Supporting Information

A Detailed Quantum Chemical Investigation on Hydrolysis Mechanism of Osmium(III) Anticancer Drug, (ImH)[*trans*-$OsCl_4$(DMSO)(Im)] (Os-NAMI-A; Im=imidazole)

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1. **Table S1.** Selected bond lengths (Å), bond angles (°) of all the stationary points involved in the first hydrolysis of Os-NAMI-A, calculated at M06- 2X/(LanL2DZ+6-31G(d, p))

Reaction	Parameters	R	RC-1_A	TS-1_A	PC-1_A	P-1A
R→ P-1A (Path-A)	Os−S(DMSO)	2.34	2.34	3.21	4.52	--
	Os−O1(wat1)	--	4.01	2.96	2.13	2.20
	∠S−Os−O1(wat1)			54.76		
R→ P-1B (Path-B)		**R**	**RC-1_B**	**TS-1_B**	**PC-1_B**	**P-1B**
	Os−Cl1	2.42	2.42	2.91	4.49	--
	Os−O1(wat1)	--	3.99	2.57	2.08	2.13
	∠Cl1−Os−O1(wat1)			62.38		

2. **Table S2.** Selected bond lengths (Å), bond angles (°) of all the stationary points involved in the second hydrolysis of Os-NAMI-A, calculated at M06- 2X/(LanL2DZ+6-31G(d, p))

Reaction	Parameters	P-1A	RC-2	TS-2	PC-2	P-2A
P-1A→ P2A (Step-2)	Os−Cl1	2.43	2.45	3.08	4.33	--
	Os−O2(wat2)	--	3.63	2.53	2.07	2.15
	∠Cl1−Os−O2(wat2)			60.64		
P-1B → P-2A (Step-3) (Path-A)		**P-1B**	**RC-2_A**	**TS-2_A**	**PC-2_A**	**P-2A**
	Os−S(DMSO)	2.31	2.34	3.25	4.67	--
	Os−O2(wat2)	--	3.69	2.79	2.09	2.18
	∠S−Os−O2(wat2)			58.04		
P-1B → P-2B (Step-3) (Path-B)		**P-1B**	**RC-2_B**	**TS-2_B**	**PC-2_B**	**P-2B**
	Os−Cl2(DMSO)	2.40	2.41	2.77	3.91	--
	Os−O2(wat2)	--	3.93	2.62	2.14	2.12
	∠Cl2−Os−O2(wat2)			64.07		
P-1B → P-2C (Step-3) (Path-C)		**P-1B**	**RC-2_C**	**TS-2_C**	**PC-2_C**	**P-2C**
	Os−Cl3(DMSO)	2.38	2.39	2.79	4.18	--
	Os−O2(wat2)	--	3.94	2.42	2.05	2.10
	∠Cl3−Os−O2(wat2)			63.44		

3. **Table S3.** Selected bond lengths (Å), bond angles (°) of all the stationary points involved in the third hydrolysis of Os-NAMI-A, calculated at M06- 2X/(LanL2DZ+6-31G(d, p))

Reaction	Parameters	P-2A	RC-3_A	TS-3_A	PC-3_A	P-2A
P-2A→ P3A (Path-A)	Os−Cl2	2.42	2.41	2.71	3.73	--
	Os−O3(wat3)	--	3.86	2.68	2.16	2.12
	∠Cl2−Os−O3(wat3)			66.19		
P-2A→ P-3B (Path-B)		**P-2A**	**RC-3_B**	**TS-3_B**	**PC-3_B**	**P-2A**
	Os−Cl3	2.38	2.38	2.78	3.95	--
	Os−O3(wat3)	--	3.86	2.50	2.11	2.09
	∠Cl3−Os−O3(wat3)			65.48		

		P-2B	RC-3	TS-3	PC-3	P-2B
P-2B → P-3A (Step-2)	Os−S(DMSO)	2.33	2.34	2.90	4.40	--
	Os−O3(wat3)	--	3.75	2.63	2.17	2.19
	∠S−Os−O3(wat3)			60.13		
		P-2C	**RC-3′**	**TS-3′**	**PC-3′**	**P-2C**
P-2B → P-3B (Step-3)	Os−S(DMSO)	2.37	2.37	2.86	4.40	--
	Os−O3(wat3)	--	3.72	2.55	2.13	2.10
	∠S−Os−O3(wat3)			63.03		

4. **Table S4.** Change of Gibbs free energies (Δ*G*) and enthalpies (Δ*H*) for the first hydrolysis of Os-NAMI-A calculated at 298.15 K in solvent medium. (Energy values are in kcal/mol)

Reaction	Species	Δ*G*(aq)	Δ*H*(aq)
R → P-1A (step-1)	$RC\text{-}1_A$	0	0
	$TS\text{-}1_A$	24.66	25.30
	$PC\text{-}1_A$	4.71	5.77
R → P-1B (step-1)	$RC\text{-}1_B$	0	0
	$TS\text{-}1_B$	28.72	27.49
	$PC\text{-}1_B$	1.24	-0.11

5. **Table S5:** Change of Gibbs free energies (Δ*G*) and enthalpies (Δ*H*) for the second hydrolysis of Os-NAMI-A calculated at 298.15 K in solvent medium. (Energy values are in kcal/mol)

Reaction	Species	Δ*G*(aq)	Δ*H*(aq)
P-1A → P-2A (step-1)	RC-2	0	0
	TS-2	25.38	24.31
	PC-2	2.99	4.06
P-1B → P-2A (step-2)	$RC\text{-}2_A$	0	0
	$TS\text{-}2_A$	24.83	26.15
	$PC\text{-}2_A$	10.22	13.73
P-1B → P-2B (step-3)	$RC\text{-}2_B$	0	0
	$TS\text{-}2_B$	22.62	21.13
	$PC\text{-}2_B$	4.87	3.17
P-1B → P-2C (step-3)	$RC\text{-}2_C$	0	0
	$TS\text{-}2_C$	29.56	28.11
	$PC\text{-}2_C$	5.82	4.08

6. **Table S6:** Change of Gibbs free energies (ΔG) and enthalpies (ΔH) for the third hydrolysis of Os-NAMI-A calculated at 298.15 K in solvent medium. (Energy values are in kcal/mol)

Reaction	Species	ΔG(aq)	ΔH(aq)
P-2A→ P3A (Path-A)	$RC\text{-}3_A$	0	0
	$TS\text{-}3_A$	17.27	14.93
	$PC\text{-}3_A$	4.93	2.35
P-2A→ P-3B (Path-B)	$RC\text{-}3_B$	0	0
	$TS\text{-}3_B$	24.86	20.82
	$PC\text{-}3_B$	3.39	2.95
P-2B → P-3A (Step-2)	RC-3	0	0
	TS-3	17.83	16.60
	PC-3	-8.56	-9.87
P-2B → P-3B (Step-3)	RC-3′	0	0
	TS-3′	23.09	20.41
	PC-3′	-5.43	-5.93

