Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information to:

Deciphering the Chemoselectivity of Nickel-dependent Quercetin 2,4-Dioxygenase

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Contents:

1. System preparation using CHARMM version 39b2

1.1 Preparation of the PDB structure.

The dimeric structure from *Streptomyces sp. FLA* (PDB ID: 5FLJ, resolution: 1.82 Å) was used for preparing the system. The original structure contains 6 dimers of 12 chains, and the C and D chains were chosen because only c-chain contains both the dioxygen and quercetin substrates. Then the C and D chains were modified as below:

(1) Delete DMS molecule in chain D.

(2) Delete A-configuration of Cys58 and B-configuration of Gln82, His122, Arg156, Arg177, His183 in chain C; Delete A-configuration of Asn51 and B-configuration of Cys58, Gln 82, His122 in chain D.

(3) Exchange all the coordination of CD1 and CD2 of all Leu residues expect Leu151 of chain C.

(4) The orientations of His, Gln and Asn side chains were adjusted manually according to their local hydrogen-bonding network if necessary. The flipped residues are His178 in both chain C and D.

(5) All Lys, Arg, Cys and Tyr residues were chosen to be protonated at their side chains, and all Asp and Glu residues were chosen to be deprotonated at their side chains except Glu74, for which both protonated and deprotonated forms were considered. The protonation states of His residues were chosen as follows:

HSD (proton at ND1): 32, 67, 69, 113, 120, 181

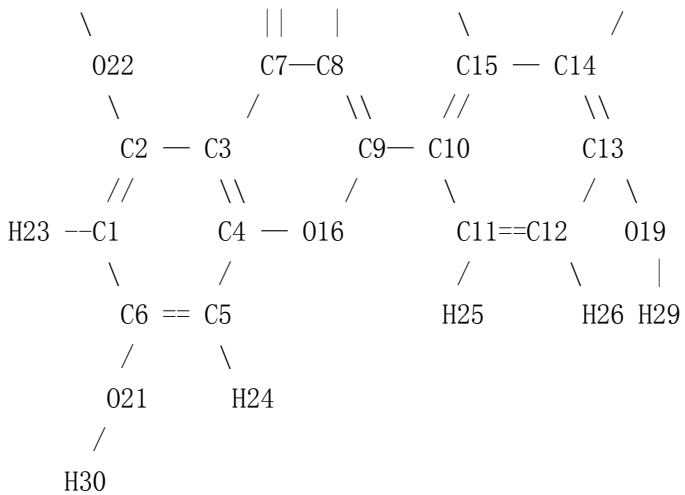
HSP (protons at both ND1 and NE2): 7, 95, 121, 178

1.2 CHARMM parameters.

Parameters for quercetin are listed below (CHELPG charges were calculated at the B3LYP/def2-SVP level)

```
RESI QUE -1.00          !                                                   H28
GROUP                   !                                                   /
ATOM C1   CA      -0.61 !         H31          O17  O20(-)  H27          O18
```

```
ATOM C2   CA       0.60 !
ATOM C3   CA      -0.53 !
ATOM C4   CA       0.48 !
ATOM C5   CA      -0.52 !
ATOM C6   CA       0.50 !
ATOM C7   CN1      0.52 !
ATOM C8   CA       0.23 !
ATOM C9   CA       0.09 !
ATOM C10  CA       0.20 !
ATOM C11  CA      -0.22 !
ATOM C12  CA      -0.24 !
ATOM C13  CA       0.27 !
ATOM C14  CA       0.17 !
ATOM C15  CA      -0.33 !
ATOM O16  OS      -0.30 !
ATOM O17  O       -0.58 !
ATOM O18  OH1     -0.59 !
ATOM O19  OH1     -0.57 !
ATOM O20  OC      -0.60 !
ATOM O21  OH1     -0.57 !
ATOM O22  OH1     -0.60 !
ATOM H23  HP       0.128 !
ATOM H24  HP       0.128 !
ATOM H25  HP       0.128 !
ATOM H26  HP       0.128 !
ATOM H27  HP       0.128 !
ATOM H28  H        0.39  !
ATOM H29  H        0.39  !
ATOM H30  H        0.39  !
ATOM H31  H        0.39  !
BOND C1 C2 C1 H23 C1 C6
BOND C2 C3 C2 O22
BOND C3 C7 C3 C4
BOND C4 C5 C4 O16
BOND C5 C6 C5 H24
BOND C6 O21
BOND C7 O17 C7 C8
BOND C8 C9 C8 O20
BOND C9 O16 C9 C10
BOND C10 C11 C10 C15
BOND C11 H25 C11 C12
BOND C12 H26 C12 C13
BOND C13 C14 C13 O19
BOND C14 C15 C14 O18
```



```
BOND C15 H27
BOND O18 H28
BOND O19 H29
BOND O21 H30
BOND O22 H31
```

1.3 System hydration.

The system with hydrogen atoms added was then hydrated using a water droplet composed of a 40 Å sphere of equilibrated TIP3 water molecules centered at nickel of chain C. All water molecules with their oxygen atoms within 2.5 Å of any protein non-hydrogen atom and cofactors and beyond 40 Å from Ni center were deleted. Then, the whole system was subjected to energy minimization [steepest descent (SD) for 1000 steps and adapted-basis Newton Raphson (ABNR) for 3000 steps] and to molecular dynamics (MD) simulations for 50 ps (20 ps heating to 300K) with a stochastic boundary potential[1] using the CHARMM force field as implemented in the CHARMM program.[2] During the minimization and simulation, all non-water heavy atoms and crystal water 189 were fixed. The water molecules were kept rigid during the heating period using the SHAKE constraint algorithm.[3] Finally, the solvated water molecules were minimized for 3000 steps using the ABNR method. The final structure then served as the starting structure for the next solvation. This procedure was repeated four times (five in total). The number of water molecules added every time is shown below:

Number of water molecules added				
Sol-1	Sol-2	Sol-3	Sol-4	Sol-5
6637	715	333	210	151

1.4 System neutralization.

To keep the total charge of the whole system to zero, 6 Na^+ counter-ions were added using the CHARMM program after the hydration. The system was then minimized (100 SD steps and 1000 ABNR steps) and equilibrated for 50ps at 300 K

(20ps heating and 30ps equilibration) with a stochastic boundary potential while the non-hydrogen atoms of the protein, cofactors, crystal water 189 and substrate were kept fixed. All Na^+ ions were located on the surface of the enzyme.

2. QM/MM Calculation

2.1 Optimized structures

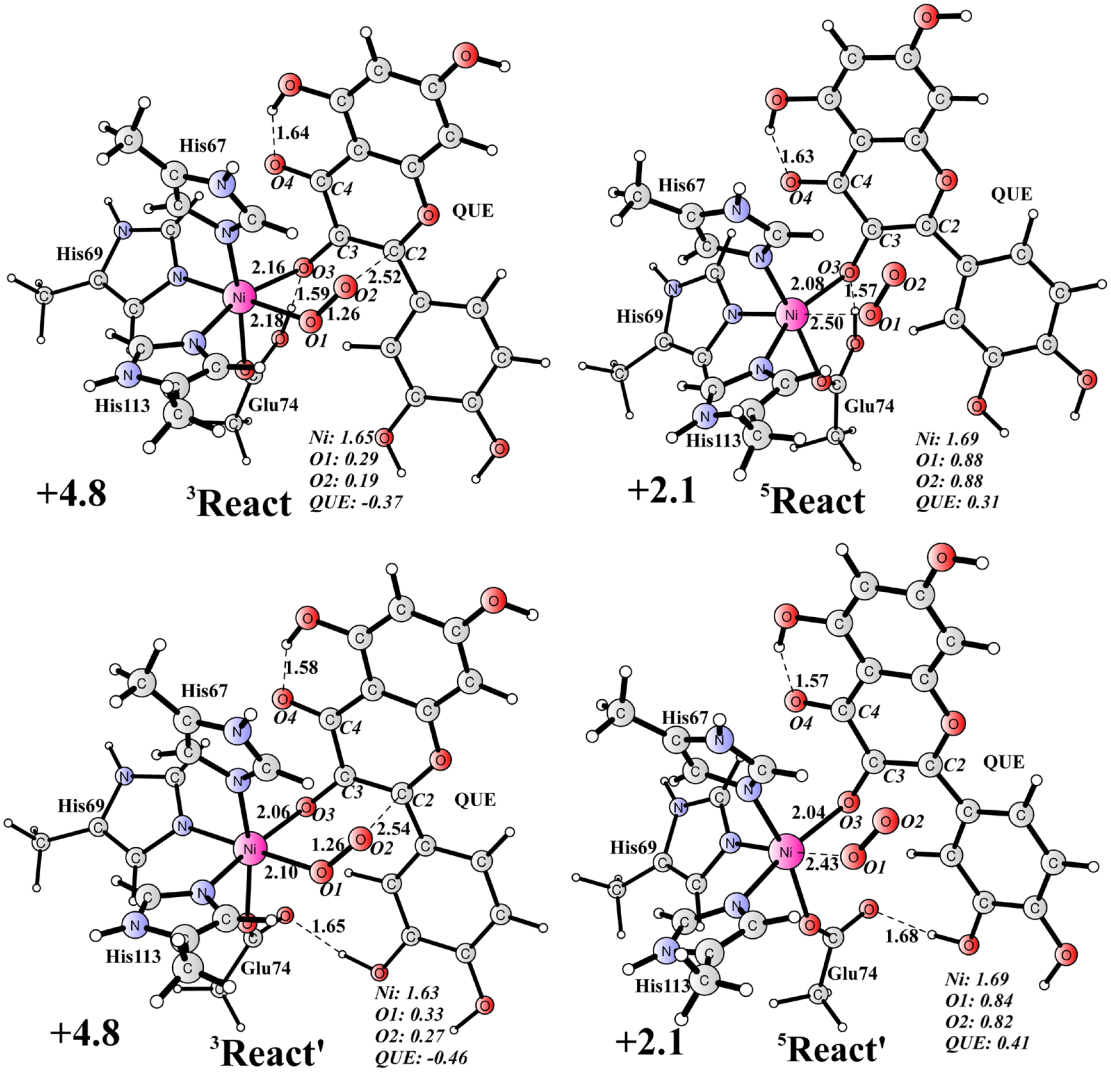


Figure S1. *Optimized structures of reactants. Distances are given in Å. Spin densities on selected atoms are indicated in italics. Superscripts indicate the multiplicity of the structures. Energies are given in kcal/mol relative to the singlet state.*

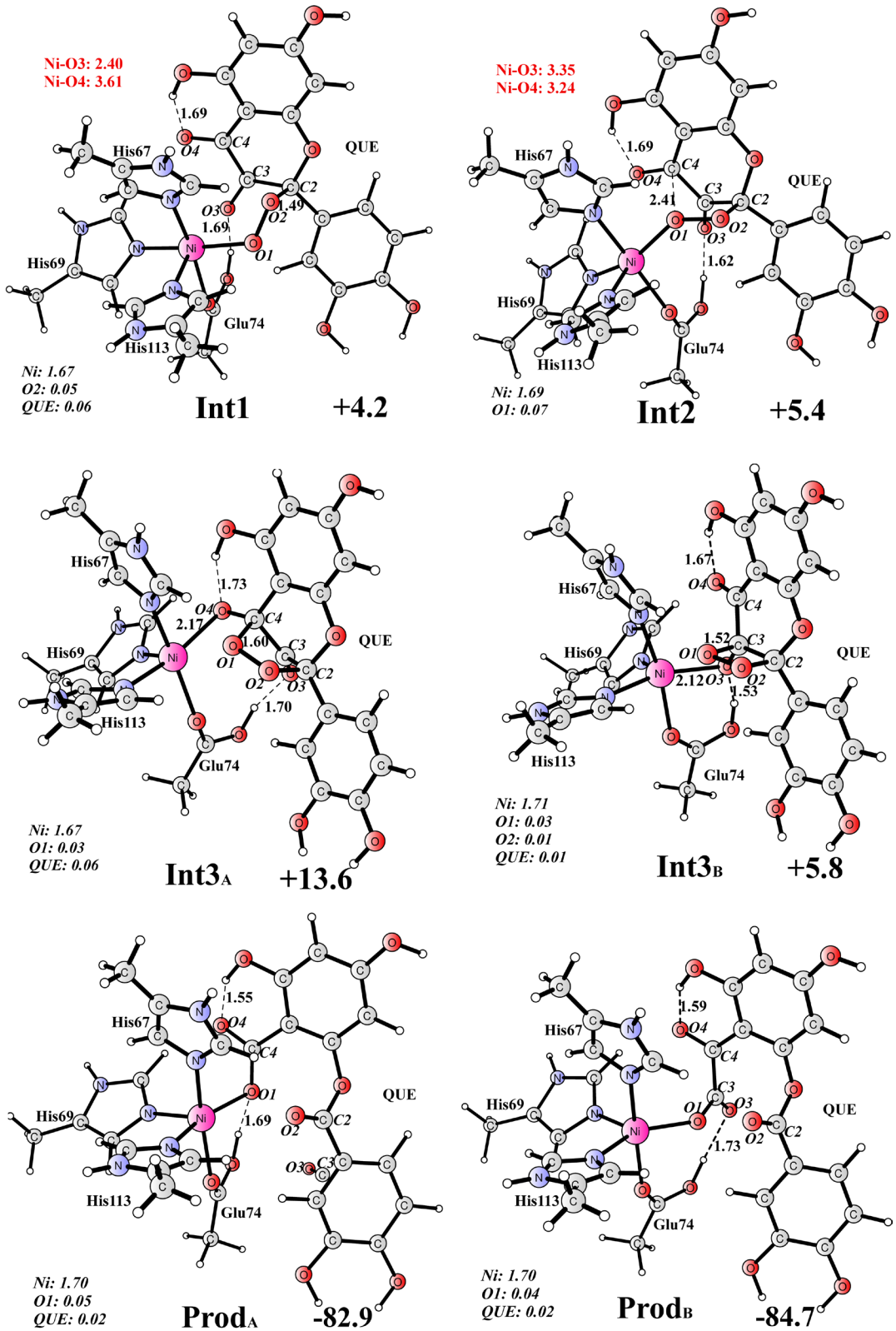


Figure S2. *Optimized structures of intermediates and products of* ***Model I*** *in 2, 4-quercetin dioxygenase. Distances are given in Å. Spin densities on selected atoms are indicated in italics. Energies are given in kcal/mol relative to the singlet state.*

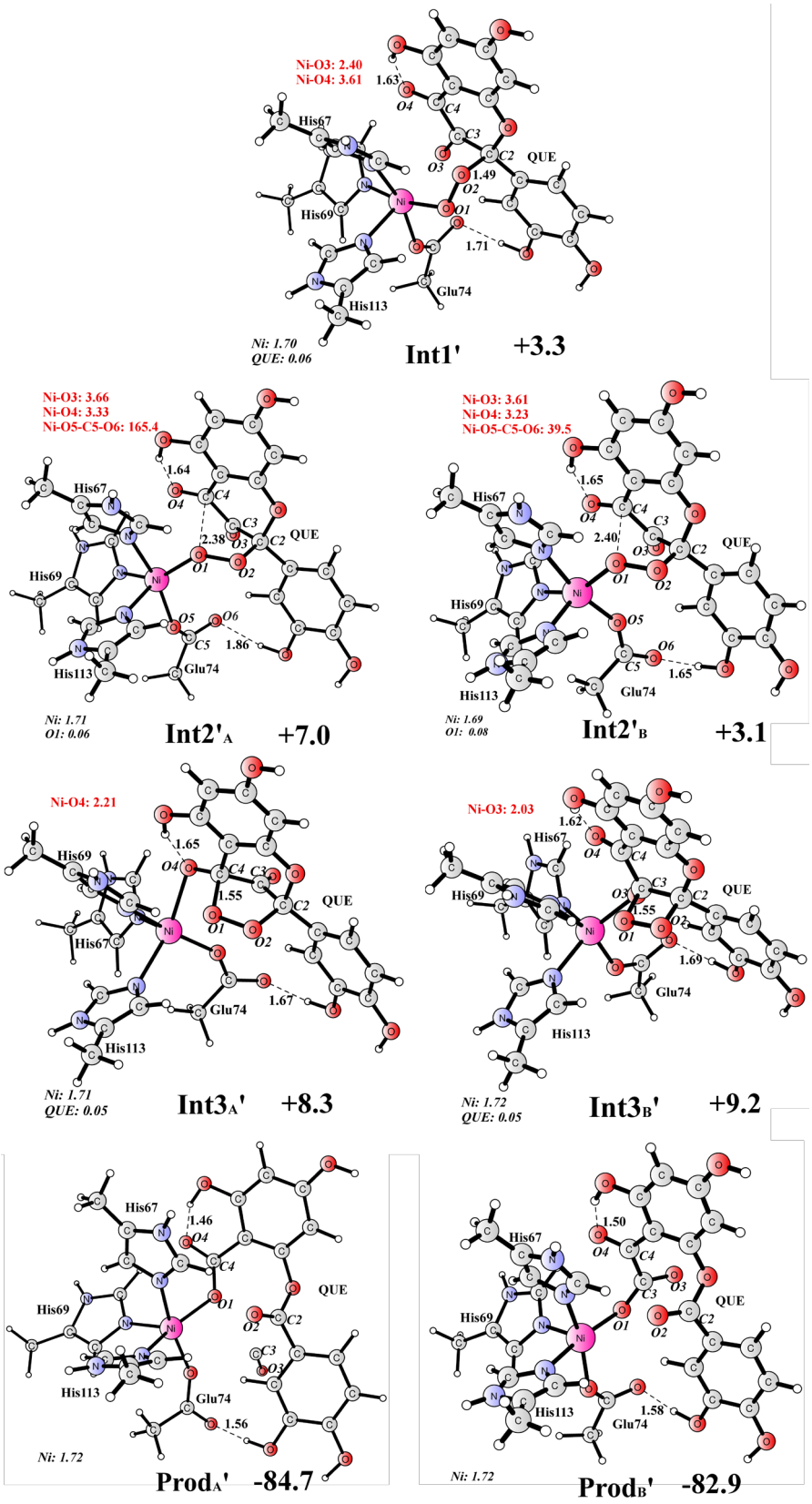


Figure S3. *Optimized structures of intermediates and products of* ***Model II*** *in 2, 4-quercetin dioxygenase. Distances are given in Å. Spin densities on selected atoms are indicated in italics. Energies are given in kcal/mol relative to the singlet state.*

