Supplementary Material (ESI) for Organic & Biomolecular Chemistry

"*In silico*" Mechanistic studies as predictive tools in Microwave Assisted Organic Synthesis

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Table S1. Total electronic energies[a] (E, in a.u.), zero-point correction of energies (ΔZPE, in a.u.), and number of imaginary frequencies[b] (NIMAG) of all stationary points discussed in the main text for the IMDA reaction of **N-Alkyl-2-cyano-1-azadienes**.

Structure	E	ΔZPE	NIMAG(ν)
1a	-498.702039	0.220191	0
1b	-498.695929	0.220062	
2a	-498.745729	0.226705	0
2a'	-498.746626	0.226548	
2b	-498.746619	0.226555	0
2b'	-498.745729	0.226705	
3a	-690.384484	0.272776	0
3b	-690.384818	0.272749	
4a	-690.427348	0.279229	0
4a'	-690.427222	0.279371	0
4b	-690.427222	0.279371	0
4b'	-690.427350	0.279227	0
5	-690.397701	0.272971	0
TS2a	-498.665294	0.221348	1(-476.6978)
TS2a'	-498.655901	0.221551	1 (-458.6955)
TS2b	-498.655902	0.221549	1(-458.6451)
TS2b'	-498.665294	0.221348	1 (-476.4700)
TS4a	-690.344238	0.273975	1 (-471.8690)
TS4a'	-690.346324	0.274184	1 (-476.2527)
TS4b	-690.346325	0.274183	1 (-476.4144)
TS4b'	-690.330774	0.274296	1 (-489.3194)

[a]Computed at the level of theory B3LYP(L1A1)/6-31G*. [b]The imaginary frequency ν (in parentheses) is given in cm^{-1}.

Table S2. Total electronic energies[a] (E, in a.u.), zero-point correction of energies (ΔZPE, in a.u.), and number of imaginary frequencies[b] (NIMAG) of all stationary points discussed in the main text for the **Intra- and intermolecular Diels-Alder reactions of 2(1H)-Pyrazinones in Ionic Liquid doped solvents**.

Structure	E	ΔZPE	NIMAG(ν)
6a	-1261.176529	0.246816	0
6b	-1300.460247	0.275567	0
7a	-1261.186855	0.252481	0
7a'	-1261.188188	0.252338	0
7b	-1300.473023	0.281700	0
7b'	-1300.472648	0.281434	0
8	-1122.271450	0.150618	0
9	-1655.272857	0.270910	0
10	-1102.289922	0.258190	0
11	-1255.693962	0.162908	0
12	-1200.835218	0.210209	0
TS7a	-1261.130632	0.248251	1 (-488.9376)
TS7a'	-1261.133016	0.248185	1 (-495.8373)
TS7b	-1300.410241	0.276958	1 (-487.8939)
TS7b'	-1300.414821	0.277350	1 (-524.3010)
TS9	-1655.198442	0.266782	1 (-395.2034)
TS10	-1655.223937	0.267352	1 (-496.8457)
TS11	-1655.237659	0.267383	1 (-488.4153)
TS12	-1200.774658	0.205000	1 (-480.8771)
bmimPF_6 (A)	-1363.776535	0.246482	0
bmimPF_6 (B)	-1363.777774	0.246426	0
bmimPF_6 (C)	-1363.776743	0.246206	0

[a]Computed at the level of theory B3LYP(L1A1)/6-31G*. [b]The imaginary frequency ν (in parentheses) is given in cm^{-1}.

Cartesian coordinates (optimized at the B3LYP(PCM)/6-31G) of all the stationary points discussed in the main text for the reaction between.

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.869864	-1.701370	0.187834
2	6	0	2.590893	-1.476161	0.509393
3	6	0	1.817998	-0.288256	0.112879
4	7	0	0.595251	-0.167929	0.477356
5	6	0	-0.205082	0.994360	0.109606
6	6	0	-1.495207	0.509528	-0.590574
7	6	0	-2.418039	-0.382621	0.261731
8	6	0	-3.565843	-0.934489	-0.539652
9	6	0	-4.856980	-0.706474	-0.296140
10	6	0	2.519639	0.711571	-0.694217
11	7	0	3.088043	1.499647	-1.332177
12	6	0	-0.478934	1.809273	1.384555
13	1	0	4.377932	-2.602800	0.515472
14	1	0	4.448551	-1.000285	-0.407746
15	1	0	2.019932	-2.182560	1.106071
16	1	0	0.329461	1.643388	-0.601537
17	1	0	-2.048618	1.396057	-0.926651
18	1	0	-1.203704	-0.035194	-1.498681
19	1	0	-1.819108	-1.207223	0.670867
20	1	0	-2.809449	0.182223	1.116253
21	1	0	-3.291263	-1.562213	-1.389952
22	1	0	-5.641702	-1.133224	-0.915198
23	1	0	-5.180199	-0.086024	0.537827
24	1	0	-1.156415	2.640641	1.159770
25	1	0	0.452971	2.224887	1.781717
26	1	0	-0.931306	1.188125	2.163048

1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.535642	-1.733026	-0.249251
2	6	0	-2.611843	-1.052020	-0.936939
3	6	0	-1.607192	-0.148079	-0.347556
4	6	0	-1.654955	-0.017901	1.110257
5	7	0	-1.720102	0.058047	2.268641
6	7	0	-0.778087	0.446949	-1.122809
7	6	0	0.264398	1.379747	-0.669022
8	6	0	-0.323186	2.637890	-0.005027
9	6	0	1.350823	0.706619	0.198923
10	6	0	2.067722	-0.464775	-0.499977
11	6	0	3.118747	-1.094088	0.373731
12	6	0	4.421400	-1.147312	0.093602
13	1	0	-4.243741	-2.380608	-0.756560
14	1	0	-3.617197	-1.668725	0.832522
15	1	0	-2.538392	-1.122040	-2.018969
16	1	0	0.754524	1.704434	-1.595587
17	1	0	2.090678	1.476448	0.453243
18	1	0	0.918751	0.370201	1.149062

19	1	0	1.322819	-1.222314	-0.782021
20	1	0	2.523943	-0.112589	-1.434543
21	1	0	2.760732	-1.524972	1.310793
22	1	0	5.134527	-1.612641	0.768885
23	1	0	4.825443	-0.730478	-0.827200
24	1	0	-1.093889	3.083182	-0.642884
25	1	0	0.470437	3.379417	0.137051
26	1	0	-0.762943	2.423380	0.972950

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.171980	-0.903885	-0.237935
2	6	0	0.775324	-1.237831	0.299301
3	7	0	-0.159295	-0.099071	0.183307
4	6	0	0.353115	1.181763	0.035279
5	6	0	1.668937	1.494220	0.159799
6	6	0	2.697344	0.415710	0.350595
7	6	0	0.045168	-2.360212	-0.452518
8	6	0	-1.434876	-2.049599	-0.203623
9	6	0	-1.524182	-0.507788	-0.211728
10	6	0	-2.617796	0.010882	0.729040
11	6	0	-0.567647	2.244779	-0.268180
12	7	0	-1.289062	3.119333	-0.530799
13	1	0	1.970873	2.531031	0.070447
14	1	0	3.635700	0.698903	-0.142291
15	1	0	2.943570	0.284977	1.416065
16	1	0	2.122167	-0.811193	-1.330244
17	1	0	2.849358	-1.734934	-0.010760
18	1	0	0.870094	-1.510050	1.363359
19	1	0	0.341468	-3.356062	-0.107697
20	1	0	0.277277	-2.291933	-1.523079
21	1	0	-2.102925	-2.496057	-0.946163
22	1	0	-1.738426	-2.426962	0.781074
23	1	0	-1.734971	-0.152458	-1.232424
24	1	0	-2.699895	1.099953	0.705293
25	1	0	-3.588066	-0.403808	0.429535
26	1	0	-2.411933	-0.301477	1.759153

2a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.534222	2.119182	0.490835
2	6	0	-0.977039	1.000475	-0.462835
3	7	0	-0.077433	-0.158871	-0.372512
4	6	0	1.273093	0.070786	-0.166413
5	6	0	1.800517	1.302285	0.051419
6	6	0	0.926932	2.516654	0.215757
7	6	0	-2.362708	0.393755	-0.187156
8	6	0	-2.204867	-1.082312	-0.595810
9	6	0	-0.771718	-1.436823	-0.149336
10	6	0	-0.699524	-1.942062	1.300842
11	6	0	2.146983	-1.069859	-0.258604

12	7	0	2.847588	-1.996969	-0.317533
13	1	0	2.878281	1.407042	0.106366
14	1	0	1.304882	3.137362	1.039586
15	1	0	0.984136	3.152380	-0.681463
16	1	0	-0.629026	1.757655	1.522655
17	1	0	-1.197609	2.985534	0.385177
18	1	0	-0.937006	1.392899	-1.492878
19	1	0	-3.156609	0.908369	-0.736718
20	1	0	-2.596957	0.471735	0.881746
21	1	0	-2.953195	-1.735970	-0.137713
22	1	0	-2.291212	-1.183337	-1.683870
23	1	0	-0.335665	-2.201808	-0.804241
24	1	0	-1.209743	-2.908743	1.387422
25	1	0	0.338547	-2.085362	1.616862
26	1	0	-1.174586	-1.239365	1.995194