7. **Table S7:** NPA charges on the central Os, incoming O (H_2O), leaving Cl or S (DMSO) atoms, calculated for each hydrolysis step of Os-NAMI-A (in the unit of electronic charge |e|)

Reaction	Atom	R	RC	TS	PC	P
DMSO Hydrolysis of R (Step-1)	Os	-0.195	-0.208	0.279	0.270	0.234
	S(DMSO)	1.521	1.511	1.259	1.196	--
	O1(wat1)	--	-0.992	-0.969	-0.881	-0.829
Cl1 Hydrolysis of R (Step-1)	Os	-0.195	-0.200	0.040	0.006	-0.023
	Cl1	-0.401	-0.404	-0.709	-0.872	--
	O1(wat1)	--	-0.981	-0.915	-0.869	-0.821
Cl1 Hydrolysis of P-1A (Step-2)	Os	0.234	0.242	0.463	0.471	0.433
	Cl1	-0.447	-0.466	-0.779	-0.869	--
	O2(wat2)	--	-0.955	-0.966	-0.867	-0.820
DMSO Hydrolysis of P-1B (Step-3)	Os	-0.023	-0.009	0.442	0.465	0.433
	S(DMSO)	1.502	1.499	1.238	1.191	--
	O2(wat2)	--	-0.955	-0.988	-0.899	-0.833
Cl2 Hydrolysis of P-1B (Step-3)	Os	-0.023	-0.026	0.153	0.213	0.196
	Cl2	-0.375	-0.380	-0.651	-0.810	--
	O2(wat2)	--	-0.973	-0.902	-0.876	-0.808
Cl3 Hydrolysis of P-1B (Step-3)	Os	-0.023	-0.027	0.183	0.237	0.232
	Cl3	-0.351	-0.359	-0.651	-0.821	--
	O2(wat2)	--	-0.907	-0.955	-0.855	-0.900
Cl2 Hydrolysis of P-2A (Step-4)	Os	0.438	0.423	0.552	0.666	0.622
	Cl2	-0.453	-0.434	-0.649	-0.838	--
	O3(wat3)	--	-0.974	-0.916	-0.857	-0.821
Cl3 Hydrolysis of P-2A (Step-4)	Os	0.438	0.423	0.610	0.678	0.554
	Cl3	-0403	-0.393	-0.671	-0.824	--
	O3(wat3)	--	-0.974	-0.894	-0.824	-0797
DMSO Hydrolysis of P-2B	Os	0.196	0.218	0.591	0.619	0.614

(Step-5)	S(DMSO) O3(wat3)	1.485 --	1.471 -0.967	1.297 -0.929	1.203 -0.876	-- -0.843
DMSO Hydrolysis of P-2C (Step-6)	Os S(DMSO) O3(wat3)	0.243 1.468 --	0.245 1.473 -0.934	0.591 1.297 -0.929	0.682 1.205 -0.851	0.554 -- -0.826

8. Table S8: The Cartesian coordinate of transition states, reactants and products intermediates, involve in first, second and third hydrolysis reaction of Os-NAMI-A

RC-1$_A$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.693865	0.504723	-0.585566
2	17	0	1.059986	0.612517	-2.668857
3	17	0	0.394997	0.298450	2.133251
4	17	0	3.112587	0.362878	0.079043
5	16	0	0.630490	-1.945742	-0.498035
6	8	0	1.922468	-2.714832	-0.600840
7	6	0	-0.339099	-2.678646	0.818635
8	1	0	-1.263907	-2.107989	0.919171
9	1	0	-0.528115	-3.722052	0.561274
10	1	0	0.274630	-2.597977	1.716950
11	6	0	-0.364092	-2.400401	-1.915716
12	1	0	0.136386	-2.002427	-2.797794
13	1	0	-0.416541	-3.489608	-1.943807
14	1	0	-1.348971	-1.945925	-1.800995
15	7	0	0.763242	2.468702	-0.121320
16	6	0	1.447715	3.219346	0.808798
17	6	0	0.121712	3.312417	-0.912056
18	1	0	2.050187	2.749902	1.569174
19	1	0	-0.506148	3.035619	-1.744163
20	1	0	1.549407	5.436527	1.055590
21	1	0	-0.001729	5.403412	-0.963162
22	7	0	0.369971	4.573658	-0.523010
23	6	0	1.208088	4.540211	0.565448
24	76	0	0.715889	0.384357	-0.276986
25	8	0	2.602792	-2.205195	2.150218
26	1	0	2.340957	-1.273491	2.135213
27	1	0	2.677041	-2.421025	1.206704

TS-1$_A$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.215945	-3.369256	0.006349
2	8	0	1.562582	-4.634204	-0.552400
3	6	0	3.668566	-3.064124	-1.007712
4	1	0	4.206987	-2.212418	-0.588637
5	1	0	4.290409	-3.960956	-1.025364
6	1	0	3.307799	-2.819432	-2.006790
7	6	0	3.048701	-3.864691	1.523543

8	1	0	2.265068	-4.096019	2.246698
9	1	0	3.661123	-4.746339	1.324579
10	1	0	3.652302	-3.029436	1.881607
11	7	0	-0.063757	1.151950	0.339375
12	6	0	0.716347	2.047107	-0.248699
13	6	0	-1.164091	1.817299	0.838229
14	1	0	1.654410	1.834362	-0.734842
15	1	0	-1.943768	1.291363	1.363610
16	1	0	0.545709	4.115979	-0.508951
17	1	0	-1.665397	3.988416	0.747175
18	76	0	0.310536	-0.824261	0.471481
19	8	0	-0.414166	-3.638564	1.074257
20	1	0	-0.055596	-4.194226	0.358431
21	17	0	2.591605	-0.313539	1.154437
22	7	0	0.152600	3.260280	-0.142734
23	6	0	-1.034169	3.141238	0.538241
24	17	0	1.011776	-0.837996	-1.861480
25	1	0	-1.224998	-3.240623	0.728276
26	17	0	-0.385640	-0.831587	2.790238
27	17	0	-1.984625	-1.282609	-0.230388

