1.50024	1.56358	-0.69131	C	1.70729	1.71735	-0.11292
C	1.98200	2.83963	-0.37417	C	2.16779	2.77910	0.67200
C	2.05577	0.90147	-1.78230	C	2.36771	1.43219	-1.30419
C	2.96101	3.44451	-1.14966	C	3.25978	3.53533	0.26817
C	3.03855	1.50246	-2.56015	C	3.45713	2.18977	-1.71555
C	3.49139	2.77825	-2.25075	C	3.90733	3.24393	-0.92953
H	1.58363	3.35741	0.49047	H	1.66277	3.01139	1.60244
H	1.72355	-0.10018	-2.00964	H	2.02499	0.59756	-1.89570
H	3.31432	4.43635	-0.89160	H	3.60629	4.35534	0.88683
H	3.45445	0.96778	-3.40622	H	3.95945	1.95177	-2.64601
H	4.25590	3.24953	-2.85732	H	4.75815	3.83614	-1.24584
C	-1.66832	2.30252	0.07156	C	-1.54480	2.37385	-0.18190
C	-1.29043	3.18945	-0.94180	C	-0.89811	3.27096	-1.04159
C	-3.02332	2.27870	0.43598	C	-2.94376	2.45930	-0.09913
C	-2.22457	4.01371	-1.56209	C	-1.61410	4.21659	-1.76698
C	-3.95355	3.10339	-0.17716	C	-3.65826	3.40647	-0.81880
C	-3.55983	3.98070	-1.18396	C	-2.99681	4.29707	-1.65782
H	-0.26252	3.23911	-1.26164	H	0.17423	3.23662	-1.14689
H	-3.35944	1.56594	1.17672	H	-3.48404	1.75040	0.51344
H	-1.89911	4.68763	-2.34653	H	-1.08143	4.89835	-2.42054
H	-4.99423	3.05168	0.12219	H	-4.73837	3.44124	-0.73131
H	-4.28558	4.62319	-1.66828	H	-3.55187	5.03752	-2.22158
TS-8a				INT-9			
C	3.24840	-0.23922	0.06524	C	3.31648	-0.90320	0.16391
C	4.58947	-0.33211	-0.34339	C	4.46151	-1.47943	-0.42269
C	3.00121	-0.25064	1.44799	C	3.26577	0.50609	0.19687
C	5.63939	-0.43262	0.54840	C	5.48915	-0.73051	-0.95893
C	4.06164	-0.33659	2.35267	C	4.32754	1.26271	-0.30525

C	5.36880	-0.42891	1.91446	C	5.42578	0.65943	-0.88383
H	4.77854	-0.31988	-1.40840	H	4.51693	-2.55956	-0.44622
H	6.65758	-0.51022	0.18689	H	6.33705	-1.22194	-1.41953
H	3.82565	-0.32670	3.40957	H	4.25230	2.34067	-0.23652
H	6.17300	-0.50224	2.63725	H	6.22789	1.27050	-1.28055
C	2.23656	-0.16250	-1.05336	C	2.38037	-1.93124	0.75454
O	2.62211	0.30055	-2.11991	O	2.85959	-2.92580	1.25360
C	0.81051	-1.76496	0.56678	C	0.80347	-1.89808	0.57075
C	0.53930	-0.31910	1.47209	C	1.05648	0.67111	1.00001
O	1.79165	-0.11007	2.08643	O	2.26771	1.27361	0.72232
O	1.20626	-2.73419	1.12282	O	0.20912	-2.84640	1.02058
C	-0.52214	-0.76840	2.41176	C	0.84953	0.03715	2.31768
C	-0.48953	-1.75654	3.38360	C	1.74007	-0.30977	3.30889
C	-1.70829	-0.07055	2.11736	C	-0.54230	-0.16504	2.44532
C	-1.65947	-2.04008	4.07996	C	1.23428	-0.87833	4.48677
C	-2.88621	-0.38428	2.80135	C	-1.02983	-0.72175	3.61209
C	-2.84786	-1.36519	3.78187	C	-0.12871	-1.07546	4.63033
H	0.42851	-2.28450	3.60312	H	2.80333	-0.13853	3.19069
H	-1.65037	-2.78873	4.86322	H	1.91125	-1.15292	5.28668
H	-3.80937	0.13704	2.58380	H	-2.08761	-0.86366	3.77823
H	-3.75029	-1.60792	4.33100	H	-0.51534	-1.50205	5.54874
C	-0.43942	-0.19931	-3.29178	C	0.97429	-0.22404	-2.73034
C	0.35481	-1.37373	-3.12540	C	0.85365	-1.58099	-2.36702
C	-1.62150	-0.12621	-2.57000	C	-0.21209	0.54717	-2.75265
C	-0.09959	-2.47574	-2.37946	C	-0.41137	-2.16123	-2.08407
C	-2.05189	-1.20838	-1.75578	C	-1.44492	-0.01086	-2.39816
C	-1.34673	-2.40989	-1.69399	C	-1.58007	-1.39218	-2.08034
H	1.30980	-1.43571	-3.62744	H	1.73922	-2.20208	-2.33176
H	-2.22874	0.76962	-2.61208	H	-0.16009	1.59875	-2.99974
H	0.48190	-3.38758	-2.35760	H	-0.44997	-3.20207	-1.79922
H	-2.96641	-1.09813	-1.19211	H	-2.32234	0.62041	-2.36437
C	0.06153	0.91946	-4.14840	C	2.28950	0.35101	-3.15668
H	1.04778	1.23330	-3.79897	H	2.37006	1.40512	-2.89407
C	-1.83448	-3.62637	-0.93861	H	3.12113	-0.18354	-2.70232
Ru	0.32489	-0.80380	-0.92006	H	2.38968	0.27314	-4.24353
C	-0.08791	0.91681	0.79335	C	-2.94849	-1.95590	-1.78640
C	-1.42001	0.97744	1.15562	H	-3.47847	-1.19154	-1.21467
C	0.66636	2.07050	0.23320	C	-2.91611	-3.23227	-0.94975
C	1.70345	2.66449	0.95894	C	-3.71333	-2.17150	-3.10202
C	0.29173	2.65765	-0.97915	H	-3.78292	-1.25028	-3.68366
C	2.36132	3.78761	0.47005	H	-3.21807	-2.92498	-3.71985

C	0.94009	3.78243	-1.46255	H	-4.72788	-2.51738	-2.89479
C	1.98675	4.35075	-0.74295	H	-2.51506	-4.07568	-1.51806
H	1.98836	2.25657	1.91739	H	-3.92953	-3.49797	-0.64539
H	-0.51946	2.22489	-1.54507	H	-2.30829	-3.10391	-0.05391
H	3.16521	4.22767	1.04886	Ru	-0.01967	-0.43668	-0.59798
H	0.63188	4.21475	-2.40739	C	-0.19772	1.27954	0.60830
H	2.50112	5.22559	-1.12303	C	-1.18336	0.38531	1.21299
C	-2.41181	1.99175	0.75678	C	-0.29135	2.69221	0.18516
C	-2.17812	3.35823	0.94890	C	-1.09832	3.56515	0.92437
C	-3.63614	1.60015	0.20438	C	0.51056	3.23195	-0.82334
C	-3.13196	4.29937	0.58685	C	-1.13248	4.92301	0.63555
C	-4.58756	2.54277	-0.16660	C	0.47992	4.58988	-1.11148
C	-4.33799	3.89708	0.02152	C	-0.34851	5.44167	-0.38900
H	-1.24601	3.68209	1.39178	H	-1.69985	3.17394	1.73478
H	-3.84467	0.54749	0.06188	H	1.17237	2.58265	-1.37560
H	-2.93405	5.35251	0.75007	H	-1.76979	5.57810	1.21831
H	-5.52613	2.21695	-0.60002	H	1.10793	4.98376	-1.90228
H	-5.08007	4.63363	-0.26350	H	-0.37640	6.50068	-0.61686
H	-0.94147	-4.13442	-0.56174	C	-2.63956	0.38075	0.97860
C	-2.54148	-4.58011	-1.91542	C	-3.29192	1.33533	0.18220
H	-3.44428	-4.11685	-2.32116	C	-3.42686	-0.66033	1.49642
H	-1.89495	-4.85073	-2.75237	C	-4.65947	1.27288	-0.04779
H	-2.83265	-5.49860	-1.40190	C	-4.79504	-0.72005	1.26976
C	-2.72837	-3.30137	0.25639	C	-5.42657	0.25218	0.50332
H	-2.24791	-2.60665	0.94426	H	-2.72689	2.13379	-0.27141
H	-3.68122	-2.86832	-0.05730	H	-2.95687	-1.46141	2.04613
H	-2.95571	-4.21675	0.80519	H	-5.12834	2.03091	-0.66517
H	0.16620	0.59302	-5.18653	H	-5.36682	-1.54232	1.68462
H	-0.61460	1.77363	-4.12557	H	-6.49446	0.20804	0.32607
TS-9				INT-10			
C	-1.53720	2.86639	-1.01578	C	-1.54623	-2.78886	-0.10062
C	-1.61002	4.24482	-0.73870	C	-2.30593	-3.91169	0.25745
C	-0.42451	2.37876	-1.73440	C	-1.50356	-2.41869	-1.45197
C	-0.63647	5.11669	-1.17051	C	-2.98771	-4.66333	-0.67949
C	0.53131	3.27773	-2.20752	C	-2.19605	-3.17704	-2.40158
C	0.43382	4.62662	-1.92484	C	-2.92486	-4.28833	-2.02223
H	-2.46479	4.59993	-0.17760	H	-2.33490	-4.17828	1.30632
H	-0.70438	6.17249	-0.93927	H	-3.56095	-5.53086	-0.37630
H	1.36476	2.88281	-2.77304	H	-2.15371	-2.86224	-3.43709
H	1.20116	5.30363	-2.28168	H	-3.45100	-4.86351	-2.77549
C	-2.66288	2.02995	-0.59117	C	-0.79182	-2.08806	0.97155