2.2 Key geometric parameters of optimized structures

Table S1. *Distances (in Å) of optimized structures of transition states and intermediates of* ***Model I****.*

species	Ni-O1	Ni-O3	Ni-O4	O1-O2	O2-C2	O1-C4	O1-C3	O3-C3	O4-C4
React	2.37	2.11	3.46	1.23	2.61	3.87	3.02	1.30	1.25
^{3}React	2.18	2.16	3.5	1.26	2.59	3.84	3.01	1.29	1.25
^{5}React	2.50	2.08	3.43	1.23	2.64	3.90	3.03	1.31	1.25
TS1	2.1	2.29	3.51	1.31	1.97	3.57	2.69	1.26	1.24
Int1	2.06	2.4	3.61	1.4	1.49	3.61	2.72	1.23	1.24
Int2	2.02	3.35	3.24	1.46	1.4	2.41	2.19	1.22	1.24
$TS2_A$	2.24	3.76	2.23	1.47	1.43	1.71	2.28	1.21	1.29
$Int3_A$	2.31	3.82	2.17	1.48	1.43	1.6	2.27	1.21	1.31
$TS3_A$	2.22	3.83	2.17	1.92	1.32	1.39	2.3	1.18	1.33
$Prod_A$	2.15	—	3.32	—	1.21	1.29	—	1.13	1.25
$TS2_B$	2.16	2.87	3.38	1.46	1.44	—	1.67	1.26	1.24
$Int3_B$	2.51	2.12	3.38	1.46	1.45	—	1.52	1.31	1.24
$TS3_B$	2.07	3.29	3.09	1.81	1.36	—	1.48	1.27	1.24
$Prod_B$	1.97	3.75	3.62	—	1.2	—	1.23	1.27	1.25

Table S2. *Distances (in Å) of optimized structures of transition states and intermediates of* ***Model II****.*

Species	Ni-O1	Ni-O3	Ni-O4	O1-O2	O2-C2	O1-C4	O1-C3	O3-C3	O4-C4
React'	2.29	2.05	3.68	1.24	2.58	3.96	3.07	1.28	1.26
^{3}React'	2.1	2.06	3.69	1.26	2.54	3.91	3.00	1.27	1.25
^{5}React'	2.43	2.04	3.64	1.24	2.6	3.91	3.04	1.28	1.26
TS1'	2.08	2.17	3.71	1.31	1.99	3.66	2.71	1.25	1.25
Int1'	2.09	2.3	3.89	1.4	1.49	3.73	2.76	1.22	1.24
Int2$_{A}$'	2.01	3.66	3.33	1.45	1.4	2.38	2.32	1.2	1.24
Int2$_{B}$'	2.03	3.61	3.23	1.45	1.4	2.4	2.39	1.2	1.24
TS2$_{A}$'	2.19	3.86	2.43	1.46	1.42	1.79	2.35	1.2	1.28
Int3$_{A}$'	2.31	3.94	2.21	1.48	1.43	1.55	2.31	1.2	1.32
TS3$_{A}$'	2.23	3.89	2.2	1.9	1.31	1.38	2.35	1.17	1.34
Prod$_{A}$'	2.08	—	3.36	2.77	1.21	1.26	—	1.13	1.27
TS2$_{B}$'	2.21	2.37	3.46	1.46	1.41	2.61	2.00	1.23	1.24
Int3$_{B}$'	2.64	2.03	3.52	1.45	1.44	2.45	1.55	1.29	1.24
TS3$_{B}$'	2.13	2.23	3.47	1.96	1.33	2.42	1.45	1.29	1.24
Prod$_{B}$'	1.99	4.16	3.7	2.95	1.21	—	1.27	1.23	1.25

2.3 Calculate energies of Model I and Model II

Table S3. *QM/MM relative energies (in kcal/mol) calculated using two different density functionals(def2-TZVPP).*

Model I			**Model II**		
	B3LYP-D3	TPSSh-D3		B3LYP-D3	TPSSh-D3
React	0	0	**React'**	0	0
^{3}React	4.8	3.1	**^{3}React'**	4.8	2.0
TS1	7.0	4.4	**TS1'**	8.1	4.5
Int1	4.2	3.4	**Int1'**	3.3	2.7
Int2	5.4	5.5	**Int2$_A$'**	7.0	7.3
TS2$_A$	13.8	11.8	**Int2$_B$'**	3.1	3.6
Int3$_A$	13.6	11.6	**TS2$_A$'**	9.3	7.5
TS3$_A$	24.8	19.4	**Int3$_A$'**	8.3	6.1
Prod $_A$	-79.6	-70.9	**TS3$_A$'**	17.4	12.1
TS2$_B$	8.6	6.6	**Prod$_A$'**	-84.7	-75.7
Int3$_B$	5.8	3.1	**TS2$_B$'**	12.9	11.3
TS3$_B$	21.8	16.9	**Int3$_B$'**	9.2	6.7
Prod$_B$	-80.7	-74.9	**TS3$_B$'**	30.6	24.2
			Prod$_B$'	-82.9	-77.1

Table S4. *QM (B3LYP-D3/def2-SVP)/MM absolute energies (in hartree) calculated for* ***Model I*** *and* ***Model II.***

Model I			**Model II**		
	QM	QM/MM		QM	QM/MM
React	-3785.031172	-3975.674442	**React'**	-3784.549268	-3975.200839
3React	-3785.020901	-3975.666092	**3React'**	-3784.540507	-3975.193374
TS1	-3785.013678	-3975.661488	**TS1'**	-3784.531241	-3975.187489
Int1	-3785.01855	-3975.665639	**Int1'**	-3784.542379	-3975.194545
Int2	-3785.014629	-3975.66183	**$Int2_A$'**	-3784.540428	-3975.193532
$TS2_A$	-3785.002562	-3975.648431	**$Int2_B$'**	-3784.530159	-3975.186601
$Int3_A$	-3785.003864	-3975.648483	**$TS2_A$'**	-3784.533031	-3975.184851
$TS3_A$	-3784.986463	-3975.628956	**$Int3_A$'**	-3784.535551	-3975.186521
$Prod_A$	-3785.163986	-3975.79289	**$TS3_A$'**	-3784.521503	-3975.17102
$TS2_B$	-3785.012708	-3975.658852	**$Prod_A$'**	-3784.678662	-3975.326792
$Int3_B$	-3785.018022	-3975.664091	**$TS2_B$'**	-3784.521778	-3975.179259
$TS3_B$	-3784.989872	-3975.63637	**$Int3_B$'**	-3784.52808	-3975.184108
$Prod_B$	-3785.161029	-3975.796999	**$TS3_B$'**	-3784.496778	-3975.15114
			$Prod_B$'	-3784.679906	-3975.328463

2.4 Dihedral angles for Ni-O5-C5-O6 of Model I and Model II

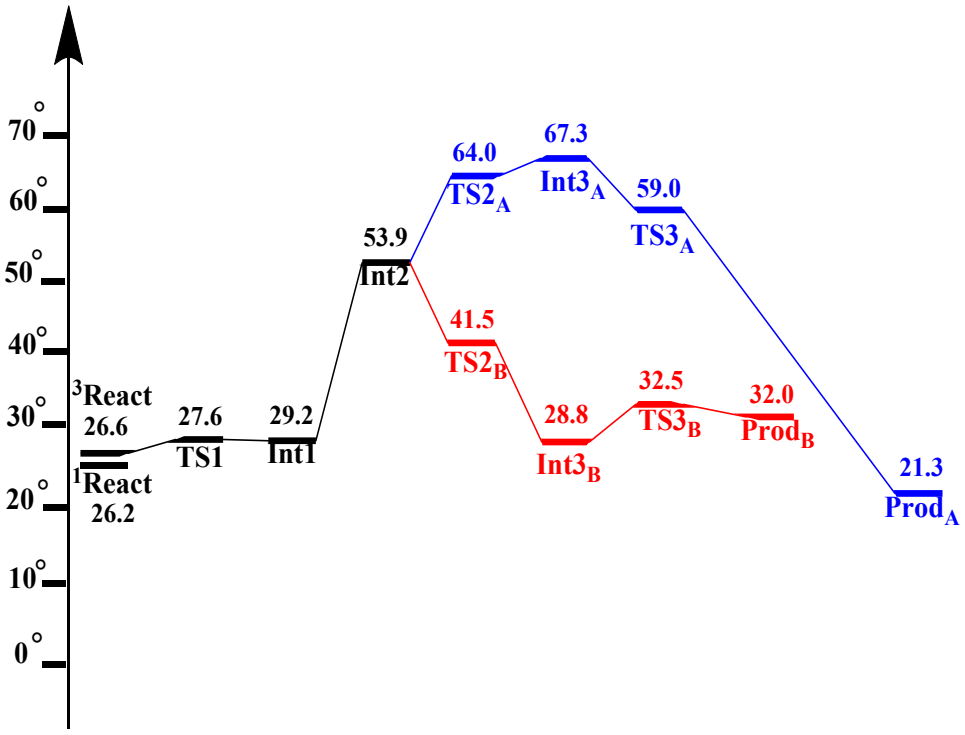


Figure S4. *Dihedral angles for Ni-O5-C5-O6 of Model I*

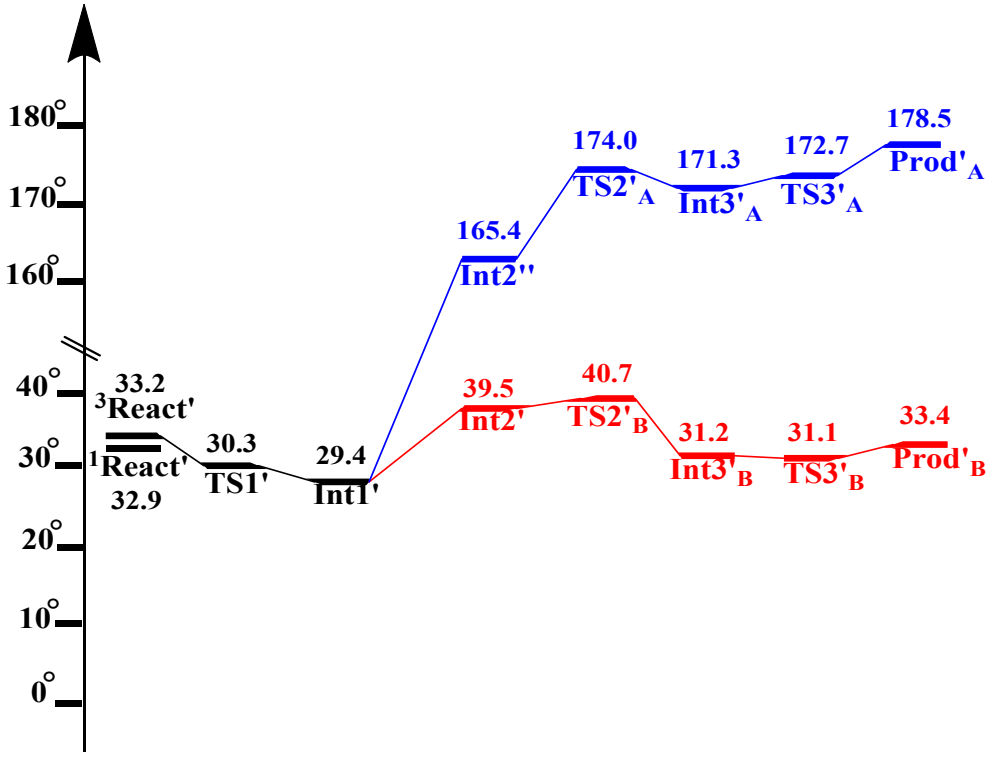


Figure S5. *Dihedral angles for Ni-O5-C5-O6 of Model II*

2.5 Potential energy profiles for Model I.

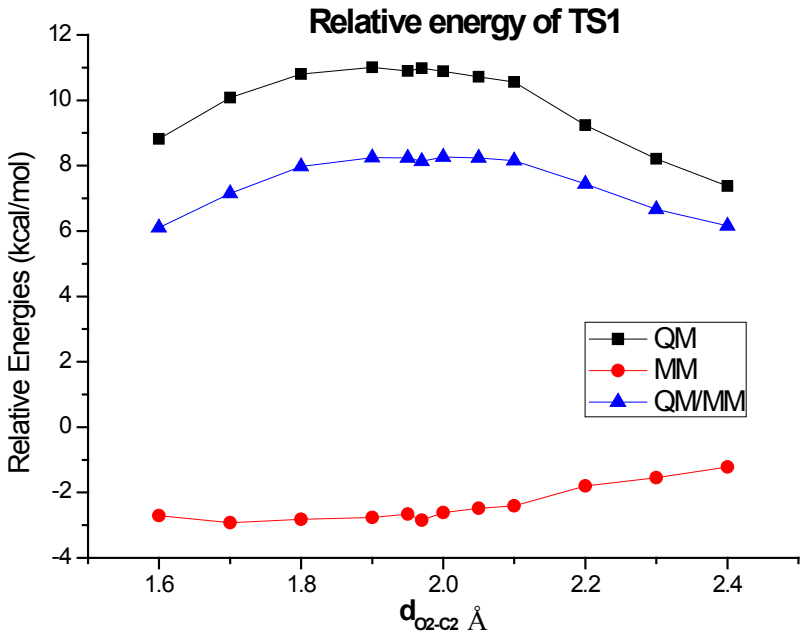


Figure S6. *QM, MM, and QM/MM relative energies as a function of d_{O2-C2} (in kcal/mol) for the first O2-C2 bond formation step.*

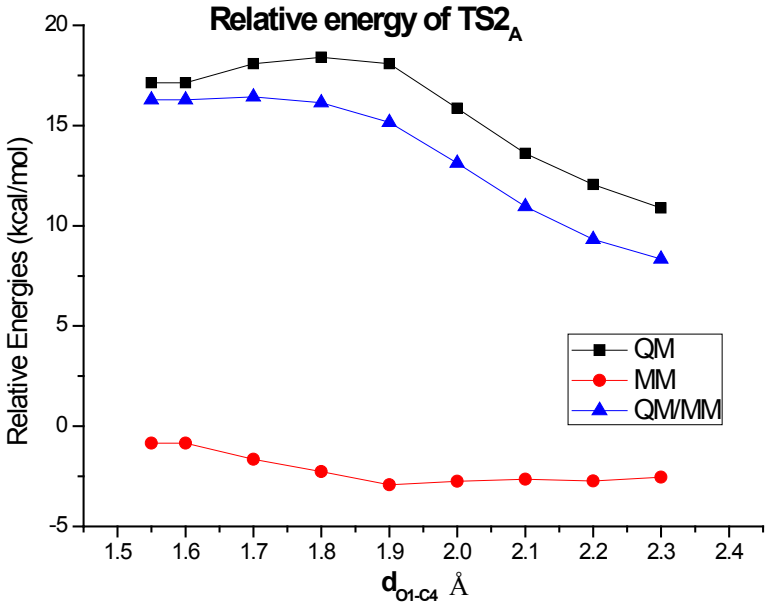


Figure S7. *QM, MM, and QM/MM relative energies as a function of d_{O1-C4} (in kcal/mol) for the nucleophilic attack step.*

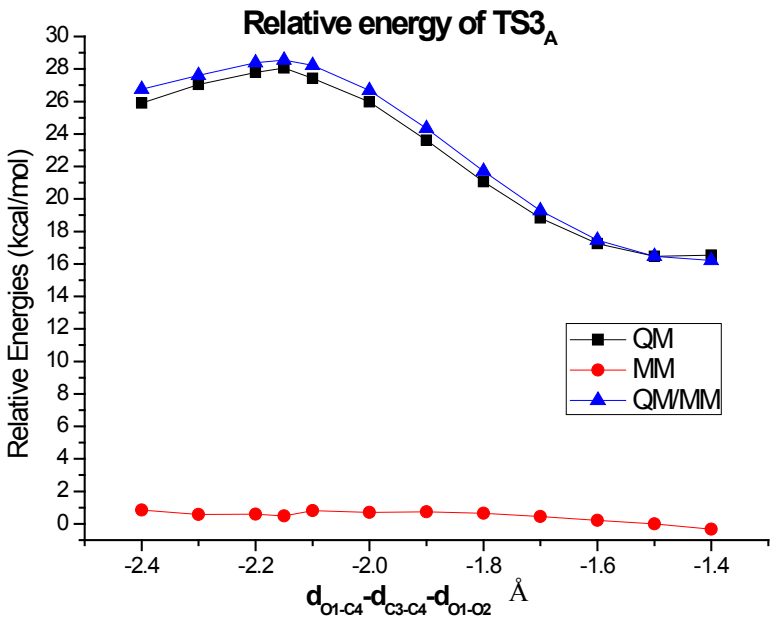


Figure S8. *QM, MM, and QM/MM relative energies as a function of* $d_{O1\text{-}C4}$ *-*$d_{C3\text{-}C4}$ *-*$d_{O1\text{-}O2}$ *(in kcal/mol) for the CO releasing step.*