PC-1$_A$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.960852	0.835894	-0.194541
2	17	0	0.136863	1.582539	-2.802664
3	7	0	0.746541	2.468017	0.339264
4	6	0	1.567257	2.758342	1.408263
5	6	0	0.175074	3.601861	-0.037900
6	1	0	2.140463	1.985818	1.893624
7	1	0	-0.521420	3.706698	-0.855145
8	1	0	1.956240	4.712737	2.414144
9	1	0	0.305889	5.566908	0.674338
10	7	0	0.595747	4.602235	0.751503
11	6	0	1.480628	4.093370	1.672396
12	76	0	0.438451	0.633003	-0.553453
13	8	0	0.128887	-1.253447	-1.515003
14	1	0	-0.261639	-1.077929	-2.382713
15	1	0	-0.489776	-1.906576	-1.007919
16	16	0	-2.740719	-2.522364	0.059595
17	8	0	-1.284394	-2.906339	-0.282257
18	6	0	-2.704813	-2.025354	1.785346
19	1	0	-3.726277	-1.823917	2.113711
20	1	0	-2.250895	-2.824244	2.375210
21	1	0	-2.097187	-1.120209	1.827389
22	6	0	-3.552565	-4.113562	0.263474
23	1	0	-3.629027	-4.572535	-0.722036
24	1	0	-2.946891	-4.732612	0.927453
25	1	0	-4.548587	-3.950874	0.678437
26	17	0	2.832185	0.431530	-0.935967
27	17	0	0.687049	-0.442401	1.643975

RC-1$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.609052	0.299773	-0.610436
2	17	0	1.185208	0.090065	-2.579681
3	17	0	0.394576	0.303962	2.212810
4	17	0	3.171169	0.096796	0.220385
5	16	0	0.606246	-2.200716	-0.093189
6	8	0	1.831374	-3.024249	0.163365
7	6	0	-0.644151	-2.683799	1.097953
8	1	0	-1.561708	-2.138969	0.868968
9	1	0	-0.781208	-3.763381	1.019881
10	1	0	-0.274169	-2.400416	2.082478
11	6	0	-0.168367	-2.811328	-1.590492
12	1	0	0.529364	-2.632748	-2.407607
13	1	0	-0.357861	-3.877671	-1.458633
14	1	0	-1.090609	-2.250286	-1.751462
15	7	0	0.898777	2.223233	-0.243228
16	6	0	1.582451	3.039604	0.630337
17	6	0	0.372113	2.999476	-1.174737
18	1	0	2.104273	2.633596	1.481795
19	1	0	-0.222600	2.662006	-2.009193
20	1	0	1.833867	5.257952	0.607511
21	1	0	0.404511	5.069533	-1.490356
22	7	0	0.686725	4.280426	-0.926420
23	6	0	1.456789	4.331025	0.208946
24	76	0	0.776636	0.138627	-0.174652
25	8	0	3.362086	2.530581	-2.056528
26	1	0	3.450133	2.145434	-1.173631
27	1	0	2.678974	1.965815	-2.444797

TS-1_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.492384	0.410650	0.636766
2	17	0	0.044468	0.167836	-2.224986
3	17	0	1.107675	0.542509	2.565312
4	17	0	3.607668	-0.399461	0.689578
5	16	0	0.869146	-2.033078	0.042117
6	8	0	1.735014	-2.686795	-0.991687
7	6	0	1.239697	-2.748897	1.641543
8	1	0	0.528394	-2.351199	2.366772
9	1	0	1.167201	-3.834183	1.551059
10	1	0	2.251052	-2.429383	1.892957
11	6	0	-0.789964	-2.669707	-0.203403
12	1	0	-1.160976	-2.228177	-1.128884
13	1	0	-0.703633	-3.754057	-0.289436
14	1	0	-1.423153	-2.377367	0.633441
15	7	0	0.805735	2.430751	0.140523
16	6	0	1.724357	3.267281	0.731105
17	6	0	-0.073445	3.190627	-0.487999
18	1	0	2.547950	2.874586	1.305922
19	1	0	-0.918728	2.833417	-1.055449
20	1	0	1.834132	5.497540	0.722278
21	1	0	-0.270328	5.266876	-0.694924
22	7	0	0.246691	4.484745	-0.319025

23	6	0	1.383373	4.557866	0.450188
24	76	0	0.843903	0.346261	0.139574
25	8	0	2.652555	1.176483	-1.495526
26	1	0	3.384466	0.638793	-1.146071
27	1	0	2.336141	0.735300	-2.296258

PC-1_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.823092	0.418571	-0.101959
2	17	0	0.743248	0.369015	-2.434000
3	17	0	0.595257	0.166492	2.393126
4	16	0	0.511955	-2.099275	-0.109406
5	8	0	1.903041	-2.683969	-0.034873
6	6	0	-0.490554	-2.821354	1.183001
7	1	0	-1.491155	-2.391261	1.103910
8	1	0	-0.502402	-3.903732	1.049224
9	1	0	-0.032454	-2.538254	2.130044
10	6	0	-0.309983	-2.728959	-1.566305
11	1	0	0.266886	-2.389409	-2.425649
12	1	0	-0.336961	-3.817507	-1.504659
13	1	0	-1.313957	-2.299446	-1.591100
14	7	0	0.746376	2.297586	0.051980
15	6	0	1.563322	3.053063	0.866035
16	6	0	0.056849	3.137385	-0.703561
17	1	0	2.243855	2.593217	1.568378
18	1	0	-0.671722	2.856275	-1.447482
19	1	0	1.787497	5.271207	0.989557
20	1	0	0.016197	5.226456	-0.838399
21	7	0	0.400565	4.399447	-0.403673
22	6	0	1.354334	4.371928	0.584925
23	76	0	0.577958	0.215721	-0.023921
24	8	0	2.652683	-0.026274	0.015914
25	17	0	4.524334	1.218824	1.890713
26	1	0	2.841868	-0.985955	0.072796
27	1	0	3.230665	0.455962	0.696977

RC-2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.821579	0.491814	-0.625749
2	17	0	0.929841	0.436295	-2.687800
3	17	0	0.237035	0.165828	2.123497
4	17	0	2.995703	0.186106	0.072665
5	7	0	0.661381	2.406117	-0.170538
6	6	0	1.358304	3.155783	0.752534
7	6	0	0.060404	3.252113	-0.991570
8	1	0	1.934136	2.683585	1.531993
9	1	0	-0.562277	2.975886	-1.827553
10	1	0	1.531021	5.373667	0.948251
11	1	0	0.009151	5.344510	-1.091037

12	7	0	0.346448	4.513320	-0.626743
13	6	0	1.166328	4.477829	0.474455
14	76	0	0.573228	0.356011	-0.268588
15	8	0	2.501095	-2.244698	-1.932116
16	8	0	0.457623	-1.831438	-0.344977
17	1	0	0.598229	-2.174518	0.548775
18	1	0	1.216968	-2.151709	-0.910749
19	1	0	3.098901	-1.693828	-1.399240
20	1	0	2.166524	-1.614844	-2.592741