O	-3.67424	2.47078	-0.06627	O	-1.15589	-2.18956	2.13464
C	-2.63859	0.45936	-0.86166	C	1.42693	-2.45469	-0.42902
C	-0.00533	0.03073	-1.11683	C	-0.22386	-0.34343	-1.16304
O	-0.26179	1.07628	-2.09982	O	-0.86382	-1.33961	-1.96773
O	-3.36150	0.01578	-1.71587	O	1.79233	-3.36367	-1.04472
C	0.03386	-1.27093	-1.82994	C	0.81170	0.37128	-1.96831
C	-0.83157	-1.80256	-2.77143	C	1.81385	-0.12193	-2.78558
C	1.19887	-1.96344	-1.44827	C	0.65127	1.75762	-1.78480
C	-0.55809	-3.06541	-3.29613	C	2.69437	0.77640	-3.38926
C	1.42573	-3.25544	-1.91887	C	1.53960	2.64954	-2.37500
C	0.54318	-3.79552	-2.85170	C	2.56733	2.14686	-3.17324
H	-1.70956	-1.25371	-3.08147	H	1.91448	-1.18687	-2.95478
H	-1.22118	-3.49283	-4.03926	H	3.48370	0.40457	-4.03205
H	2.28607	-3.82584	-1.59311	H	1.42864	3.71835	-2.24202
H	0.72238	-4.78986	-3.24416	H	3.26221	2.83158	-3.64547
C	-2.33874	-1.90007	1.24391	C	0.99337	0.17957	2.95316
C	-0.92945	-1.96699	1.40708	C	1.84298	-0.95001	2.89716
C	-3.00703	-0.83341	1.91360	C	1.22190	1.20175	2.02946
C	-0.24171	-1.14172	2.34971	C	2.92090	-0.99276	2.00701
C	-2.28998	0.08546	2.68652	C	2.32245	1.16523	1.14784
C	-0.90149	-0.10875	2.99194	C	3.21407	0.09516	1.14260
H	-0.36655	-2.71866	0.87609	H	1.66953	-1.78340	3.56588
H	-4.06766	-0.68474	1.76295	H	0.56338	2.06043	2.01025
H	0.81822	-1.28874	2.50111	H	3.56321	-1.86414	2.01269
H	-2.80865	0.93420	3.11360	H	2.48011	1.98772	0.46264
C	-3.14744	-2.92468	0.47600	C	-0.12532	0.23607	3.94498
H	-3.73467	-2.37653	-0.26715	H	-0.60145	1.21558	3.95407
C	-0.21293	0.81573	3.94757	H	-0.87068	-0.52220	3.69689
H	-0.50534	1.85208	3.76952	H	0.24660	0.02528	4.95009
Ru	-1.42131	0.01438	0.54675	C	4.46277	0.12801	0.28844
C	1.35342	0.11817	-0.46040	H	4.33965	0.95605	-0.41475
C	2.00181	-1.07996	-0.59456	C	4.68219	-1.14708	-0.52776
C	1.89536	1.35094	0.12806	C	5.68337	0.43151	1.17267
C	1.13976	2.17321	0.96951	H	5.55102	1.36125	1.72914
C	3.19087	1.77246	-0.20257	H	5.85304	-0.37226	1.89364
C	1.64594	3.36561	1.46442	H	6.58074	0.52618	0.55800
C	3.70157	2.96420	0.28974	H	4.81334	-2.02193	0.11297
C	2.93229	3.76847	1.12523	H	5.58479	-1.04747	-1.13372
H	0.13636	1.86542	1.24306	H	3.84442	-1.33393	-1.19694
H	3.79083	1.16481	-0.86702	Ru	0.86802	-1.03777	0.55993
H	1.03248	3.98335	2.10937	C	-1.12625	0.77498	-0.68540

H	4.70292	3.27270	0.01176	C	-0.56355	1.97922	-0.98621
H	3.33053	4.70243	1.50392	C	-2.39570	0.56571	0.03767
C	3.29385	-1.45900	0.00143	C	-2.56948	1.04700	1.33759
C	3.59679	-1.15647	1.33459	C	-3.46664	-0.09410	-0.57309
C	4.26442	-2.12609	-0.75719	C	-3.76582	0.85975	2.01598
C	4.81753	-1.51127	1.89080	C	-4.66560	-0.27992	0.10214
C	5.48880	-2.47738	-0.20250	C	-4.81851	0.19089	1.40154
C	5.77065	-2.17544	1.12507	H	-1.75747	1.57496	1.81672
H	2.87020	-0.62754	1.93643	H	-3.36285	-0.45296	-1.58795
H	4.06868	-2.34798	-1.79831	H	-3.87571	1.23484	3.02694
H	5.02612	-1.26887	2.92659	H	-5.48373	-0.79307	-0.38991
H	6.22718	-2.98511	-0.81260	H	-5.75308	0.04195	1.92978
H	6.72435	-2.45256	1.55867	C	-1.06175	3.31452	-0.61204
C	-2.29451	-3.95961	-0.24995	C	-0.20089	4.26360	-0.04820
H	-1.75241	-4.59040	0.45990	C	-2.39923	3.67279	-0.81612
H	-2.93597	-4.61276	-0.84412	C	-0.66454	5.52249	0.31441
H	-1.57693	-3.50011	-0.92390	C	-2.86075	4.93276	-0.46095
C	-4.12481	-3.62602	1.43461	C	-1.99666	5.86263	0.10889
H	-4.73437	-4.34456	0.88339	H	0.83928	4.01247	0.11901
H	-3.58044	-4.17069	2.21041	H	-3.07682	2.95742	-1.26319
H	-4.79884	-2.92265	1.92529	H	0.01773	6.23912	0.75716
H	-0.49536	0.57082	4.97575	H	-3.89913	5.19176	-0.63339
H	0.87039	0.74317	3.86433	H	-2.35817	6.84583	0.38650
TS-10				INT-11			
C	0.35493	2.72373	0.41934	C	1.91558	2.92005	-0.07154
C	0.22840	3.79156	1.29782	C	2.20993	4.19268	0.41441
C	0.60182	2.96445	-0.92124	C	2.13849	2.59611	-1.40788
C	0.32638	5.08982	0.80673	C	2.72410	5.12943	-0.46509
C	0.70663	4.24479	-1.43594	C	2.65896	3.52277	-2.30408
C	0.56122	5.31016	-0.55074	C	2.94346	4.78850	-1.80871
H	0.04980	3.60350	2.34993	H	2.03102	4.43188	1.45586
H	0.22521	5.93300	1.47943	H	2.95941	6.12943	-0.12279
H	0.90357	4.40318	-2.48916	H	2.83409	3.26306	-3.34045
H	0.64139	6.32418	-0.92463	H	3.34837	5.53533	-2.48224
C	0.27042	1.27411	0.73808	C	1.39890	1.72840	0.58568
O	0.76008	0.79260	1.76729	O	1.19729	1.53278	1.76543
C	-2.25379	1.79591	-0.44033	C	-1.48209	2.57642	0.40795
C	0.72599	0.65407	-0.94840	C	1.22342	0.67306	-0.53030
O	0.73636	1.84687	-1.70448	O	1.83262	1.31570	-1.72352
O	-2.71456	2.75088	-0.90567	O	-1.23751	3.71218	0.43866
C	-0.19447	-0.39244	-1.47731	C	-0.19513	0.22482	-0.91614

C	-1.25792	-0.29928	-2.39095	C	-1.14616	0.94498	-1.71929
C	0.42546	-1.65415	-1.23076	C	-0.08852	-1.20847	-1.14769
C	-1.81661	-1.47496	-2.88215	C	-1.99372	0.20391	-2.60934
C	-0.17629	-2.82005	-1.69344	C	-0.93082	-1.87733	-1.98605
C	-1.30714	-2.71805	-2.50091	C	-1.91739	-1.15495	-2.71608
H	-1.59704	0.66495	-2.74288	H	-0.97913	1.98580	-1.96078
H	-2.64736	-1.42415	-3.57497	H	-2.69583	0.75905	-3.22056
H	0.26514	-3.78855	-1.49504	H	-0.80243	-2.93889	-2.15793
H	-1.76356	-3.62066	-2.89086	H	-2.57084	-1.68488	-3.39858
C	-1.73501	-0.93548	2.60656	C	-2.21748	0.14111	2.58913
C	-2.63045	0.13171	2.34820	C	-3.26976	0.99291	2.14680
C	-1.70556	-1.97324	1.67946	C	-2.01512	-1.03553	1.85502
C	-3.58426	0.01409	1.29757	C	-4.15876	0.63704	1.09830
C	-2.70312	-2.12017	0.67266	C	-2.85055	-1.34797	0.75762
C	-3.69714	-1.17174	0.50599	C	-3.97036	-0.56216	0.39500
H	-2.67817	0.97775	3.02029	H	-3.42323	1.93345	2.65995
H	-0.95192	-2.74460	1.77655	H	-1.19180	-1.69168	2.10529
H	-4.32508	0.79482	1.19217	H	-4.97159	1.30444	0.85240
H	-2.67607	-2.99008	0.03099	H	-2.62749	-2.22835	0.17112
C	-0.78825	-0.87016	3.75844	C	-1.38094	0.49298	3.78048
H	-0.23183	-1.80068	3.86784	H	-0.35482	0.15516	3.64394
H	-0.07678	-0.05922	3.59384	H	-1.36349	1.57106	3.93778
H	-1.33048	-0.67761	4.68718	H	-1.78648	0.02647	4.68348
C	-4.83604	-1.38072	-0.46523	C	-4.88165	-1.03252	-0.71210
H	-4.54039	-2.20569	-1.11953	H	-4.23515	-1.50997	-1.45449
C	-5.12114	-0.16171	-1.34591	C	-5.64035	0.09429	-1.41031
C	-6.09771	-1.81177	0.29979	C	-5.85077	-2.10016	-0.17946
H	-5.91511	-2.70988	0.89258	H	-5.31512	-2.93274	0.28007
H	-6.43135	-1.02180	0.97764	H	-6.52099	-1.67455	0.57177
H	-6.91160	-2.02163	-0.39740	H	-6.46243	-2.49727	-0.99256
H	-5.46373	0.69127	-0.75607	H	-6.37782	0.55574	-0.74905
H	-5.90874	-0.39772	-2.06424	H	-6.18130	-0.30065	-2.27214
H	-4.23225	0.14278	-1.89689	H	-4.96072	0.87215	-1.76081
Ru	-1.63332	0.25769	0.29535	Ru	-1.94251	0.80868	0.36907
C	1.99099	-0.05720	-0.66227	C	1.94024	-0.63280	-0.21467
C	1.74972	-1.41045	-0.68880	C	1.16542	-1.68620	-0.57419
C	3.20556	0.63011	-0.20523	C	3.26555	-0.66387	0.41844
C	3.85195	0.24894	0.97633	C	3.51971	-1.53300	1.48803
C	3.73767	1.69408	-0.94313	C	4.29838	0.18260	-0.00437
C	5.00147	0.90133	1.39807	C	4.76215	-1.56245	2.10370
C	4.89042	2.34491	-0.52139	C	5.54223	0.15221	0.61387