2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.544045	2.114188	0.491007
2	6	0	-0.981260	0.995551	-0.465388
3	7	0	-0.076287	-0.160302	-0.378105
4	6	0	1.272813	0.075553	-0.168395
5	6	0	1.794363	1.309044	0.052019
6	6	0	0.915158	2.519167	0.217303
7	6	0	-2.364782	0.382820	-0.190921
8	6	0	-2.199872	-1.093831	-0.594584
9	6	0	-0.765266	-1.439853	-0.146561
10	6	0	-0.690607	-1.936088	1.306642
11	6	0	2.152026	-1.061098	-0.260046
12	7	0	2.856951	-1.984998	-0.317855
13	1	0	2.871581	1.418572	0.108528
14	1	0	1.289789	3.140570	1.042111
15	1	0	0.969813	3.156250	-0.679116
16	1	0	-0.637418	1.749969	1.522029
17	1	0	-1.211599	2.977540	0.387073
18	1	0	-0.942477	1.390382	-1.494439
19	1	0	-3.159729	0.892096	-0.743908
20	1	0	-2.602121	0.463200	0.877093
21	1	0	-2.945225	-1.749422	-0.134446
22	1	0	-2.285317	-1.199048	-1.682307
23	1	0	-0.326085	-2.206872	-0.796941
24	1	0	-1.197137	-2.904142	1.399337
25	1	0	0.348093	-2.073585	1.623168
26	1	0	-1.167985	-1.231121	1.997088

2b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.172317	-0.903210	-0.237916
2	6	0	-0.775850	-1.237667	0.299475
3	7	0	0.159280	-0.099056	0.183868
4	6	0	-0.352760	1.181891	0.035330

5	6	0	-1.668439	1.494721	0.159429
6	6	0	-2.697138	0.416602	0.350403
7	6	0	-0.045950	-2.360268	-0.452365
8	6	0	1.434222	-2.050001	-0.203756
9	6	0	1.523945	-0.508214	-0.211763
10	6	0	2.617986	0.010005	0.728628
11	6	0	0.568372	2.244595	-0.267992
12	7	0	1.290021	3.118983	-0.530557
13	1	0	-1.970012	2.531630	0.069892
14	1	0	-2.943310	0.286081	1.415924
15	1	0	-3.635486	0.700043	-0.142399
16	1	0	-2.850045	-1.733968	-0.010639
17	1	0	-2.122442	-0.810691	-1.330269
18	1	0	-0.870874	-1.509936	1.363499
19	1	0	-0.342391	-3.356037	-0.107403
20	1	0	-0.278220	-2.292108	-1.522928
21	1	0	2.101979	-2.496595	-0.946495
22	1	0	1.737962	-2.427529	0.780843
23	1	0	1.734451	-0.152829	-1.232521
24	1	0	2.700269	1.099083	0.705120
25	1	0	3.588066	-0.404766	0.428613
26	1	0	2.412524	-0.302581	1.758753

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.428767	-3.304435	0.111676
2	6	0	1.914139	-2.833867	-1.099215
3	6	0	1.098272	-1.703661	-1.123966
4	6	0	0.784824	-1.026604	0.062909
5	6	0	1.295756	-1.510539	1.272119
6	6	0	2.117103	-2.640051	1.297770
7	6	0	-0.088551	0.223150	0.045285
8	7	0	-1.288421	-0.059152	-0.737369
9	6	0	0.613713	1.439655	-0.609060
10	6	0	1.863465	1.910668	0.157187
11	6	0	2.537834	3.072022	-0.521619
12	6	0	2.695396	4.286269	0.006366
13	6	0	-2.461741	0.062409	-0.235167
14	6	0	-3.646034	-0.224985	-1.059104
15	6	0	-4.912755	-0.130187	-0.639133
16	6	0	-2.706470	0.482036	1.144896
17	7	0	-2.908444	0.817599	2.239294
18	1	0	3.064134	-4.185898	0.129549
19	1	0	2.146359	-3.351085	-2.026600
20	1	0	0.683771	-1.351143	-2.063772
21	1	0	1.048415	-1.001926	2.201117
22	1	0	2.506893	-3.001447	2.245711
23	1	0	-0.330244	0.489635	1.085635
24	1	0	-0.108269	2.263759	-0.666066
25	1	0	0.877310	1.179099	-1.641607
26	1	0	2.568302	1.071365	0.236946
27	1	0	1.587374	2.191241	1.182235
28	1	0	2.910765	2.879443	-1.529420
29	1	0	3.190508	5.087287	-0.536134
30	1	0	2.338324	4.525344	1.006354
31	1	0	-3.402481	-0.532576	-2.072477

32	1	0	-5.740085	-0.359423	-1.303208
33	1	0	-5.165323	0.175932	0.372594

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.406787	0.148096	-0.279143
2	6	0	-3.868511	0.064924	1.005233
3	6	0	-2.484018	0.079807	1.186126
4	6	0	-1.623011	0.186924	0.088634
5	6	0	-2.170698	0.265459	-1.198953
6	6	0	-3.553111	0.245657	-1.380646
7	6	0	-0.115085	0.249774	0.309689
8	7	0	0.539734	-0.643514	-0.640675
9	6	0	0.422700	1.684783	0.095494
10	6	0	1.925941	1.833759	0.393702
11	6	0	2.387230	3.263078	0.298355
12	6	0	3.296018	3.721584	-0.562878
13	6	0	1.217991	-1.660121	-0.253433
14	6	0	1.853268	-2.540661	-1.246168
15	6	0	2.587517	-3.620093	-0.953469
16	6	0	1.407712	-2.011943	1.154328
17	7	0	1.566080	-2.297067	2.269970
18	1	0	-5.483933	0.131910	-0.422305
19	1	0	-4.523861	-0.018389	1.868247
20	1	0	-2.069645	0.005747	2.189082
21	1	0	-1.507843	0.326304	-2.056745
22	1	0	-3.965033	0.304331	-2.384814
23	1	0	0.092052	-0.039392	1.351818
24	1	0	-0.155504	2.351056	0.748556
25	1	0	0.216498	1.992363	-0.936123
26	1	0	2.505133	1.211968	-0.299116
27	1	0	2.124189	1.451624	1.407376
28	1	0	1.915842	3.961190	0.992918
29	1	0	3.584536	4.769059	-0.588307
30	1	0	3.790748	3.064077	-1.275324
31	1	0	1.673207	-2.234339	-2.273121
32	1	0	3.027774	-4.225985	-1.739011
33	1	0	2.772212	-3.933611	0.070568

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.460153	1.233392	-0.165267
2	6	0	-2.603163	1.490410	0.519559
3	6	0	-3.465214	0.386783	1.074970
4	6	0	-2.743899	-0.976042	1.047776
5	6	0	-1.985090	-1.151674	-0.272163
6	7	0	-1.034174	-0.053795	-0.452747
7	6	0	-1.087626	-2.384828	-0.412996
8	6	0	-0.050556	-1.931721	-1.455283
9	6	0	0.211597	-0.432811	-1.120219
10	6	0	1.468837	-0.219165	-0.280490

11	6	0	2.689388	0.007018	-0.929909
12	6	0	3.871745	0.144138	-0.203885
13	6	0	3.849680	0.064217	1.190123
14	6	0	2.637700	-0.149177	1.847483
15	6	0	1.456119	-0.289044	1.116953
16	6	0	-0.659143	2.324333	-0.651929
17	7	0	-0.023136	3.212426	-1.052133
18	1	0	-2.897824	2.522501	0.672076
19	1	0	-3.759880	0.628545	2.105511
20	1	0	-4.407445	0.326675	0.508749
21	1	0	-2.025327	-1.033096	1.875005
22	1	0	-3.461721	-1.793465	1.182289
23	1	0	-2.722315	-1.136917	-1.096201
24	1	0	-0.601347	-2.605406	0.545014
25	1	0	-1.643545	-3.274664	-0.723671
26	1	0	-0.477221	-2.008525	-2.462393
27	1	0	0.870987	-2.518360	-1.434583
28	1	0	0.335754	0.135253	-2.052849
29	1	0	2.711426	0.084570	-2.015166
30	1	0	4.807940	0.324957	-0.725547
31	1	0	4.768467	0.178350	1.759076
32	1	0	2.608703	-0.201102	2.932898
33	1	0	0.513192	-0.434705	1.635614

4a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.293829	1.231432	-0.091657
2	6	0	2.481672	1.768179	0.285288
3	6	0	3.620023	0.893213	0.728201
4	6	0	3.456764	-0.510632	0.124786
5	6	0	2.055716	-1.070758	0.395464
6	7	0	0.987699	-0.121402	0.011218
7	6	0	1.700097	-2.336648	-0.398379
8	6	0	0.173409	-2.270186	-0.508005
9	6	0	-0.131749	-0.763628	-0.700685
10	6	0	-1.511622	-0.387283	-0.180935
11	6	0	-2.584974	-0.282733	-1.071495
12	6	0	-3.873247	-0.014697	-0.606984
13	6	0	-4.101649	0.160125	0.758332
14	6	0	-3.034347	0.064885	1.654102
15	6	0	-1.749226	-0.209099	1.187543
16	6	0	0.288824	2.112516	-0.625021
17	7	0	-0.476027	2.860717	-1.081730
18	1	0	2.611871	2.842043	0.219878
19	1	0	4.574690	1.330051	0.409272
20	1	0	3.669316	0.831526	1.826647
21	1	0	3.616720	-0.454206	-0.959459
22	1	0	4.202947	-1.203749	0.529859
23	1	0	1.969512	-1.276142	1.474892
24	1	0	2.159465	-2.285575	-1.393998
25	1	0	2.057609	-3.249040	0.089558
26	1	0	-0.292637	-2.616597	0.421284
27	1	0	-0.236667	-2.868527	-1.326538
28	1	0	-0.089396	-0.519040	-1.773692
29	1	0	-2.409332	-0.401446	-2.138603
30	1	0	-4.694868	0.069532	-1.313335

31	1	0	-5.102323	0.378143	1.121710
32	1	0	-3.202247	0.209300	2.718310
33	1	0	-0.917475	-0.269595	1.884471