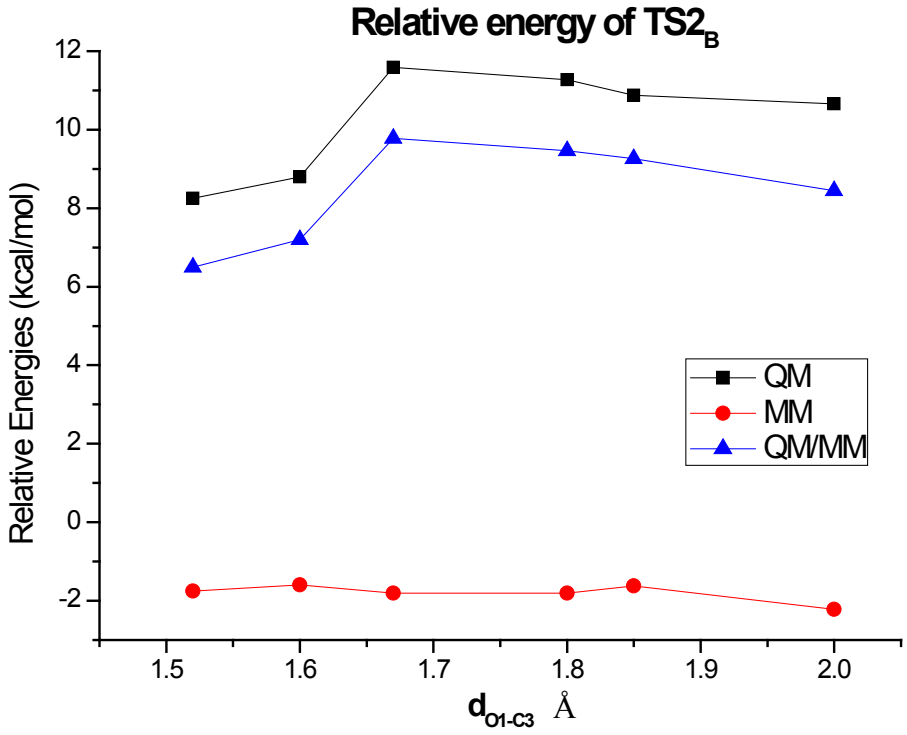


Figure S9. *QM, MM, and QM/MM relative energies as a function of* $d_{O1\text{-}C4}$*3(in kcal/mol) for the nucleophilic attack step.*

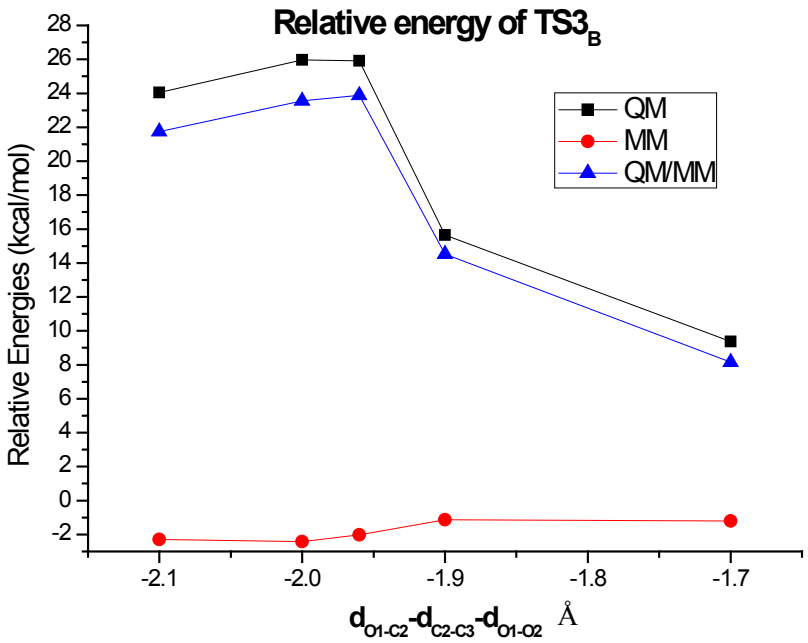


Figure S10. *QM, MM, and QM/MM relative energies as a function of* $d_{O1\text{-}C2}$ *-*$d_{C2\text{-}C3}$ *-*$d_{O1\text{-}O2}$ *(in kcal/mol) for the 2,3-dioxygenolytic cleavage of quercetin step.*

2.6 Reaction in the singlet state

Here, the relative energies of all intermediates in the singlet states are shown for both **Model I** and **Model II**. As shown in Table S4, the singlet energies are all higher than those for the triplet.

Table S5. *QM (B3LYP-D3/def2-SVP)/MM relative energies (in kcal/mol) calculated for* ***Model I*** *and* ***Model II.***

Model I			**Model II**		
	triplet	singlet(closed shell)		triplet	singlet(closed shell)
React	5.2	29.5	**React'**	4.7	27.2
Int1	5.5	18.5	**Int1'**	3.9	26.7
Int2	7.9	35.9	**Int2$_A$'**	4.6	32.7
Int3$_A$	16.3	43.1	**Int2$_B$'**	8.9	24.9
Prod $_A$	-74.3	-52.0	**Int3$_A$'**	9.0	[a]¬
Int3$_B$	6.5	34.4	**Prod$_A$'**	-79.0	-54.4
Prod$_B$	-76.9	-62.9	**Int3$_B$'**	10.5	36.5
			Prod$_B$'	-80.1	-59.3

[a]¬ Not stable, optimization leads to **Int2$_A$'.**

Reference

(1) Brooks, C. L.; Karplus, M. Deformable stochastic boundaries in molecular dynamics. *J. Chem. Phys.* **1983**, *79*, 6312-6325.

(2) Brooks, B. R.; Brooks, C. L., 3rd; Mackerell, A. D., Jr.; Nilsson, L.; Petrella, R. J.; Roux, B.; Won, Y.; Archontis, G.; Bartels, C.; Boresch, S.; Caflisch, A.; Caves, L.; Cui, Q.; Dinner, A. R.; Feig, M.; Fischer, S.; Gao, J.; Hodoscek, M.; Im, W.; Kuczera, K.; Lazaridis, T.; Ma, J.; Ovchinnikov, V.; Paci, E.; Pastor, R. W.; Post, C. B.; Pu, J. Z.; Schaefer, M.; Tidor, B.; Venable, R. M.; Woodcock, H. L.; Wu, X.; Yang, W.; York, D. M.; Karplus, M. CHARMM: the biomolecular simulation program. *J. Comput. Chem.* **2009**, *30*, 1545-1614.

(3) Ryckaert, J.-P.; Ciccotti, G.; Berendsen, H. J. C. Numerical integration of the Cartesian Equations of Motion of a System with Constraints: Molecular Dynamics of n-Alkanes. *J. Comput. Chem.* **1977**, *23*, 327-341.

3. Cartesian Coordinates for QM regions

Model I

React

C	-3.486416	-3.151650	3.202264
H	-4.287207	-3.108039	2.450626
H	-3.941528	-2.923066	4.178840
N	-1.518211	-1.610795	3.747893
H	-1.469816	-1.803776	4.755578
C	-2.435026	-2.146526	2.862578
C	-0.712527	-0.767096	3.063010
H	0.099070	-0.211146	3.521562
N	-1.057810	-0.728877	1.785789
C	-2.129349	-1.580828	1.648282
H	-2.612501	-1.751812	0.691957
C	-3.091859	-2.315326	-4.137328
H	-2.178685	-2.624521	-4.669443
H	-3.755755	-1.787044	-4.839087
N	-3.517955	-0.609854	-2.283148
H	-4.486726	-0.416358	-2.559190
C	-2.676796	-1.450212	-2.988279
C	-2.816326	-0.027188	-1.283083
H	-3.203921	0.682565	-0.553759
N	-1.562832	-0.459086	-1.304738
C	-1.453345	-1.324651	-2.373100
H	-0.501971	-1.762145	-2.659528
C	1.481865	0.984062	-3.952288
H	1.252031	1.860303	-4.567713
H	0.981873	0.110352	-4.399046
C	0.928395	1.170855	-2.569965
O	1.137873	0.351513	-1.668375
O	0.216397	2.259853	-2.387311
H	-0.100029	2.295346	-1.428137
C	3.266131	-4.369908	1.562074
H	4.106474	-3.735016	1.878194
H	3.682722	-5.149584	0.904823
N	1.265326	-4.078631	0.010372
H	1.190588	-5.057508	-0.295193
C	2.236284	-3.558379	0.845975
C	0.474721	-3.070837	-0.410793

H	-0.372041	-3.217701	-1.074981
N	0.887390	-1.921380	0.095537
C	1.984428	-2.209038	0.876973
H	2.522175	-1.440797	1.422218
Ni	-0.058216	-0.045180	0.052001
O	1.658527	0.621886	1.422073
O	1.484202	1.296768	2.438082
C	-2.769820	2.856339	5.589398
C	-2.761060	2.374475	4.288566
C	-1.767966	2.819438	3.366879
C	-0.798705	3.734079	3.817949
C	-0.812932	4.262668	5.108773
C	-1.808160	3.810017	5.997771
C	-1.755994	2.351406	2.004928
C	-0.548491	2.670710	1.214557
C	0.396033	3.564152	1.747898
C	1.640420	4.036277	1.126774
C	2.397403	5.066955	1.733656
C	3.594860	5.490389	1.164806
C	4.081970	4.936710	-0.027725
C	3.332871	3.912768	-0.646228
C	2.152617	3.464445	-0.057348
O	0.196964	4.117934	2.978718
O	-2.680622	1.655988	1.529360
O	3.715649	3.338474	-1.821782
O	5.245653	5.417359	-0.528547
O	-0.400766	2.036526	0.087579
O	-1.901239	4.228710	7.261634
O	-3.667419	1.472728	3.881826
H	-3.534033	2.523969	6.293353
H	-0.048200	4.972964	5.426231
H	2.052307	5.522109	2.661839
H	4.203626	6.262421	1.637993
H	1.653141	2.626874	-0.520396
H	4.656239	3.491270	-2.028230
H	5.599134	4.885617	-1.265327
H	-1.281396	4.979380	7.470714
H	-3.521602	1.348992	2.894968
h	-3.108895	-4.171503	3.276052
h	-3.601726	-3.215280	-3.793549
h	2.556408	0.801857	-3.937306
h	2.858338	-4.912478	2.414945

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^{3}React

C	-3.494614	-3.161750	3.210519
H	-4.300298	-3.118857	2.464155
H	-3.944898	-2.937076	4.190494
N	-1.526891	-1.617764	3.746492
H	-1.464916	-1.818835	4.751389
C	-2.449946	-2.151708	2.865836
C	-0.727115	-0.770363	3.058587
H	0.086440	-0.206526	3.503271
N	-1.083337	-0.727821	1.784584
C	-2.153990	-1.580677	1.651256
H	-2.640799	-1.752694	0.696646
C	-3.081638	-2.313682	-4.135502
H	-2.168115	-2.624729	-4.665746
H	-3.743642	-1.785086	-4.838879
N	-3.511663	-0.608796	-2.283652
H	-4.480975	-0.419485	-2.560455
C	-2.667701	-1.447766	-2.986871
C	-2.810155	-0.020694	-1.286125
H	-3.202228	0.689086	-0.559768
N	-1.555036	-0.446734	-1.306465
C	-1.444053	-1.314659	-2.372862
H	-0.492102	-1.750276	-2.660713
C	1.494778	0.986585	-3.965424
H	1.266244	1.859883	-4.585636
H	0.994460	0.111595	-4.408802
C	0.944055	1.182060	-2.583925
O	1.149912	0.373794	-1.675518
O	0.235357	2.279179	-2.412561
H	-0.081909	2.321787	-1.461803
C	3.269448	-4.357531	1.570478
H	4.107221	-3.722427	1.892825
H	3.692208	-5.132167	0.911038
N	1.272638	-4.072331	0.013968
H	1.203374	-5.051877	-0.290211
C	2.239352	-3.546875	0.852515
C	0.478662	-3.067955	-0.409741
H	-0.365942	-3.218255	-1.076033
N	0.885738	-1.917399	0.097325
C	1.981698	-2.197949	0.882709
H	2.507403	-1.418501	1.425429
Ni	-0.040192	-0.036990	0.071329
O	1.588589	0.641610	1.358589

O	1.339384	1.327950	2.380422
C	-2.749805	2.863648	5.595212
C	-2.739181	2.381809	4.294185
C	-1.746275	2.828478	3.373711
C	-0.773664	3.738841	3.826679
C	-0.788858	4.266722	5.115495
C	-1.789200	3.816442	6.003597
C	-1.741441	2.369486	2.011658
C	-0.535373	2.697403	1.211300
C	0.422283	3.590375	1.754074
C	1.656637	4.061590	1.127490
C	2.421291	5.087453	1.734461
C	3.618216	5.503003	1.162314
C	4.093823	4.948494	-0.035929
C	3.335761	3.930455	-0.655382
C	2.157904	3.487253	-0.061345
O	0.224639	4.126087	2.986597
O	-2.666849	1.685691	1.528293
O	3.710022	3.359508	-1.834308
O	5.256453	5.421697	-0.540107
O	-0.406923	2.095835	0.081899
O	-1.884039	4.237894	7.264893
O	-3.644519	1.480614	3.887855
H	-3.514875	2.531681	6.298178
H	-0.023502	4.975562	5.434236
H	2.081147	5.540113	2.665879
H	4.236018	6.268555	1.634328
H	1.655941	2.647401	-0.517520
H	4.654814	3.492131	-2.036006
H	5.600642	4.893132	-1.284161
H	-1.265338	4.990165	7.473276
H	-3.506368	1.359582	2.901108
h	-3.113581	-4.180497	3.281477
h	-3.593955	-3.212156	-3.791493
h	2.569771	0.807259	-3.948142
h	2.860386	-4.905898	2.419022

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^{5}React

C	-3.479351	-3.160925	3.207774
H	-4.282097	-3.114117	2.458384
H	-3.931126	-2.929071	4.185012
N	-1.515193	-1.608323	3.744722
H	-1.472439	-1.787427	4.755470
C	-2.424539	-2.160884	2.862882
C	-0.704983	-0.775841	3.050443
H	0.099092	-0.205511	3.504579
N	-1.040885	-0.761764	1.769725
C	-2.108482	-1.619570	1.640699
H	-2.582183	-1.812080	0.683887
C	-3.133588	-2.342261	-4.145602
H	-2.222577	-2.644540	-4.685388
H	-3.806399	-1.814936	-4.839559
N	-3.552898	-0.644567	-2.285307
H	-4.519948	-0.444422	-2.563797
C	-2.714035	-1.482301	-2.996078
C	-2.850481	-0.073401	-1.280121
H	-3.235567	0.631432	-0.545014
N	-1.599146	-0.511104	-1.304512
C	-1.490900	-1.367151	-2.379594
H	-0.541442	-1.806183	-2.669651
C	1.469388	0.976143	-3.938717
H	1.246306	1.861348	-4.543712
H	0.967023	0.109234	-4.394956
C	0.919861	1.153652	-2.553971
O	1.092320	0.300260	-1.675053
O	0.257942	2.266352	-2.340159
H	-0.041534	2.289355	-1.373108
C	3.263686	-4.385347	1.565619
H	4.104369	-3.749852	1.879646
H	3.682289	-5.167619	0.912606
N	1.269091	-4.107174	0.002973
H	1.197525	-5.087445	-0.299424
C	2.233570	-3.580061	0.841503
C	0.476865	-3.104179	-0.426420
H	-0.365472	-3.257881	-1.094791
N	0.880505	-1.950671	0.077822
C	1.975411	-2.231579	0.866359
H	2.507465	-1.460716	1.412489
Ni	-0.090883	-0.095891	0.018052
O	1.764026	0.630019	1.532862

O	1.606119	1.318906	2.533218
C	-2.783457	2.866660	5.577873
C	-2.759854	2.378595	4.279754
C	-1.754533	2.816620	3.367602
C	-0.793692	3.738765	3.823271
C	-0.822336	4.271255	5.112864
C	-1.824195	3.819835	5.993790
C	-1.718515	2.327199	2.013202
C	-0.495183	2.632231	1.247123
C	0.421495	3.554984	1.769056
C	1.669033	4.023523	1.150993
C	2.402845	5.085442	1.730453
C	3.597987	5.510195	1.156722
C	4.101907	4.930891	-0.016153
C	3.378674	3.871199	-0.603189
C	2.203509	3.419972	-0.007080
O	0.203924	4.126541	2.990537
O	-2.637405	1.628265	1.529087
O	3.780866	3.255924	-1.750494
O	5.257341	5.422286	-0.528232
O	-0.301942	1.971472	0.137784
O	-1.925555	4.238808	7.257400
O	-3.662146	1.475040	3.866855
H	-3.555500	2.538043	6.274943
H	-0.061701	4.984053	5.434155
H	2.041717	5.563287	2.641097
H	4.190368	6.307259	1.608356
H	1.727103	2.554136	-0.443126
H	4.704082	3.460088	-1.987985
H	5.621216	4.879429	-1.251355
H	-1.302728	4.985545	7.470840
H	-3.501911	1.342787	2.883161
h	-3.105465	-4.182068	3.282226
h	-3.634851	-3.245010	-3.796537
h	2.543314	0.790326	-3.923861
h	2.854807	-4.925288	2.419638

TS1

C	-3.530036	-3.185566	3.232552
H	-4.341795	-3.156521	2.492288
H	-3.976464	-2.969680	4.216420
N	-1.571765	-1.618394	3.742081
H	-1.485681	-1.827849	4.743328
C	-2.509096	-2.155787	2.877657
C	-0.803332	-0.748860	3.045712
H	0.011243	-0.171244	3.471050
N	-1.194589	-0.695967	1.782472
C	-2.253494	-1.564876	1.663540
H	-2.758015	-1.735777	0.717617
C	-3.100635	-2.318290	-4.126477
H	-2.182485	-2.625711	-4.650933
H	-3.763180	-1.797479	-4.835203
N	-3.551953	-0.611316	-2.282308
H	-4.520386	-0.426401	-2.566398
C	-2.698218	-1.444894	-2.979449
C	-2.859275	-0.016571	-1.282640
H	-3.264185	0.693019	-0.563370
N	-1.601091	-0.432465	-1.294520
C	-1.479047	-1.300905	-2.358951
H	-0.523073	-1.731513	-2.640901
C	1.504310	0.943143	-3.927703
H	1.300042	1.813763	-4.560876
H	0.983882	0.074482	-4.360228
C	0.950382	1.177845	-2.554060
O	1.100445	0.374583	-1.633383
O	0.295197	2.313574	-2.407071
H	-0.039368	2.380728	-1.472057
C	3.269336	-4.276638	1.591525
H	4.098045	-3.636621	1.927654
H	3.704355	-5.030581	0.915585
N	1.306714	-4.011984	0.004134
H	1.275979	-4.988566	-0.314636
C	2.224997	-3.470704	0.886549
C	0.475439	-3.033225	-0.407128
H	-0.344414	-3.201734	-1.099386
N	0.813603	-1.883958	0.149857
C	1.898383	-2.135853	0.958280
H	2.353722	-1.341251	1.543908
Ni	-0.107680	-0.026484	0.115427
O	1.327571	0.886533	1.347817