C	5.52724	1.95045	0.64976	C	5.78125	-0.71996	1.66941
H	3.43739	-0.55425	1.56930	H	2.72847	-2.18027	1.84269
H	3.25148	2.00059	-1.85943	H	4.13675	0.85093	-0.83839
H	5.48607	0.59540	2.31826	H	4.93351	-2.23884	2.93334
H	5.29259	3.16102	-1.11056	H	6.32912	0.81100	0.26487
H	6.42553	2.45914	0.98019	H	6.75115	-0.74124	2.15237
C	2.68604	-2.49516	-0.34412	C	1.52754	-3.11467	-0.52704
C	2.28398	-3.53834	0.49608	C	0.65043	-4.05098	0.02853
C	3.98276	-2.52449	-0.86777	C	2.73984	-3.56633	-1.05765
C	3.15493	-4.57338	0.81383	C	0.98555	-5.39868	0.07323
C	4.85191	-3.56027	-0.55357	C	3.06994	-4.91411	-1.02302
C	4.44286	-4.58817	0.29039	C	2.19630	-5.83502	-0.45307
H	1.28477	-3.52923	0.91381	H	-0.29451	-3.71807	0.44003
H	4.30574	-1.73090	-1.52943	H	3.42216	-2.85352	-1.50300
H	2.82704	-5.36881	1.47327	H	0.29851	-6.10933	0.51800
H	5.85158	-3.56789	-0.97270	H	4.01118	-5.24769	-1.44452
H	5.12213	-5.39634	0.53526	H	2.45595	-6.88680	-0.42353
LRu(CO)(HOAc)				LRu(CO)			
C	-1.87269	0.93263	1.16622	C	-2.34975	-1.29604	-0.06178
O	-2.83088	1.22151	1.77452	O	-3.37312	-1.86125	0.02280
Ru	-0.40616	0.39496	0.22378	Ru	-0.71187	-0.53812	-0.27000
C	1.83378	0.77547	0.86102	C	0.89665	0.29070	1.23836
C	1.89420	-0.18797	-0.15240	C	1.51319	0.31051	-0.02543
C	1.27001	0.09591	-1.40693	C	0.88952	1.01766	-1.09800
C	0.60728	1.30332	-1.66373	C	-0.35444	1.64104	-0.95121
C	0.45837	2.24765	-0.61121	C	-1.05465	1.51299	0.28688
C	1.06543	1.95426	0.64666	C	-0.40571	0.83432	1.37776
H	2.31787	0.61817	1.81353	H	1.37052	-0.18851	2.08223
H	1.29524	-0.66424	-2.17781	H	1.37789	1.02715	-2.06469
H	0.19178	1.50236	-2.64218	H	-0.79358	2.18996	-1.77350
H	0.97083	2.67333	1.44960	H	-0.90251	0.78838	2.33792
C	2.61549	-1.50991	0.00820	C	2.85426	-0.34759	-0.28637
C	2.62374	-2.04342	1.44026	C	3.09989	-1.61274	0.53688
C	4.04439	-1.39542	-0.54497	C	3.98566	0.67035	-0.07661
H	2.07444	-2.23242	-0.61167	H	2.85529	-0.63515	-1.34306
H	1.61273	-2.10669	1.84481	H	2.29419	-2.33733	0.40540
H	3.06662	-3.04111	1.46352	H	4.03533	-2.08292	0.22726
H	3.21777	-1.41025	2.10346	H	3.18522	-1.39182	1.60316
H	4.04488	-1.05133	-1.58105	H	3.84043	1.55959	-0.69286
H	4.62897	-0.68558	0.04586	H	4.02801	0.98763	0.96846
H	4.54924	-2.36343	-0.50856	H	4.95125	0.23073	-0.33662

C	-0.23418	3.55889	-0.83891	C	-2.37428	2.19404	0.49678
H	-1.04982	3.45094	-1.55447	H	-2.95487	2.21810	-0.42583
H	-0.64423	3.95272	0.09116	H	-2.96271	1.68410	1.25982
H	0.46777	4.29875	-1.23540	H	-2.21914	3.22592	0.82656
H	-2.29649	-0.16456	-0.99791				
O	-2.79669	-1.03560	-1.15306				
O	-1.16797	-1.67966	0.22873				
C	-2.16250	-1.94736	-0.44952				
C	-2.73434	-3.32330	-0.53295				
H	-2.78666	-3.63677	-1.57689				
H	-2.12529	-4.01775	0.03875				
H	-3.75426	-3.31487	-0.14316				
³pre-CAT				¹pre-CAT			
C	2.43693	0.90365	0.08823	C	2.18963	-0.94561	-0.72763
O	3.54292	1.21824	0.19150	O	3.16514	-1.24645	-1.25471
Ru	0.65902	0.37884	-0.04726	Ru	0.62401	-0.40825	0.11481
C	-0.92026	-0.91163	1.15995	C	-0.84965	0.79311	-1.15074
C	-1.50460	-0.61138	-0.10351	C	-1.54760	0.55529	0.06869
C	-0.83031	-1.01749	-1.27207	C	-0.91489	0.91945	1.26279
C	0.45673	-1.58434	-1.20001	C	0.36569	1.54434	1.27411
C	1.06083	-1.84114	0.05984	C	1.00587	1.88780	0.07086
C	0.32897	-1.53348	1.24244	C	0.38839	1.46584	-1.13902
H	-1.42800	-0.63160	2.07157	H	-1.27534	0.49218	-2.09662
H	-1.26818	-0.80971	-2.24046	H	-1.38105	0.66693	2.20686
H	0.98448	-1.84252	-2.10841	H	0.83048	1.78603	2.22086
H	0.76199	-1.74731	2.21101	H	0.89792	1.64204	-2.07792
C	-2.85528	0.06500	-0.22359	C	-2.90343	-0.10991	0.09254
C	-3.15974	1.04876	0.90717	C	-3.00159	-1.31457	-0.84629
C	-3.95759	-0.99982	-0.33592	C	-3.98781	0.93448	-0.21510
H	-2.83307	0.62985	-1.16073	H	-3.05487	-0.46794	1.11472
H	-2.36650	1.78755	1.02181	H	-2.22008	-2.04139	-0.62459
H	-4.08989	1.57724	0.69104	H	-3.97283	-1.79673	-0.72142
H	-3.29562	0.53665	1.86270	H	-2.91715	-1.01941	-1.89449
H	-3.77954	-1.67402	-1.17569	H	-3.94583	1.77342	0.48206
H	-4.00844	-1.60065	0.57573	H	-3.87409	1.32828	-1.22817
H	-4.92964	-0.52432	-0.48159	H	-4.97669	0.47836	-0.14028
C	2.40350	-2.50419	0.14507	C	2.30779	2.62900	0.05417
H	3.00884	-2.28254	-0.73358	H	2.87676	2.44454	0.96488
H	2.94769	-2.18170	1.03278	H	2.91632	2.34249	-0.80330
H	2.28046	-3.58922	0.20345	H	2.11971	3.70414	-0.01591
O	-0.03585	2.66901	-0.88282	O	0.80584	-1.86833	1.50212