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.729865	0.554059	-0.184234
2	17	0	0.614859	0.270561	-2.656836
3	17	0	0.553020	0.009893	2.267239
4	17	0	3.549192	0.930938	0.494909
5	7	0	0.792069	2.289263	-0.209513
6	6	0	1.158850	3.082075	0.859093
7	6	0	0.432252	3.099367	-1.195607
8	1	0	1.498983	2.644129	1.782446
9	1	0	0.080693	2.785459	-2.164491
10	1	0	1.210563	5.305392	1.029210
11	1	0	0.359757	5.181100	-1.370075
12	7	0	0.565499	4.372462	-0.800373
13	6	0	1.023127	4.388048	0.497139
14	76	0	0.613662	0.237317	-0.173945
15	8	0	2.464864	-1.330204	-0.923263
16	8	0	0.120282	-1.909551	-0.034739
17	1	0	-0.036686	-2.074172	0.909675
18	1	0	0.957918	-2.350530	-0.260328
19	1	0	3.184944	-0.797935	-0.518061
20	1	0	2.444823	-1.095799	-1.864180

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.704343	0.178594	-0.371942
2	17	0	1.120568	0.225389	-2.391358
3	17	0	0.442285	-0.267659	2.413502
4	7	0	0.801017	2.136608	0.154191
5	6	0	1.256444	2.851801	1.243123
6	6	0	0.450678	3.011973	-0.778188
7	1	0	1.597434	2.355664	2.137735
8	1	0	0.053360	2.764089	-1.749575
9	1	0	1.434063	5.057969	1.518273
10	1	0	0.475871	5.100938	-0.840537
11	7	0	0.666751	4.253335	-0.324231
12	6	0	1.178112	4.179912	0.949780
13	76	0	0.672874	0.102761	0.007685

14	8	0	2.718573	-0.055485	0.345520
15	17	0	4.486676	2.081008	-0.540135
16	1	0	2.923749	-0.256704	1.271139
17	1	0	3.314668	0.710740	0.032172
18	8	0	0.607190	-2.066139	-0.117277
19	1	0	-0.008902	-2.388103	-0.791735
20	1	0	0.312647	-2.425361	0.734847

RC-2_A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.779591	0.458103	-0.524368
2	17	0	1.065843	0.586681	-2.590601
3	17	0	0.515529	0.200716	2.173007
4	16	0	0.485921	-1.981040	-0.421597
5	8	0	1.773100	-2.763150	-0.279996
6	6	0	-0.689851	-2.661075	0.741024
7	1	0	-1.646036	-2.155310	0.595547
8	1	0	-0.763329	-3.733566	0.555386
9	1	0	-0.300688	-2.457419	1.738465
10	6	0	-0.258969	-2.466804	-1.973262
11	1	0	0.418629	-2.147708	-2.764279
12	1	0	-0.379365	-3.550681	-1.962635
13	1	0	-1.217050	-1.950758	-2.060356
14	7	0	0.690060	2.424257	-0.080086
15	6	0	1.507030	3.141233	0.766296
16	6	0	0.002236	3.296167	-0.799093
17	1	0	2.171955	2.646077	1.455071
18	1	0	-0.726737	3.051217	-1.555607
19	1	0	1.730267	5.350680	0.993728
20	1	0	-0.035537	5.389324	-0.839666
21	7	0	0.347087	4.542930	-0.441754
22	6	0	1.298479	4.471114	0.546702
23	76	0	0.596575	0.352246	-0.240066
24	8	0	3.266849	-1.466968	1.555863
25	1	0	2.668784	-1.286697	2.296816
26	1	0	2.813843	-2.156668	1.022175
27	8	0	2.707667	0.436669	0.010360
28	1	0	3.039712	-0.317378	0.629584
29	1	0	3.150393	0.357284	-0.848009

TS-2_A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.050219	-3.531661	0.830920
2	8	0	1.240028	-4.726170	1.356289
3	6	0	3.007121	-4.143085	-0.563045
4	1	0	3.681685	-3.351840	-0.893117
5	1	0	3.557251	-5.034330	-0.255633
6	1	0	2.299594	-4.384352	-1.356985
7	6	0	3.394734	-3.263240	1.989496
8	1	0	2.942636	-2.959913	2.933459
9	1	0	3.964984	-4.186671	2.103643

10	1	0	4.018420	-2.455641	1.600832
11	7	0	-0.028805	1.138682	0.423593
12	6	0	0.842596	2.049916	0.832127
13	6	0	-1.164362	1.799640	0.000755
14	1	0	1.826444	1.845912	1.222718
15	1	0	-2.016637	1.263762	-0.384835
16	1	0	0.761935	4.137233	0.920474
17	1	0	-1.587579	3.987792	-0.048037
18	76	0	0.228528	-0.856325	0.448856
19	8	0	-0.904059	-3.398531	0.645341
20	1	0	-0.253913	-4.074513	0.976931
21	8	0	-1.706739	-1.080433	1.308486
22	17	0	1.023686	-0.706227	2.726608
23	1	0	-1.758788	-0.731143	2.211166
24	1	0	-1.803809	-2.060441	1.340463
25	7	0	0.303016	3.268590	0.683189
26	6	0	-0.960324	3.137929	0.161986
27	17	0	2.413388	-0.567464	-0.500094
28	1	0	-1.041331	-3.558717	-0.297524
29	17	0	-0.826202	-1.148716	-1.692576

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.675222	2.317627	-2.169821
2	17	0	1.732690	1.910618	-2.717856
3	7	0	0.439391	2.310247	0.268584
4	6	0	0.313594	2.129882	1.632824
5	6	0	0.902556	3.539849	0.073694
6	1	0	-0.052507	1.202647	2.042405
7	1	0	1.112865	3.981579	-0.887757
8	1	0	0.765024	3.542314	3.298404
9	1	0	1.409191	5.088904	1.379864
10	7	0	1.069381	4.145088	1.254280
11	6	0	0.709129	3.273708	2.256932
12	76	0	0.040437	0.950187	-1.222381
13	8	0	-0.183247	-0.524542	-2.689134
14	1	0	0.154634	-0.220827	-3.544233
15	1	0	-1.157065	-0.904468	-2.809719
16	16	0	-2.897104	-2.584531	-2.063275
17	8	0	-2.473164	-1.388693	-2.950123
18	6	0	-1.364116	-3.382186	-1.558279
19	1	0	-1.612864	-4.322176	-1.062937
20	1	0	-0.745764	-3.554327	-2.441482
21	1	0	-0.873228	-2.703828	-0.859947
22	6	0	-3.446117	-3.819275	-3.250559
23	1	0	-4.350963	-3.434176	-3.720405
24	1	0	-2.662841	-3.969064	-3.995293
25	1	0	-3.668187	-4.745446	-2.718106
26	17	0	-1.500847	-0.291530	0.243905
27	8	0	1.544654	-0.288373	-0.385510
28	1	0	1.180187	-1.043559	0.102696
29	1	0	2.216567	-0.610470	-1.005225