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.293606	1.231536	-0.091469
2	6	0	-2.481438	1.768356	0.285474
3	6	0	-3.620075	0.893516	0.727848
4	6	0	-3.456790	-0.510345	0.124551
5	6	0	-2.055821	-1.070572	0.395301
6	7	0	-0.987832	-0.121410	0.010772
7	6	0	-1.700320	-2.336634	-0.398255
8	6	0	-0.173649	-2.270319	-0.507985
9	6	0	0.131685	-0.763825	-0.700885
10	6	0	1.511557	-0.387500	-0.181112
11	6	0	2.584761	-0.282057	-1.071736
12	6	0	3.873026	-0.013997	-0.607204
13	6	0	4.101556	0.159948	0.758199
14	6	0	3.034396	0.063800	1.654050
15	6	0	1.749299	-0.210223	1.187468
16	6	0	-0.288382	2.112685	-0.624292
17	7	0	0.476655	2.860959	-1.080568
18	1	0	-2.611255	2.842319	0.220759
19	1	0	-3.670207	0.832060	1.826278
20	1	0	-4.574504	1.330388	0.408225
21	1	0	-4.202995	-1.203423	0.529635
22	1	0	-3.616760	-0.453979	-0.959698
23	1	0	-1.969636	-1.275744	1.474779
24	1	0	-2.057858	-3.248893	0.089942
25	1	0	-2.159742	-2.285796	-1.393861
26	1	0	0.236334	-2.868787	-1.326490
27	1	0	0.292417	-2.616680	0.421319
28	1	0	0.089433	-0.519423	-1.773945
29	1	0	2.409012	-0.400084	-2.138902
30	1	0	4.694531	0.070943	-1.313606
31	1	0	5.102217	0.377987	1.121601
32	1	0	3.202400	0.207524	2.718336
33	1	0	0.917662	-0.271469	1.884473

4b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460201	1.233079	-0.166148
2	6	0	2.602436	1.490192	0.519988
3	6	0	3.464044	0.386555	1.075981
4	6	0	2.742214	-0.976106	1.048790
5	6	0	1.984576	-1.152288	-0.271792
6	7	0	1.034662	-0.053911	-0.454532
7	6	0	1.086412	-2.385035	-0.412253
8	6	0	0.050178	-1.932081	-1.455411
9	6	0	-0.211631	-0.433012	-1.120934

10	6	0	-1.468419	-0.218984	-0.280595
11	6	0	-2.689509	0.005653	-0.929560
12	6	0	-3.871487	0.143100	-0.203000
13	6	0	-3.848522	0.065086	1.191110
14	6	0	-2.636026	-0.146739	1.847999
15	6	0	-1.454808	-0.286951	1.116926
16	6	0	0.659707	2.324016	-0.653565
17	7	0	0.024067	3.212094	-1.054378
18	1	0	2.896909	2.522299	0.672785
19	1	0	4.406554	0.325964	0.510248
20	1	0	3.758244	0.628387	2.106643
21	1	0	3.459574	-1.793746	1.184439
22	1	0	2.022923	-1.032409	1.875447
23	1	0	2.722703	-1.138861	-1.095039
24	1	0	1.641990	-3.275446	-0.721898
25	1	0	0.599377	-2.604577	0.545615
26	1	0	-0.871573	-2.518422	-1.435087
27	1	0	0.477485	-2.009318	-2.462224
28	1	0	-0.336262	0.134689	-2.053716
29	1	0	-2.712268	0.081706	-2.014912
30	1	0	-4.808104	0.322686	-0.724333
31	1	0	-4.767024	0.179472	1.760473
32	1	0	-2.606322	-0.197185	2.933467
33	1	0	-0.511510	-0.431429	1.635250

5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.526293	-0.639975	-0.204194
2	6	0	-3.662074	-1.640162	-0.660215
3	6	0	-2.287182	-1.501737	-0.507308
4	6	0	-1.738207	-0.360737	0.108053
5	6	0	-2.619349	0.636865	0.559364
6	6	0	-3.999193	0.497456	0.405744
7	6	0	-0.255814	-0.246126	0.260225
8	7	0	0.422915	-1.309483	-0.007925
9	6	0	0.322159	1.077134	0.732828
10	6	0	0.327505	2.185684	-0.354231
11	6	0	0.849910	3.489052	0.188621
12	6	0	2.019874	4.033908	-0.146911
13	6	0	1.822618	-1.417029	0.005526
14	6	0	2.400483	-2.565699	0.429523
15	6	0	3.864004	-2.860804	0.486712
16	6	0	2.650862	-0.374589	-0.554885
17	7	0	3.305286	0.453584	-1.046867
18	1	0	-5.600863	-0.747442	-0.325411
19	1	0	-4.063415	-2.528895	-1.139976
20	1	0	-1.609501	-2.271460	-0.858679
21	1	0	-2.239972	1.531068	1.041758
22	1	0	-4.660574	1.280854	0.765681
23	1	0	1.343468	0.930264	1.090850
24	1	0	-0.254047	1.423545	1.599439
25	1	0	-0.693236	2.318936	-0.736240
26	1	0	0.946823	1.859735	-1.195114
27	1	0	0.216125	3.991866	0.922151
28	1	0	2.357120	4.973000	0.284361
29	1	0	2.685692	3.553882	-0.860653

30	1	0	1.714464	-3.336466	0.775417
31	1	0	4.093927	-3.769833	-0.085221
32	1	0	4.470313	-2.041289	0.091615
33	1	0	4.180457	-3.055912	1.520446

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.209122	-1.317872	-0.351882
2	6	0	0.897897	-1.725398	-0.153541
3	7	0	-0.247707	0.074870	0.638796
4	6	0	0.350181	1.176607	0.218067
5	6	0	1.742268	1.358148	0.404665
6	6	0	2.482950	0.331968	0.971295
7	6	0	-0.200071	-1.814521	-1.178004
8	6	0	-1.558633	-1.613193	-0.497315
9	6	0	-1.603254	-0.217559	0.172254
10	6	0	-2.589978	-0.170965	1.344871
11	6	0	-0.324647	2.178464	-0.594451
12	7	0	-0.858303	3.002593	-1.219000
13	1	0	2.228992	2.168681	-0.129010
14	1	0	3.565694	0.421736	1.012658
15	1	0	2.032656	-0.255769	1.763200
16	1	0	2.504867	-0.889053	-1.306401
17	1	0	3.002506	-1.831061	0.184200
18	1	0	0.704597	-2.299106	0.752413
19	1	0	-0.171677	-2.808483	-1.651306
20	1	0	-0.040678	-1.082244	-1.980612
21	1	0	-2.390700	-1.722733	-1.202240
22	1	0	-1.686185	-2.388831	0.270743
23	1	0	-1.927701	0.510689	-0.585856
24	1	0	-2.657761	0.840174	1.759193
25	1	0	-3.591028	-0.472841	1.015122
26	1	0	-2.266519	-0.847468	2.143575

TS2a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.517100	-0.833822	0.287328
2	6	0	-1.294366	-1.459114	0.085541
3	7	0	0.073147	-0.024783	-0.895890
4	6	0	-0.043288	1.113866	-0.235294
5	6	0	-1.321204	1.732552	-0.181602
6	6	0	-2.394044	1.088824	-0.769900
7	6	0	-0.259420	-1.642983	1.171129
8	6	0	1.203825	-1.559498	0.651025
9	6	0	1.229258	-0.915961	-0.760866
10	6	0	2.586720	-0.314373	-1.147785
11	6	0	0.975515	1.686587	0.627256
12	7	0	1.779099	2.168275	1.318196
13	1	0	-1.469557	2.553993	0.513118
14	1	0	-3.397549	1.487530	-0.646184
15	1	0	-2.214914	0.499459	-1.661181

16	1	0	-2.758503	-0.427413	1.265638
17	1	0	-3.371279	-1.119696	-0.319207
18	1	0	-1.201998	-2.109446	-0.781589
19	1	0	-0.423297	-2.610598	1.667096
20	1	0	-0.431090	-0.881939	1.942096
21	1	0	1.808101	-0.971817	1.351276
22	1	0	1.667769	-2.551465	0.595237
23	1	0	1.026944	-1.718066	-1.483232
24	1	0	3.344153	-1.106975	-1.152232
25	1	0	2.542263	0.114510	-2.154461
26	1	0	2.917860	0.461003	-0.453510

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.517039	-0.833952	0.287361
2	6	0	1.294305	-1.459212	0.085532
3	7	0	-0.073172	-0.024711	-0.895964
4	6	0	0.043356	1.113904	-0.235316
5	6	0	1.321313	1.732525	-0.181633
6	6	0	2.394154	1.088738	-0.769901
7	6	0	0.259322	-1.643069	1.171095
8	6	0	-1.203934	-1.559342	0.651016
9	6	0	-1.229325	-0.915862	-0.760908
10	6	0	-2.586789	-0.314215	-1.147835
11	6	0	-0.975384	1.686570	0.627342
12	7	0	-1.778954	2.168178	1.318353
13	1	0	1.469689	2.553966	0.513077
14	1	0	2.215082	0.499523	-1.661284
15	1	0	3.397685	1.487319	-0.645996
16	1	0	3.371208	-1.119765	-0.319213
17	1	0	2.758441	-0.427611	1.265698
18	1	0	1.201944	-2.109566	-0.781582
19	1	0	0.423073	-2.610794	1.666895
20	1	0	0.431096	-0.882158	1.942171
21	1	0	-1.808078	-0.971502	1.351254
22	1	0	-1.668075	-2.551221	0.595314
23	1	0	-1.027054	-1.718003	-1.483245
24	1	0	-3.344277	-1.106768	-1.152101
25	1	0	-2.542378	0.114517	-2.154579
26	1	0	-2.917818	0.461290	-0.453653