O	0.02586	2.31270	0.37933	O	0.05478	-2.32586	0.38954
TS-1c				INT-1c			
C	-1.33330	0.22542	1.60064	C	1.47038	0.69188	-1.53506
O	-2.11675	0.41039	2.40924	O	2.16838	1.04377	-2.37064
Ru	-0.03404	0.01141	0.25446	Ru	0.23932	0.21927	-0.21418
C	1.93996	0.75955	0.85410	C	-1.89748	0.74966	-0.81503
C	2.23619	0.13022	-0.39291	C	-2.09129	-0.02967	0.36123
C	1.43910	0.48145	-1.48299	C	-1.37807	0.34225	1.50368
C	0.45999	1.52676	-1.40585	C	-0.56749	1.51610	1.52622
C	0.28078	2.26984	-0.24030	C	-0.47117	2.36457	0.41952
C	0.99250	1.81674	0.91498	C	-1.11003	1.91789	-0.77770
H	2.46198	0.47326	1.75445	H	-2.36017	0.46137	-1.74638
H	1.53406	-0.07044	-2.40962	H	-1.41856	-0.28281	2.38667
H	-0.15919	1.72580	-2.27022	H	-0.00613	1.74511	2.42296
H	0.80705	2.29386	1.86893	H	-0.99032	2.49547	-1.68611
C	3.29309	-0.93862	-0.52857	C	-2.98216	-1.24851	0.39041
C	3.45637	-1.81161	0.71651	C	-3.15999	-1.92265	-0.96941
C	4.62269	-0.27282	-0.92094	C	-4.33933	-0.85472	0.99876
H	2.97664	-1.58108	-1.35534	H	-2.50208	-1.96319	1.06544
H	2.50373	-2.24658	1.01772	H	-2.19307	-2.14336	-1.42062
H	4.15637	-2.62068	0.50134	H	-3.70964	-2.85670	-0.84140
H	3.86694	-1.24499	1.55573	H	-3.73995	-1.29878	-1.65439
H	4.52680	0.30597	-1.84128	H	-4.22693	-0.42988	1.99775
H	4.96915	0.39811	-0.13087	H	-4.84667	-0.11844	0.37043
H	5.38802	-1.03560	-1.07516	H	-4.98101	-1.73468	1.07246
C	-0.68471	3.41045	-0.16175	C	0.29476	3.65067	0.46266
H	-1.50963	3.26605	-0.85816	H	1.07393	3.61693	1.22343
H	-1.09011	3.51769	0.84422	H	0.75444	3.87160	-0.50063
H	-0.17790	4.34493	-0.41823	H	-0.37971	4.47656	0.70618
O	-0.56384	-2.13276	-0.49840	O	0.66538	-2.68771	-0.32983
O	0.06335	-1.93103	0.77253	O	0.13310	-1.61044	-1.12836
H	-1.59213	-2.09235	-0.29411	H	1.61828	-2.61296	-0.52851
O	-3.03319	-1.88457	-0.20042	O	3.14360	-1.26764	-0.40938
O	-2.38410	0.11299	-0.97081	O	1.74109	-0.37178	1.09720
C	-3.26476	-0.74842	-0.72275	C	2.84560	-0.93558	0.74245
C	-4.71388	-0.42555	-1.04146	C	3.79786	-1.21140	1.88973
H	-5.27540	-0.35352	-0.10693	H	4.82598	-1.09641	1.54932
H	-4.80029	0.51295	-1.58511	H	3.60422	-0.56211	2.74119

H	-5.15600	-1.23608	-1.62290	H	3.66536	-2.24817	2.20911
TS-2c				INT-2c			
C	-0.36822	0.60125	-2.00664	C	0.78952	-1.46877	-2.03896
O	-0.57311	1.07439	-3.02142	O	1.12009	-1.99082	-2.99774
Ru	0.02761	-0.34111	-0.41624	Ru	0.30526	-0.63405	-0.43216
C	2.11517	-0.78989	-1.12381	C	2.24896	-1.21535	0.55305
C	2.20129	-0.48725	0.24151	C	1.95450	0.09997	0.94750
C	1.49617	-1.34417	1.16402	C	0.74859	0.31244	1.69712
C	0.63459	-2.32688	0.72713	C	-0.15811	-0.70921	1.91082
C	0.38090	-2.49828	-0.67619	C	0.07412	-2.02496	1.38650
C	1.19186	-1.77228	-1.58475	C	1.31269	-2.26502	0.76974
H	2.65598	-0.20117	-1.85042	H	3.16045	-1.43333	0.01497
H	1.56239	-1.13099	2.22227	H	0.51117	1.31141	2.03154
H	0.04912	-2.88828	1.44045	H	-1.09366	-0.49068	2.40049
H	1.06762	-1.92629	-2.64898	H	1.53493	-3.25417	0.38911
C	3.06376	0.61870	0.79644	C	2.88409	1.26419	0.70395
C	3.32037	1.75668	-0.18858	C	3.69503	1.14682	-0.58499
C	4.37929	0.01397	1.31555	C	3.79568	1.44379	1.92867
H	2.51146	1.02579	1.64797	H	2.24548	2.14816	0.62216
H	2.38283	2.17752	-0.55273	H	3.04258	1.01033	-1.44744
H	3.87734	2.54924	0.31383	H	4.27387	2.05930	-0.73578
H	3.92428	1.43053	-1.03918	H	4.40540	0.31774	-0.54573
H	4.20393	-0.77712	2.04731	H	3.21855	1.56413	2.84745
H	4.96317	-0.40688	0.49329	H	4.45364	0.57998	2.05108
H	4.97836	0.78930	1.79580	H	4.41908	2.33050	1.80238
C	-0.62533	-3.49641	-1.15030	C	-0.92341	-3.12126	1.59129
H	-1.49130	-3.50729	-0.49037	H	-1.93297	-2.73778	1.46297
H	-0.95229	-3.27508	-2.16533	H	-0.75450	-3.93883	0.89119
H	-0.18109	-4.49609	-1.14385	H	-0.83052	-3.51791	2.60667
O	-0.72000	0.10855	2.93757	O	-3.53414	1.69089	1.87772
O	-0.21545	0.83216	1.77945	O	-2.18619	2.03554	2.30345
H	-1.28231	-0.57705	2.50617	H	-3.39317	0.78682	1.50961
O	-2.22344	-1.66084	1.53828	O	-2.79326	-0.62585	0.68664
O	-2.06571	-0.47250	-0.36143	O	-1.63238	-0.68366	-1.23495
C	-2.72401	-1.08293	0.56311	C	-2.71367	-0.57709	-0.54911
C	-4.22583	-1.02529	0.39548	C	-3.96061	-0.35314	-1.37883
H	-4.50719	-0.87723	-0.64488	H	-4.24947	0.69622	-1.27838
H	-4.67919	-1.93220	0.79255	H	-3.79172	-0.57241	-2.43049

H	-4.59989	-0.17891	0.97730	H	-4.77784	-0.95972	-0.98911
H	-0.88267	1.60174	1.63140	H	-1.73981	2.19777	1.44550
O	-1.66972	2.79091	1.12139	O	-0.78712	2.32495	-0.04636
O	-0.08142	2.38493	-0.39803	O	0.32919	1.12182	-1.57882
C	-1.03797	3.07164	0.06527	C	-0.27435	2.18264	-1.16022
C	-1.44024	4.31354	-0.70961	C	-0.33167	3.30145	-2.17969
H	-2.18042	4.89879	-0.16744	H	-1.29162	3.24082	-2.69878
H	-0.56004	4.92452	-0.91469	H	-0.28192	4.26660	-1.67768
H	-1.85485	4.01098	-1.67413	H	0.46286	3.21144	-2.91756
INT-3c				TS-3c			
C	0.27604	-0.19908	2.29055	C	-0.34161	-2.39030	0.01200
O	0.30407	-0.19893	3.43224	C	0.17577	-1.87215	-1.21151
Ru	0.17531	-0.25116	0.42543	C	0.33865	-2.07063	1.20598
C	-1.60546	-1.63598	0.49342	C	1.35589	-1.08552	-1.22532
C	-1.84791	-0.69183	-0.51774	C	1.49478	-1.24756	1.17462
C	-0.94759	-0.67445	-1.63617	C	2.05737	-0.76835	-0.03289
C	0.19534	-1.45097	-1.65200	H	-0.37782	-2.01529	-2.12675
C	0.52538	-2.30509	-0.54687	H	-0.07983	-2.36640	2.15768
C	-0.42588	-2.43194	0.47768	H	1.66002	-0.64372	-2.16271
H	-2.27715	-1.71773	1.33625	H	1.92211	-0.91596	2.11292
H	-1.12514	0.02804	-2.43625	C	-1.60884	-3.18304	0.03122
H	0.90069	-1.35009	-2.46137	H	-2.11552	-3.08841	0.99119
H	-0.22809	-3.09647	1.30941	H	-2.27702	-2.85156	-0.76054
C	-3.05817	0.21100	-0.52820	H	-1.37640	-4.24025	-0.12750
C	-3.49488	0.66812	0.86289	C	3.30904	0.07853	0.00357
C	-4.20354	-0.48815	-1.27771	H	3.25146	0.67304	0.92036
H	-2.76745	1.09701	-1.09841	C	3.44143	1.04189	-1.17506
H	-2.67376	1.15498	1.38891	C	4.53838	-0.83765	0.10415
H	-4.31551	1.38159	0.77211	H	4.47862	-1.49539	0.97337
H	-3.85769	-0.16417	1.47062	H	4.62859	-1.46303	-0.78774
H	-3.90361	-0.78548	-2.28447	H	5.44847	-0.24099	0.19194
H	-4.52768	-1.38363	-0.74164	H	3.60857	0.50841	-2.11402
H	-5.05914	0.18381	-1.36438	H	4.30031	1.69639	-1.01845
C	1.78691	-3.10960	-0.55297	H	2.55384	1.66284	-1.28857
H	2.60857	-2.51214	-0.94204	Ru	-0.08996	-0.19024	0.11421
H	2.03455	-3.45693	0.44956	O	-2.67411	-0.67253	-1.87241
H	1.66365	-3.98593	-1.19626	C	-2.96005	-0.07192	-0.83698
O	2.78191	-0.16288	-1.57694	O	-2.14711	0.19080	0.13689
O	2.14891	0.44414	0.49968	C	-4.36376	0.46109	-0.60772
C	2.97744	0.38743	-0.49481	H	-4.66400	0.33987	0.43281
C	4.28226	1.11589	-0.21975	H	-5.07073	-0.03841	-1.26723