RC-2_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.472912	0.492489	0.524069
2	17	0	0.265634	0.229124	-2.493457
3	17	0	1.654803	0.641418	2.093604
4	16	0	0.910418	-1.935258	0.042258
5	8	0	2.295903	-2.416485	-0.328162
6	6	0	0.492914	-2.535302	1.672122
7	1	0	-0.508754	-2.169784	1.909213
8	1	0	0.534576	-3.624981	1.663336
9	1	0	1.222794	-2.110734	2.360212
10	6	0	-0.295407	-2.784113	-0.965818
11	1	0	-0.084443	-2.514513	-2.000106
12	1	0	-0.191715	-3.857325	-0.801139
13	1	0	-1.284061	-2.423481	-0.673915
14	7	0	0.904841	2.443173	-0.374942
15	6	0	1.931005	3.270582	0.027709
16	6	0	-0.043347	3.210341	-0.886767
17	1	0	2.822699	2.877428	0.489818
18	1	0	-0.982244	2.862176	-1.288064
19	1	0	2.098146	5.492797	-0.101302
20	1	0	-0.207456	5.279054	-1.154756
21	7	0	0.339604	4.493742	-0.830275
22	6	0	1.583280	4.559181	-0.253679
23	76	0	0.817582	0.375117	-0.153634
24	8	0	2.856140	0.211123	-0.755388
25	1	0	3.060333	-0.754203	-0.766851
26	1	0	3.031791	0.568729	-1.639751
27	8	0	-0.499127	3.218338	2.232749
28	1	0	0.379073	2.817044	2.271403
29	1	0	-1.001945	2.560486	1.733368

TS-2_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.700410	0.416783	-1.057069
2	17	0	1.331926	0.328226	-2.290967
3	17	0	1.076755	0.049639	2.639724
4	16	0	0.532713	-1.927470	-0.023946
5	8	0	1.949819	-2.418897	0.159237
6	6	0	-0.523448	-2.649589	1.224329
7	1	0	-1.539236	-2.293628	1.038083
8	1	0	-0.460539	-3.736065	1.148786
9	1	0	-0.160220	-2.288082	2.185569
10	6	0	-0.138758	-2.666463	-1.506397
11	1	0	0.465997	-2.307123	-2.338376
12	1	0	-0.071471	-3.750154	-1.402563
13	1	0	-1.170896	-2.329342	-1.613612
14	7	0	0.707529	2.481550	-0.091373
15	6	0	1.179134	3.273168	0.932436
16	6	0	0.367482	3.282478	-1.087280
17	1	0	1.502202	2.844918	1.869206
18	1	0	-0.042034	2.965968	-2.033838

19	1	0	1.394132	5.492571	1.030688
20	1	0	0.434620	5.362240	-1.324307
21	7	0	0.607575	4.556490	-0.739421
22	6	0	1.122805	4.576284	0.533902
23	76	0	0.521735	0.412967	-0.057135
24	8	0	-1.265605	1.347646	1.616425
25	1	0	-1.026831	0.930377	2.456311
26	1	0	-2.073707	0.916490	1.307683
27	8	0	2.681084	0.280595	0.294495
28	1	0	2.816865	0.455919	1.243639
29	1	0	2.845420	-0.685167	0.199322

PC-2_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.376694	0.261117	1.166474
2	17	0	-0.065169	0.250633	-2.140152
3	16	0	0.898534	-2.010218	0.083743
4	8	0	2.029222	-2.578080	-0.711534
5	6	0	0.948325	-2.655518	1.753335
6	1	0	0.086304	-2.262449	2.297338
7	1	0	0.917763	-3.745103	1.700514
8	1	0	1.887837	-2.318141	2.194245
9	6	0	-0.632562	-2.735817	-0.496131
10	1	0	-0.776361	-2.392337	-1.520457
11	1	0	-0.519582	-3.820151	-0.454817
12	1	0	-1.447188	-2.389280	0.141492
13	7	0	0.660797	2.414344	0.061101
14	6	0	1.508759	3.274145	0.729785
15	6	0	-0.222752	3.157677	-0.586316
16	1	0	2.308116	2.908933	1.354561
17	1	0	-1.024098	2.785910	-1.205160
18	1	0	1.512448	5.504494	0.794075
19	1	0	-0.501341	5.226265	-0.738277
20	7	0	0.030255	4.454943	-0.358171
21	6	0	1.120905	4.555379	0.468611
22	76	0	0.743411	0.323910	0.092693
23	8	0	2.718497	0.458136	-0.608793
24	1	0	3.058532	1.357696	-0.731769
25	8	0	1.614759	0.581025	2.033932
26	1	0	1.015085	0.447044	2.782782
27	1	0	2.458549	0.056163	2.163963
28	17	0	4.148366	-0.839981	1.644510
29	1	0	3.360786	-0.050723	-0.031036

RC-2_C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.470682	0.110821	0.762402
2	17	0	0.106496	0.214379	-2.341697
3	17	0	1.727038	0.326676	2.186045
4	16	0	1.023847	-2.108714	-0.055410
5	8	0	2.393502	-2.466071	-0.589696
6	6	0	0.796987	-2.879676	1.538557
7	1	0	-0.199837	-2.612815	1.896849
8	1	0	0.907186	-3.958274	1.419105
9	1	0	1.558241	-2.468634	2.200492
10	6	0	-0.223678	-2.939392	-1.026713
11	1	0	-0.124405	-2.570214	-2.046836
12	1	0	-0.050830	-4.014689	-0.968147
13	1	0	-1.197819	-2.663276	-0.617098
14	7	0	0.729675	2.279550	-0.069689
15	6	0	1.722227	3.136923	0.354052
16	6	0	-0.289614	3.022325	-0.468748
17	1	0	2.659836	2.766931	0.737628
18	1	0	-1.225567	2.648121	-0.853130
19	1	0	1.747541	5.368474	0.403721
20	1	0	-0.594952	5.090569	-0.550476
21	7	0	0.016023	4.319153	-0.320796
22	6	0	1.281928	4.418893	0.199824
23	76	0	0.783660	0.198135	-0.030180
24	8	0	2.788271	0.213386	-0.756626
25	1	0	3.033126	-0.733963	-0.889255
26	1	0	2.889389	0.675693	-1.603070
27	8	0	-0.579879	2.721938	2.674022
28	1	0	0.318555	2.371561	2.609630
29	1	0	-1.087950	2.076285	2.164481