TS2b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.211432	-1.315710	-0.351434
2	6	0	-0.900508	-1.724421	-0.152968
3	7	0	0.247922	0.074652	0.639075
4	6	0	-0.348370	1.177273	0.218144
5	6	0	-1.740241	1.360669	0.404080
6	6	0	-2.482684	0.335715	0.970750
7	6	0	0.196916	-1.814530	-1.177816
8	6	0	1.555957	-1.615345	-0.497604

9	6	0	1.602946	-0.219826	0.172036
10	6	0	2.590370	-0.175009	1.344147
11	6	0	0.328063	2.178274	-0.594107
12	7	0	0.863017	3.001980	-1.218103
13	1	0	-2.225458	2.171989	-0.129773
14	1	0	-2.033272	-0.252532	1.762784
15	1	0	-3.565278	0.427316	1.012045
16	1	0	-3.005104	-1.827712	0.185366
17	1	0	-2.506794	-0.887295	-1.306251
18	1	0	-0.707641	-2.298208	0.753027
19	1	0	0.167040	-2.808045	-1.651978
20	1	0	0.038128	-1.081401	-1.979777
21	1	0	2.387543	-1.725968	-1.202934
22	1	0	1.682765	-2.391251	0.270295
23	1	0	1.928247	0.507835	-0.586258
24	1	0	2.659222	0.835680	1.759391
25	1	0	3.590970	-0.477329	1.013455
26	1	0	2.266955	-0.852031	2.142433

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.464573	1.208375	0.394804
2	6	0	-2.524797	1.092957	1.330412
3	6	0	-2.766841	-0.148440	1.891805
4	6	0	-3.215711	-1.549111	0.235239
5	6	0	-2.300799	-1.265568	-0.768488
6	7	0	-0.829942	0.102491	0.057268
7	6	0	-1.113898	-2.098576	-1.171346
8	6	0	-0.060607	-1.197537	-1.832943
9	6	0	0.235065	0.053215	-0.933424
10	6	0	1.594520	-0.039899	-0.244505
11	6	0	2.679863	0.677149	-0.761209
12	6	0	3.946370	0.571659	-0.183282
13	6	0	4.142642	-0.250545	0.926643
14	6	0	3.063441	-0.962231	1.455227
15	6	0	1.799216	-0.857214	0.875280
16	6	0	-1.241146	2.475928	-0.274238
17	7	0	-1.032489	3.483397	-0.817949
18	1	0	-3.232858	1.910741	1.427218
19	1	0	-1.919861	-0.803086	2.058524
20	1	0	-3.627400	-0.293522	2.538979
21	1	0	-3.088788	-2.442016	0.843293
22	1	0	-4.234169	-1.188566	0.142450
23	1	0	-2.622697	-0.549069	-1.524650
24	1	0	-0.707310	-2.614996	-0.293854
25	1	0	-1.422284	-2.877065	-1.884790
26	1	0	-0.453334	-0.849001	-2.796760
27	1	0	0.860789	-1.747241	-2.046327
28	1	0	0.250021	0.949336	-1.571342
29	1	0	2.531629	1.327904	-1.620129
30	1	0	4.776279	1.138681	-0.596938
31	1	0	5.126435	-0.330643	1.381384
32	1	0	3.205174	-1.597881	2.325703
33	1	0	0.958911	-1.395772	1.302166

TS4a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.475811	1.089782	-0.510793
2	6	0	-2.648290	1.024690	-1.301146
3	6	0	-3.053393	-0.202556	-1.803712
4	6	0	-3.367190	-1.405803	-0.071143
5	6	0	-2.097419	-1.669875	0.420986
6	7	0	-0.737479	0.010649	-0.311722
7	6	0	-1.553226	-1.339987	1.783961
8	6	0	-0.036092	-1.141046	1.700259
9	6	0	0.279161	0.041682	0.740246
10	6	0	1.688687	-0.052361	0.170462
11	6	0	2.728459	0.668058	0.768404
12	6	0	4.037161	0.558689	0.293953
13	6	0	4.320141	-0.269331	-0.792518
14	6	0	3.286102	-0.984384	-1.401676
15	6	0	1.980492	-0.877636	-0.923464
16	6	0	-1.245156	2.343227	0.191717
17	7	0	-1.060172	3.358660	0.728797
18	1	0	-3.330319	1.868873	-1.275025
19	1	0	-4.010245	-0.274860	-2.314803
20	1	0	-2.295431	-0.905157	-2.130843
21	1	0	-4.053896	-0.789440	0.504107
22	1	0	-3.841718	-2.142349	-0.713453
23	1	0	-1.522744	-2.426447	-0.112636
24	1	0	-2.054496	-0.455207	2.198346
25	1	0	-1.771853	-2.173348	2.470075
26	1	0	0.423132	-2.056216	1.305758
27	1	0	0.413453	-0.956468	2.682101
28	1	0	0.214631	0.968524	1.327818
29	1	0	2.511899	1.325231	1.607888
30	1	0	4.832082	1.127628	0.769134
31	1	0	5.336915	-0.351740	-1.167331
32	1	0	3.496484	-1.624006	-2.255196
33	1	0	1.173917	-1.419063	-1.408678

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.475272	1.089946	-0.510571
2	6	0	2.647595	1.025781	-1.301184
3	6	0	3.053343	-0.201065	-1.804111
4	6	0	3.367682	-1.404441	-0.071794
5	6	0	2.098075	-1.669526	0.420269
6	7	0	0.737506	0.010388	-0.311597
7	6	0	1.553724	-1.340821	1.783501
8	6	0	0.036523	-1.142467	1.699697
9	6	0	-0.278984	0.040798	0.740557
10	6	0	-1.688566	-0.052855	0.170803
11	6	0	-2.727773	0.669665	0.767141
12	6	0	-4.036494	0.560628	0.292622
13	6	0	-4.319995	-0.269049	-0.792433
14	6	0	-3.286475	-0.986150	-1.400094

15	6	0	-1.980901	-0.879810	-0.921739
16	6	0	1.244213	2.343079	0.192388
17	7	0	1.058836	3.358279	0.729778
18	1	0	3.329256	1.870278	-1.274873
19	1	0	2.295814	-0.904074	-2.131366
20	1	0	4.010215	-0.272702	-2.315273
21	1	0	3.842630	-2.140503	-0.714367
22	1	0	4.054055	-0.787896	0.503633
23	1	0	1.523763	-2.426218	-0.113587
24	1	0	1.772573	-2.174659	2.468958
25	1	0	2.054602	-0.456123	2.198515
26	1	0	-0.413425	-0.959100	2.681581
27	1	0	-0.422162	-2.057524	1.304261
28	1	0	-0.214612	0.967335	1.328618
29	1	0	-2.510780	1.328237	1.605413
30	1	0	-4.831000	1.131083	0.766678
31	1	0	-5.336753	-0.351182	-1.167352
32	1	0	-3.497264	-1.627078	-2.252533
33	1	0	-1.174735	-1.422823	-1.405870

TS4b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.993829	1.212162	0.239758
2	6	0	-2.188023	1.954238	0.032349
3	6	0	-3.408265	1.421472	0.424993
4	6	0	-3.620835	-0.342964	-0.677302
5	6	0	-2.729211	-1.229488	-0.090288
6	7	0	-1.060119	0.044150	0.848757
7	6	0	-1.596046	-1.969233	-0.735593
8	6	0	-0.513001	-2.260944	0.310126
9	6	0	0.035252	-0.935648	0.936351
10	6	0	1.424146	-0.559915	0.427307
11	6	0	2.334852	0.018119	1.322088
12	6	0	3.622494	0.365061	0.915914
13	6	0	4.024630	0.130206	-0.399233
14	6	0	3.133581	-0.457653	-1.298362
15	6	0	1.847088	-0.801895	-0.887226
16	6	0	0.172137	1.837399	-0.373567
17	7	0	0.990454	2.497177	-0.872835
18	1	0	-2.147049	2.794253	-0.653949
19	1	0	-3.449880	0.855625	1.349543
20	1	0	-4.317535	1.961510	0.171117
21	1	0	-4.663021	-0.379892	-0.371682
22	1	0	-3.459436	-0.013232	-1.701134
23	1	0	-3.027806	-1.639403	0.874727
24	1	0	-1.967755	-2.927321	-1.133336
25	1	0	-1.206275	-1.406108	-1.592959
26	1	0	0.304792	-2.858694	-0.102574
27	1	0	-0.968190	-2.861510	1.107199
28	1	0	0.149740	-1.120413	2.012568
29	1	0	2.026440	0.201649	2.349355
30	1	0	4.310754	0.816302	1.625629
31	1	0	5.026534	0.400601	-0.721407
32	1	0	3.439756	-0.645163	-2.324109
33	1	0	1.166755	-1.252997	-1.604322

6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.539803	2.402732	0.141573
2	6	0	1.541094	1.491281	0.236359
3	7	0	1.241829	0.152860	0.039655
4	6	0	-0.060462	-0.286024	-0.261368
5	6	0	-1.048776	0.824496	-0.296585
6	7	0	-0.744240	2.077490	-0.118420
7	1	0	2.566205	1.734422	0.476400
8	8	0	-0.323147	-1.464242	-0.481722
9	17	0	0.893879	4.105229	0.389412
10	6	0	2.322664	-0.801473	0.044699
11	6	0	3.459357	-0.545967	-0.726462
12	6	0	2.242783	-1.953412	0.831698
13	6	0	4.529744	-1.440364	-0.696585
14	1	0	3.498025	0.337570	-1.356775
15	6	0	3.314471	-2.843672	0.848914
16	1	0	1.351115	-2.149285	1.414480
17	6	0	4.459792	-2.589963	0.090326
18	1	0	5.412051	-1.239750	-1.297467
19	1	0	3.253521	-3.738749	1.461214
20	1	0	5.291472	-3.288419	0.109705
21	8	0	-2.327198	0.577151	-0.612732
22	6	0	-2.988819	-0.672174	-0.294311
23	6	0	-4.488630	-0.387654	-0.362055
24	1	0	-2.696740	-1.003554	0.706592
25	1	0	-2.686300	-1.439185	-1.009046
26	6	0	-5.297395	-1.639753	-0.153211
27	1	0	-4.751361	0.370388	0.384339
28	1	0	-4.705650	0.042682	-1.349933
29	6	0	-6.158997	-1.835211	0.845293
30	1	0	-5.144954	-2.434722	-0.885274
31	1	0	-6.718636	-2.761385	0.944786
32	1	0	-6.344833	-1.071677	1.598250