H	4.14347	2.17471	-0.45222	H	-4.37349	1.53089	-0.83077
H	4.56512	1.03933	0.82908	O	-0.15343	1.53553	-1.12487
H	5.07211	0.72420	-0.85799	C	0.10947	2.50250	-0.32847
O	-0.12720	2.17891	-1.61140	O	0.41203	2.29223	0.86264
O	-0.18336	1.80473	0.60631	C	0.02700	3.90142	-0.88149
C	-0.20398	2.56272	-0.44610	H	0.25486	3.91582	-1.94616
C	-0.31928	4.03937	-0.11197	H	0.69951	4.56300	-0.33836
H	0.67547	4.41941	0.13350	H	-0.99373	4.26887	-0.74935
H	-0.69893	4.59067	-0.97010	C	-0.87055	0.71676	2.51148
H	-0.95790	4.19758	0.75609	O	-1.40454	1.34400	3.27915

Table S3 Frequencies of all stationary points for the overall catalytic cycle, computed at B3LYP-D3a+IDSCRF/TZP-DKH(-dfg) level in tert-butanol

Species	Fequencies(cm ⁻¹)
1a	46 54 100 110 137 194 263 282 297 325 352 378 415 440 448 485 518 535 549 592 636 645 670 689 706 716 725 772 789 813 855 859 884 913 949 984 1000 1011 1016 1016 1024 1052 1059 1110 1135 1148 1176 1185 1210 1223 1251 1263 1312 1336 1340 1368 1376 1436 1485 1504 1514 1533 1598 1616 1628 1644 1653 1667 3161 3169 3170 3180 3182 3190 3194 3205 3235 3463
2a	41 47 48 138 156 261 285 409 413 414 478 526 551 566 576 637 644 706 707 718 776 776 855 855 860 937 937 993 993 1011 1011 1019 1020 1049 1051 1102 1103 1163 1182 1182 1200 1201 1311 1313 1340 1358 1358 1477 1479 1521 1538 1608 1609 1636 1644 2292 3159 3159 3167 3167 3176 3177 3183 3183 3187 3187
3a	28 30 49 53 57 63 79 95 103 138 189 195 209 215 228 259 282 291 302 332 393 414 417 420 428 450 492 523 530 546 561 597 601 633 635 641 653 655 688 706 714 716 717 725 758 768 770 775 786 812 821 861 862 867 870 884 892 909 942 947 963 965 978 996 997 1001 1003 1009 1012 1012 1024 1024 1034 1042 1052 1053 1071 1098 1105 1109 1128 1142 1171 1182 1182 1182 1196 1204 1206 1220 1228 1255 1268 1311 1317 1322 1328 1358 1361 1362 1369 1381 1479 1481 1495 1495 1500 1512 1528 1536 1612 1616 1627 1633 1640 1643 1645 1646 1650 1752 3157 3157 3161 3165 3166 3166 3168 3173 3176 3178 3180 3181 3186 3187 3189 3191 3192 3203
AcOH	66 433 543 589 649 869 1004 1069 1197 1345 1410 1467 1473 1769 3051 3108 3159 3492
³ O ₂	1613
H ₂ O ₂	376 950 1339 1393 3545 3561
CO	2206
CAT	25 33 41 50 63 68 77 98 114 120 135 175 184 198 215 218 237 243 265 268 285 299 330 354 394 405 437 445 450 486 525 532 582 623 626 648 675 677 690 696 818 896 904 915 936 942 963 973 979 988 1010 1018 1021 1033 1055 1063 1070 1081 1114 1136 1172 1182 1227 1240 1310 1335 1341 1358 1384 1390 1403 1418 1418 1423 1426 1448 1465 1466 1474 1476

	1486 1488 1492 1499 1502 1504 1513 1523 1533 1568 1646 3020 3026 3035 3035 3044 3048 3088 3094 3097 3098 3102 3111 3111 3128 3137 3143 3174 3195 3217 3234
TS-1	-70 15 23 30 35 47 53 60 62 68 70 74 82 90 98 109 116 129 133 143 152 165 176 183 205 206 219 220 233 248 259 266 272 279 289 294 301 325 327 341 358 382 385 409 414 427 430 450 456 457 468 489 492 519 525 528 550 570 592 616 630 633 646 649 671 673 679 689 691 703 710 718 726 773 791 815 817 858 863 885 897 906 915 922 940 943 951 970 972 975 985 986 1001 1010 1010 1013 1018 1020 1025 1025 1033 1052 1057 1064 1065 1072 1084 1107 1113 1136 1142 1159 1168 1174 1184 1193 1208 1229 1230 1243 1256 1259 1312 1318 1335 1336 1341 1360 1366 1367 1375 1386 1390 1402 1418 1420 1425 1430 1434 1443 1467 1471 1478 1481 1484 1489 1492 1494 1503 1504 1506 1506 1510 1514 1529 1534 1537 1576 1605 1617 1637 1644 1645 1656 1669 3027 3031 3032 3040 3041 3051 3089 3094 3095 3102 3109 3110 3114 3129 3149 3151 3161 3167 3171 3176 3179 3182 3189 3194 3199 3215 3217 3231 3245 3526
INT-1	24 34 46 48 52 56 57 62 63 66 70 75 83 96 107 117 120 134 140 145 169 172 185 190 201 206 217 226 247 251 257 265 277 284 286 288 306 319 333 357 371 397 402 412 418 429 448 450 457 480 503 517 520 521 534 552 574 592 620 627 633 645 665 669 670 677 683 691 698 711 716 729 774 791 815 818 859 866 887 889 903 916 931 934 938 944 954 976 977 985 988 1002 1007 1011 1012 1019 1023 1026 1033 1036 1052 1056 1061 1063 1065 1084 1105 1113 1135 1142 1167 1167 1173 1184 1188 1204 1216 1225 1226 1241 1245 1262 1272 1315 1324 1330 1339 1339 1362 1362 1370 1380 1389 1403 1415 1418 1421 1428 1430 1437 1467 1471 1476 1478 1482 1483 1489 1493 1495 1501 1503 1508 1508 1516 1532 1541 1566 1574 1608 1618 1638 1643 1649 1655 1673 2101 3026 3031 3034 3041 3045 3048 3088 3094 3099 3101 3107 3107 3115 3139 3143 3144 3162 3168 3172 3179 3181 3189 3189 3192 3194 3200 3214 3231 3241
TS-2	-719 24 33 35 38 45 56 57 63 64 69 73 79 82 95 114 120 123 139 145 157 171 176 186 193 207 211 226 242 246 254 260 269 281 284 286 299 312 323 340 356 371 399 411

	413	416	442	449	458	465	495	507	517	520	522
	554	571	590	600	621	625	633	645	663	669	671
	680	691	697	698	711	732	774	774	792	818	819
	863	866	886	890	902	918	930	936	940	943	953
	975	976	984	988	1001	1009	1009	1012	1018	1024	1026
	1041	1052	1056	1061	1064	1066	1083	1104	1113	1135	1142
	1174	1183	1189	1203	1225	1227	1241	1250	1260	1315	1323
	1339	1340	1359	1361	1362	1371	1386	1389	1403	1415	1418
	1427	1430	1453	1467	1469	1476	1478	1481	1488	1489	1492
	1501	1503	1507	1508	1514	1532	1542	1565	1574	1604	1618
	1640	1647	1648	1661	1680	3026	3032	3034	3041	3047	3050
	3095	3099	3101	3107	3109	3115	3139	3144	3148	3161	3167
	3179	3181	3188	3188	3193	3194	3198	3212	3232	3241	
INT-2	29	34	43	47	52	55	63	64	65	73	77
	81	85	98	111	120	121	133	142	151	171	173
	186	193	203	206	215	228	233	251	256	259	279
	280	284	290	314	319	334	357	371	395	404	412
	413	432	449	458	460	488	500	513	518	520	527
	557	572	592	617	622	633	644	658	660	667	672
	680	691	698	711	730	736	773	790	819	821	861
	865	884	892	903	916	929	931	937	942	951	973
	975	983	986	1000	1007	1008	1011	1016	1024	1026	1032
	1051	1055	1061	1064	1066	1083	1103	1113	1135	1142	1165
	1182	1189	1201	1203	1223	1225	1241	1252	1256	1315	1321
	1339	1341	1360	1362	1370	1376	1389	1402	1408	1414	1418
	1427	1430	1457	1467	1474	1476	1479	1481	1489	1492	1495
	1502	1504	1508	1508	1514	1531	1543	1573	1586	1617	1629
	1645	1645	1662	1666	2086	3026	3033	3034	3041	3049	3051
	3095	3100	3100	3107	3110	3115	3138	3144	3155	3160	3166
	3178	3180	3187	3188	3194	3194	3197	3210	3234	3243	
TS-3	-78	22	29	31	35	48	50	55	58	61	68
	71	74	80	85	91	98	104	107	113	123	132
	141	146	147	181	192	197	220	241	244	265	275
	280	282	290	303	315	345	362	376	390	407	418
	427	441	448	452	455	459	497	507	514	515	529
	557	577	579	592	615	625	635	639	641	667	672
	681	690	699	722	731	733	752	773	786	817	827
	861	875	884	894	895	918	926	939	940	947	951
	972	975	984	995	1005	1009	1010	1012	1019	1025	1025
	1031	1050	1055	1064	1065	1067	1084	1103	1104	1136	1139
	1174	1180	1183	1199	1221	1226	1238	1250	1260	1276	1314
										1324	