TS-2$_C$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.846502	0.074618	-1.608207
2	17	0	1.274721	0.430758	-2.313744
3	17	0	0.655408	0.296353	2.468329
4	16	0	0.408042	-1.975702	0.087516
5	8	0	1.734801	-2.469586	0.625622
6	6	0	-0.932611	-2.577832	1.099997
7	1	0	-1.857354	-2.217703	0.642947
8	1	0	-0.892728	-3.666984	1.138859
9	1	0	-0.796372	-2.130075	2.084776
10	6	0	0.103997	-2.793772	-1.469536
11	1	0	0.891131	-2.463264	-2.147631
12	1	0	0.148164	-3.870221	-1.298110
13	1	0	-0.870494	-2.468979	-1.835997
14	7	0	0.550648	2.418255	-0.002405
15	6	0	1.286392	3.226003	0.837057
16	6	0	-0.071282	3.204779	-0.866763
17	1	0	1.879695	2.810530	1.636047
18	1	0	-0.722681	2.866875	-1.659298
19	1	0	1.482601	5.449917	0.855491
20	1	0	-0.112360	5.282398	-1.120985
21	7	0	0.236182	4.484596	-0.607526
22	6	0	1.095064	4.524455	0.463761

23	76	0	0.426929	0.338887	0.004479
24	8	0	2.515589	0.123552	0.257205
25	1	0	2.934483	0.225195	-0.617396
26	1	0	2.642182	-0.816022	0.539149
27	8	0	-1.705309	0.787294	1.058280
28	1	0	-1.563263	1.510416	1.685020
29	1	0	-2.312074	1.088591	0.364393

PC-2_C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.244315	0.275259	-2.228488
2	17	0	0.870335	0.516713	2.532708
3	16	0	0.692917	-1.986629	0.190615
4	8	0	2.065856	-2.330229	-0.362142
5	6	0	0.529653	-2.770113	1.783390
6	1	0	-0.482324	-2.572069	2.146904
7	1	0	0.715547	-3.836130	1.642887
8	1	0	1.276044	-2.315929	2.434416
9	6	0	-0.543014	-2.836822	-0.774920
10	1	0	-0.504749	-2.412203	-1.777786
11	1	0	-0.290713	-3.898491	-0.779225
12	1	0	-1.509934	-2.651574	-0.298546
13	7	0	0.581875	2.443805	0.043935
14	6	0	1.375778	3.290997	0.789798
15	6	0	-0.129647	3.196943	-0.784904
16	1	0	2.046508	2.913038	1.544242
17	1	0	-0.835592	2.832946	-1.515322
18	1	0	1.533596	5.515102	0.724356
19	1	0	-0.231286	5.262840	-1.092912
20	7	0	0.177010	4.486515	-0.590028
21	6	0	1.128687	4.572653	0.395877
22	76	0	0.520852	0.365406	0.164769
23	8	0	2.594763	0.210874	-0.152197
24	1	0	2.772563	-0.741923	-0.382791
25	1	0	2.946261	0.784957	-0.849107
26	8	0	-1.503797	0.584343	0.425983
27	1	0	-2.006027	-0.167112	0.920922
28	1	0	-1.758276	1.437380	0.809386
29	17	0	-2.829905	-1.570489	1.758532

RC-3_A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.599061	0.121279	0.575851
2	17	0	0.332501	0.269356	-2.360917
3	17	0	1.455546	0.120641	2.320856
4	7	0	0.687000	2.311176	0.050788
5	6	0	1.645213	3.133547	0.605781
6	6	0	-0.286441	3.084649	-0.404261
7	1	0	2.540983	2.731219	1.051633
8	1	0	-1.187505	2.739356	-0.886182

9	1	0	1.683268	5.358201	0.766237
10	1	0	-0.561184	5.157988	-0.415874
11	7	0	0.017750	4.368129	-0.166518
12	6	0	1.231465	4.425846	0.471915
13	76	0	0.719478	0.273807	0.023234
14	8	0	2.794886	0.464528	-0.476345
15	1	0	3.370711	-0.295531	-0.306887
16	1	0	2.926061	0.733986	-1.399290
17	8	0	-0.814041	2.588472	2.710941
18	1	0	0.066064	2.191903	2.754810
19	1	0	-1.283615	1.979703	2.124413
20	8	0	0.759662	-1.918105	-0.002093
21	1	0	1.038922	-2.318079	-0.837837
22	1	0	1.303467	-2.301574	0.701344

TS-3$_A$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.634580	0.320285	-1.126004
2	17	0	1.618342	0.246046	-2.169065
3	17	0	0.546431	-0.606169	2.461866
4	7	0	0.736074	2.445249	-0.097713
5	6	0	1.519405	3.233181	0.717599
6	6	0	0.071244	3.250275	-0.912333
7	1	0	2.159748	2.803040	1.469320
8	1	0	-0.634930	2.934798	-1.664569
9	1	0	1.726482	5.453590	0.768145
10	1	0	0.038744	5.330252	-1.134238
11	7	0	0.403015	4.522196	-0.648803
12	6	0	1.315025	4.537726	0.378425
13	76	0	0.552709	0.409114	-0.057405
14	8	0	-1.234455	1.570694	1.574612
15	1	0	-1.233948	0.897373	2.269536
16	1	0	-1.985320	1.353180	1.003254
17	8	0	2.590381	0.516265	0.704176
18	1	0	2.662496	-0.054947	1.488447
19	1	0	3.238819	0.220379	0.046323
20	8	0	0.419550	-1.793618	-0.206608
21	1	0	1.003672	-2.144705	-0.895044
22	1	0	0.681753	-2.186461	0.642182

PC-3$_A$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.368316	0.295742	1.370508
2	17	0	-0.102343	0.110996	-1.965124
3	7	0	0.648852	2.483176	0.145460
4	6	0	1.379367	3.377456	0.906339
5	6	0	-0.100660	3.189574	-0.695677
6	1	0	2.060110	3.035762	1.668756
7	1	0	-0.780214	2.776199	-1.424305
8	1	0	1.395733	5.604930	0.837987

9	1	0	-0.322738	5.241104	-1.004516
10	7	0	0.124193	4.490356	-0.495024
11	6	0	1.056355	4.637810	0.507547
12	76	0	0.743028	0.457907	0.283632
13	8	0	2.659250	0.542114	-0.589810
14	1	0	2.664087	0.280209	-1.524459
15	8	0	1.612191	0.688900	2.251984
16	1	0	0.964718	0.473001	2.941194
17	1	0	2.376425	0.074223	2.348812
18	17	0	3.800848	-1.310814	1.489306
19	1	0	3.311444	-0.009581	-0.086777
20	8	0	0.996371	-1.658198	0.394716
21	1	0	1.896990	-1.900027	0.719190
22	1	0	0.820178	-2.114045	-0.442450