6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.144718	2.419843	0.238782
2	6	0	2.010338	1.378162	0.324077
3	7	0	1.546254	0.104853	0.033875
4	6	0	0.214753	-0.138378	-0.347740
5	6	0	-0.613754	1.096916	-0.367423
6	7	0	-0.154495	2.285840	-0.100807
7	1	0	3.044149	1.466433	0.625726
8	8	0	-0.190123	-1.259213	-0.642104
9	17	0	1.706472	4.042961	0.607096
10	6	0	2.489433	-0.985696	0.033014
11	6	0	3.687392	-0.848061	-0.672706
12	6	0	2.219009	-2.152996	0.751909
13	6	0	4.628001	-1.878185	-0.644586
14	1	0	3.873533	0.051951	-1.251271
15	6	0	3.162057	-3.178606	0.767782

16	1	0	1.281038	-2.255081	1.283706
17	6	0	4.367739	-3.044449	0.075002
18	1	0	5.558383	-1.768832	-1.194314
19	1	0	2.953207	-4.085793	1.327428
20	1	0	5.098405	-3.848016	0.092860
21	8	0	-1.895202	1.048020	-0.753184
22	6	0	-2.727549	-0.130408	-0.610602
23	6	0	-4.166960	0.356815	-0.712045
24	1	0	-2.525563	-0.604743	0.353413
25	1	0	-2.483424	-0.845517	-1.399048
26	6	0	-5.198497	-0.792904	-0.698573
27	1	0	-4.372982	1.050806	0.111191
28	1	0	-4.272821	0.923865	-1.645046
29	6	0	-5.218572	-1.592638	0.578581
30	1	0	-6.193470	-0.366553	-0.873800
31	1	0	-4.333223	-2.194014	0.790167
32	1	0	-4.990628	-1.462944	-1.546582
33	6	0	-6.228054	-1.609863	1.449865
34	1	0	-7.136360	-1.033628	1.282625
35	1	0	-6.190307	-2.200892	2.361127

7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.146425	0.974280	0.809243
2	6	0	-1.837903	-0.329362	-0.467667
3	6	0	-0.393410	-0.891538	-0.654583
4	6	0	-1.030384	1.720735	-0.181231
5	1	0	0.603447	1.599964	1.285445
6	6	0	-2.205224	-0.403547	1.044313
7	1	0	-3.125312	0.184896	1.134854
8	6	0	-1.081058	0.271325	1.849296
9	1	0	-1.474098	1.002932	2.561687
10	1	0	-0.470127	-0.447306	2.405295
11	7	0	0.506712	-0.097503	0.029899
12	6	0	1.922827	-0.266080	0.018431
13	6	0	2.759764	0.858540	0.019015
14	6	0	2.487150	-1.549656	0.009883
15	6	0	4.144866	0.700034	0.035896
16	1	0	2.334924	1.857268	-0.018785
17	6	0	3.873761	-1.693790	0.011342
18	1	0	1.842419	-2.417973	-0.017482
19	6	0	4.709242	-0.575852	0.032581
20	1	0	4.781302	1.580659	0.037039
21	1	0	4.301077	-2.692804	0.002336
22	1	0	5.788606	-0.697442	0.039120
23	8	0	-0.140772	-1.904335	-1.280867
24	17	0	-0.859835	3.461543	-0.326863
25	7	0	-1.874479	1.076301	-0.869189
26	6	0	-2.552374	-1.889572	1.165272
27	1	0	-3.257388	-2.102604	1.974125
28	1	0	-1.652146	-2.490375	1.335805
29	6	0	-3.159978	-2.191395	-0.234441
30	8	0	-2.782256	-1.111258	-1.118367
31	1	0	-4.254493	-2.220757	-0.212612
32	1	0	-2.787544	-3.134252	-0.645361

7a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.116238	0.969550	0.630762
2	6	0	-1.638713	-0.748538	-0.360723
3	6	0	-0.165132	-1.121483	-0.600882
4	6	0	-1.098929	1.440635	-0.420381
5	1	0	0.583836	1.739583	0.945409
6	6	0	-1.837600	-0.718360	1.190576
7	1	0	-1.440229	-1.669061	1.562940
8	6	0	-1.030099	0.448645	1.786181
9	1	0	-1.666005	1.267988	2.138946
10	1	0	-0.411808	0.119225	2.626264
11	7	0	0.626797	-0.153965	0.016207
12	6	0	2.050740	-0.205711	0.062290
13	6	0	2.785508	-0.700585	-1.024525
14	6	0	2.727381	0.248004	1.203458
15	6	0	4.177391	-0.733028	-0.959334
16	1	0	2.267774	-1.064847	-1.901718
17	6	0	4.120929	0.224621	1.249832
18	1	0	2.170169	0.604553	2.065006
19	6	0	4.853468	-0.267559	0.169885
20	1	0	4.736177	-1.119090	-1.807470
21	1	0	4.630304	0.582502	2.140433
22	1	0	5.938701	-0.291398	0.208832
23	8	0	0.229869	-2.118270	-1.169657
24	17	0	-1.168934	3.149727	-0.821615
25	7	0	-1.891398	0.600587	-0.928402
26	6	0	-3.369580	-0.770414	1.253719
27	1	0	-3.793294	0.232726	1.138869
28	1	0	-3.745353	-1.194874	2.189456
29	6	0	-3.711926	-1.658310	0.030132
30	8	0	-2.547891	-1.676114	-0.830276
31	1	0	-4.567641	-1.272564	-0.533235
32	1	0	-3.917571	-2.696179	0.312620

7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.180212	1.084834	0.826786
2	6	0	-1.691025	0.013428	-0.473798
3	6	0	-0.323750	-0.718504	-0.671946
4	6	0	-0.594198	1.959130	-0.136962
5	1	0	1.015061	1.583572	1.312118
6	6	0	-2.035267	-0.082577	1.051974
7	1	0	-2.932014	0.533596	1.178524
8	6	0	-0.867801	0.557897	1.845808
9	1	0	-1.211629	1.381919	2.479071
10	1	0	-0.373915	-0.176244	2.490757
11	7	0	0.666269	-0.068405	0.044338
12	6	0	2.049122	-0.417867	0.006976
13	6	0	3.024932	0.587738	-0.026904
14	6	0	2.441186	-1.763745	0.009815
15	6	0	4.377984	0.250126	-0.033582

16	1	0	2.732503	1.632796	-0.072329
17	6	0	3.796680	-2.088167	-0.012583
18	1	0	1.688408	-2.540991	0.011095
19	6	0	4.770800	-1.088404	-0.026320
20	1	0	5.123643	1.039976	-0.059307
21	1	0	4.090359	-3.134359	-0.012362
22	1	0	5.825020	-1.349973	-0.038243
23	8	0	-0.185450	-1.733657	-1.327461
24	17	0	-0.200212	3.669116	-0.251133
25	7	0	-1.530844	1.445214	-0.807283
26	6	0	-2.366154	-1.536642	1.450602
27	1	0	-2.951982	-1.515065	2.377267
28	1	0	-1.440230	-2.074974	1.684199
29	6	0	-3.693029	-1.301586	-0.698481
30	8	0	-2.656284	-0.531793	-1.314217
31	1	0	-4.442191	-0.635374	-0.242969
32	1	0	-4.177369	-1.827447	-1.525183
33	6	0	-3.130415	-2.282362	0.325957
34	1	0	-2.448806	-2.955564	-0.203030
35	1	0	-3.943018	-2.890684	0.739630

7b’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.158506	0.939821	0.741814
2	6	0	-1.477141	-0.596401	-0.400766
3	6	0	-0.001790	-1.078536	-0.547870
4	6	0	-0.758196	1.549217	-0.298720
5	1	0	0.886344	1.632577	1.155991
6	6	0	-1.806981	-0.576080	1.130691
7	1	0	-1.668807	-1.605556	1.478320
8	6	0	-0.780305	0.350639	1.830744
9	1	0	-1.278879	1.166289	2.365606
10	1	0	-0.164570	-0.194509	2.552428
11	7	0	0.848100	-0.184842	0.083425
12	6	0	2.270788	-0.286326	0.072309
13	6	0	3.054451	0.866236	-0.075810
14	6	0	2.893977	-1.533550	0.218458
15	6	0	4.445784	0.774456	-0.053087
16	1	0	2.582771	1.831962	-0.232599
17	6	0	4.285533	-1.613772	0.223707
18	1	0	2.289902	-2.426724	0.309428
19	6	0	5.068344	-0.464875	0.096763
20	1	0	5.040760	1.676368	-0.167759
21	1	0	4.758921	-2.585411	0.335849
22	1	0	6.152234	-0.535656	0.107851
23	8	0	0.327152	-2.104065	-1.108501
24	17	0	-0.682653	3.283411	-0.596013
25	7	0	-1.583140	0.805739	-0.896693
26	6	0	-3.284492	-0.169541	1.352270
27	1	0	-3.358651	0.917530	1.463001
28	1	0	-3.620563	-0.603415	2.301828
29	6	0	-3.554498	-1.794316	-0.567837
30	8	0	-2.290395	-1.440034	-1.141892
31	1	0	-4.171920	-2.107198	-1.414044
32	1	0	-3.428135	-2.665954	0.093239
33	6	0	-4.189295	-0.630422	0.185788