O	0.855047	1.614633	2.328574
C	-2.786031	2.877131	5.643134
C	-2.789978	2.404154	4.337785
C	-1.790129	2.830473	3.416153
C	-0.775253	3.691721	3.879863
C	-0.778359	4.214753	5.165087
C	-1.799864	3.799624	6.052579
C	-1.823754	2.402450	2.046638
C	-0.620765	2.734613	1.216038
C	0.467088	3.481264	1.839211
C	1.662669	4.000940	1.166153
C	2.400762	5.063001	1.738960
C	3.579692	5.494435	1.141144
C	4.055312	4.919278	-0.047980
C	3.315597	3.871165	-0.634723
C	2.157673	3.407081	-0.012172
O	0.256706	4.046016	3.052613
O	-2.766256	1.763341	1.550694
O	3.688398	3.286961	-1.808228
O	5.207372	5.401019	-0.571483
O	-0.535795	2.224333	0.071855
O	-1.881796	4.227428	7.310193
O	-3.723213	1.532163	3.932598
H	-3.561614	2.564507	6.343213
H	0.014931	4.888973	5.491202
H	2.058595	5.531535	2.662192
H	4.180739	6.290314	1.583656
H	1.685636	2.530799	-0.429342
H	4.641411	3.382363	-1.990316
H	5.529328	4.882958	-1.332784
H	-1.254108	4.974876	7.512773
H	-3.604989	1.413050	2.946983
h	-3.129962	-4.197403	3.297312
h	-3.608120	-3.219468	-3.782380
h	2.574016	0.734893	-3.907021
h	2.867469	-4.852569	2.425115

Int1

C	-3.510687	-3.154625	3.233249
H	-4.325010	-3.126658	2.495626
H	-3.956115	-2.941007	4.217945
N	-1.538206	-1.591587	3.722060
H	-1.433489	-1.812030	4.718966
C	-2.497639	-2.118065	2.873408
C	-0.790842	-0.707311	3.020986
H	0.043139	-0.142316	3.425721
N	-1.219288	-0.632056	1.770525
C	-2.277619	-1.504259	1.664219
H	-2.804531	-1.662026	0.728473
C	-3.082223	-2.302483	-4.122231
H	-2.161890	-2.609593	-4.643109
H	-3.744449	-1.785255	-4.833571
N	-3.546391	-0.593396	-2.283764
H	-4.514530	-0.414084	-2.571861
C	-2.686800	-1.425636	-2.975000
C	-2.859852	0.007915	-1.284102
H	-3.271332	0.722578	-0.573359
N	-1.600006	-0.404833	-1.287760
C	-1.470910	-1.275705	-2.349554
H	-0.512332	-1.703728	-2.626738
C	1.488366	0.918328	-3.950627
H	1.260329	1.761998	-4.611778
H	0.985810	0.019806	-4.339771
C	0.955865	1.198717	-2.577653
O	1.067796	0.401460	-1.646712
O	0.374237	2.374587	-2.439080
H	0.035464	2.461184	-1.514583
C	3.273104	-4.235036	1.604973
H	4.103776	-3.599966	1.945547
H	3.704590	-4.980366	0.917234
N	1.299348	-3.961408	0.038112
H	1.262436	-4.938524	-0.276794
C	2.226375	-3.420459	0.912899
C	0.468120	-2.982165	-0.369283
H	-0.357990	-3.149347	-1.054139
N	0.815222	-1.832744	0.182111
C	1.905992	-2.083297	0.984136
H	2.360633	-1.280090	1.559362
Ni	-0.105498	0.004792	0.124375
O	1.293746	0.925052	1.331595

O	0.796177	1.770925	2.336192
C	-2.841109	2.863945	5.627489
C	-2.859119	2.398363	4.320528
C	-1.842130	2.791230	3.399074
C	-0.772211	3.587511	3.875132
C	-0.768490	4.107280	5.160690
C	-1.820728	3.748107	6.038667
C	-1.922858	2.413249	2.020536
C	-0.718597	2.747364	1.159012
C	0.536657	3.172728	1.892527
C	1.692527	3.824394	1.171774
C	2.333841	4.950565	1.718878
C	3.475930	5.468502	1.107386
C	3.993649	4.915652	-0.069921
C	3.327054	3.814166	-0.644829
C	2.211234	3.269348	-0.007661
O	0.279439	3.890385	3.063963
O	-2.889866	1.828738	1.510359
O	3.734364	3.245392	-1.814907
O	5.114165	5.469433	-0.602323
O	-0.686558	2.329302	0.001767
O	-1.894836	4.189061	7.290489
O	-3.826087	1.564950	3.913685
H	-3.632486	2.583125	6.323201
H	0.055798	4.737517	5.498601
H	1.964638	5.404620	2.637756
H	4.012508	6.313927	1.539877
H	1.806083	2.349317	-0.404359
H	4.670047	3.428786	-2.018951
H	5.497995	4.932492	-1.318809
H	-1.256558	4.928443	7.491792
H	-3.729728	1.454343	2.928148
h	-3.111413	-4.166919	3.295751
h	-3.590262	-3.203596	-3.778779
h	2.562347	0.733292	-3.930833
h	2.876305	-4.822634	2.432830

Int2

C	-3.640064	-3.307444	3.241762
H	-4.459622	-3.310730	2.510767
H	-4.079342	-3.092768	4.228840
N	-1.748089	-1.669995	3.728516
H	-1.674892	-1.844491	4.738648
C	-2.651419	-2.258484	2.863427
C	-0.982696	-0.811078	3.022973
H	-0.189982	-0.192538	3.431147
N	-1.341394	-0.819364	1.746901
C	-2.377672	-1.714303	1.630881
H	-2.855495	-1.931055	0.679255
C	-3.091443	-2.331384	-4.099003
H	-2.168552	-2.641717	-4.613310
H	-3.748208	-1.815846	-4.816653
N	-3.568652	-0.626226	-2.260838
H	-4.537482	-0.452074	-2.551408
C	-2.701980	-1.449597	-2.953571
C	-2.890089	-0.021433	-1.259798
H	-3.307555	0.695504	-0.555720
N	-1.624977	-0.421401	-1.263745
C	-1.487522	-1.288538	-2.328714
H	-0.528157	-1.713184	-2.606946
C	1.459570	0.845332	-3.774471
H	1.175822	1.555444	-4.560712
H	1.006382	-0.131867	-4.000095
C	0.925538	1.335357	-2.458721
O	0.997512	0.680263	-1.414859
O	0.406340	2.539883	-2.505348
H	0.081376	2.828352	-1.612159
C	3.276965	-4.232037	1.596724
H	4.108565	-3.600194	1.941079
H	3.709293	-4.977065	0.909214
N	1.308866	-3.948956	0.024980
H	1.272779	-4.925473	-0.292700
C	2.235780	-3.412549	0.901702
C	0.481872	-2.967923	-0.384343
H	-0.347174	-3.135472	-1.065235
N	0.831982	-1.816718	0.165949
C	1.918912	-2.074175	0.971647
H	2.383431	-1.287923	1.562316
Ni	-0.193758	-0.046824	0.190132
O	0.365259	1.156008	1.719646

O	1.417271	2.107167	2.050143
C	-2.583637	2.856672	5.447312
C	-2.538915	2.413890	4.132626
C	-1.527636	2.884629	3.246335
C	-0.509299	3.728412	3.755774
C	-0.569565	4.217259	5.054133
C	-1.625433	3.788182	5.896842
C	-1.580890	2.564289	1.851198
C	-0.424422	3.070689	0.999896
C	0.885037	3.378051	1.784866
C	1.964756	4.149334	1.062692
C	2.663790	5.224723	1.623114
C	3.817375	5.692103	0.985989
C	4.263485	5.143515	-0.221909
C	3.508219	4.113371	-0.824690
C	2.408844	3.601471	-0.146422
O	0.535824	4.113016	2.969661
O	-2.499658	1.930137	1.310267
O	3.818142	3.567242	-2.035049
O	5.414964	5.625869	-0.752781
O	-0.563719	3.260288	-0.192894
O	-1.761743	4.207154	7.153398
O	-3.450743	1.535177	3.685906
H	-3.374934	2.518816	6.117408
H	0.209398	4.884902	5.425008
H	2.343258	5.652317	2.573341
H	4.431277	6.480801	1.423771
H	1.945001	2.704743	-0.541930
H	4.755275	3.702994	-2.273927
H	5.754537	5.075617	-1.482706
H	-1.156917	4.963775	7.387116
H	-3.319361	1.447878	2.702359
h	-3.202365	-4.303169	3.312604
h	-3.603395	-3.230209	-3.755367
h	2.542748	0.724663	-3.759305
h	2.875404	-4.819836	2.422137

$TS2_A$

C	-3.622448	-3.368898	3.337788
H	-4.448225	-3.337148	2.614524
H	-4.046622	-3.164969	4.333268
N	-1.650516	-1.811781	3.805206
H	-1.573392	-1.974519	4.819064
C	-2.606935	-2.345617	2.964009
C	-0.854444	-0.997255	3.080250
H	-0.034013	-0.408533	3.479900
N	-1.246910	-0.990236	1.817964
C	-2.334619	-1.818569	1.725405
H	-2.845010	-2.003041	0.783968
C	-3.178708	-2.379686	-4.110302
H	-2.252889	-2.676302	-4.627394
H	-3.844556	-1.871029	-4.824780
N	-3.684179	-0.699020	-2.265476
H	-4.648895	-0.522523	-2.571967
C	-2.802820	-1.502057	-2.959935
C	-3.026283	-0.112275	-1.242916
H	-3.458488	0.589500	-0.534398
N	-1.759644	-0.504016	-1.235956
C	-1.598708	-1.346405	-2.315736
H	-0.633973	-1.757109	-2.594038
C	1.342361	0.878980	-3.668761
H	1.025664	1.508510	-4.509301
H	0.960310	-0.140576	-3.832659
C	0.732448	1.418887	-2.403497
O	0.804525	0.864816	-1.307038
O	0.120548	2.576682	-2.561558
H	-0.239671	2.904044	-1.703569
C	3.248959	-4.143775	1.582602
H	4.073823	-3.505956	1.932457
H	3.691817	-4.876085	0.887411
N	1.264784	-3.874490	0.032523
H	1.220370	-4.856098	-0.264234
C	2.203772	-3.326296	0.888442
C	0.453327	-2.890472	-0.402863
H	-0.386313	-3.072639	-1.065840
N	0.820300	-1.725504	0.106071
C	1.907737	-1.979664	0.914578
H	2.392505	-1.187118	1.480457
Ni	-0.415797	-0.013829	0.230989
O	0.424066	1.307308	1.846900

O	1.555069	2.230004	2.037211
C	-2.494106	2.793736	5.083820
C	-2.274259	2.296549	3.797236
C	-1.233651	2.818646	2.998975
C	-0.384802	3.794839	3.555680
C	-0.586093	4.309327	4.829920
C	-1.651942	3.796023	5.602712
C	-0.948928	2.284081	1.641862
C	-0.128802	3.283587	0.858925
C	1.118516	3.548536	1.699574
C	2.254619	4.244077	1.020806
C	3.064225	5.186761	1.661422
C	4.209645	5.646809	1.009895
C	4.543349	5.207695	-0.276889
C	3.682633	4.308450	-0.944894
C	2.575070	3.815012	-0.272170
O	0.692996	4.280913	2.839785
O	-1.794914	1.548884	0.997831
O	3.872769	3.898852	-2.233183
O	5.683587	5.680596	-0.830057
O	-0.379836	3.724124	-0.236247
O	-1.899790	4.212823	6.850462
O	-3.055020	1.305097	3.315027
H	-3.310106	2.398882	5.690743
H	0.101763	5.053510	5.235173
H	2.818831	5.523872	2.668899
H	4.896920	6.344061	1.491886
H	1.978226	3.064297	-0.779196
H	4.815438	3.942038	-2.488224
H	5.972418	5.157840	-1.602098
H	-1.309281	4.960455	7.133063
H	-2.781333	1.147986	2.371762
h	-3.200066	-4.372918	3.377840
h	-3.673960	-3.283630	-3.755791
h	2.430853	0.830836	-3.638203
h	2.861094	-4.749047	2.401914

$Int2_A$

C	-3.627262	-3.387999	3.347380
H	-4.453990	-3.353284	2.625412
H	-4.047478	-3.181113	4.343850
N	-1.653038	-1.834783	3.814075
H	-1.582248	-1.989779	4.829937
C	-2.607232	-2.369822	2.971809
C	-0.849327	-1.029205	3.088025
H	-0.031674	-0.439384	3.491945
N	-1.234339	-1.029945	1.823675
C	-2.325695	-1.853148	1.730996
H	-2.831352	-2.040512	0.787531
C	-3.201394	-2.389037	-4.106090
H	-2.277053	-2.683283	-4.627431
H	-3.870758	-1.880193	-4.817075
N	-3.696874	-0.707816	-2.257515
H	-4.660525	-0.524799	-2.563427
C	-2.820593	-1.513679	-2.955400
C	-3.033544	-0.124878	-1.236134
H	-3.459069	0.579149	-0.525497
N	-1.769338	-0.523312	-1.232820
C	-1.614277	-1.364317	-2.314111
H	-0.651770	-1.777736	-2.595836
C	1.341248	0.863790	-3.641441
H	1.017629	1.477874	-4.490785
H	0.957789	-0.158611	-3.782082
C	0.742111	1.427719	-2.381403
O	0.796887	0.880893	-1.280421
O	0.162305	2.600996	-2.547987
H	-0.199553	2.936995	-1.694392
C	3.250727	-4.151475	1.581699
H	4.071273	-3.507753	1.930934
H	3.700629	-4.885569	0.892961
N	1.268773	-3.894800	0.024445
H	1.226515	-4.877470	-0.270183
C	2.205328	-3.341471	0.879579
C	0.456928	-2.913895	-0.417435
H	-0.381266	-3.100695	-1.081135
N	0.821303	-1.745847	0.086237
C	1.906983	-1.995408	0.898574
H	2.389936	-1.200904	1.463328
Ni	-0.429886	-0.039647	0.233181
O	0.423125	1.339812	1.876692

O	1.558330	2.262605	2.085291
C	-2.486116	2.796085	5.065888
C	-2.246333	2.296679	3.782813
C	-1.202464	2.827471	2.996154
C	-0.378038	3.819689	3.558063
C	-0.596432	4.334580	4.829794
C	-1.660149	3.806607	5.594067
C	-0.867202	2.258370	1.650612
C	-0.099591	3.303391	0.868419
C	1.135699	3.584765	1.722077
C	2.282442	4.260502	1.044572
C	3.091460	5.211818	1.672454
C	4.231602	5.668859	1.009811
C	4.561332	5.215363	-0.273350
C	3.703577	4.301789	-0.925629
C	2.600263	3.814149	-0.242634
O	0.700207	4.322931	2.848819
O	-1.726708	1.520337	0.997353
O	3.891668	3.870208	-2.206252
O	5.696334	5.687517	-0.836682
O	-0.366890	3.757859	-0.216107
O	-1.921492	4.217621	6.842151
O	-3.010655	1.294570	3.295270
H	-3.304654	2.393679	5.664398
H	0.078337	5.088248	5.239725
H	2.843037	5.563625	2.674334
H	4.916659	6.377893	1.477353
H	2.006032	3.051981	-0.736011
H	4.831536	3.922979	-2.469518
H	5.979957	5.165098	-1.610925
H	-1.334135	4.964135	7.132793
H	-2.722475	1.139794	2.353874
h	-3.207566	-4.393210	3.385763
h	-3.692060	-3.295039	-3.750459
h	2.429883	0.814948	-3.617896
h	2.862236	-4.754200	2.402591

$TS3_A$

C	-3.673545	-3.434479	3.359528
H	-4.503404	-3.413160	2.641402
H	-4.094135	-3.238220	4.358000
N	-1.710952	-1.868377	3.812485
H	-1.624785	-2.028054	4.826484
C	-2.678228	-2.396237	2.980793
C	-0.924371	-1.051422	3.083391
H	-0.095218	-0.470694	3.477226
N	-1.336008	-1.034984	1.826316
C	-2.425585	-1.860170	1.742069
H	-2.946422	-2.040281	0.805058
C	-3.199663	-2.408637	-4.121949
H	-2.274686	-2.707675	-4.639295
H	-3.867292	-1.904463	-4.837994
N	-3.700100	-0.715213	-2.288891
H	-4.663064	-0.532936	-2.599360
C	-2.821468	-1.526205	-2.977235
C	-3.042479	-0.131423	-1.265052
H	-3.471558	0.575440	-0.559090
N	-1.779392	-0.532705	-1.253582
C	-1.618717	-1.378873	-2.328947
H	-0.655390	-1.798695	-2.598891
C	1.362736	0.906415	-3.680846
H	1.040322	1.562357	-4.498432
H	0.984958	-0.108543	-3.880958
C	0.747807	1.389505	-2.395528
O	0.848274	0.818226	-1.314087
O	0.079737	2.527125	-2.523829
H	-0.295038	2.795985	-1.659361
C	3.240743	-4.164554	1.583942
H	4.063908	-3.521506	1.928091
H	3.683863	-4.898316	0.890595
N	1.253866	-3.913599	0.035040
H	1.222134	-4.894367	-0.267229
C	2.187341	-3.356592	0.891461
C	0.425903	-2.939329	-0.391155
H	-0.412562	-3.128200	-1.054167
N	0.777880	-1.773277	0.124329
C	1.871821	-2.014659	0.927141
H	2.347431	-1.216481	1.493410
Ni	-0.475318	-0.062066	0.247872
O	0.322461	1.219774	1.874158

