Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

On the Mechanism of the Dakin-West Reaction

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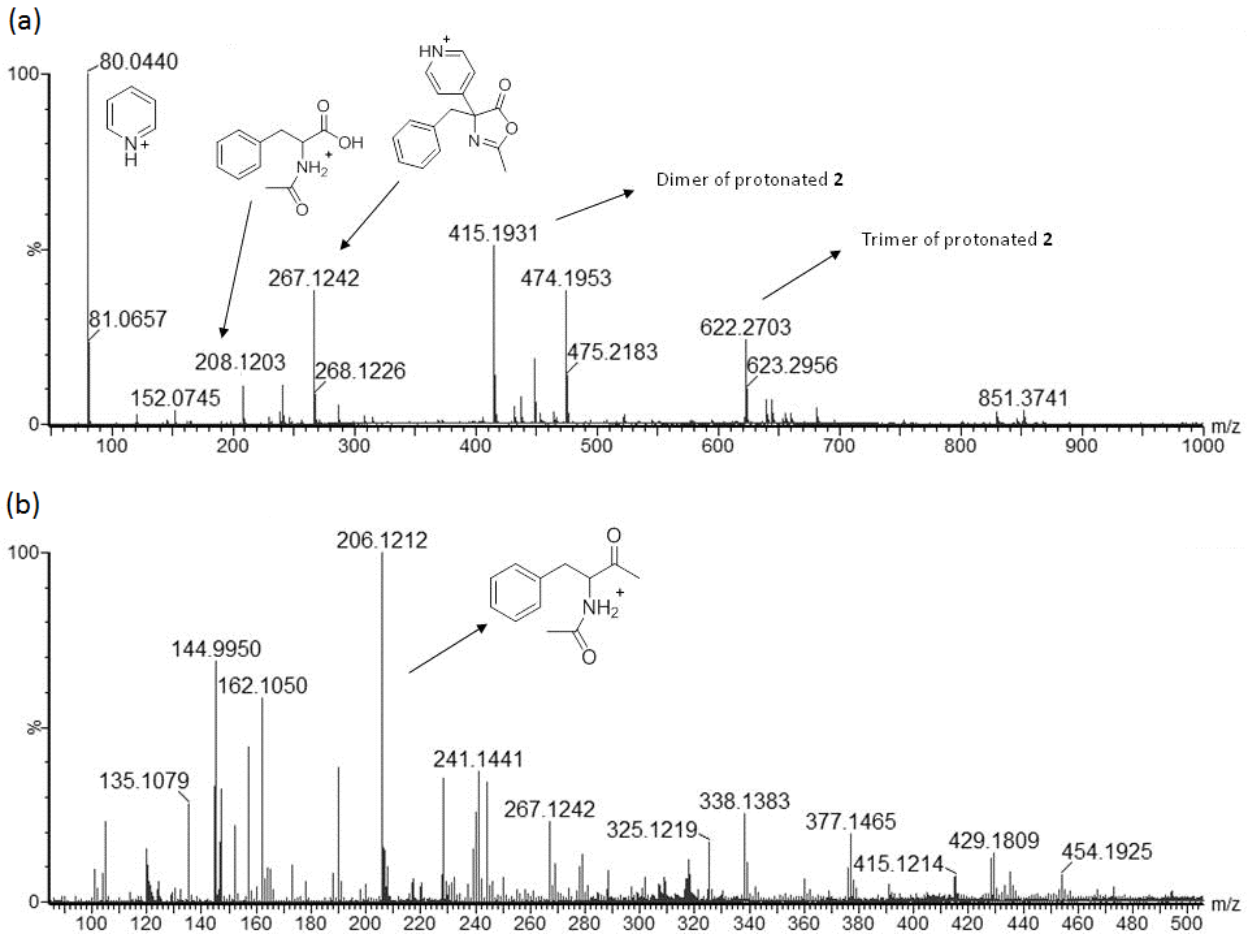

Figure S1. ESI-MS spectra of the reaction mixture after the addition of water, immediately analyzed after the addition (a) and after 3 h (b).

Cartesian coordinates, energies, and imaginary frequency (transition states) for all the calculated structures.