RC-3_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.599061	0.121279	0.575851
2	17	0	0.332501	0.269356	-2.360917
3	17	0	1.455546	0.120641	2.320856
4	7	0	0.687000	2.311176	0.050788
5	6	0	1.645213	3.133547	0.605781
6	6	0	-0.286441	3.084649	-0.404261
7	1	0	2.540983	2.731219	1.051633
8	1	0	-1.187505	2.739356	-0.886182
9	1	0	1.683268	5.358201	0.766237
10	1	0	-0.561184	5.157988	-0.415874
11	7	0	0.017750	4.368129	-0.166518
12	6	0	1.231465	4.425846	0.471915
13	76	0	0.719478	0.273807	0.023234
14	8	0	2.794886	0.464528	-0.476345
15	1	0	3.370711	-0.295531	-0.306887
16	1	0	2.926061	0.733986	-1.399290
17	8	0	-0.814041	2.588472	2.710941
18	1	0	0.066064	2.191903	2.754810
19	1	0	-1.283615	1.979703	2.124413
20	8	0	0.759662	-1.918105	-0.002093
21	1	0	1.038922	-2.318079	-0.837837
22	1	0	1.303467	-2.301574	0.701344

TS-3_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.726343	0.353294	-2.016131
2	17	0	-1.071475	0.319797	1.983976
3	7	0	0.560269	2.467122	-0.076839
4	6	0	0.741776	3.179223	1.089953
5	6	0	0.698963	3.310644	-1.086854
6	1	0	0.667881	2.702948	2.054765
7	1	0	0.611591	3.057180	-2.131229
8	1	0	1.201653	5.344464	1.370185
9	1	0	1.111913	5.359320	-1.173467
10	7	0	0.962517	4.534504	-0.608649
11	6	0	0.998847	4.477765	0.763936
12	76	0	0.107387	0.470307	-0.178032
13	8	0	1.834632	0.222566	0.958140
14	1	0	2.612340	0.149258	0.375382
15	1	0	1.827006	-0.533960	1.566455
16	8	0	-1.996486	1.807385	-0.467848
17	17	0	-1.576763	-0.448239	-2.196964
18	1	0	-2.343331	1.772190	0.436356
19	1	0	-2.532870	1.186501	-0.986008
20	8	0	-0.048053	-1.715142	-0.059077
21	1	0	-0.522411	-1.975783	-0.871450
22	1	0	-0.632409	-1.937927	0.684311

PC-3_B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.342305	0.346466	-2.353696
2	17	0	0.815519	0.450002	2.462063
3	7	0	0.600483	2.501616	0.002618
4	6	0	1.497322	3.337526	0.639453
5	6	0	-0.257065	3.266488	-0.665677
6	1	0	2.290768	2.946765	1.255855
7	1	0	-1.076998	2.906296	-1.267126
8	1	0	1.600850	5.563957	0.634234
9	1	0	-0.436541	5.334423	-0.876909
10	7	0	0.060184	4.549304	-0.476897
11	6	0	1.164831	4.623271	0.342795
12	76	0	0.550426	0.471452	0.053863
13	8	0	2.667836	0.371396	-0.112541
14	1	0	3.108091	0.062389	0.694663
15	1	0	2.994643	-0.158258	-0.855551
16	8	0	-1.553575	0.611826	0.205129
17	1	0	-1.984385	-0.233567	-0.119987
18	1	0	-1.840712	0.736971	1.122953
19	17	0	-2.360420	-2.128392	-0.600934
20	8	0	0.485207	-1.657021	0.132580
21	1	0	0.709087	-2.012194	1.006090
22	1	0	-0.413100	-2.010085	-0.128752

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Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	17	0	-1.385833	0.745481	1.724952
2	17	0	-0.794506	0.556837	-1.791074
3	16	0	0.604793	-1.828771	0.380988
4	8	0	2.091192	-2.019305	0.641905
5	6	0	-0.316668	-2.640008	1.676224
6	1	0	-1.371506	-2.585478	1.405295
7	1	0	0.037719	-3.670338	1.733202
8	1	0	-0.117337	-2.101443	2.602860
9	6	0	0.143704	-2.768621	-1.064206
10	1	0	0.625653	-2.300483	-1.922802
11	1	0	0.498060	-3.790107	-0.917598
12	1	0	-0.942537	-2.719798	-1.148208
13	7	0	0.606408	2.567520	0.151871
14	6	0	1.776139	3.280381	0.313878
15	6	0	-0.367190	3.439710	-0.059830
16	1	0	2.717075	2.787302	0.500196
17	1	0	-1.404957	3.196612	-0.225994
18	1	0	2.111261	5.485219	0.252994
19	1	0	-0.396657	5.528074	-0.174957
20	7	0	0.137965	4.680804	-0.039118
21	6	0	1.488999	4.608156	0.195081
22	76	0	0.430160	0.506005	0.231238
23	8	0	2.283442	0.377606	-0.826216
24	1	0	2.713557	-0.490328	-0.697296
25	1	0	2.294266	0.609066	-1.767821
26	8	0	1.830349	0.524512	1.844177
27	1	0	1.533923	0.861325	2.703975
28	1	0	2.254504	-0.347466	1.964157
29	8	0	-2.689134	-1.540312	-0.192183
30	1	0	-2.462573	-0.983058	-0.949838
31	1	0	-2.733633	-0.905603	0.536267

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-1.804321	0.121760	-0.374877
2	16	0	1.299717	-1.924987	2.359052
3	8	0	2.349706	-1.185870	3.210659
4	6	0	0.149086	-2.705201	3.483564
5	1	0	-0.554177	-3.287793	2.885823
6	1	0	0.706500	-3.339285	4.174314
7	1	0	-0.368992	-1.901787	4.005824
8	6	0	2.129694	-3.356774	1.669671
9	1	0	2.846297	-2.984523	0.936539
10	1	0	2.640912	-3.881437	2.478048
11	1	0	1.385530	-3.989008	1.186017
12	7	0	0.336438	2.224734	0.239502
13	6	0	1.309652	2.953587	-0.419227
14	6	0	-0.640837	3.061307	0.578501
15	1	0	2.202688	2.493643	-0.808379
16	1	0	-1.538331	2.789277	1.110550
17	1	0	1.353905	5.128616	-0.894729
18	1	0	-0.898720	5.109475	0.292112
19	7	0	-0.324519	4.286998	0.159358
20	6	0	0.898269	4.248984	-0.472525

21	76	0	0.398463	0.261677	0.666106
22	8	0	-0.069780	-2.230785	-0.049796
23	1	0	0.356501	-2.588270	-0.840277
24	1	0	-0.998012	-2.093392	-0.295258
25	8	0	2.283799	0.655771	1.555336
26	1	0	3.051206	0.630974	0.966431
27	1	0	2.458716	0.006573	2.353476
28	8	0	1.378020	0.084256	-1.258794
29	1	0	0.759292	0.094308	-2.005784
30	1	0	2.001586	-0.640610	-1.409266
31	17	0	-0.618428	0.660325	2.821926