O	1.797811	2.424233	2.116527
C	-2.465489	2.830993	5.048833
C	-2.199485	2.315237	3.779033
C	-1.109145	2.794375	3.022005
C	-0.309799	3.813638	3.574727
C	-0.560556	4.347477	4.835444
C	-1.635494	3.832971	5.588228
C	-0.728756	2.109967	1.722881
C	0.016297	3.286668	0.902974
C	1.287743	3.593946	1.790521
C	2.338942	4.364189	1.020842
C	3.164156	5.300998	1.647142
C	4.294361	5.753959	0.966573
C	4.605811	5.295557	-0.319416
C	3.725097	4.402806	-0.969645
C	2.625777	3.922887	-0.274367
O	0.738809	4.367687	2.861570
O	-1.688724	1.597528	0.949894
O	3.892527	3.975859	-2.254875
O	5.748310	5.742246	-0.886300
O	-0.296594	3.744174	-0.139190
O	-1.917901	4.255277	6.828297
O	-2.979457	1.324557	3.284772
H	-3.306702	2.448914	5.629111
H	0.097212	5.120092	5.237847
H	2.942361	5.631250	2.662556
H	4.992688	6.453664	1.427192
H	2.027481	3.158655	-0.762667
H	4.833582	3.998944	-2.519293
H	6.024303	5.204866	-1.653088
H	-1.325900	4.995758	7.125261
H	-2.718566	1.185996	2.337964
h	-3.233097	-4.430873	3.395178
h	-3.692268	-3.310117	-3.757611
h	2.451533	0.863511	-3.653537
h	2.856521	-4.766875	2.407137

$Prod_A$

C	-3.556967	-3.250323	3.328558
H	-4.381342	-3.215624	2.603097
H	-3.986017	-3.055320	4.324036
N	-1.618117	-1.650366	3.826893
H	-1.543654	-1.832657	4.838258
C	-2.552031	-2.208464	2.971571
C	-0.865869	-0.776526	3.122375
H	-0.065330	-0.161965	3.526256
N	-1.263329	-0.754712	1.859690
C	-2.310263	-1.635241	1.748875
H	-2.817233	-1.814694	0.805398
C	-3.054689	-2.371842	-4.136044
H	-2.133061	-2.698534	-4.641605
H	-3.703659	-1.854744	-4.860149
N	-3.567457	-0.676925	-2.317125
H	-4.534497	-0.513376	-2.622342
C	-2.675289	-1.486245	-2.991539
C	-2.931942	-0.078514	-1.290628
H	-3.369802	0.617803	-0.575828
N	-1.661015	-0.465482	-1.259513
C	-1.479739	-1.321454	-2.330761
H	-0.508456	-1.733050	-2.586867
C	1.569431	1.598550	-3.357485
H	1.983798	2.619911	-3.378558
H	0.822610	1.532632	-4.166276
C	0.816172	1.458193	-2.062587
O	1.033562	0.580036	-1.220018
O	-0.110216	2.372374	-1.879391
H	-0.547923	2.270258	-0.979997
C	3.262631	-4.204997	1.616558
H	4.088738	-3.564700	1.958698
H	3.696239	-4.937268	0.916332
N	1.268116	-3.939307	0.077101
H	1.242092	-4.914474	-0.244947
C	2.201101	-3.393625	0.941318
C	0.418326	-2.968793	-0.311089
H	-0.418802	-3.143439	-0.980477
N	0.759818	-1.815634	0.237896
C	1.865795	-2.059554	1.021840
H	2.332397	-1.266359	1.603114
Ni	-0.300838	-0.028956	0.231333
O	-0.938234	1.986097	0.637504

O	1.248543	1.544317	2.284424
C	-2.733261	2.665355	5.142774
C	-2.762165	2.148576	3.844888
C	-1.745042	2.463449	2.884350
C	-0.693363	3.268168	3.370177
C	-0.676687	3.838567	4.642895
C	-1.719063	3.544304	5.545763
C	-1.926055	1.989246	1.474565
C	0.877786	4.954628	-1.225800
C	1.267774	2.740008	2.072649
C	2.292141	3.465392	1.288355
C	2.671890	4.779282	1.608567
C	3.670998	5.398257	0.866332
C	4.255319	4.763721	-0.238625
C	3.813793	3.470885	-0.602207
C	2.875850	2.822295	0.195398
O	0.366680	3.628382	2.556189
O	-3.060646	1.556498	1.168768
O	4.238721	2.815667	-1.716363
O	5.216420	5.448501	-0.906504
O	0.084872	5.290819	-1.959814
O	-1.799935	4.038444	6.786155
O	-3.777630	1.332612	3.528697
H	-3.546634	2.421809	5.828072
H	0.149826	4.488608	4.937058
H	2.205478	5.296752	2.447456
H	4.028672	6.400726	1.110676
H	2.592675	1.803796	-0.063079
H	5.019260	3.237344	-2.120185
H	5.659124	4.917634	-1.597348
H	-1.181898	4.789614	6.980141
H	-3.742972	1.249266	2.523621
h	-3.140496	-4.257043	3.362229
h	-3.581704	-3.257294	-3.780660
h	2.376085	0.888652	-3.540296
h	2.877771	-4.806081	2.440359

$TS2_B$

C	-3.576812	-3.241961	3.204637
H	-4.401201	-3.239294	2.478603
H	-4.005557	-3.004596	4.191027
N	-1.654703	-1.625398	3.656413
H	-1.584152	-1.786893	4.667559
C	-2.571896	-2.214118	2.806872
C	-0.894728	-0.772228	2.936417
H	-0.101275	-0.154860	3.345667
N	-1.267889	-0.787182	1.664103
C	-2.309015	-1.679274	1.567893
H	-2.800746	-1.898531	0.624465
C	-3.136487	-2.349642	-4.139276
H	-2.223160	-2.656471	-4.672852
H	-3.808650	-1.834778	-4.842864
N	-3.566410	-0.628108	-2.303225
H	-4.534692	-0.435914	-2.585446
C	-2.722828	-1.469976	-3.002806
C	-2.867337	-0.032328	-1.312011
H	-3.258717	0.692878	-0.600184
N	-1.611733	-0.459880	-1.332700
C	-1.498668	-1.332279	-2.393648
H	-0.547561	-1.770538	-2.678984
C	1.500299	0.878125	-3.826634
H	1.236138	1.666812	-4.540941
H	1.027486	-0.062376	-4.148096
C	0.966635	1.242773	-2.470814
O	1.069127	0.466119	-1.504034
O	0.417496	2.415724	-2.381384
H	0.083189	2.590347	-1.425887
C	3.281372	-4.258073	1.597377
H	4.112069	-3.623502	1.938843
H	3.715338	-5.009247	0.917977
N	1.321556	-3.986348	0.011580
H	1.286443	-4.964375	-0.303388
C	2.242274	-3.445801	0.891429
C	0.498304	-3.007925	-0.410379
H	-0.323786	-3.176993	-1.099678
N	0.844587	-1.855644	0.137975
C	1.925612	-2.107114	0.951994
H	2.392619	-1.319385	1.538988
Ni	-0.166907	-0.087497	0.043888
O	0.449576	1.273956	1.602768

O	1.414149	2.089155	2.333215
C	-2.622507	2.902021	5.556053
C	-2.590851	2.430197	4.252078
C	-1.563093	2.846419	3.353994
C	-0.557035	3.722898	3.831972
C	-0.606612	4.242379	5.119160
C	-1.650420	3.828784	5.982529
C	-1.598650	2.434075	1.981228
C	-0.341296	2.666849	1.134749
C	0.856902	3.353337	1.913520
C	1.908030	4.102013	1.135395
C	2.589025	5.210735	1.656644
C	3.731790	5.682109	1.005472
C	4.190087	5.103273	-0.183397
C	3.458260	4.036220	-0.747913
C	2.365143	3.522825	-0.055710
O	0.464690	4.129337	3.020765
O	-2.554713	1.830688	1.470788
O	3.786577	3.460436	-1.938890
O	5.330369	5.594388	-0.732636
O	-0.531448	2.751685	-0.106364
O	-1.772067	4.261593	7.235370
O	-3.529771	1.571705	3.826164
H	-3.420708	2.597784	6.233968
H	0.168528	4.929152	5.462254
H	2.259560	5.664960	2.591434
H	4.326615	6.499983	1.414851
H	1.915235	2.611494	-0.433166
H	4.718459	3.614763	-2.184568
H	5.673196	5.036843	-1.455050
H	-1.158658	5.015459	7.456538
H	-3.403290	1.471274	2.839330
h	-3.159928	-4.245887	3.284693
h	-3.636745	-3.249669	-3.781842
h	2.580512	0.732772	-3.817753
h	2.875404	-4.837810	2.426330

$Int2_B$

C	-3.571801	-3.255185	3.177325
H	-4.376972	-3.238642	2.430112
H	-4.022858	-3.014862	4.153207
N	-1.600647	-1.726899	3.685670
H	-1.544652	-1.911381	4.693721
C	-2.538824	-2.242160	2.813782
C	-0.803283	-0.881199	3.001327
H	0.011765	-0.326220	3.450119
N	-1.172826	-0.818037	1.728589
C	-2.251995	-1.663743	1.599418
H	-2.749073	-1.828750	0.648436
C	-3.150785	-2.354814	-4.147142
H	-2.239974	-2.656269	-4.687990
H	-3.827473	-1.834951	-4.843104
N	-3.573725	-0.650105	-2.294521
H	-4.542532	-0.453167	-2.571381
C	-2.732056	-1.484133	-3.005763
C	-2.867759	-0.061328	-1.302623
H	-3.256562	0.646768	-0.573513
N	-1.612641	-0.484451	-1.335282
C	-1.504497	-1.349011	-2.402501
H	-0.552550	-1.778987	-2.697626
C	1.522806	0.937164	-3.915241
H	1.291864	1.805952	-4.541462
H	1.028189	0.053247	-4.346264
C	0.975352	1.148156	-2.535527
O	1.110855	0.295001	-1.647310
O	0.359954	2.287326	-2.340397
H	0.055053	2.336100	-1.375343
C	3.273150	-4.272582	1.591661
H	4.098725	-3.630071	1.930579
H	3.713786	-5.025637	0.918761
N	1.321990	-4.021665	-0.008942
H	1.294380	-5.000875	-0.321298
C	2.231458	-3.472681	0.876979
C	0.498303	-3.047841	-0.443479
H	-0.314491	-3.222687	-1.142484
N	0.831413	-1.893022	0.104294
C	1.905303	-2.136479	0.929644
H	2.360161	-1.345526	1.522169
Ni	-0.140513	-0.085088	0.002648
O	0.622503	1.211415	2.007200

O	1.560040	2.183160	2.556023
C	-2.643298	2.951288	5.603294
C	-2.623414	2.447473	4.312162
C	-1.583109	2.817126	3.410553
C	-0.591961	3.728294	3.844969
C	-0.632108	4.285194	5.116265
C	-1.660875	3.878592	6.002899
C	-1.562002	2.280028	2.081608
C	-0.205798	2.294147	1.344620
C	0.864070	3.307355	1.966495
C	1.850694	4.070134	1.119319
C	2.526175	5.188164	1.635085
C	3.667262	5.663016	0.986586
C	4.135604	5.078720	-0.195929
C	3.406416	4.010592	-0.761337
C	2.312384	3.491596	-0.070571
O	0.379898	4.153604	2.977381
O	-2.535793	1.726319	1.556994
O	3.741853	3.437238	-1.951097
O	5.279225	5.569411	-0.737420
O	-0.338979	2.028179	0.072944
O	-1.768657	4.326368	7.250906
O	-3.574782	1.590018	3.910868
H	-3.438559	2.671173	6.294624
H	0.132687	4.997232	5.429782
H	2.195893	5.645297	2.568127
H	4.255462	6.486249	1.395190
H	1.864787	2.580304	-0.449571
H	4.674428	3.594003	-2.191999
H	5.633678	5.007333	-1.450922
H	-1.147460	5.076655	7.462998
H	-3.455209	1.461158	2.929743
h	-3.168843	-4.263888	3.267928
h	-3.646665	-3.257802	-3.791075
h	2.598680	0.762892	-3.901423
h	2.868132	-4.848721	2.423581

$TS3_B$

C	-3.545185	-3.217085	3.289574
H	-4.387563	-3.194393	2.584585
H	-3.948431	-2.997780	4.290576
N	-1.612888	-1.578323	3.698203
H	-1.516761	-1.732708	4.709496
C	-2.543637	-2.190886	2.878656
C	-0.862948	-0.743598	2.938677
H	-0.064977	-0.103943	3.311635
N	-1.261358	-0.801062	1.677694
C	-2.303087	-1.690882	1.622613
H	-2.807483	-1.936485	0.692558
C	-3.220174	-2.423176	-4.182103
H	-2.302816	-2.724694	-4.712052
H	-3.898404	-1.921011	-4.889005
N	-3.680915	-0.718518	-2.345611
H	-4.645050	-0.523225	-2.644491
C	-2.820333	-1.538290	-3.047969
C	-3.003276	-0.139457	-1.332975
H	-3.413576	0.570873	-0.618211
N	-1.744933	-0.555878	-1.345301
C	-1.606045	-1.402527	-2.421417
H	-0.645221	-1.821420	-2.702615
C	1.473404	0.973389	-3.915675
H	1.242405	1.793014	-4.605793
H	1.009544	0.048386	-4.287521
C	0.906185	1.286468	-2.559471
O	0.888945	0.426295	-1.668027
O	0.475540	2.503893	-2.402972
H	0.156120	2.703007	-1.448948
C	3.258650	-4.222127	1.579281
H	4.073616	-3.567391	1.920647
H	3.713525	-4.967693	0.907216
N	1.311803	-4.006125	-0.029589
H	1.298570	-4.988383	-0.334172
C	2.208395	-3.437551	0.857531
C	0.478226	-3.049084	-0.479035
H	-0.327118	-3.243333	-1.181469
N	0.792838	-1.883563	0.059399
C	1.865686	-2.104125	0.893979
H	2.310069	-1.298075	1.473829
Ni	-0.285762	-0.119572	-0.007866
O	0.580772	1.416595	1.072205

O	1.440879	2.163121	2.485135
C	-2.597474	2.880729	5.419258
C	-2.498143	2.419166	4.114244
C	-1.453344	2.880303	3.255436
C	-0.502153	3.790842	3.784489
C	-0.616479	4.294781	5.072738
C	-1.673560	3.835635	5.893114
C	-1.399532	2.453536	1.890612
C	-0.115504	2.722893	1.048973
C	1.037326	3.373529	2.000584
C	2.126888	4.091441	1.230855
C	2.841968	5.170787	1.765821
C	3.957829	5.658996	1.080753
C	4.358707	5.119591	-0.146811
C	3.601154	4.072122	-0.710489
C	2.528808	3.548955	0.004301
O	0.531064	4.223436	3.015586
O	-2.297323	1.800597	1.337465
O	3.874516	3.528028	-1.930885
O	5.465890	5.635765	-0.739954
O	-0.358919	3.164825	-0.120146
O	-1.845654	4.249921	7.146213
O	-3.382463	1.518182	3.656604
H	-3.403927	2.532764	6.066026
H	0.126622	4.999025	5.450086
H	2.548460	5.600390	2.724281
H	4.572262	6.463246	1.488728
H	2.045523	2.666753	-0.401361
H	4.799954	3.678382	-2.202533
H	5.785824	5.088617	-1.480535
H	-1.237415	4.998131	7.399023
H	-3.213965	1.410766	2.680587
h	-3.134714	-4.225824	3.334572
h	-3.707228	-3.323118	-3.806672
h	2.552830	0.827515	-3.875338
h	2.861880	-4.806834	2.409195

$Prod_B$

C	-3.474294	-3.150400	3.232950
H	-4.308103	-3.124236	2.517103
H	-3.888168	-2.909991	4.224717
N	-1.554069	-1.495276	3.657202
H	-1.483453	-1.633345	4.671229
C	-2.448977	-2.144156	2.823504
C	-0.791320	-0.666121	2.900144
H	-0.023553	0.005830	3.283876
N	-1.143233	-0.765563	1.627142
C	-2.169379	-1.674656	1.564315
H	-2.644870	-1.946377	0.626432
C	-3.156049	-2.419382	-4.165568
H	-2.238132	-2.733399	-4.687188
H	-3.822971	-1.914846	-4.881746
N	-3.612853	-0.704106	-2.332581
H	-4.583692	-0.526286	-2.614706
C	-2.754698	-1.526263	-3.036209
C	-2.924526	-0.095008	-1.342777
H	-3.336791	0.620301	-0.632282
N	-1.660589	-0.496749	-1.367864
C	-1.532566	-1.364995	-2.429779
H	-0.572104	-1.782220	-2.715607
C	1.542727	1.035131	-3.924611
H	1.351752	1.899250	-4.570600
H	1.016798	0.159337	-4.332337
C	1.009561	1.304069	-2.543112
O	0.996685	0.407180	-1.693838
O	0.597422	2.532130	-2.361072
H	0.168143	2.761312	-1.483835
C	3.259356	-4.272081	1.567832
H	4.068117	-3.606360	1.902566
H	3.723962	-5.027409	0.913830
N	1.328022	-4.088115	-0.069706
H	1.314941	-5.075240	-0.359790
C	2.212301	-3.506948	0.820827
C	0.506921	-3.136686	-0.554029
H	-0.285088	-3.340662	-1.269597
N	0.815043	-1.962904	-0.032690
C	1.872602	-2.173538	0.825593
H	2.311280	-1.362940	1.404387
Ni	-0.148634	-0.163166	-0.074514
O	0.031585	1.679746	0.586815