34	1	0	-5.180419	-0.924321	0.550422
35	1	0	-4.330774	0.193234	-0.522062

8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.829020	-1.197686	-0.107386
2	6	0	-0.458770	-1.199296	-0.143032
3	7	0	0.230834	-0.023551	-0.050650
4	6	0	-0.445142	1.230134	0.055397
5	6	0	-1.909957	1.069586	0.092950
6	7	0	-2.551083	-0.073138	0.015030
7	1	0	0.126744	-2.102074	-0.259327
8	8	0	0.147086	2.292508	0.111963
9	17	0	-2.696077	-2.712312	-0.234415
10	6	0	1.673275	-0.057379	-0.015634
11	6	0	2.306496	-0.931227	0.872201
12	6	0	2.417234	0.758333	-0.872099
13	6	0	3.699195	-1.003974	0.888245
14	1	0	1.716389	-1.531890	1.558285
15	6	0	3.808209	0.679792	-0.842392
16	1	0	1.915477	1.444224	-1.542927
17	6	0	4.451435	-0.199976	0.031258
18	1	0	4.191935	-1.681193	1.579489
19	1	0	4.390378	1.310501	-1.507570
20	1	0	5.536057	-0.253162	0.048440
21	6	0	-2.681089	2.274554	0.226949
22	7	0	-3.309972	3.246072	0.334795

9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642688	0.488469	0.811503
2	6	0	0.736902	-1.516551	0.311164
3	6	0	-0.644056	-1.527761	-0.480883
4	6	0	-0.276988	-0.406292	1.995214
5	1	0	-1.247514	1.358122	1.047747
6	6	0	1.425699	-0.210565	-0.133730
7	6	0	0.691991	0.867474	0.180026
8	7	0	-1.355029	-0.409619	-0.128086
9	6	0	-2.693610	-0.144966	-0.554126
10	6	0	-3.624885	0.371244	0.354434
11	6	0	-3.068851	-0.396647	-1.879124
12	6	0	-4.923656	0.652310	-0.068241
13	1	0	-3.347475	0.537312	1.391275
14	6	0	-4.375362	-0.127066	-2.283683
15	1	0	-2.349212	-0.807431	-2.575975
16	6	0	-5.304635	0.402781	-1.386942
17	1	0	-5.639349	1.055687	0.642393
18	1	0	-4.662421	-0.326017	-3.312322
19	1	0	-6.318586	0.616242	-1.712460
20	8	0	-0.963887	-2.414627	-1.239953
21	17	0	-0.818910	0.003787	3.593470

22	7	0	0.402231	-1.448976	1.766631
23	6	0	1.510197	-2.726387	0.028597
24	7	0	2.149120	-3.664378	-0.204062
25	6	0	1.004484	2.304636	-0.003669
26	8	0	0.220940	3.191580	0.275016
27	8	0	2.237234	2.502437	-0.494911
28	6	0	2.719424	-0.267190	-0.897120
29	8	0	2.793433	-0.136560	-2.095683
30	8	0	3.733260	-0.548096	-0.071273
31	6	0	2.600806	3.876382	-0.731482
32	1	0	1.905127	4.335601	-1.437647
33	1	0	2.588556	4.437839	0.205917
34	1	0	3.606510	3.839833	-1.148711
35	6	0	5.011470	-0.764564	-0.707460
36	1	0	4.944405	-1.608541	-1.397483
37	1	0	5.319417	0.131518	-1.251157
38	1	0	5.702452	-0.983451	0.105607

10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.690464	0.963960	-0.123131
2	6	0	0.474069	-1.529895	-0.023765
3	6	0	-0.988433	-1.457300	0.010712
4	1	0	-1.171743	1.933351	-0.175463
5	6	0	1.281073	-0.412797	-0.105335
6	6	0	0.683537	0.881960	-0.146263
7	7	0	-1.501924	-0.115903	-0.048129
8	6	0	-2.931750	0.084180	0.028400
9	6	0	-3.443325	0.939477	1.006155
10	6	0	-3.778881	-0.552463	-0.881138
11	6	0	-4.817261	1.175998	1.061811
12	1	0	-2.774392	1.403984	1.724838
13	6	0	-5.149975	-0.313812	-0.812138
14	1	0	-3.369748	-1.225972	-1.624349
15	6	0	-5.671494	0.550371	0.153784
16	1	0	-5.215815	1.841888	1.821507
17	1	0	-5.812282	-0.805619	-1.518411
18	1	0	-6.741533	0.730763	0.200823
19	8	0	-1.737925	-2.413867	0.080487
20	6	0	1.034695	-2.844587	0.019857
21	7	0	1.518058	-3.901974	0.053281
22	6	0	1.402533	2.181343	-0.191122
23	8	0	0.851567	3.253933	-0.352422
24	8	0	2.727606	2.043487	-0.003921
25	6	0	2.771424	-0.620896	-0.268297
26	8	0	3.323304	-0.584875	-1.342054
27	8	0	3.348083	-0.910419	0.902834
28	6	0	3.493793	3.259886	-0.064406
29	1	0	3.361196	3.743867	-1.034801
30	1	0	3.180092	3.945491	0.726584
31	1	0	4.530741	2.955726	0.075879
32	6	0	4.752239	-1.232874	0.834237
33	1	0	4.903043	-2.115945	0.209189
34	1	0	5.313590	-0.391880	0.420033
35	1	0	5.052147	-1.431899	1.862542

11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.608173	-1.205283	0.021865
2	6	0	-0.819117	1.405911	0.019861
3	6	0	-2.498254	-0.130530	-0.065267
4	1	0	-1.955474	-2.231027	0.034624
5	6	0	0.179770	0.417713	0.096763
6	6	0	-0.247980	-0.922681	0.088919
7	17	0	-4.212874	-0.461341	-0.181954
8	7	0	-2.133574	1.135392	-0.066265
9	6	0	-0.495357	2.812603	0.074652
10	7	0	-0.257948	3.947799	0.137615
11	6	0	0.684292	-2.104929	0.138604
12	8	0	0.412877	-3.133216	0.717221
13	8	0	1.792934	-1.896783	-0.584291
14	6	0	1.622970	0.775534	0.327300
15	8	0	2.281318	0.318796	1.235006
16	8	0	2.052720	1.674046	-0.566261
17	6	0	2.764254	-2.961931	-0.550224
18	1	0	3.141570	-3.088538	0.467203
19	1	0	2.313523	-3.896287	-0.892035
20	1	0	3.562022	-2.646174	-1.221612
21	6	0	3.391675	2.168979	-0.360166
22	1	0	3.470098	2.644499	0.620069
23	1	0	4.109919	1.348329	-0.425831
24	1	0	3.554583	2.894586	-1.155904

12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.869535	-1.683271	0.187003
2	6	0	2.598139	-1.461428	0.520481
3	6	0	1.811846	-0.282110	0.120805
4	7	0	0.602577	-0.161509	0.495898
5	6	0	-0.204766	0.989303	0.120434
6	6	0	-1.482711	0.493158	-0.584809
7	6	0	-2.413296	-0.387763	0.264743
8	6	0	-3.556980	-0.938810	-0.539465
9	6	0	-4.844617	-0.699504	-0.310516
10	6	0	2.501125	0.711067	-0.708567
11	7	0	3.067114	1.481958	-1.360655
12	6	0	-0.490521	1.806930	1.385619
13	1	0	4.384282	-2.576984	0.518729
14	1	0	4.436119	-0.987019	-0.422851
15	1	0	2.040032	-2.163390	1.131558
16	1	0	0.326353	1.638096	-0.590344
17	1	0	-2.033260	1.372535	-0.937280
18	1	0	-1.180464	-0.059743	-1.481765
19	1	0	-1.824437	-1.211937	0.684540
20	1	0	-2.808611	0.183739	1.110789
21	1	0	-3.281936	-1.578154	-1.378799
22	1	0	-5.624753	-1.126921	-0.931645
23	1	0	-5.169807	-0.068284	0.512320

24	1	0	-1.169985	2.632311	1.154544
25	1	0	0.434654	2.229207	1.785768
26	1	0	-0.942549	1.187967	2.163366

TS7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.124854	1.241716	0.363265
2	6	0	-1.710366	-0.492225	-0.722472
3	6	0	-0.253480	-0.837786	-0.804241
4	6	0	-1.320703	1.646691	-0.258812
5	1	0	0.510701	1.945260	0.882640
6	6	0	-1.989042	-0.778843	1.365234
7	1	0	-3.006643	-0.394519	1.311214
8	6	0	-1.067271	0.041838	2.015388
9	1	0	-1.418129	0.908382	2.566363
10	1	0	-0.108475	-0.358010	2.337608
11	7	0	0.538146	0.154145	-0.240790
12	6	0	1.961581	0.038282	-0.124200
13	6	0	2.752315	1.175300	-0.333091
14	6	0	2.564134	-1.181246	0.208776
15	6	0	4.136487	1.098475	-0.185808
16	1	0	2.287368	2.110400	-0.630396
17	6	0	3.950058	-1.247495	0.343628
18	1	0	1.956075	-2.066896	0.336214
19	6	0	4.740616	-0.112509	0.153994
20	1	0	4.741284	1.985610	-0.351088
21	1	0	4.412630	-2.196307	0.600686
22	1	0	5.819791	-0.173659	0.261419
23	8	0	0.168238	-1.887828	-1.278500
24	17	0	-1.873126	3.302211	-0.029841
25	7	0	-2.124840	0.787263	-0.825584
26	6	0	-1.891581	-2.270868	1.141004
27	1	0	-2.462865	-2.805517	1.910726
28	1	0	-0.851796	-2.603168	1.225235
29	6	0	-2.469808	-2.638101	-0.259138
30	8	0	-2.576905	-1.459943	-1.090413
31	1	0	-3.491772	-3.020146	-0.191701
32	1	0	-1.837354	-3.376080	-0.756856