CO_2

```
E(RM062X) =  -188.570158140
Zero-point correction=                           0.012046 (Hartree/Particle)
Thermal correction to Energy=                    0.014648
Thermal correction to Enthalpy=                  0.015592
Thermal correction to Gibbs Free Energy=        -0.009284
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.000028
2	8	0	0.000000	0.000000	1.154482
3	8	0	0.000000	0.000000	-1.154461

Structure 3

```
E(RM062X) =  -629.013460028
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.050012	1.318375	0.245253
2	7	0	1.790049	0.216506	-0.327481
3	6	0	1.701172	-1.024640	0.204115
4	8	0	0.982671	-1.241541	1.174563
5	6	0	-0.419797	0.976648	0.430817
6	6	0	1.173765	2.552868	-0.644569
7	6	0	2.518899	-2.102302	-0.454553
8	8	0	-1.102511	1.389354	1.320613
9	1	0	2.224684	2.833874	-0.733535
10	1	0	0.629168	3.389987	-0.206447
11	1	0	0.775241	2.351652	-1.641468
12	1	0	1.856250	-2.923280	-0.733133
13	1	0	3.237908	-2.485798	0.272159
14	1	0	3.051583	-1.747993	-1.336707
15	1	0	2.328935	0.371486	-1.168181
16	8	0	-0.908007	0.251413	-0.614579
17	6	0	-2.077185	-0.492703	-0.522695
18	8	0	-2.680735	-0.669811	-1.535994
19	6	0	-2.419917	-1.072129	0.813171
20	1	0	-1.520009	-1.319487	1.376303
21	1	0	-2.996278	-0.340911	1.382305
22	1	0	-3.030457	-1.957545	0.645331
23	1	0	1.419584	1.540442	1.249678