O	1.513237	2.109241	2.814906
C	-2.626425	2.804099	5.310089
C	-2.656451	2.348354	3.994153
C	-1.693048	2.793392	3.031303
C	-0.660241	3.636480	3.520469
C	-0.642286	4.132829	4.814137
C	-1.654633	3.728167	5.721253
C	-1.883626	2.422507	1.635310
C	-0.820528	2.624331	0.551840
C	1.391395	3.212724	2.352977
C	2.343124	3.894061	1.438597
C	2.943593	5.101289	1.824146
C	3.977844	5.621571	1.049167
C	4.385026	4.991377	-0.131886
C	3.714382	3.823822	-0.560025
C	2.724472	3.267624	0.247886
O	0.340199	4.049039	2.655979
O	-2.886057	1.780653	1.266040
O	3.995787	3.203940	-1.736229
O	5.412453	5.554690	-0.815484
O	-0.846408	3.512424	-0.298035
O	-1.735783	4.159054	6.977878
O	-3.612601	1.477986	3.647010
H	-3.396411	2.475279	6.009169
H	0.153929	4.807958	5.134790
H	2.635871	5.595823	2.747610
H	4.519074	6.523941	1.338284
H	2.248828	2.338329	-0.063201
H	4.851027	3.484541	-2.111336
H	5.758532	4.985367	-1.528506
H	-1.144799	4.932124	7.190120
H	-3.571198	1.388025	2.649791
h	-3.087364	-4.167128	3.300881
h	-3.659561	-3.314338	-3.800060
h	2.610610	0.817086	-3.912428
h	2.859739	-4.843246	2.405772

Model II

React'

C	-3.481341	-3.143306	3.212706
H	-4.274549	-3.098884	2.452487
H	-3.950502	-2.920716	4.184292
N	-1.528112	-1.588057	3.783646
H	-1.474131	-1.791931	4.786781
C	-2.432502	-2.130167	2.887389
C	-0.732102	-0.725467	3.103418
H	0.066933	-0.152293	3.563963
N	-1.072310	-0.682067	1.828455
C	-2.124961	-1.550393	1.679810
H	-2.602342	-1.716655	0.719486
C	-3.058427	-2.281448	-4.095610
H	-2.136281	-2.585882	-4.614705
H	-3.711725	-1.752382	-4.807303
N	-3.521218	-0.604204	-2.219449
H	-4.489310	-0.419311	-2.495855
C	-2.660750	-1.415341	-2.939408
C	-2.820584	-0.002766	-1.225519
H	-3.217819	0.692456	-0.485880
N	-1.559383	-0.396868	-1.265111
C	-1.434894	-1.252212	-2.336972
H	-0.469534	-1.647329	-2.638844
C	1.702337	0.588292	-3.866030
H	1.292350	1.191068	-4.688153
H	1.430876	-0.468011	-4.016557
C	1.129601	1.123060	-2.560110
O	1.159326	0.342402	-1.562332
O	0.709158	2.308597	-2.557996
C	3.287862	-4.315718	1.573557
H	4.132358	-3.691669	1.900789
H	3.703304	-5.083219	0.899756
N	1.298030	-3.996816	0.020556
H	1.228693	-4.970587	-0.294063
C	2.260600	-3.485577	0.873528
C	0.498647	-2.978896	-0.373094
H	-0.345927	-3.109523	-1.043691
N	0.895042	-1.843371	0.166384
C	1.990608	-2.138555	0.941328
H	2.510934	-1.368871	1.504334
Ni	-0.046751	0.119613	0.067506

O	1.572154	0.730405	1.561856
O	1.424337	1.464120	2.551277
C	-2.930092	2.847125	5.880472
C	-2.953382	2.361344	4.579518
C	-1.974206	2.788667	3.635916
C	-0.991467	3.702908	4.056988
C	-0.965745	4.221737	5.355006
C	-1.939149	3.779305	6.265537
C	-1.991545	2.291316	2.280488
C	-0.830408	2.633983	1.435614
C	0.097857	3.587699	1.932786
C	1.253679	4.118019	1.219842
C	2.199006	4.964893	1.846618
C	3.364373	5.330331	1.171276
C	3.616606	4.898829	-0.140760
C	2.623636	4.141734	-0.808140
C	1.478032	3.749726	-0.122774
O	-0.034216	4.102712	3.193512
O	-2.925184	1.568862	1.853506
O	2.844899	3.813161	-2.101878
O	4.788351	5.216420	-0.736119
O	-0.709137	2.047473	0.305306
O	-1.983258	4.195521	7.540561
O	-3.880211	1.476238	4.183810
H	-3.687876	2.531102	6.598975
H	-0.184426	4.924037	5.648638
H	2.033561	5.313626	2.866528
H	4.131752	5.935359	1.661856
H	0.759107	3.129418	-0.652629
H	2.053554	3.288726	-2.419272
H	4.922698	4.667717	-1.533248
H	-1.342280	4.933536	7.716185
H	-3.718442	1.338917	3.188588
h	-3.104789	-4.163240	3.290227
h	-3.572185	-3.185488	-3.768761
h	2.789635	0.664001	-3.876956
h	2.881879	-4.878257	2.414268

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^{3}React'

C	-3.498570	-3.150238	3.205378
H	-4.295930	-3.113350	2.449180
H	-3.964226	-2.927853	4.178888
N	-1.546651	-1.589694	3.761417
H	-1.480535	-1.797240	4.762388
C	-2.457576	-2.132007	2.871570
C	-0.758368	-0.723787	3.076524
H	0.044749	-0.146364	3.524477
N	-1.109395	-0.677775	1.804015
C	-2.161709	-1.548412	1.662637
H	-2.646114	-1.716745	0.706041
C	-3.035602	-2.269785	-4.087677
H	-2.113475	-2.577199	-4.604929
H	-3.684952	-1.737820	-4.800838
N	-3.498200	-0.590213	-2.212972
H	-4.465569	-0.403815	-2.489583
C	-2.638312	-1.404665	-2.929823
C	-2.796846	0.008549	-1.216734
H	-3.196995	0.704046	-0.479181
N	-1.537018	-0.389657	-1.249689
C	-1.414030	-1.245034	-2.322287
H	-0.449501	-1.643736	-2.622108
C	1.706168	0.548014	-3.836649
H	1.288232	1.135383	-4.666151
H	1.441749	-0.512321	-3.970628
C	1.133037	1.101050	-2.537387
O	1.152308	0.338774	-1.529490
O	0.720200	2.292480	-2.556961
C	3.280456	-4.291838	1.566490
H	4.122470	-3.664384	1.893739
H	3.697500	-5.053014	0.886267
N	1.280052	-3.979698	0.027411
H	1.215404	-4.953123	-0.288259
C	2.245332	-3.463744	0.874997
C	0.470266	-2.966469	-0.356698
H	-0.379509	-3.101867	-1.019519
N	0.863475	-1.829347	0.181680
C	1.967506	-2.118503	0.947295
H	2.486025	-1.342042	1.503202
Ni	-0.033220	0.106076	0.108040
O	1.480641	0.720437	1.430924
O	1.282139	1.400901	2.477402

C	-2.923886	2.844474	5.869375
C	-2.953195	2.357261	4.568897
C	-1.975748	2.779898	3.622055
C	-0.984319	3.685505	4.040431
C	-0.952784	4.207254	5.335318
C	-1.928659	3.772762	6.249589
C	-2.004130	2.288410	2.266231
C	-0.838384	2.621788	1.414323
C	0.103751	3.574970	1.913290
C	1.254301	4.101335	1.201261
C	2.200769	4.948788	1.830174
C	3.365878	5.309933	1.156847
C	3.618648	4.873292	-0.155113
C	2.624847	4.117703	-0.825574
C	1.477789	3.730836	-0.141187
O	-0.025166	4.081049	3.173156
O	-2.945260	1.582756	1.836315
O	2.847512	3.789981	-2.117233
O	4.790896	5.187147	-0.745071
O	-0.725995	2.033742	0.294588
O	-1.969138	4.194304	7.521604
O	-3.885988	1.476957	4.178658
H	-3.680779	2.532609	6.590350
H	-0.166935	4.905223	5.627149
H	2.034455	5.297816	2.849641
H	4.134809	5.913591	1.646417
H	0.761375	3.109228	-0.673214
H	2.056422	3.259235	-2.434325
H	4.929230	4.642045	-1.544878
H	-1.327727	4.933014	7.694394
H	-3.736811	1.341343	3.184007
h	-3.116349	-4.167890	3.285121
h	-3.554811	-3.172142	-3.764816
h	2.792819	0.631414	-3.853994
h	2.881505	-4.861634	2.405678

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[5]React'

C	-3.490255	-3.152213	3.210499
H	-4.291293	-3.112829	2.458278
H	-3.949369	-2.926775	4.186098
N	-1.540388	-1.584951	3.757178
H	-1.483140	-1.778599	4.761781
C	-2.445675	-2.139904	2.870358
C	-0.745447	-0.731191	3.063954
H	0.049936	-0.149467	3.519833
N	-1.087104	-0.707208	1.788481
C	-2.140324	-1.576972	1.654475
H	-2.619114	-1.758812	0.697676
C	-3.084295	-2.304909	-4.123871
H	-2.161572	-2.607538	-4.643292
H	-3.742932	-1.784207	-4.836778
N	-3.554036	-0.632335	-2.247632
H	-4.521423	-0.445676	-2.528186
C	-2.689559	-1.434923	-2.971163
C	-2.860266	-0.042813	-1.243145
H	-3.262726	0.642857	-0.497570
N	-1.598884	-0.436034	-1.282188
C	-1.466992	-1.278882	-2.361673
H	-0.498839	-1.670524	-2.659126
C	1.696093	0.594153	-3.871461
H	1.293323	1.207731	-4.689358
H	1.419653	-0.458997	-4.033598
C	1.119108	1.119628	-2.563548
O	1.110199	0.313579	-1.584417
O	0.733593	2.315480	-2.540498
C	3.278709	-4.312422	1.564806
H	4.119030	-3.681845	1.890182
H	3.698788	-5.079741	0.893693
N	1.292560	-4.011390	0.005143
H	1.231276	-4.986693	-0.306914
C	2.246879	-3.490827	0.861235
C	0.489205	-3.000733	-0.398120
H	-0.349755	-3.142373	-1.073645
N	0.874049	-1.860130	0.139270
C	1.967733	-2.145156	0.921996
H	2.481267	-1.372133	1.486138
Ni	-0.095170	0.071950	0.025085
O	1.585909	0.736023	1.650839
O	1.506491	1.521941	2.601714

C	-2.913892	2.856003	5.872982
C	-2.927770	2.372836	4.571302
C	-1.946180	2.808019	3.632868
C	-0.973389	3.731835	4.059304
C	-0.958908	4.248046	5.358926
C	-1.930470	3.794142	6.264444
C	-1.945583	2.301225	2.281363
C	-0.771073	2.639021	1.455626
C	0.126581	3.625126	1.942789
C	1.283395	4.154102	1.229016
C	2.230944	4.999616	1.852832
C	3.398821	5.357813	1.176484
C	3.651064	4.921362	-0.133685
C	2.655451	4.166612	-0.799126
C	1.508064	3.782620	-0.113192
O	-0.017394	4.143426	3.202025
O	-2.872419	1.573351	1.845258
O	2.875903	3.828561	-2.091578
O	4.826650	5.229041	-0.728222
O	-0.591757	2.022826	0.350752
O	-1.980627	4.204881	7.541359
O	-3.845628	1.479835	4.170033
H	-3.671776	2.532311	6.587882
H	-0.184812	4.955873	5.658049
H	2.066876	5.350179	2.872513
H	4.169418	5.959375	1.666191
H	0.790398	3.159431	-0.640382
H	2.087667	3.298468	-2.403824
H	4.957291	4.677664	-1.524258
H	-1.339956	4.941955	7.721468
H	-3.676465	1.343497	3.176216
h	-3.110641	-4.171089	3.286995
h	-3.591188	-3.208757	-3.785959
h	2.783820	0.663977	-3.877842
h	2.877317	-4.875883	2.407101

TS1'

C	-3.515690	-3.149300	3.211514
H	-4.320139	-3.122628	2.462470
H	-3.975067	-2.930882	4.189125
N	-1.565552	-1.576152	3.739992
H	-1.474363	-1.795509	4.736019
C	-2.492891	-2.117050	2.865763
C	-0.809281	-0.685791	3.049432
H	-0.009538	-0.090132	3.479316
N	-1.196328	-0.623396	1.788070
C	-2.238376	-1.508618	1.659448
H	-2.742566	-1.673449	0.712327
C	-3.057198	-2.276086	-4.094074
H	-2.130299	-2.580292	-4.604758
H	-3.707019	-1.752664	-4.813157
N	-3.543480	-0.595453	-2.228224
H	-4.510711	-0.417515	-2.512725
C	-2.671842	-1.402205	-2.939125
C	-2.851297	0.016708	-1.233999
H	-3.264554	0.713318	-0.505328
N	-1.586675	-0.365438	-1.261739
C	-1.451016	-1.224153	-2.329865
H	-0.480187	-1.611519	-2.624124
C	1.697004	0.564414	-3.840011
H	1.283973	1.168850	-4.659823
H	1.425829	-0.491781	-3.991188
C	1.129594	1.102512	-2.531778
O	1.101743	0.309687	-1.548083
O	0.765992	2.309365	-2.519971
C	3.272342	-4.207904	1.592328
H	4.104143	-3.574147	1.933444
H	3.703468	-4.944944	0.894362
N	1.293934	-3.917699	0.034435
H	1.262292	-4.889164	-0.291282
C	2.221529	-3.386321	0.915051
C	0.457387	-2.926592	-0.348416
H	-0.370053	-3.075905	-1.035984
N	0.798490	-1.789637	0.223014
C	1.891614	-2.052075	1.011879
H	2.356590	-1.259715	1.594741
Ni	-0.078043	0.124356	0.103832
O	1.289975	1.015935	1.386662
O	0.835146	1.653585	2.433801

C	-2.906978	2.866319	5.886463
C	-2.938549	2.388563	4.582265
C	-1.946852	2.792222	3.643148
C	-0.920649	3.655170	4.076155
C	-0.891667	4.171537	5.369608
C	-1.893955	3.768838	6.274295
C	-2.007969	2.342793	2.276065
C	-0.846114	2.688096	1.401205
C	0.230383	3.498108	1.980413
C	1.345975	4.082855	1.246334
C	2.268600	4.962503	1.860523
C	3.419369	5.344908	1.173404
C	3.676286	4.897085	-0.134546
C	2.701128	4.110814	-0.788532
C	1.574407	3.689964	-0.085269
O	0.071739	4.027057	3.228921
O	-2.969613	1.691352	1.824944
O	2.913469	3.780119	-2.081883
O	4.836733	5.237283	-0.738019
O	-0.774380	2.169437	0.270511
O	-1.936753	4.196243	7.541943
O	-3.895165	1.536725	4.186229
H	-3.678576	2.572394	6.599041
H	-0.086660	4.842381	5.672683
H	2.094131	5.324946	2.874163
H	4.173078	5.979498	1.647349
H	0.870418	3.049540	-0.609105
H	2.117864	3.253231	-2.393215
H	4.981889	4.683329	-1.530586
H	-1.292162	4.932923	7.715548
H	-3.765115	1.411757	3.193215
h	-3.122330	-4.162946	3.288048
h	-3.571016	-3.180340	-3.767912
h	2.784067	0.642628	-3.855598
h	2.883024	-4.805893	2.416286

Int1'

C	-3.508042	-3.129068	3.212779
H	-4.312273	-3.104848	2.463399
H	-3.969065	-2.916843	4.190853
N	-1.535665	-1.570289	3.722357
H	-1.422689	-1.805959	4.712300
C	-2.494196	-2.087974	2.865983
C	-0.798285	-0.666028	3.028802
H	0.030656	-0.097497	3.43949
N	-1.231024	-0.569755	1.784694
C	-2.280593	-1.447833	1.668332
H	-2.815013	-1.586145	0.733380
C	-3.042040	-2.282838	-4.111679
H	-2.115965	-2.595246	-4.618770
H	-3.689343	-1.762569	-4.835098
N	-3.521298	-0.580955	-2.264405
H	-4.487828	-0.401667	-2.551041
C	-2.654507	-1.402486	-2.963201
C	-2.828275	0.036556	-1.274856
H	-3.239540	0.749866	-0.561277
N	-1.566633	-0.358264	-1.292768
C	-1.434472	-1.229543	-2.350888
H	-0.466082	-1.629350	-2.636736
C	1.702586	0.548588	-3.867218
H	1.283955	1.149826	-4.686301
H	1.450502	-0.511469	-4.025725
C	1.113355	1.063309	-2.560985
O	1.159540	0.285990	-1.562589
O	0.655165	2.236454	-2.557771
C	3.287155	-4.201869	1.613710
H	4.119006	-3.571705	1.961111
H	3.718626	-4.935540	0.912593
N	1.321712	-3.904104	0.045039
H	1.295614	-4.873632	-0.286904
C	2.238276	-3.375893	0.939534
C	0.479169	-2.916875	-0.331700
H	-0.341100	-3.062789	-1.028436
N	0.807329	-1.785869	0.258750
C	1.896506	-2.045698	1.053495
H	2.340098	-1.248594	1.647569
Ni	-0.039041	0.131144	0.094023
O	1.262301	1.072447	1.425693
O	0.702875	1.844808	2.457367