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-2.120734	0.975047	-0.502924
2	17	0	0.262613	1.982970	-2.867007
3	7	0	0.647992	2.350147	0.274989
4	6	0	1.657800	2.451419	1.211141
5	6	0	0.018635	3.514923	0.244284
6	1	0	2.323253	1.627890	1.420774
7	1	0	-0.823021	3.757106	-0.385144
8	1	0	2.233837	4.180491	2.498376
9	1	0	0.294995	5.304302	1.294780
10	7	0	0.589024	4.352224	1.124319
11	6	0	1.625631	3.705225	1.747321
12	76	0	0.215379	0.697292	-0.857354
13	8	0	2.285515	0.306815	-1.096451
14	1	0	2.467112	-0.456185	-1.668146
15	1	0	2.818932	1.048862	-1.420752
16	8	0	0.328489	-0.531788	0.832181
17	1	0	0.166478	-0.114386	1.690195
18	1	0	-0.282468	-1.337294	0.702228
19	8	0	-0.104397	-1.110817	-2.020179
20	1	0	-0.638884	-0.953269	-2.810850
21	1	0	-0.591688	-1.754052	-1.431615
22	16	0	-2.679699	-2.466715	0.150887
23	8	0	-1.125604	-2.397101	-0.011426
24	6	0	-2.989382	-1.729044	1.758398
25	1	0	-4.037021	-1.891950	2.016610
26	1	0	-2.327689	-2.194785	2.491068
27	1	0	-2.789079	-0.661553	1.662268
28	6	0	-2.961544	-4.189172	0.570801
29	1	0	-2.694202	-4.779009	-0.305550
30	1	0	-2.333803	-4.454428	1.422471
31	1	0	-4.019868	-4.320580	0.801169

RC-3′

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	17	0	2.132108	0.524324	-1.431280
2	16	0	1.080297	-2.093413	0.495917
3	8	0	2.116301	-2.201130	1.601134
4	6	0	-0.274782	-3.189549	0.883479
5	1	0	-0.994652	-3.146512	0.063666
6	1	0	0.130522	-4.194549	1.007659
7	1	0	-0.723669	-2.821214	1.805072
8	6	0	1.756983	-2.846141	-0.973998
9	1	0	2.647035	-2.273173	-1.233363
10	1	0	2.006846	-3.880744	-0.735181
11	1	0	1.015063	-2.775279	-1.772361
12	7	0	0.146007	2.229632	0.307138
13	6	0	0.065633	3.048046	1.413887
14	6	0	-0.042969	2.985896	-0.762741
15	1	0	0.177706	2.657063	2.412824
16	1	0	-0.037352	2.642491	-1.785015
17	1	0	-0.303979	5.245927	1.527972
18	1	0	-0.410673	5.031189	-1.004906
19	7	0	-0.240459	4.255283	-0.379824
20	6	0	-0.174854	4.321680	0.990442
21	76	0	0.504204	0.191498	0.303842
22	8	0	-0.006576	-1.191293	-3.110218
23	8	0	1.949896	0.378441	1.802006
24	1	0	2.667168	1.009810	1.639573
25	8	0	-0.986663	0.122878	-1.187594
26	1	0	-1.814803	-0.253511	-0.852686
27	1	0	-0.689244	-0.420995	-2.000511
28	1	0	2.322568	-0.532490	1.968596
29	17	0	-1.209099	-0.067268	1.951316
30	1	0	-0.487974	-1.233318	-3.947003
31	1	0	0.830885	-0.738937	-3.293167

TS-3′

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	1.100283	0.695954	-1.944864
2	7	0	-0.052740	2.431641	0.437490
3	6	0	-1.012378	2.972676	1.278570
4	6	0	0.356226	3.401589	-0.381647
5	1	0	-1.482339	2.391147	2.054318
6	1	0	1.084425	3.296284	-1.169841
7	1	0	-1.810945	5.048583	1.353268
8	1	0	-0.177109	5.405030	-0.568902
9	7	0	-0.301815	4.522105	-0.090153
10	6	0	-1.172458	4.281660	0.948539
11	76	0	0.632690	0.532655	0.451372
12	8	0	2.580818	1.356603	0.614948
13	1	0	2.957382	1.464955	-0.276293
14	8	0	-1.417724	-0.091720	0.293409
15	1	0	-1.969650	0.397282	-0.337098
16	1	0	-1.859711	-0.080485	1.160157
17	1	0	3.112944	0.667171	1.059624
18	17	0	0.173322	0.342009	2.841893
19	16	0	0.444084	-2.207261	-0.370226

20	8	0	1.755583	-2.978475	-0.361360
21	6	0	-0.718205	-3.121647	0.649496
22	1	0	-1.713808	-2.695828	0.523530
23	1	0	-0.691583	-4.167323	0.338496
24	1	0	-0.389910	-3.019929	1.684829
25	6	0	-0.311533	-2.417510	-1.979119
26	1	0	0.366062	-1.975111	-2.708237
27	1	0	-0.451603	-3.483931	-2.161208
28	1	0	-1.265109	-1.886445	-1.981181
29	8	0	2.401839	-1.072512	1.356325
30	1	0	2.503118	-1.900573	0.830940
31	1	0	2.113411	-1.313441	2.248569

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.718865	-0.704164	-1.128075
2	17	0	2.722058	0.637502	2.057724
3	7	0	0.631965	2.024258	0.006184
4	6	0	1.495647	3.094602	0.159301
5	6	0	-0.514596	2.504324	-0.470433
6	1	0	2.492134	2.961670	0.547390
7	1	0	-1.387351	1.916012	-0.706519
8	1	0	1.162894	5.254680	-0.274604
9	1	0	-1.144510	4.429893	-0.967178
10	7	0	-0.410211	3.826435	-0.621496
11	6	0	0.849538	4.225003	-0.235761
12	76	0	0.978378	0.064590	0.456616
13	8	0	2.406602	-0.149545	-1.062081
14	1	0	2.064546	-0.280872	-1.959962
15	1	0	3.161853	0.456049	-1.092984
16	8	0	-0.428446	0.127386	1.953440
17	1	0	-0.858652	-0.821733	2.042168
18	1	0	-0.072081	0.420040	2.806003
19	8	0	1.314100	-1.985062	0.957991
20	1	0	2.011697	-2.100729	1.621323
21	1	0	0.474685	-2.376271	1.310176
22	16	0	-2.397541	-2.670766	1.161639
23	8	0	-1.119680	-2.240187	1.958194
24	6	0	-3.264634	-3.715848	2.336707
25	1	0	-4.103652	-4.190291	1.825092
26	1	0	-2.568130	-4.457878	2.729176
27	1	0	-3.630290	-3.068645	3.133398
28	6	0	-1.785272	-3.935484	0.046929
29	1	0	-1.147460	-3.428588	-0.677634
30	1	0	-1.223412	-4.669809	0.626941
31	1	0	-2.636312	-4.397702	-0.455649