	1328 1333 1351 1357 1360 1373 1385 1397 1402 1410 1417 1419 1421 1427 1444 1465 1471 1472 1475 1476 1478 1489 1491 1493 1501 1503 1506 1507 1515 1524 1541 1560 1565 1610 1623 1629 1637 1638 1657 1741 3030 3034 3037 3043 3046 3049 3094 3100 3102 3103 3105 3110 3135 3139 3149 3150 3163 3167 3177 3179 3188 3191 3192 3194 3199 3204 3212 3214 3216 3311
INT-3	19 31 35 39 46 51 55 61 63 67 75 78 87 89 96 100 103 105 108 123 129 134 142 161 171 187 192 210 221 231 236 247 269 270 273 288 298 317 341 355 372 391 397 420 434 439 445 446 454 468 497 512 519 523 534 550 581 589 600 613 616 619 635 641 670 671 681 689 698 726 730 738 771 781 817 823 861 883 885 888 898 905 923 931 934 941 946 951 974 981 984 991 1004 1008 1013 1014 1018 1026 1027 1034 1038 1053 1058 1060 1061 1068 1080 1100 1106 1136 1138 1171 1173 1175 1185 1185 1210 1224 1238 1240 1253 1261 1287 1310 1333 1335 1336 1340 1357 1373 1376 1386 1387 1399 1408 1412 1421 1426 1435 1445 1466 1469 1471 1474 1475 1477 1488 1488 1493 1501 1503 1507 1507 1511 1531 1534 1563 1567 1605 1619 1626 1640 1641 1661 1731 3027 3036 3039 3043 3046 3049 3061 3091 3097 3099 3103 3106 3109 3112 3130 3136 3137 3152 3163 3166 3173 3178 3185 3187 3191 3192 3194 3202 3210 3232
TS-4	-1352 14 25 32 33 46 59 61 67 72 76 81 84 89 90 101 118 121 125 134 140 148 151 163 172 185 201 214 214 234 234 257 267 279 284 297 303 313 321 346 362 376 384 398 411 438 446 449 455 463 472 499 514 519 540 550 559 578 594 596 618 628 630 645 654 670 688 690 697 699 727 735 765 771 790 817 818 846 866 882 894 896 898 904 922 925 943 952 973 975 982 983 987 1006 1012 1013 1016 1025 1025 1028 1042 1052 1061 1067 1069 1071 1083 1112 1115 1137 1142 1166 1171 1174 1186 1186 1202 1223 1228 1240 1249 1264 1285 1289 1317 1317 1338 1341 1361 1376 1379 1388 1393 1401 1414 1417 1419 1422 1427 1447 1456 1464 1470 1473 1473 1478 1490 1490 1493 1497 1501 1502 1506 1508 1509 1514 1545 1553 1575 1594 1611 1617 1622 1636 1656 1739 3026 3033 3034 3048 3049 3054 3090 3096 3098 3099 3107 3116 3120 3139 3149 3150 3152 3161 3165 3166 3176 3177 3182 3187 3193 3197 3209 3213 3218
INT-4	14 25 34 45 57 60 69 77 85 100 102

	112	128	138	147	156	174	180	192	201	225	231
	240	249	262	269	290	294	305	308	317	335	357
	365	398	400	413	435	447	455	459	481	510	513
	522	523	533	556	576	595	622	648	655	659	663
	676	680	695	702	730	734	763	773	799	816	817
	865	882	884	893	897	912	920	930	940	970	973
	974	979	983	1002	1007	1010	1011	1026	1038	1047	1053
	1069	1074	1076	1112	1125	1135	1136	1141	1165	1172	1180
	1218	1218	1238	1252	1255	1276	1303	1312	1329	1335	1357
	1372	1400	1406	1411	1417	1419	1421	1424	1457	1459	1473
	1478	1483	1489	1492	1497	1499	1504	1507	1513	1516	1546
	1578	1595	1618	1625	1632	1656	1670	2097	3024	3027	3031
	3051	3088	3089	3094	3096	3108	3121	3128	3145	3158	3162
	3166	3171	3176	3178	3185	3187	3189	3189	3193	3210	
INT-5	18	25	26	29	35	39	43	50	55	57	65
	70	75	80	86	92	100	111	112	120	126	131
	134	142	147	159	167	169	187	189	191	200	225
	242	247	248	258	272	277	293	293	314	320	328
	350	365	378	384	390	393	408	410	417	430	441
	446	455	468	487	504	512	517	518	522	536	555
	562	568	569	589	597	605	620	638	639	644	654
	656	679	682	696	699	707	712	730	733	735	754
	770	773	773	792	810	820	856	860	864	867	877
	884	888	891	896	912	919	936	943	950	974	975
	982	983	992	998	1002	1006	1007	1008	1010	1012	1018
	1022	1023	1024	1039	1051	1053	1053	1057	1065	1069	1080
	1082	1104	1106	1111	1127	1136	1144	1163	1167	1172	1181
	1182	1182	1186	1191	1202	1205	1227	1231	1242	1253	1255
	1278	1284	1298	1305	1315	1317	1319	1331	1335	1357	1360
	1363	1370	1384	1399	1408	1415	1418	1425	1433	1435	1458
	1468	1475	1477	1478	1479	1482	1488	1490	1493	1498	1504
	1505	1506	1515	1523	1533	1543	1566	1591	1595	1611	1613
	1619	1625	1631	1638	1641	1655	1743	2093	2973	3027	3035
	3038	3049	3053	3090	3097	3100	3102	3106	3130	3133	3151
	3153	3158	3158	3166	3167	3167	3170	3176	3177	3178	3180
	3183	3185	3187	3188	3191	3193	3194	3196	3205	3211	3220
TS-5	-365	13	22	24	29	34	39	44	47	55	57
	60	63	68	80	86	88	93	108	116	124	132
	138	140	159	162	163	177	190	194	195	204	210
	230	242	251	271	273	278	280	291	305	313	330
	344	355	371	379	392	394	403	418	420	438	440
	445	447	456	485	494	514	517	523	529	541	557

	563	577	593	599	609	623	632	635	638	639	651
	672	676	680	692	696	707	713	724	734	738	771
	772	778	781	785	812	818	853	859	862	878	884
	887	890	890	900	921	922	939	942	948	972	974
	976	983	994	997	1003	1005	1006	1006	1007	1010	1014
	1018	1021	1024	1024	1048	1051	1052	1059	1061	1069	1075
	1102	1106	1114	1121	1136	1144	1165	1167	1173	1180	1181
	1182	1186									
	1195	1197	1203	1228	1236	1248	1250	1258	1275	1284	1287
	1312										
	1316	1320	1323	1337	1351	1355	1356	1362	1372	1388	1402
	1410										
	1419	1422	1423	1430	1446	1455	1468	1475	1477	1478	1480
	1489										
	1490	1492	1494	1500	1505	1507	1508	1514	1520	1528	1540
	1567										
	1585	1592	1609	1613	1617	1623	1634	1636	1640	1660	1726
	1811										
	2897	3023	3030	3037	3048	3053	3085	3093	3094	3098	3106
	3106										
	3131	3151	3156	3158	3159	3165	3165	3168	3173	3177	3177
	3180										
	3181	3185	3186	3187	3189	3191	3194	3202	3205	3208	3214
	3215										
INT-6	19	23	26	35	40	40	45	54	57	65	67
	69	76	85	89	96	101	107	114	117	123	125
	135	140	149	156	165	181	187	193	202	208	220
	233	240	248	255	266	277	281	301	306	324	331
	337	351	379	397	404	415	417	443	446	450	453
	459	465	484	496	511	515	525	533	553	555	566
	592	602	608	609	621	634	637	641	644	660	680
	682	692	692	698	710	715	728	731	742	758	773
	773	788	809	817	819	848	853	856	872	881	884
	888	891	897	918	922	931	934	940	956	970	974
	978	984	986	990	991	999	1000	1004	1006	1007	1009
	1015										
	1021	1021	1023	1027	1050	1052	1053	1055	1058	1069	1083
	1101										
	1108	1112	1123	1135	1136	1161	1168	1173	1178	1179	1181
	1189	1191									
	1199	1207	1223	1226	1239	1243	1244	1255	1275	1277	1299
	1308										
	1316	1319	1330	1335	1345	1353	1363	1365	1373	1384	1402
	1412										
	1419	1420	1421	1425	1435	1460	1468	1474	1474	1479	1480
	1486										
	1488	1493	1497	1500	1504	1505	1506	1512	1522	1532	1548
	1566										
	1578	1600	1611	1613	1630	1635	1639	1641	1644	1665	1669
	1733										
	3025	3033	3035	3048	3074	3079	3087	3094	3096	3101	3105
	3111										
	3129	3153	3153	3153	3160	3161	3161	3165	3168	3173	3175
	3177										
	3178	3180	3184	3185	3187	3193	3197	3198	3203	3209	3209
	3216										
TS-6	-216	15	23	27	32	36	40	41	43	49	56
	62	62	69	79	85	88	92	100	105	115	120
	126	136	144	163	174	185	189	191	204	213	218
	231	234	252	254	259	282	286	298	306	319	326
	329	345	360	383	399	416	420	422	426	433	446