C	-2.955864	2.875201	5.888971
C	-3.013352	2.399856	4.585591
C	-2.020162	2.772524	3.634145
C	-0.942165	3.586053	4.058301
C	-0.898494	4.107726	5.347758
C	-1.912567	3.748326	6.261051
C	-2.138300	2.357792	2.263882
C	-0.977192	2.686968	1.348785
C	0.289994	3.204845	2.015496
C	1.350778	3.920940	1.225505
C	2.235871	4.830121	1.831636
C	3.353400	5.284392	1.123047
C	3.599940	4.872342	-0.194006
C	2.639789	4.062326	-0.838887
C	1.554638	3.572516	-0.112956
O	0.063180	3.911477	3.213681
O	-3.124031	1.753905	1.809981
O	2.824516	3.765313	-2.148883
O	4.736047	5.270220	-0.818025
O	-0.976579	2.224933	0.216442
O	-1.933811	4.187374	7.522955
O	-4.004583	1.581835	4.203292
H	-3.730297	2.608479	6.608804
H	-0.064909	4.744435	5.647937
H	2.070163	5.170974	2.853522
H	4.086414	5.945484	1.593709
H	0.875285	2.905723	-0.633274
H	2.031502	3.240909	-2.451155
H	4.910582	4.703251	-1.593585
H	-1.279963	4.918870	7.687041
H	-3.908351	1.460729	3.210913
H	-3.112071	-4.141913	3.286387
H	-3.560299	-3.181883	-3.778225
H	2.788491	0.642366	-3.876259
H	2.892787	-4.804213	2.432075

Int2'

C	-3.631848	-3.261137	3.232891
H	-4.449337	-3.271840	2.498756
H	-4.078698	-3.050489	4.218133
N	-1.762401	-1.598372	3.729848
H	-1.678148	-1.783531	4.734772
C	-2.651540	-2.201759	2.859072
C	-1.018207	-0.714536	3.023529
H	-0.240951	-0.074651	3.430515
N	-1.374424	-0.721749	1.750240
C	-2.387339	-1.640163	1.631197
H	-2.862778	-1.858711	0.678165
C	-3.042515	-2.306702	-4.070662
H	-2.110636	-2.619478	-4.566445
H	-3.681390	-1.786838	-4.801894
N	-3.558836	-0.626616	-2.216154
H	-4.528478	-0.466353	-2.504935
C	-2.671152	-1.421834	-2.919893
C	-2.882374	0.009072	-1.229005
H	-3.310189	0.716187	-0.519832
N	-1.607393	-0.344817	-1.253576
C	-1.453319	-1.211513	-2.314619
H	-0.474665	-1.584357	-2.602308
C	1.728088	0.575505	-3.702369
H	1.290370	1.153468	-4.528781
H	1.446055	-0.483429	-3.806391
C	1.207946	1.179707	-2.399956
O	1.106736	0.396849	-1.401199
O	0.955320	2.405269	-2.402539
C	3.267821	-4.217469	1.598783
H	4.103251	-3.587259	1.937368
H	3.691156	-4.953262	0.895209
N	1.283760	-3.916490	0.050993
H	1.256682	-4.884921	-0.285589
C	2.213179	-3.392070	0.933084
C	0.438316	-2.928173	-0.314696
H	-0.391865	-3.071654	-1.000221
N	0.776724	-1.796226	0.271027
C	1.876087	-2.061481	1.049928
H	2.343290	-1.281252	1.647454
Ni	-0.126880	0.074760	0.162692
O	0.299357	1.261459	1.734366
O	1.288726	2.268502	2.083119

C	-2.634501	2.801021	5.568832
C	-2.575390	2.372349	4.246463
C	-1.583934	2.879757	3.364072
C	-0.602838	3.767029	3.871637
C	-0.673006	4.229103	5.184614
C	-1.700406	3.751479	6.026020
C	-1.658169	2.597655	1.949476
C	-0.609820	3.297363	1.093467
C	0.732422	3.536193	1.851514
C	1.790878	4.329130	1.131497
C	2.697815	5.201415	1.743271
C	3.850483	5.579701	1.038006
C	4.101528	5.120864	-0.263457
C	3.116778	4.339383	-0.910610
C	2.006604	3.928701	-0.188019
O	0.410447	4.216282	3.092952
O	-2.578413	1.948901	1.426947
O	3.295528	3.967187	-2.206280
O	5.279412	5.428231	-0.854872
O	-0.842011	3.660668	-0.028983
O	-1.834231	4.152752	7.297881
O	-3.472345	1.484420	3.781994
H	-3.418720	2.433903	6.232268
H	0.083658	4.922537	5.554270
H	2.538122	5.534902	2.769888
H	4.621347	6.198709	1.505398
H	1.317895	3.253631	-0.690785
H	2.499049	3.440773	-2.466443
H	5.432758	4.858951	-1.639104
H	-1.229346	4.908112	7.522340
H	-3.327506	1.425989	2.791095
h	-3.194379	-4.256469	3.310364
h	-3.566544	-3.205237	-3.744938
h	2.813759	0.650089	-3.764192
h	2.879867	-4.815941	2.423034

Int2''

C	-3.579319	-3.218497	3.178654
H	-4.397870	-3.219513	2.445079
H	-4.017555	-2.976785	4.160391
N	-1.657696	-1.608991	3.649132
H	-1.592893	-1.771329	4.658494
C	-2.561718	-2.199953	2.784843
C	-0.865843	-0.781278	2.928123
H	-0.076943	-0.150640	3.327389
N	-1.204585	-0.812003	1.648960
C	-2.255944	-1.689711	1.543894
H	-2.730705	-1.915571	0.592513
C	-3.100367	-2.342184	-4.108622
H	-2.187530	-2.652937	-4.640801
H	-3.764584	-1.817678	-4.813389
N	-3.516351	-0.644373	-2.239627
H	-4.491156	-0.459731	-2.491589
C	-2.678459	-1.465210	-2.970742
C	-2.784442	-0.018744	-1.285339
H	-3.168262	0.705806	-0.569008
N	-1.519647	-0.408186	-1.351126
C	-1.435696	-1.286711	-2.409872
H	-0.490055	-1.691055	-2.753359
C	1.781411	0.061480	-3.076826
H	1.156848	-0.058481	-3.975546
H	1.583662	-0.777003	-2.394450
C	1.403462	1.372880	-2.383513
O	0.858933	1.304036	-1.229575
O	1.641856	2.455696	-2.957494
C	3.326680	-4.172042	1.606869
H	4.154881	-3.551545	1.979334
H	3.776726	-4.918515	0.931264
N	1.424755	-3.849961	-0.037709
H	1.367357	-4.827854	-0.340381
C	2.326334	-3.332109	0.877173
C	0.653191	-2.841449	-0.494890
H	-0.150954	-2.985250	-1.209675
N	1.011894	-1.695972	0.059427
C	2.048579	-1.982818	0.919029
H	2.506343	-1.205617	1.526828
Ni	-0.039015	0.106017	0.073329
O	0.436927	1.215596	1.706112
O	1.419465	2.274500	1.875759

C	-2.566716	2.781700	5.415446
C	-2.496558	2.337602	4.099155
C	-1.505625	2.845320	3.215749
C	-0.529999	3.740180	3.718654
C	-0.613255	4.219990	5.026496
C	-1.642674	3.745721	5.867031
C	-1.559673	2.544460	1.806412
C	-0.529396	3.267897	0.941900
C	0.815707	3.517911	1.677857
C	1.856962	4.362708	0.985859
C	2.751046	5.186517	1.680099
C	3.929559	5.602075	1.043544
C	4.221933	5.210128	-0.267609
C	3.255019	4.483344	-1.004263
C	2.101206	4.054811	-0.358371
O	0.485225	4.177995	2.942857
O	-2.461530	1.864258	1.287822
O	3.524085	4.188801	-2.294498
O	5.424438	5.513438	-0.804946
O	-0.779017	3.625340	-0.178360
O	-1.792260	4.159575	7.133148
O	-3.382782	1.434534	3.641891
H	-3.349409	2.414732	6.080621
H	0.137684	4.920356	5.394619
H	2.561564	5.453599	2.720053
H	4.687619	6.179696	1.579455
H	1.413329	3.423454	-0.909497
H	2.830191	3.551774	-2.623953
H	5.569428	4.977527	-1.616824
H	-1.195145	4.918834	7.363938
H	-3.227327	1.359271	2.654968
h	-3.168441	-4.223773	3.271747
h	-3.612567	-3.241202	-3.765863
h	2.830627	0.024218	-3.369784
h	2.900536	-4.767178	2.414508

$TS2_A'$

C	-3.538900	-3.249870	3.232666
H	-4.360234	-3.217760	2.502869
H	-3.965022	-3.003016	4.218055
N	-1.539435	-1.721705	3.684317
H	-1.481305	-1.864481	4.698656
C	-2.488484	-2.265145	2.838789
C	-0.726190	-0.928049	2.948917
H	0.080950	-0.321347	3.348866
N	-1.092785	-0.944404	1.679235
C	-2.184222	-1.770147	1.592821
H	-2.685454	-1.970045	0.649893
C	-3.152510	-2.390854	-4.124316
H	-2.237030	-2.695357	-4.655584
H	-3.820784	-1.871434	-4.829269
N	-3.599462	-0.724535	-2.242564
H	-4.571552	-0.539889	-2.509663
C	-2.742949	-1.515954	-2.982553
C	-2.889191	-0.112082	-1.267431
H	-3.286349	0.596941	-0.545095
N	-1.618804	-0.482232	-1.328427
C	-1.508578	-1.333388	-2.406514
H	-0.553556	-1.711016	-2.753842
C	1.713020	0.136124	-2.997944
H	1.088542	0.014773	-3.897303
H	1.509059	-0.702443	-2.318936
C	1.315354	1.444708	-2.305981
O	0.669227	1.375752	-1.202003
O	1.621107	2.531055	-2.840344
C	3.316360	-4.109651	1.600433
H	4.140297	-3.488662	1.981823
H	3.774934	-4.846417	0.919537
N	1.416342	-3.785277	-0.043245
H	1.351457	-4.765040	-0.335330
C	2.318924	-3.265802	0.869145
C	0.662448	-2.771781	-0.519894
H	-0.140682	-2.920459	-1.233999
N	1.028750	-1.620541	0.017866
C	2.057286	-1.911295	0.887379
H	2.526936	-1.136906	1.489608
Ni	-0.215571	0.123656	0.079948
O	0.429103	1.351367	1.768560
O	1.501680	2.333257	1.926916

C	-2.495883	2.693275	5.147795
C	-2.288533	2.226991	3.844794
C	-1.276022	2.783522	3.036179
C	-0.439262	3.773066	3.586743
C	-0.634061	4.258237	4.879757
C	-1.668897	3.709420	5.662619
C	-1.069214	2.328284	1.635092
C	-0.305945	3.389814	0.859406
C	0.991856	3.632146	1.652061
C	2.088486	4.395963	0.985241
C	3.012594	5.188460	1.673123
C	4.170611	5.599549	1.001643
C	4.419404	5.216277	-0.322146
C	3.429987	4.499454	-1.038602
C	2.286412	4.093893	-0.364541
O	0.597139	4.300485	2.865545
O	-1.913076	1.572815	1.043221
O	3.647119	4.201148	-2.338379
O	5.604502	5.531433	-0.884610
O	-0.682835	3.950513	-0.129950
O	-1.904544	4.111545	6.927028
O	-3.064835	1.241187	3.343688
H	-3.295032	2.272302	5.760139
H	0.042461	5.014446	5.282110
H	2.849350	5.448353	2.719696
H	4.948828	6.170558	1.514409
H	1.558016	3.506134	-0.913316
H	2.929501	3.579219	-2.636016
H	5.737256	5.005040	-1.705907
H	-1.322962	4.867688	7.194014
H	-2.794849	1.131710	2.382015
h	-3.153444	-4.266549	3.309183
h	-3.655359	-3.291521	-3.772169
h	2.762016	0.091362	-3.290638
h	2.895217	-4.718767	2.400234

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C	-3.520532	-3.268299	3.241734
H	-4.337646	-3.220290	2.507979
H	-3.945589	-3.012647	4.225031
N	-1.490786	-1.778341	3.697238
H	-1.449929	-1.901974	4.715377
C	-2.445778	-2.308305	2.850531
C	-0.646055	-1.022748	2.956982
H	0.168165	-0.429590	3.363211
N	-0.998068	-1.052771	1.684580
C	-2.112670	-1.845182	1.599991
H	-2.610121	-2.041145	0.654364
C	-3.178122	-2.400444	-4.125465
H	-2.263927	-2.700650	-4.661550
H	-3.851364	-1.882620	-4.826634
N	-3.617917	-0.741129	-2.234552
H	-4.589645	-0.551367	-2.499495
C	-2.764791	-1.528014	-2.983545
C	-2.903711	-0.138411	-1.256155
H	-3.294816	0.567219	-0.526598
N	-1.635141	-0.511115	-1.325873
C	-1.528388	-1.352647	-2.410532
H	-0.574955	-1.728290	-2.763955
C	1.681672	0.193254	-2.992895
H	1.066378	0.113203	-3.903054
H	1.459155	-0.664343	-2.345241
C	1.295170	1.484220	-2.261511
O	0.665269	1.392519	-1.149971
O	1.598049	2.582521	-2.775377
C	3.321812	-4.124698	1.588757
H	4.142112	-3.498802	1.969970
H	3.788310	-4.867766	0.920170
N	1.426236	-3.817276	-0.065832
H	1.355300	-4.801212	-0.343208
C	2.332592	-3.288839	0.837400
C	0.692550	-2.803625	-0.574083
H	-0.106792	-2.961054	-1.290711
N	1.071537	-1.644673	-0.063573
C	2.091599	-1.930637	0.817738
H	2.575441	-1.151262	1.402090
Ni	-0.251430	0.090874	0.075209
O	0.447646	1.432681	1.827130
O	1.530088	2.424493	2.001400

C	-2.488293	2.667770	5.089158
C	-2.224903	2.197272	3.794944
C	-1.205821	2.778224	3.017460
C	-0.436759	3.811043	3.580937
C	-0.677900	4.293936	4.866840
C	-1.706260	3.707105	5.627328
C	-0.855811	2.243502	1.641146
C	-0.257189	3.419479	0.878417
C	1.016790	3.725342	1.686564
C	2.115731	4.469150	1.010968
C	3.059188	5.242327	1.693387
C	4.221985	5.627091	1.015997
C	4.454038	5.237779	-0.309682
C	3.447574	4.537446	-1.019403
C	2.297689	4.160557	-0.339556
O	0.596849	4.387511	2.880266
O	-1.706163	1.453317	1.018415
O	3.653351	4.227367	-2.317778
O	5.639717	5.531584	-0.879774
O	-0.709206	4.001588	-0.062880
O	-1.975124	4.099178	6.890873
O	-2.946705	1.177055	3.278700
H	-3.289644	2.221654	5.680525
H	-0.038465	5.076675	5.279297
H	2.908481	5.499070	2.742999
H	5.013918	6.183376	1.522909
H	1.557105	3.585363	-0.886815
H	2.926864	3.610607	-2.606135
H	5.758200	5.005876	-1.703993
H	-1.398998	4.853055	7.172397
H	-2.629338	1.061863	2.327673
h	-3.151141	-4.290960	3.317761
h	-3.674078	-3.303779	-3.770387
h	2.733386	0.143791	-3.274882
h	2.896295	-4.726875	2.391493

$TS3_A'$

C	-3.581006	-3.336159	3.275766
H	-4.406733	-3.299902	2.551655
H	-3.998447	-3.089545	4.264826
N	-1.553714	-1.842964	3.706386
H	-1.494369	-1.971717	4.723169
C	-2.528716	-2.358377	2.873948
C	-0.724196	-1.080233	2.959215
H	0.104487	-0.499483	3.353953
N	-1.107221	-1.088796	1.694351
C	-2.225636	-1.876292	1.622634
H	-2.743066	-2.061754	0.684868
C	-3.198245	-2.424988	-4.121391
H	-2.283878	-2.724498	-4.657685
H	-3.872875	-1.910028	-4.823589
N	-3.638523	-0.757685	-2.238689
H	-4.608701	-0.564169	-2.507675
C	-2.785670	-1.549734	-2.982452
C	-2.924136	-0.152675	-1.261821
H	-3.313397	0.557508	-0.535417
N	-1.656920	-0.528924	-1.328510
C	-1.549829	-1.376317	-2.407612
H	-0.596035	-1.759067	-2.753146
C	1.678895	0.199034	-2.958428
H	1.054514	0.119322	-3.862702
H	1.454444	-0.655073	-2.305812
C	1.304663	1.491745	-2.221903
O	0.653095	1.400600	-1.125086
O	1.633181	2.591003	-2.722465
C	3.313397	-4.143816	1.598509
H	4.135676	-3.517444	1.974507
H	3.774525	-4.887358	0.926616
N	1.412495	-3.841427	-0.048508
H	1.350709	-4.824184	-0.332607
C	2.316993	-3.310000	0.855015
C	0.664375	-2.831946	-0.544098
H	-0.138503	-2.991123	-1.256644
N	1.033824	-1.674131	-0.025262
C	2.061212	-1.954155	0.848485
H	2.536336	-1.171281	1.435870
Ni	-0.296821	0.068985	0.105859
O	0.355682	1.279243	1.864608
O	1.741232	2.554722	2.076096

C	-2.485731	2.684723	5.093745
C	-2.197072	2.198047	3.812243
C	-1.140236	2.740445	3.056190
C	-0.392669	3.794804	3.611062
C	-0.665080	4.296626	4.885658
C	-1.703321	3.721129	5.637752
C	-0.744488	2.098847	1.727055
C	-0.141000	3.371666	0.920524
C	1.171844	3.698307	1.782584
C	2.183986	4.528731	1.029890
C	3.134197	5.309342	1.695681
C	4.275715	5.704991	0.991441
C	4.492118	5.298847	-0.332177
C	3.478172	4.588813	-1.021854
C	2.343072	4.208117	-0.318833
O	0.617389	4.409275	2.910594
O	-1.702697	1.515556	0.995983
O	3.667381	4.262801	-2.316875
O	5.673294	5.579161	-0.915189
O	-0.610066	3.941490	0.012545
O	-1.991510	4.126991	6.893206
O	-2.931579	1.187000	3.289327
H	-3.308147	2.256641	5.669420
H	-0.041294	5.095307	5.291948
H	3.005292	5.557377	2.750381
H	5.070998	6.272608	1.479133
H	1.614243	3.602304	-0.849662
H	2.949198	3.625129	-2.584701
H	5.784182	5.040448	-1.732415
H	-1.408853	4.874271	7.178747
H	-2.639880	1.089504	2.333225
h	-3.191879	-4.351950	3.345158
h	-3.691533	-3.327793	-3.761284
h	2.727381	0.139868	-3.250394
h	2.891300	-4.744960	2.403820