TS7a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.050007	1.191864	0.027266
2	6	0	-1.475264	-0.886381	-0.597627
3	6	0	-0.008970	-1.122541	-0.666305
4	6	0	-1.292381	1.341083	-0.614394
5	1	0	0.533209	2.057282	0.309904
6	6	0	-1.575698	-0.763267	1.536398
7	1	0	-0.961434	-1.646738	1.703892
8	6	0	-1.022031	0.467213	1.901989
9	1	0	-1.664512	1.323351	2.090750
10	1	0	-0.070429	0.481942	2.424281

11	7	0	0.691105	0.053495	-0.330847
12	6	0	2.107037	0.019781	-0.099901
13	6	0	2.942563	-0.656519	-0.997897
14	6	0	2.660886	0.678016	1.005043
15	6	0	4.319243	-0.667968	-0.782247
16	1	0	2.514100	-1.171376	-1.846995
17	6	0	4.041608	0.667189	1.204340
18	1	0	2.023719	1.190344	1.718536
19	6	0	4.876427	-0.006756	0.313855
20	1	0	4.959594	-1.194773	-1.484115
21	1	0	4.459108	1.181951	2.065176
22	1	0	5.950915	-0.017762	0.472495
23	8	0	0.517570	-2.192966	-0.920701
24	17	0	-1.992568	2.951863	-0.737766
25	7	0	-2.016301	0.308306	-0.937878
26	6	0	-3.064382	-1.033062	1.444321
27	1	0	-3.610768	-0.085293	1.462242
28	1	0	-3.387294	-1.608780	2.320822
29	6	0	-3.423697	-1.832404	0.149118
30	8	0	-2.248762	-1.986836	-0.666582
31	1	0	-4.202100	-1.312114	-0.417289
32	1	0	-3.756545	-2.851385	0.357887

TS7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.191460	1.375256	0.345153
2	6	0	-1.619373	-0.128548	-0.800237
3	6	0	-0.219682	-0.659032	-0.860675
4	6	0	-0.958483	1.938619	-0.236037
5	1	0	0.923114	1.985566	0.857038
6	6	0	-1.813246	-0.425479	1.443640
7	1	0	-2.820314	-0.024692	1.355129
8	6	0	-0.866680	0.428658	2.008869
9	1	0	-1.181998	1.371651	2.444640
10	1	0	0.044268	0.007221	2.430261
11	7	0	0.694090	0.222825	-0.277419
12	6	0	2.089636	-0.084646	-0.163303
13	6	0	3.025574	0.929616	-0.400062
14	6	0	2.522908	-1.366279	0.197342
15	6	0	4.387491	0.670500	-0.251641
16	1	0	2.688873	1.911468	-0.719403
17	6	0	3.887559	-1.616277	0.332864
18	1	0	1.800554	-2.157797	0.346889
19	6	0	4.823319	-0.602835	0.116297
20	1	0	5.106089	1.463506	-0.438358
21	1	0	4.219068	-2.612522	0.611994
22	1	0	5.884729	-0.806904	0.224576
23	8	0	0.093724	-1.737965	-1.347820
24	17	0	-1.310631	3.636234	0.070896
25	7	0	-1.865447	1.197042	-0.809284
26	6	0	-1.733701	-1.938397	1.524373
27	1	0	-2.263047	-2.229940	2.443674
28	1	0	-0.691379	-2.244407	1.673874
29	6	0	-3.249251	-1.897846	-0.586706
30	8	0	-2.563444	-0.912033	-1.381469
31	1	0	-4.046163	-1.398357	-0.017065

32	1	0	-3.725419	-2.545424	-1.326601
33	6	0	-2.339400	-2.719873	0.322064
34	1	0	-1.541197	-3.129536	-0.300659
35	1	0	-2.927973	-3.565509	0.698380

TS7b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.243919	1.167666	0.282421
2	6	0	-1.332762	-0.620477	-0.764061
3	6	0	0.115321	-0.979934	-0.812670
4	6	0	-0.952211	1.551234	-0.345809
5	1	0	0.891769	1.894973	0.752340
6	6	0	-1.379071	-0.913095	1.429345
7	1	0	-0.797887	-1.828084	1.341449
8	6	0	-0.706286	0.194453	1.958833
9	1	0	-1.275206	1.016235	2.389788
10	1	0	0.283654	0.058641	2.385711
11	7	0	0.898807	0.053150	-0.284028
12	6	0	2.315924	-0.082045	-0.118856
13	6	0	3.137274	1.018132	-0.394878
14	6	0	2.882076	-1.282434	0.327911
15	6	0	4.515068	0.926311	-0.201946
16	1	0	2.699803	1.935305	-0.778124
17	6	0	4.262188	-1.365841	0.506526
18	1	0	2.250754	-2.142321	0.509854
19	6	0	5.082613	-0.265661	0.249824
20	1	0	5.143819	1.785196	-0.419290
21	1	0	4.696464	-2.300009	0.851625
22	1	0	6.156933	-0.339667	0.392615
23	8	0	0.553962	-2.039554	-1.231702
24	17	0	-1.526659	3.205637	-0.160138
25	7	0	-1.740446	0.664572	-0.886623
26	6	0	-2.884039	-1.159172	1.604191
27	1	0	-3.219412	-0.650873	2.516737
28	1	0	-3.015405	-2.232556	1.789670
29	6	0	-3.557566	-1.399596	-0.885523
30	8	0	-2.151791	-1.608099	-1.158356
31	1	0	-3.994600	-0.814508	-1.702339
32	1	0	-3.971117	-2.411357	-0.920196
33	6	0	-3.835241	-0.733625	0.466893
34	1	0	-4.860275	-0.997809	0.757241
35	1	0	-3.805233	0.352682	0.357069

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.761698	0.583972	1.143128
2	6	0	1.190923	-1.129029	1.437531
3	6	0	-0.064668	-1.697259	0.874388
4	6	0	0.236510	0.771194	2.140909
5	1	0	-1.549422	1.315247	1.005414
6	6	0	1.278387	0.256246	-0.660795

7	6	0	0.427214	1.140083	-0.400317
8	7	0	-1.087022	-0.732697	0.828524
9	6	0	-2.300795	-0.995620	0.099597
10	6	0	-3.522536	-0.663511	0.689203
11	6	0	-2.247181	-1.544638	-1.185371
12	6	0	-4.706182	-0.871599	-0.018769
13	1	0	-3.544070	-0.259618	1.697405
14	6	0	-3.437873	-1.755942	-1.878300
15	1	0	-1.291598	-1.799109	-1.630210
16	6	0	-4.665169	-1.420086	-1.301213
17	1	0	-5.657306	-0.613913	0.437831
18	1	0	-3.403621	-2.182115	-2.876690
19	1	0	-5.587609	-1.588954	-1.849499
20	8	0	-0.191220	-2.849477	0.504416
21	17	0	0.257708	2.252024	3.056373
22	7	0	1.228693	-0.068283	2.266428
23	6	0	2.341388	-1.988261	1.413747
24	7	0	3.285637	-2.663729	1.355715
25	6	0	-0.095926	2.444028	-0.861624
26	8	0	-1.086303	2.995768	-0.426279
27	8	0	0.681653	2.936763	-1.837824
28	6	0	2.131134	-0.617667	-1.448298
29	8	0	1.673904	-1.417039	-2.241598
30	8	0	3.425873	-0.437965	-1.166477
31	6	0	0.262501	4.209563	-2.371488
32	1	0	-0.734411	4.127420	-2.811323
33	1	0	0.248821	4.965560	-1.582716
34	1	0	1.002318	4.456312	-3.132350
35	6	0	4.336785	-1.331698	-1.845112
36	1	0	4.132508	-2.362396	-1.549297
37	1	0	4.235086	-1.226085	-2.927604
38	1	0	5.328971	-1.026864	-1.515188

TS10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.603585	-0.723234	-0.090911
2	6	0	-0.579018	1.590525	0.222302
3	6	0	0.880847	1.656902	-0.087192
4	6	0	0.298249	-0.599194	1.791189
5	1	0	1.094472	-1.677317	-0.246093
6	6	0	-1.387710	0.575164	-0.346391
7	6	0	-0.766575	-0.648631	-0.519686
8	7	0	1.426529	0.389626	-0.330094
9	6	0	2.848589	0.228489	-0.480784
10	6	0	3.540685	-0.729904	0.265611
11	6	0	3.528619	1.027486	-1.406538
12	6	0	4.912333	-0.897696	0.072569
13	1	0	3.025879	-1.335441	1.004007
14	6	0	4.900364	0.857518	-1.581670
15	1	0	2.988889	1.773695	-1.975524
16	6	0	5.596632	-0.105326	-0.848476
17	1	0	5.443611	-1.644340	0.655650
18	1	0	5.424098	1.480492	-2.300919
19	1	0	6.665466	-0.234281	-0.991954
20	8	0	1.509066	2.697227	-0.122352
21	17	0	0.701701	-2.093554	2.555677