	455	460	466	482	498	507	515	536	538	553	564
	585	591	603	614	619	626	635	636	641	657	670
	678	682	693	702	712	720	721	734	749	759	769
	773	782	796	812	817	856	860	867	879	882	883
	886	889	900	908	921	938	943	948	950	957	964
	968	969	982	994	998	1000	1001	1005	1007	1010	1013
	1020	1023	1026	1027	1049	1053	1054	1055	1057	1069	1070
	1107	1118	1121	1127	1135	1146	1154	1172	1172	1180	1180
	1181	1181	1181	1181	1181	1181	1181	1181	1181	1181	1181
	1198	1207	1221	1229	1239	1241	1247	1260	1276	1299	1304
	1308	1319	1326	1331	1340	1342	1354	1357	1365	1365	1385
	1397	1403	1415	1419	1421	1425	1438	1449	1466	1471	1474
	1479	1481	1483	1484	1486	1488	1492	1497	1501	1506	1507
	1514	1521	1527	1531	1534	1565	1596	1608	1609	1617	1626
	1629	1635	1641	1654	1736	3025	3028	3034	3040	3049	3090
	3094	3099	3101	3106	3118	3127	3135	3154	3155	3157	3160
	3164	3165	3166	3167	3177	3178	3179	3179	3181	3187	3189
	3189	3189	3191	3193	3197	3208	3215	3220			
INT-7	21	24	26	35	41	47	58	58	65	78	91
	101	110	120	126	133	150	175	177	190	195	206
	213	222	228	236	244	252	253	264	266	271	288
	307	310	314	333	339	363	386	403	417	422	423
	430	440	444	454	483	494	501	515	523	528	536
	557	563	581	597	612	632	635	637	641	660	669
	680	693	694	704	720	724	727	734	742	762	767
	772	785	802	809	819	864	864	870	873	874	878
	883	900	902	921	936	941	945	952	963	963	968
	971	982	995	999	1002	1004	1004	1006	1011	1013	1019
	1025	1027	1029	1053	1055	1057	1059	1064	1074	1083	1098
	1109	1112	1128	1132	1135	1143	1169	1173	1178	1181	1182
	1187	1197	1205	1218	1224	1227	1236	1242	1249	1283	1299
	1311	1313	1315	1328	1337	1342	1350	1352	1358	1361	1367
	1380	1395	1402	1417	1419	1426	1471	1477	1478	1483	1487
	1488	1492	1492	1494	1502	1503	1506	1511	1523	1530	1537
	1538	1569	1604	1605	1616	1618	1628	1632	1641	1642	1652
	3021	3025	3032	3034	3086	3092	3095	3101	3115	3142	3153
	3155	3159	3160	3162	3164	3171	3173	3178	3179	3179	3182
	3186	3187	3187	3187	3193	3203	3205	3215	3231	3259	
TS-7	-250	26	31	38	44	53	57	62	67	76	82
	93	100	112	120	133	141	160	169	177	182	194
	202	209	223	230	237	249	260	263	264	279	283
	297	305	316	320	331	356	363	377	400	405	422
	426	430	437	445	455	457	491	497	510	524	531
	535	554	586	595	611	634	635	641	643	645	671

	676	685	688	698	710	721	727	732	748	763	765
	774	786	799	805	820	842	859	864	866	870	871
	880	886	901	916	930	940	942	946	952	960	965
	971	978	986	990	994	998	1000	1005	1008	1009	1010
	1024	1027	1053	1054	1056	1057	1058	1064	1071	1099	1103
	1120	1133	1134	1141	1172	1176	1178	1179	1180	1183	1195
	1199	1208	1214	1225	1239	1240	1253	1273	1295	1306	1312
	1317	1330	1335	1339	1346	1353	1355	1359	1372	1373	1401
	1408	1416	1419	1428	1476	1477	1480	1489	1490	1491	1493
	1496	1502	1504	1508	1509	1513	1524	1530	1535	1573	1602
	1611	1617	1618	1635	1640	1641	1643	1653	1710	3019	3023
	3027	3035	3082	3089	3095	3100	3136	3140	3152	3153	3156
	3159	3161	3164	3167	3172	3177	3178	3179	3180	3181	3181
	3192	3193	3193	3198	3203	3205	3218	3251			
INT-8	20	23	28	39	53	53	61	67	71	81	91
	105	110	117	123	136	161	167	176	187	191	200
	217	221	231	241	251	258	261	280	282	294	295
	309	317	327	345	356	365	390	402	411	421	422
	425	428	434	444	446	472	502	509	525	530	538
	564	569	584	603	618	632	635	639	641	651	678
	683	687	698	704	710	720	724	734	741	764	770
	776	790	796	812	820	855	864	868	870	872	880
	892	895	902	917	942	943	947	953	955	964	971
	975	977	997	998	998	1002	1004	1004	1010	1012	1025
	1027	1029	1040	1053	1056	1058	1058	1064	1078	1096	1100
	1109	1110	1110	1130	1137	1138	1154	1169	1173	1180	1181
	1182	1183	1188	1199	1204	1213	1223	1233	1241	1249	1266
	1298	1312	1315	1317	1323	1334	1352	1353	1360	1363	1370
	1386	1402	1402	1415	1419	1427	1430	1478	1480	1483	1485
	1491	1492	1494	1496	1505	1507	1509	1515	1524	1531	1536
	1538	1574	1612	1615	1618	1628	1640	1641	1643	1648	1667
	3022	3026	3033	3035	3085	3092	3097	3103	3126	3143	3155
	3155	3157	3163	3163	3164	3168	3172	3177	3178	3180	3180
	3180	3180	3187	3190	3191	3193	3209	3211	3215	3225	3238
TS-8	-267	6	23	35	41	50	53	57	62	69	75
	82	108	112	122	128	135	154	171	177	187	197
	206	210	218	231	242	246	249	251	262	269	273
	289	296	311	327	333	341	353	365	378	395	402
	415	420	422	428	442	448	458	486	499	518	524
	543	560	567	593	612	616	620	630	637	641	649
	677	682	683	692	701	717	721	726	755	763	766
	777	785	791	799	821	829	849	863	864	875	881
	889	890	899	906	923	940	944	947	952	956	964

	971 980 983 990 999 1002 1003 1007 1008 1010 1013 1023 1027 1033 1040 1052 1054 1055 1060 1061 1080 1100 1102 1109 1111 1129 1132 1134 1153 1167 1176 1179 1180 1181 1190 1195 1198 1211 1224 1234 1238 1242 1258 1300 1316 1319 1320 1322 1334 1337 1350 1354 1361 1363 1381 1387 1389 1402 1414 1417 1427 1478 1480 1486 1488 1490 1492 1493 1495 1501 1503 1509 1512 1524 1533 1536 1559 1574 1613 1617 1619 1626 1640 1641 1644 1647 1651 1690 3015 3023 3029 3033 3085 3088 3090 3093 3117 3122 3154 3154 3156 3162 3163 3168 3171 3171 3177 3179 3180 3182 3184 3190 3190 3196 3200 3200 3207 3211 3234 3236
TS-8a	-133 20 23 32 47 56 60 63 68 75 78 89 94 103 108 112 123 131 144 149 160 173 182 202 208 218 228 235 243 252 257 265 269 275 283 305 317 319 336 350 364 394 401 417 418 422 430 445 451 459 469 499 519 523 525 536 573 577 589 601 617 620 636 639 646 647 657 663 685 687 696 707 709 718 720 745 759 765 773 776 794 801 819 834 846 860 863 864 869 884 888 894 899 905 932 940 942 943 956 967 973 978 981 995 997 999 1000 1004 1008 1010 1023 1026 1037 1038 1049 1053 1062 1066 1071 1080 1091 1104 1108 1112 1125 1138 1145 1163 1166 1177 1181 1181 1186 1190 1191 1204 1208 1218 1226 1240 1241 1247 1296 1310 1315 1321 1323 1338 1341 1356 1358 1361 1366 1379 1383 1403 1410 1419 1429 1464 1471 1476 1479 1483 1487 1490 1494 1497 1502 1504 1507 1512 1520 1534 1556 1576 1596 1605 1609 1610 1616 1619 1636 1643 1644 1648 1806 3024 3027 3029 3038 3084 3089 3094 3097 3117 3126 3157 3157 3160 3162 3165 3166 3174 3175 3175 3177 3179 3184 3185 3188 3190 3195 3195 3199 3205 3212 3213 3216
INT-9	29 40 44 46 57 59 60 66 75 79 89 103 115 122 130 137 156 158 171 174 191 202 210 213 224 237 241 254 256 270 274 279 286 290 303 311 324 333 353 357 386 394 412 414 415 419 427 431 439 443 477 502 502 519 530 546 553 568 591 605 609 628 634 637 641 656 662 682 693 699 715 720 722 724 739 760 765 770 780 784 796 807 818 858 860 863 865 873 875 887 896 900 915 939 943 948 949 953 957 972 975 980 980 986 1001 1002 1004 1005 1009 1014 1024 1025 1028 1045 1053 1056 1057 1073 1084 1086 1103 1109 1113 1123 1132 1141 1142 1166 1179 1180 1181 1181 1189 1193 1198 1206