$Prod_A'$

C	-3.464982	-3.148727	3.211753
H	-4.288366	-3.108151	2.483880
H	-3.889114	-2.904292	4.197942
N	-1.525209	-1.530032	3.675659
H	-1.475976	-1.662423	4.690247
C	-2.411815	-2.163342	2.821385
C	-0.728812	-0.720335	2.933003
H	0.027676	-0.045033	3.328575
N	-1.049634	-0.816293	1.653068
C	-2.087880	-1.707479	1.568324
H	-2.554528	-1.961460	0.622069
C	-3.188536	-2.390540	-4.156076
H	-2.265271	-2.681236	-4.681489
H	-3.860930	-1.881698	-4.864967
N	-3.688743	-0.777655	-2.242817
H	-4.666000	-0.618259	-2.509358
C	-2.803650	-1.512467	-3.008591
C	-3.006293	-0.156632	-1.255983
H	-3.420304	0.486914	-0.476535
N	-1.720706	-0.465670	-1.341690
C	-1.574503	-1.287427	-2.439190
H	-0.604602	-1.615934	-2.795351
C	1.742487	0.034364	-3.146881
H	1.149099	-0.100758	-4.065247
H	1.525010	-0.800439	-2.468101
C	1.312988	1.338367	-2.477619
O	0.612487	1.267952	-1.414836
O	1.658606	2.437386	-2.963903
C	3.285790	-4.034839	1.559987
H	4.084456	-3.384426	1.946421
H	3.777384	-4.755659	0.884891
N	1.403694	-3.777240	-0.118832
H	1.364478	-4.762764	-0.396976
C	2.269682	-3.226764	0.811207
C	0.638305	-2.787476	-0.628356
H	-0.136073	-2.963365	-1.368706
N	0.961474	-1.621817	-0.094314
C	1.973677	-1.879051	0.806041
H	2.403282	-1.084093	1.411928
Ni	-0.290375	0.171590	-0.034641
O	-1.000578	1.912757	0.844397
O	1.272542	1.780525	2.421354

C	-2.750172	2.677606	5.323968
C	-2.789018	2.143854	4.031159
C	-1.804691	2.480231	3.046647
C	-0.785285	3.355102	3.479674
C	-0.762432	3.933269	4.753545
C	-1.757823	3.593995	5.689310
C	-1.961664	1.896227	1.662184
C	-0.053293	4.251378	-1.178566
C	1.196194	2.961715	2.161319
C	2.186937	3.719421	1.351785
C	2.846399	4.848889	1.855008
C	3.903038	5.403140	1.122019
C	4.245748	4.897844	-0.136258
C	3.481004	3.845972	-0.702386
C	2.509422	3.223717	0.080666
O	0.227321	3.787213	2.634840
O	-3.080793	1.353038	1.406088
O	3.771254	3.502419	-1.970390
O	5.282892	5.430805	-0.815219
O	-0.047650	4.954352	-2.068337
O	-1.816136	4.087269	6.939670
O	-3.782735	1.297570	3.733738
H	-3.534819	2.406753	6.032516
H	0.041600	4.624450	5.016039
H	2.572399	5.264267	2.827109
H	4.495002	6.233332	1.515011
H	1.946511	2.379941	-0.313090
H	2.969292	3.078886	-2.403633
H	5.480760	4.877680	-1.604224
H	-1.201310	4.844721	7.106182
H	-3.706604	1.172646	2.710682
h	-3.092033	-4.170388	3.283755
h	-3.678092	-3.298104	-3.802905
h	2.801267	0.004754	-3.404126
h	2.883914	-4.660092	2.357245

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C	-3.636128	-3.260578	3.184127
H	-4.443469	-3.269540	2.438818
H	-4.094012	-3.038690	4.161874
N	-1.737676	-1.653369	3.706570
H	-1.661851	-1.855651	4.707496
C	-2.640894	-2.210898	2.821834
C	-0.972296	-0.771456	3.026286
H	-0.174739	-0.171878	3.451934
N	-1.327783	-0.727032	1.750945
C	-2.363876	-1.619761	1.609601
H	-2.846907	-1.801788	0.653252
C	-3.044050	-2.295437	-4.086415
H	-2.118340	-2.607124	-4.594659
H	-3.690031	-1.770870	-4.807907
N	-3.528094	-0.608138	-2.227921
H	-4.497014	-0.434587	-2.510791
C	-2.655854	-1.416600	-2.936386
C	-2.836531	0.016022	-1.243011
H	-3.247991	0.721394	-0.522139
N	-1.569115	-0.360931	-1.273198
C	-1.432508	-1.227329	-2.335434
H	-0.462607	-1.615289	-2.632094
C	1.755919	0.493860	-3.729580
H	1.297212	1.020671	-4.578558
H	1.513505	-0.578374	-3.786009
C	1.220918	1.138909	-2.454601
O	1.141116	0.396102	-1.424325
O	0.943813	2.358967	-2.512317
C	3.276638	-4.192207	1.607381
H	4.116570	-3.571309	1.952047
H	3.695507	-4.923059	0.896016
N	1.292197	-3.866987	0.068117
H	1.254162	-4.834350	-0.268128
C	2.228992	-3.351899	0.948587
C	0.458288	-2.868099	-0.296364
H	-0.377537	-3.003466	-0.975882
N	0.810659	-1.739717	0.287170
C	1.906459	-2.016856	1.066469
H	2.376012	-1.240840	1.667518
Ni	-0.112609	0.125971	0.122800
O	0.530708	1.116369	1.990002
O	1.434564	2.209606	2.325354

C	-2.712026	2.877549	5.745278
C	-2.701806	2.389857	4.446307
C	-1.685749	2.789524	3.530646
C	-0.674070	3.682850	3.963314
C	-0.704915	4.212282	5.253102
C	-1.725480	3.803662	6.139385
C	-1.750084	2.363009	2.163670
C	-0.545846	2.639594	1.269083
C	0.694368	3.346117	1.956583
C	1.625247	4.218513	1.144740
C	2.515654	5.118629	1.749154
C	3.649211	5.537110	1.038474
C	3.904879	5.087007	-0.264061
C	2.929075	4.295475	-0.912737
C	1.827311	3.850528	-0.188284
O	0.303212	4.099693	3.127752
O	-2.725092	1.764853	1.681529
O	3.124915	3.945197	-2.208657
O	5.075908	5.413594	-0.861338
O	-0.667796	2.433694	0.066622
O	-1.817088	4.248312	7.397141
O	-3.653861	1.535909	4.036882
H	-3.500134	2.585629	6.440133
H	0.073251	4.908132	5.569838
H	2.362796	5.441502	2.779962
H	4.404951	6.174455	1.505836
H	1.144486	3.167632	-0.688525
H	2.349617	3.385286	-2.483204
H	5.238737	4.834929	-1.634786
H	-1.189486	4.995204	7.590296
H	-3.528232	1.427256	3.046655
h	-3.205869	-4.257843	3.275810
h	-3.565300	-3.194887	-3.758764
h	2.838080	0.608021	-3.792516
h	2.886600	-4.797756	2.425457

$Int2_B'$

C	-3.561003	-3.253946	3.184965
H	-4.359801	-3.227872	2.430431
H	-4.022235	-3.015269	4.156943
N	-1.565607	-1.759764	3.709095
H	-1.496925	-1.963039	4.710415
C	-2.517391	-2.246267	2.833717
C	-0.765636	-0.908767	3.027666
H	0.056871	-0.363650	3.475083
N	-1.145569	-0.810768	1.763684
C	-2.230554	-1.644999	1.629339
H	-2.742694	-1.781210	0.681519
C	-3.117686	-2.327703	-4.119414
H	-2.196103	-2.625111	-4.643938
H	-3.781831	-1.808520	-4.828705
N	-3.583442	-0.661935	-2.236631
H	-4.553401	-0.478491	-2.510669
C	-2.718877	-1.455478	-2.970546
C	-2.880006	-0.056510	-1.248467
H	-3.279681	0.629620	-0.503588
N	-1.614769	-0.431405	-1.306066
C	-1.488853	-1.277718	-2.383393
H	-0.519647	-1.653421	-2.697137
C	1.718471	0.642087	-3.902625
H	1.310210	1.284487	-4.695477
H	1.432401	-0.403193	-4.093052
C	1.172923	1.140240	-2.571046
O	1.100388	0.280183	-1.636450
O	0.879374	2.354963	-2.487752
C	3.270234	-4.232132	1.586278
H	4.097282	-3.592731	1.928111
H	3.710419	-4.975130	0.900781
N	1.312412	-3.959320	-0.001265
H	1.280414	-4.935670	-0.314878
C	2.229129	-3.419794	0.884406
C	0.501732	-2.967230	-0.432327
H	-0.310866	-3.123425	-1.136052
N	0.845212	-1.820719	0.118609
C	1.915069	-2.079596	0.940269
H	2.382577	-1.292347	1.528667
Ni	-0.098946	0.057978	-0.041233
O	0.583780	1.259164	2.203440
O	1.484146	2.297141	2.680154

C	-2.750754	2.935982	5.807453
C	-2.727079	2.427857	4.515909
C	-1.691865	2.799190	3.611287
C	-0.717049	3.735491	4.029717
C	-0.758620	4.286958	5.308995
C	-1.768945	3.865839	6.200775
C	-1.664291	2.238451	2.284729
C	-0.330661	2.295781	1.509584
C	0.712330	3.368697	2.110446
C	1.620673	4.186816	1.234814
C	2.522700	5.102665	1.801430
C	3.631684	5.520027	1.056540
C	3.847613	5.057120	-0.248290
C	2.857621	4.254524	-0.860817
C	1.778797	3.803067	-0.100559
O	0.231596	4.186012	3.169358
O	-2.639984	1.656558	1.789741
O	3.023002	3.909178	-2.160184
O	4.995650	5.388414	-0.886015
O	-0.460938	2.031992	0.258293
O	-1.860593	4.308264	7.459824
O	-3.677331	1.569257	4.109985
H	-3.543369	2.651580	6.500271
H	0.001649	5.007372	5.614894
H	2.393977	5.440615	2.830888
H	4.395459	6.170026	1.492430
H	1.073997	3.112509	-0.562272
H	2.235484	3.355270	-2.425624
H	5.142546	4.799349	-1.653389
H	-1.222964	5.045618	7.656012
H	-3.527775	1.436158	3.125722
h	-3.169495	-4.266973	3.277508
h	-3.617944	-3.234326	-3.779055
h	2.805999	0.713310	-3.919246
h	2.873515	-4.822136	2.412459

$TS3_B'$

C	-3.623800	-3.295622	3.208548
H	-4.443653	-3.293566	2.477102
H	-4.060781	-3.062308	4.192938
N	-1.678782	-1.721390	3.676441
H	-1.594928	-1.902988	4.680270
C	-2.616046	-2.267260	2.821047
C	-0.901948	-0.874420	2.959680
H	-0.093891	-0.283719	3.379345
N	-1.284561	-0.846261	1.694494
C	-2.346102	-1.707919	1.590951
H	-2.853508	-1.893330	0.647225
C	-3.108589	-2.339486	-4.124983
H	-2.187418	-2.646445	-4.644772
H	-3.768987	-1.824338	-4.840669
N	-3.572858	-0.666361	-2.248381
H	-4.548017	-0.497109	-2.513625
C	-2.706978	-1.455542	-2.985988
C	-2.867044	-0.040021	-1.276333
H	-3.267597	0.648754	-0.534179
N	-1.596476	-0.396703	-1.348584
C	-1.471656	-1.254280	-2.417820
H	-0.500240	-1.620610	-2.736450
C	1.742462	0.664284	-3.943918
H	1.340403	1.312505	-4.735032
H	1.446265	-0.378188	-4.133221
C	1.209869	1.168171	-2.611890
O	1.117714	0.299210	-1.682881
O	0.952435	2.386886	-2.511387
C	3.259089	-4.200870	1.583504
H	4.088364	-3.564144	1.925111
H	3.695340	-4.939109	0.890110
N	1.289898	-3.921230	0.012403
H	1.251675	-4.898568	-0.296181
C	2.214620	-3.383223	0.891466
C	0.483439	-2.926433	-0.419562
H	-0.334182	-3.080138	-1.117965
N	0.838057	-1.779549	0.124516
C	1.909995	-2.040066	0.943199
H	2.384606	-1.249941	1.521667
Ni	-0.073707	0.111482	-0.094334
O	0.468333	1.074918	1.723450
O	1.539308	2.348698	2.767566

C	-2.689457	2.890752	5.754243
C	-2.645320	2.378531	4.465445
C	-1.607083	2.765707	3.567540
C	-0.663444	3.735960	3.987393
C	-0.728433	4.288770	5.266749
C	-1.734034	3.847228	6.152160
C	-1.593660	2.236000	2.230915
C	-0.272946	2.274165	1.397344
C	0.853457	3.303483	2.155243
C	1.756286	4.120040	1.245222
C	2.649816	5.045214	1.813865
C	3.741170	5.492003	1.062907
C	3.954591	5.043130	-0.247615
C	2.975901	4.224574	-0.856851
C	1.916080	3.742329	-0.086888
O	0.256377	4.204627	3.119272
O	-2.579819	1.674711	1.734664
O	3.130068	3.899403	-2.162901
O	5.091131	5.401426	-0.890909
O	-0.520960	2.280384	0.133675
O	-1.851660	4.294938	7.407061
O	-3.581249	1.503964	4.058782
H	-3.483462	2.592817	6.439987
H	0.010636	5.030885	5.573379
H	2.516650	5.375959	2.844964
H	4.494571	6.155021	1.497315
H	1.216768	3.052289	-0.557439
H	2.334320	3.364157	-2.435160
H	5.244215	4.822946	-1.666069
H	-1.226998	5.041180	7.611216
H	-3.442651	1.389169	3.072107
h	-3.203811	-4.297929	3.292557
h	-3.614942	-3.240327	-3.778346
h	2.830658	0.725007	-3.958358
h	2.870234	-4.797972	2.408323

$Prod_B'$

C	-3.464639	-3.135023	3.236714
H	-4.274106	-3.092389	2.493516
H	-3.912291	-2.913149	4.218017
N	-1.537371	-1.515411	3.755718
H	-1.470597	-1.692858	4.761902
C	-2.424856	-2.121778	2.882460
C	-0.763755	-0.657646	3.039021
H	-0.005439	-0.002856	3.460729
N	-1.102200	-0.688717	1.762894
C	-2.127373	-1.593653	1.650880
H	-2.598374	-1.816419	0.699125
C	-3.146992	-2.399053	-4.153856
H	-2.222909	-2.705300	-4.669121
H	-3.808366	-1.887354	-4.870476
N	-3.626792	-0.726620	-2.285412
H	-4.594237	-0.545863	-2.571182
C	-2.756128	-1.522240	-3.007160
C	-2.941085	-0.131077	-1.281314
H	-3.355508	0.553993	-0.541831
N	-1.677873	-0.520958	-1.315558
C	-1.536010	-1.359860	-2.395216
H	-0.563939	-1.739497	-2.695227
C	1.687678	0.695278	-3.865120
H	1.305256	1.382438	-4.632905
H	1.349612	-0.328103	-4.084961
C	1.183923	1.175635	-2.510280
O	1.035702	0.284881	-1.614228
O	1.009902	2.405063	-2.354722
C	3.289785	-4.238485	1.607538
H	4.118460	-3.602906	1.952603
H	3.728006	-4.982325	0.921848
N	1.334374	-3.961689	0.018618
H	1.300677	-4.937507	-0.296919
C	2.249588	-3.424553	0.906317
C	0.518485	-2.970332	-0.403782
H	-0.295661	-3.126883	-1.105596
N	0.857317	-1.825193	0.152864
C	1.930131	-2.085599	0.969763
H	2.401864	-1.302903	1.560861
Ni	-0.190218	0.056397	-0.034952
O	-0.877841	1.921632	0.050604
O	0.862040	1.976040	2.431163

C	-2.829869	2.746772	5.776860
C	-2.847358	2.238480	4.476885
C	-1.889679	2.636272	3.485675
C	-0.873670	3.533368	3.938299
C	-0.869141	4.062523	5.225120
C	-1.859915	3.680801	6.152121
C	-2.116593	2.159676	2.108250
C	-1.350004	2.720880	0.911455
C	0.938822	3.186257	2.386003
C	1.894371	3.935541	1.542288
C	2.707565	4.964489	2.041490
C	3.760811	5.437731	1.250769
C	3.956617	4.956500	-0.049193
C	3.022383	4.045456	-0.606453
C	2.045160	3.490029	0.219992
O	0.158812	3.999125	3.154081
O	-3.076188	1.408599	1.838266
O	3.161039	3.747466	-1.912594
O	5.021381	5.380129	-0.765036
O	-1.375573	3.946756	0.858966
O	-1.913319	4.152474	7.404407
O	-3.815056	1.365118	4.169474
H	-3.605827	2.439852	6.479516
H	-0.071431	4.751984	5.508329
H	2.559862	5.346548	3.053349
H	4.480522	6.164913	1.634822
H	1.359179	2.749970	-0.193681
H	2.336199	3.247289	-2.208206
H	5.147954	4.806418	-1.547920
H	-1.283502	4.904364	7.561564
H	-3.722982	1.188729	3.171966
h	-3.087412	-4.155452	3.303719
h	-3.650757	-3.298957	-3.801066
h	2.777218	0.716941	-3.887484
h	2.889573	-4.828247	2.432206