22	7	0	-0.092125	0.468906	2.201958
23	6	0	-1.168384	2.810416	0.677102
24	7	0	-1.681918	3.784578	1.048966
25	6	0	-1.421071	-1.942000	-0.855402
26	8	0	-0.837235	-3.008412	-0.828805
27	8	0	-2.710567	-1.792971	-1.192484
28	6	0	-2.849779	0.854540	-0.609213
29	8	0	-3.275216	1.189234	-1.688470
30	8	0	-3.561471	0.745980	0.518176
31	6	0	-3.403071	-3.000028	-1.565362
32	1	0	-2.896156	-3.482498	-2.404164
33	1	0	-3.440201	-3.690361	-0.719173
34	1	0	-4.404552	-2.680053	-1.850671
35	6	0	-4.954750	1.105178	0.407327
36	1	0	-5.049393	2.143053	0.080303
37	1	0	-5.457795	0.449548	-0.307563
38	1	0	-5.364504	0.976442	1.408417

TS11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.593017	-0.202048	1.076055
2	6	0	1.240799	-1.628688	-0.097385
3	6	0	-0.656508	-1.013371	-1.407066
4	6	0	-0.331396	-1.577953	1.517937
5	1	0	-1.352262	0.370850	1.597282
6	6	0	1.550929	-0.234145	0.064586
7	6	0	0.655852	0.501502	0.812123
8	7	0	-1.322235	-0.458274	-0.478067
9	6	0	-2.618970	0.122978	-0.710543
10	6	0	-3.678325	-0.219906	0.133117
11	6	0	-2.795697	1.023117	-1.763653
12	6	0	-4.930137	0.355118	-0.083744
13	1	0	-3.525682	-0.932831	0.937560
14	6	0	-4.056552	1.580665	-1.975093
15	1	0	-1.957991	1.284688	-2.402837
16	6	0	-5.122868	1.252213	-1.136375
17	1	0	-5.757102	0.092736	0.569515
18	1	0	-4.199086	2.280239	-2.793412
19	1	0	-6.100953	1.694085	-1.301794
20	8	0	-0.473979	-1.412458	-2.500156
21	17	0	-1.286232	-2.261557	2.813502
22	7	0	0.505028	-2.302151	0.872417
23	6	0	2.017033	-2.448879	-0.978952
24	7	0	2.619393	-3.086086	-1.743197
25	6	0	0.734365	1.926742	1.179847
26	8	0	-0.212686	2.567678	1.600301
27	8	0	1.974352	2.431513	1.025840
28	6	0	2.710225	0.358214	-0.696089
29	8	0	2.572823	1.081534	-1.655968
30	8	0	3.878922	-0.072675	-0.206847
31	6	0	2.113874	3.830549	1.326214
32	1	0	1.471453	4.427111	0.673655
33	1	0	1.847036	4.024499	2.368070
34	1	0	3.163729	4.062059	1.147063
35	6	0	5.049012	0.361770	-0.928485
36	1	0	5.012774	-0.005474	-1.956760

37	1	0	5.107736	1.452869	-0.932708
38	1	0	5.893831	-0.070786	-0.393569

TS12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.309634	1.092494	0.237186
2	6	0	-1.785039	-0.962012	-0.373360
3	6	0	-0.319780	-1.189374	-0.499815
4	6	0	-1.616482	1.268211	-0.278103
5	1	0	0.291365	1.943832	0.528815
6	6	0	-1.610558	-0.841516	1.910885
7	6	0	-0.947525	0.357297	2.163919
8	7	0	0.402105	-0.015000	-0.227231
9	6	0	1.837190	-0.001939	-0.165017
10	6	0	2.519783	1.101323	-0.690833
11	6	0	2.546014	-1.054456	0.425487
12	6	0	3.909746	1.163752	-0.603681
13	1	0	1.966790	1.895265	-1.184510
14	6	0	3.936580	-0.984634	0.497405
15	1	0	2.018433	-1.921747	0.800430
16	6	0	4.621872	0.121530	-0.008737
17	1	0	4.433679	2.021844	-1.014583
18	1	0	4.485440	-1.803068	0.954221
19	1	0	5.705399	0.166313	0.051594
20	8	0	0.193923	-2.260218	-0.779275
21	17	0	-2.314577	2.876324	-0.268034
22	7	0	-2.365813	0.249567	-0.577533
23	6	0	-2.616880	-2.119604	-0.580318
24	7	0	-3.304758	-3.048703	-0.697071
25	1	0	-2.692027	-0.891299	1.974958
26	1	0	-1.516005	1.228773	2.475772
27	1	0	0.082997	0.328284	2.509063
28	1	0	-1.092109	-1.791450	1.997745

bmimPF_6 (A)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.960008	1.366933	0.304158
2	6	0	2.695689	2.129014	-0.830261
3	6	0	2.050912	3.199925	-0.282948
4	7	0	0.967173	2.700242	0.418784
5	1	0	0.216320	0.699234	0.720998
6	1	0	3.572079	2.077719	-1.457627
7	1	0	2.261137	4.256920	-0.336547
8	7	0	1.999812	0.994821	-0.451186
9	6	0	-0.038173	3.479171	1.152448
10	1	0	-0.318470	4.347321	0.552470
11	1	0	-0.916387	2.849776	1.301046
12	1	0	0.370258	3.804674	2.112885
13	6	0	2.269199	-0.397210	-0.883349
14	6	0	2.501234	-1.349641	0.292466
15	1	0	3.148461	-0.347228	-1.532145

16	1	0	1.409582	-0.716726	-1.478407
17	6	0	2.789130	-2.777351	-0.195071
18	1	0	3.339006	-0.983554	0.902898
19	1	0	1.607986	-1.361330	0.928386
20	6	0	2.998754	-3.760414	0.962301
21	1	0	1.950943	-3.119577	-0.816475
22	1	0	3.679241	-2.773734	-0.841373
23	1	0	3.202331	-4.769685	0.587274
24	1	0	3.845750	-3.460873	1.592935
25	1	0	2.107445	-3.814196	1.598543
26	15	0	-2.174252	-0.508646	-0.106790
27	9	0	-2.064867	1.130241	0.194979
28	9	0	-0.934649	-0.330553	-1.209959
29	9	0	-0.996469	-0.732360	1.074895
30	9	0	-3.327449	-0.642516	1.026641
31	9	0	-2.187697	-2.109460	-0.383530
32	9	0	-3.265681	-0.233915	-1.272432

bmimPF_6 (B)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.648453	1.686732	0.613100
2	6	0	2.606593	2.101699	-0.319734
3	6	0	1.759104	3.117163	-0.652843
4	7	0	0.538873	2.836791	-0.060965
5	1	0	-0.152310	1.186417	1.136707
6	1	0	3.639441	1.930715	-0.580478
7	1	0	1.913251	3.999552	-1.254546
8	7	0	1.893621	1.219739	0.475076
9	6	0	-0.697938	3.618295	-0.188438
10	1	0	-0.798000	3.948523	-1.224219
11	1	0	-1.539066	2.970228	0.062532
12	1	0	-0.664231	4.484340	0.478066
13	6	0	2.359253	-0.097359	0.963363
14	6	0	2.474288	-1.124195	-0.168172
15	1	0	1.627324	-0.429135	1.701986
16	1	0	3.318039	0.063227	1.468085
17	6	0	2.877911	-2.505275	0.368005
18	1	0	1.507310	-1.190642	-0.678788
19	1	0	3.214372	-0.781909	-0.906096
20	6	0	3.000742	-3.549779	-0.747625
21	1	0	3.832650	-2.430155	0.910083
22	1	0	2.126621	-2.838126	1.096310
23	1	0	3.275644	-4.529078	-0.339625
24	1	0	2.050889	-3.664205	-1.282548
25	1	0	3.768196	-3.264492	-1.478694
26	15	0	-1.973999	-0.711188	-0.028815
27	9	0	-1.599232	-2.193935	-0.581177
28	9	0	-0.824895	-0.047945	-1.039240
29	9	0	-3.105848	-0.502715	-1.172540
30	9	0	-3.059958	-1.312963	1.013730
31	9	0	-2.264818	0.832424	0.552845
32	9	0	-0.779475	-0.848959	1.139575

bmimPF_6 (C)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.610725	1.250745	0.319383
2	6	0	-2.060447	2.382073	-0.904977
3	6	0	-1.175667	3.272572	-0.371289
4	7	0	-0.279016	2.543664	0.391327
5	1	0	-0.059466	0.442872	0.778868
6	1	0	-2.904373	2.530766	-1.560788
7	1	0	-1.099015	4.343794	-0.476415
8	7	0	-1.687423	1.123509	-0.463762
9	6	0	0.909033	3.063231	1.081139
10	1	0	0.601388	3.754907	1.869376
11	1	0	1.457313	2.219845	1.501002
12	1	0	1.547465	3.572116	0.355816
13	6	0	-2.327285	-0.163686	-0.807296
14	6	0	-3.393555	-0.583864	0.209310
15	1	0	-1.523735	-0.901420	-0.874175
16	1	0	-2.757511	-0.040528	-1.805808
17	6	0	-4.048911	-1.917665	-0.177401
18	1	0	-2.927456	-0.675786	1.199548
19	1	0	-4.159997	0.200358	0.288181
20	6	0	-5.105671	-2.371982	0.835928
21	1	0	-4.509960	-1.823068	-1.171087
22	1	0	-3.272002	-2.688714	-0.268447
23	1	0	-5.556287	-3.323462	0.532529
24	1	0	-4.665614	-2.514385	1.830546
25	1	0	-5.913048	-1.634524	0.929131
26	15	0	2.298883	-0.872222	-0.064769
27	9	0	0.713673	-1.355232	-0.304416
28	9	0	1.919915	0.558407	-0.829186
29	9	0	2.722554	-1.531315	-1.484528
30	9	0	3.805220	-0.329538	0.207837
31	9	0	2.595894	-2.253396	0.732340
32	9	0	1.787576	-0.159837	1.371455