	1214 1227 1227 1244 1249 1303 1306 1311 1323 1323 1330 1341 1341 1358 1362 1369 1376 1394 1399 1403 1413 1420 1422 1428 1470 1478 1482 1484 1487 1490 1491 1493 1494 1504 1507 1513 1525 1536 1538 1551 1588 1600 1612 1618 1629 1638 1642 1643 1644 1692 1718 3025 3030 3033 3062 3087 3095 3097 3099 3115 3141 3156 3158 3158 3163 3166 3166 3169 3178 3179 3179 3182 3184 3186 3187 3190 3195 3201 3203 3216 3222 3225 3229
TS-9	-36 26 36 40 44 57 60 66 71 85 90 91 95 106 113 121 126 130 141 152 160 173 185 198 216 226 228 237 256 259 267 273 277 285 295 310 320 326 346 359 371 377 408 413 422 425 432 434 451 460 463 491 502 505 526 532 537 568 573 604 609 636 637 640 645 665 672 675 677 690 699 710 718 719 729 745 763 771 780 794 809 813 829 839 857 860 863 864 873 890 894 898 906 922 939 940 943 958 962 965 973 985 993 993 997 997 998 1003 1008 1009 1014 1025 1025 1027 1046 1053 1054 1059 1063 1076 1084 1106 1109 1112 1132 1133 1140 1164 1174 1178 1180 1181 1185 1193 1204 1206 1215 1218 1237 1239 1240 1256 1304 1310 1315 1318 1326 1332 1349 1356 1357 1359 1370 1376 1393 1400 1412 1418 1427 1475 1476 1480 1481 1481 1486 1489 1494 1495 1499 1500 1506 1517 1524 1533 1542 1583 1592 1597 1612 1614 1621 1630 1638 1641 1644 1661 1720 3025 3028 3030 3036 3084 3086 3093 3102 3125 3126 3156 3156 3157 3158 3164 3166 3168 3171 3177 3179 3179 3180 3183 3190 3190 3191 3194 3195 3196 3205 3208 3226
INT-10	26 33 34 39 47 55 56 62 69 76 82 89 96 99 104 108 118 126 133 148 153 158 178 206 210 216 223 231 239 242 260 269 271 279 290 307 315 334 360 376 399 407 413 418 419 430 445 448 459 502 526 529 538 540 548 551 563 572 591 608 621 634 637 644 648 665 672 679 685 697 704 712 717 718 742 758 764 765 775 779 788 807 843 851 860 861 868 875 881 884 889 894 907 939 940 942 957 960 962 971 976 982 992 993 996 996 1001 1007 1009 1017 1024 1026 1036 1042 1048 1053 1056 1067 1070 1091 1098 1104 1108 1124 1131 1135 1140 1170 1178 1180 1181 1186 1194 1200 1204 1204 1207 1232 1244 1247 1254 1303 1309 1312 1316 1322 1335 1344 1352 1358 1360 1360 1372 1379 1399 1404 1412 1423 1440 1477 1478 1480 1481 1486 1488 1492 1494 1496 1503 1506 1509 1526

	1531 1536 1583 1601 1609 1611 1615 1618 1624 1626 1639 1645 1647 1652 1972 3026 3035 3038 3041 3088 3095 3096 3098 3123 3129 3156 3156 3157 3159 3163 3166 3170 3173 3174 3177 3178 3180 3181 3181 3182 3186 3189 3190 3191 3195 3196 3206
TS-10	-235 23 29 34 39 48 50 54 59 63 70 76 80 89 99 107 113 118 125 138 152 162 168 196 199 216 222 227 229 236 240 257 262 262 282 304 305 313 331 350 356 389 395 415 418 420 438 444 447 465 492 509 528 534 538 546 555 571 584 597 600 602 621 635 636 637 645 660 681 689 691 698 709 712 715 745 759 763 766 767 780 805 823 829 849 856 858 860 861 871 880 882 898 906 932 937 939 945 948 953 960 969 986 987 991 992 994 1007 1008 1012 1024 1024 1038 1040 1043 1049 1053 1059 1062 1066 1103 1105 1111 1114 1120 1124 1164 1167 1168 1178 1180 1181 1186 1193 1203 1204 1215 1222 1232 1242 1246 1266 1305 1311 1312 1319 1327 1341 1351 1355 1358 1361 1367 1371 1393 1400 1402 1420 1425 1453 1477 1479 1481 1487 1488 1488 1491 1493 1501 1505 1507 1515 1522 1536 1550 1574 1578 1586 1592 1615 1619 1620 1629 1644 1645 1649 1962 3025 3031 3035 3038 3087 3094 3097 3098 3118 3121 3155 3155 3159 3160 3163 3164 3170 3174 3175 3176 3176 3179 3181 3184 3184 3185 3186 3195 3195 3196 3197 3202
INT-11	17 20 28 31 33 44 49 52 61 64 70 88 97 99 110 118 124 132 143 160 173 185 193 196 200 209 216 232 237 244 261 271 275 283 295 298 305 327 356 364 405 409 413 415 416 421 438 442 484 496 518 524 528 532 545 552 561 565 588 605 614 619 633 636 637 648 656 681 683 700 703 708 713 714 722 747 761 769 771 779 799 815 819 855 857 859 861 870 879 894 899 902 907 917 925 938 939 940 952 955 972 973 978 981 992 993 1004 1004 1007 1010 1020 1024 1026 1033 1035 1051 1053 1061 1062 1081 1082 1104 1107 1107 1124 1128 1135 1164 1166 1173 1181 1182 1187 1188 1200 1203 1206 1224 1224 1243 1253 1270 1292 1314 1317 1318 1331 1335 1354 1358 1359 1363 1370 1383 1391 1399 1415 1420 1422 1423 1461 1478 1480 1482 1486 1488 1493 1495 1502 1510 1512 1528 1528 1535 1538 1547 1579 1610 1617 1633 1635 1640 1645 1646 1649 1753 1932 3023 3028 3028 3034 3085 3091 3096 3097 3105 3130 3155 3156 3157 3163 3165 3165 3167 3174 3175 3175 3178

	3179 3182 3183 3185 3186 3187 3190 3190 3198 3207 3211
³Pre-CAT	26 44 72 75 97 105 143 159 169 193 205 211 240 266 269 283 324 358 377 388 418 444 479 501 521 553 570 640 679 690 805 853 878 900 941 959 968 972 1005 1010 1062 1076 1112 1137 1166 1172 1183 1226 1242 1309 1338 1347 1393 1404 1420 1422 1429 1480 1487 1488 1492 1502 1509 1512 1520 1582 1966 3023 3026 3035 3036 3088 3094 3095 3098 3116 3122 3177 3185 3193 3210
¹Pre-CAT	34 39 74 93 118 143 153 179 189 197 216 235 257 280 300 323 361 393 437 444 477 490 494 533 564 578 597 645 692 704 820 879 899 910 942 958 973 974 984 1006 1031 1062 1073 1110 1128 1177 1186 1222 1243 1311 1337 1360 1389 1402 1418 1423 1425 1483 1486 1489 1491 1501 1508 1516 1548 1575 2010 3027 3032 3035 3037 3090 3096 3096 3100 3117 3126 3179 3181 3194 3213
TS-1c	-183 29 33 35 50 64 75 82 95 102 130 137 164 174 185 201 228 241 257 271 283 311 333 350 384 387 439 443 458 480 507 528 550 569 588 630 637 656 685 701 824 898 900 915 932 939 944 966 974 995 1005 1028 1037 1063 1066 1073 1104 1129 1170 1185 1213 1221 1244 1310 1334 1364 1368 1386 1403 1413 1418 1422 1425 1452 1477 1481 1487 1490 1491 1500 1507 1511 1515 1557 1569 1579 2059 2283 3027 3030 3036 3037 3041 3090 3096 3098 3100 3102 3120 3129 3135 3180 3181 3197 3219
INT-1c	33 34 47 56 69 77 93 99 115 132 153 158 170 186 204 214 222 238 250 274 276 286 320 337 362 398 437 443 475 497 518 524 538 547 565 580 638 640 685 687 708 819 883 897 899 914 945 946 974 976 999 1006 1031 1035 1063 1063 1078 1106 1135 1174 1190 1224 1246 1315 1332 1355 1360 1364 1389 1390 1401 1415 1423 1424 1468 1478 1483 1486 1491 1492 1503 1512 1519 1559 1580 1626 2043 3027 3028 3035 3035 3045 3088 3095 3096 3101 3107 3122 3126 3139 3178 3181 3191 3223 3583
TS-2c	-132 35 43 44 48 57 62 69 78 84 86 109 119 127 146 156 161 172 178 188 201 206 215 234 241 250 260 281 288 332 346 354 384 418 434 449 454 470 502 518 520 560 569 626 627 640 659 678 682 694 701 805 872 896 918 930 940 947 948 977 995 1004 1007 1015 1028 1033 1035

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INT-2c	33 34 45 49 53 60 64 66 71 76 88 105 108 113 128 137 144 157 168 184 189 209 217 240 244 250 262 273 283 287 322 346 370 412 435 448 464 512 520 522 532 562 576 582 620 630 639 682 687 688 701 750 810 874 897 933 944 945 948 952 975 988 1002 1010 1020 1033 1036 1062 1065 1066 1082 1114 1141 1170 1198 1226 1244 1316 1342 1355 1362 1370 1391 1395 1403 1413 1417 1425 1434 1461 1467 1470 1475 1479 1481 1487 1491 1495 1498 1504 1505 1512 1552 1599 1608 1635 2067 3028 3034 3035 3041 3045 3046 3092 3097 3102 3103 3107 3110 3117 3143 3145 3147 3181 3207 3218 3242 3394 3528
INT-3c	35 38 40 47 54 56 68 78 90 91 109 125 141 147 159 169 186 211 216 240 241 260 271 280 282 320 345 369 412 435 449 470 520 522 527 535 560 578 619 624 640 678 685 688 698 810 855 897 929 936 940 944 974 980 992 1008 1021 1030 1032 1060 1061 1065 1081 1115 1142 1171 1203 1226 1245 1317 1330 1343 1345 1363 1386 1387 1403 1414 1417 1424 1435 1466 1466 1476 1477 1478 1488 1492 1495 1505 1506 1512 1552 1601 1641 1656 2057 3027 3034 3034 3044 3045 3045 3091 3096 3101 3102 3107 3107 3116 3139 3139 3144 3181 3205 3222 3239
TS-3c	-185 20 32 37 45 48 55 63 65 82 96 106 119 139 151 160 175 181 198 218 230 240 249 264 267 271 287 321 358 390 400 425 442 448 487 515 525 572 620 626 641 662 669 685 695 821 898 910 927 934 939 952 973 978 993 1013 1026 1027 1030 1059 1061 1067 1080 1110 1137 1170 1185 1225 1242 1311 1335 1336 1360 1378 1388 1402 1411 1415 1420 1426 1430 1465 1465 1474 1477 1480 1488 1493 1498 1503 1510 1512 1527 1562 1589 1645 2194 3024 3028 3035 3038 3043 3046 3089 3095 3098 3102 3103 3108 3126 3136 3140 3143 3174 3196 3206 3221