TS $3 \rightarrow 3^{-}/PyH^{+}$

```
Imaginary Freq: -912.3848
E(RM062X) =  -877.229016264
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.685073	0.343263	1.416570
2	7	0	-1.532318	1.406501	0.954693
3	6	0	-1.594493	1.811019	-0.331502
4	8	0	-0.862170	1.352749	-1.207789
5	6	0	-1.070446	-0.991115	1.130172
6	6	0	0.001036	0.628005	2.733196
7	6	0	-2.642604	2.849630	-0.644415
8	8	0	-0.556842	-2.027698	1.516380
9	1	0	0.744677	1.425920	2.631391
10	1	0	0.511643	-0.265820	3.095533
11	1	0	-0.714675	0.940868	3.504167
12	1	0	-2.226699	3.576692	-1.342115
13	1	0	-3.010000	3.359430	0.246715
14	1	0	-3.482386	2.352060	-1.136630
15	1	0	-2.216130	1.792356	1.595625
16	8	0	-2.160779	-1.079233	0.226885
17	6	0	-2.029915	-1.669768	-0.983414
18	8	0	-3.028114	-1.915430	-1.607902
19	6	0	-0.636401	-1.930378	-1.478333
20	1	0	-0.067632	-0.998836	-1.440595
21	1	0	-0.144242	-2.668703	-0.844566
22	1	0	-0.691717	-2.293295	-2.502133
23	1	0	0.587588	0.304983	0.534739
24	7	0	1.709325	0.240931	0.115671
25	6	0	2.500043	-0.705498	0.634859
26	6	0	2.150204	1.088700	-0.818289
27	6	0	3.811551	-0.839838	0.214310
28	1	0	2.046680	-1.345456	1.383550
29	6	0	3.454392	1.013390	-1.277557
30	1	0	1.426064	1.804627	-1.186532
31	6	0	4.293034	0.034837	-0.754995
32	1	0	4.437236	-1.613526	0.639137
33	1	0	3.799403	1.707059	-2.032955
34	1	0	5.316404	-0.046966	-1.102090

TS 3^{-}/PyH^{+}→7

Imaginary Freq: -120.5529
E(RM062X) = -1029.85866530

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.514996	-1.467880	-0.567863
2	7	0	0.945865	-1.454932	0.781247
3	6	0	2.108102	-0.937283	1.257860
4	8	0	2.958337	-0.419433	0.545975
5	6	0	0.451803	-0.283347	-1.299167
6	6	0	0.525732	-2.804303	-1.246892
7	6	0	2.261417	-1.000688	2.759758
8	8	0	0.155320	-0.118087	-2.481868
9	1	0	1.546685	-3.199954	-1.311687
10	1	0	0.124107	-2.735138	-2.258086
11	1	0	-0.066458	-3.534090	-0.680645

12	1	0	1.558239	-1.690633	3.228442
13	1	0	2.093384	0.001262	3.164009
14	1	0	3.283251	-1.292713	3.002961
15	1	0	0.357146	-1.958137	1.440005
16	8	0	0.609811	0.873250	-0.484188
17	6	0	1.538765	1.807755	-0.766966
18	8	0	1.545666	2.816866	-0.106916
19	6	0	2.499452	1.534456	-1.887842
20	1	0	2.834385	0.498033	-1.863039
21	1	0	1.999078	1.713567	-2.841011
22	1	0	3.345518	2.210967	-1.785632
23	6	0	-2.257681	0.924151	-0.552467
24	6	0	-2.233542	2.270274	-0.258689
25	6	0	-1.811058	2.686690	0.997921
26	6	0	-1.430642	1.734821	1.936341
27	6	0	-1.478201	0.400019	1.601031
28	7	0	-1.881786	0.013673	0.371811
29	1	0	-1.782313	3.741198	1.244188
30	1	0	-2.578683	0.551522	-1.513044
31	1	0	-2.546195	2.975339	-1.016949
32	1	0	-1.100967	2.015933	2.927469
33	1	0	-1.218315	-0.396198	2.282646
34	6	0	-1.873568	-1.461482	0.073914
35	8	0	-1.784384	-2.194793	1.031532
36	6	0	-2.403061	-1.840943	-1.272244
37	1	0	-3.463222	-1.571200	-1.321569
38	1	0	-1.868913	-1.355176	-2.090354
39	1	0	-2.318369	-2.921620	-1.363559

TS 3→4

Imaginary Freq: -170.6486
E(RM062X) = -628.967703417

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.525125	-1.112719	-0.085146
2	7	0	-1.882660	0.205516	-0.602925
3	6	0	-1.354600	1.158056	0.101669
4	8	0	-0.629598	0.729946	1.097502
5	6	0	-0.420413	-0.727821	0.891095
6	6	0	-1.195181	-2.146365	-1.138636
7	6	0	-1.502793	2.602626	-0.137659
8	8	0	0.120448	-1.358731	1.731013
9	1	0	-2.104725	-2.431289	-1.669886
10	1	0	-0.796398	-3.034319	-0.644735
11	1	0	-0.453342	-1.759474	-1.832002
12	1	0	-0.513863	3.010810	-0.361975
13	1	0	-1.870576	3.079939	0.772555
14	1	0	-2.183895	2.788714	-0.965351
15	1	0	-2.450374	0.371079	-1.427862
16	8	0	0.881395	-0.276078	-0.667852
17	6	0	2.080903	0.144503	-0.510364
18	8	0	2.810127	0.507876	-1.438857
19	6	0	2.619981	0.183671	0.915246
20	1	0	1.966867	0.786427	1.550323
21	1	0	2.634015	-0.824306	1.334302
22	1	0	3.627030	0.598004	0.926271

23	1	0	-2.351725	-1.459990	0.547151

TS 4→5/PyH$^+$

Imaginary Freq: -915.0594
E(RM062X) = -648.141471949

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.316094	-0.626144	0.780458
2	7	0	-1.598707	0.764281	0.950051
3	6	0	-2.073784	1.163204	-0.169021
4	8	0	-2.226732	0.180717	-1.102554
5	6	0	-1.843051	-1.025573	-0.480789
6	6	0	-1.219400	-1.537451	1.970608
7	6	0	-2.475545	2.535188	-0.569932
8	8	0	-1.954041	-2.082088	-1.077320
9	1	0	0.119709	-0.469135	0.350162
10	1	0	-0.478706	-1.170216	2.687128
11	1	0	-0.906715	-2.534743	1.651886
12	1	0	-2.173970	-1.638549	2.499400
13	1	0	-3.531157	2.555627	-0.852392
14	1	0	-1.892061	2.872753	-1.430093
15	1	0	-2.312988	3.217102	0.263555
16	7	0	1.284805	-0.206794	0.139529
17	6	0	1.949230	-0.862203	-0.816738
18	6	0	1.873119	0.734978	0.882428
19	6	0	3.281110	-0.583206	-1.069687
20	1	0	1.388703	-1.608263	-1.367628
21	6	0	3.202841	1.063766	0.683265
22	1	0	1.250015	1.210783	1.631219
23	6	0	3.913758	0.393067	-0.307236
24	1	0	3.805631	-1.120831	-1.848506
25	1	0	3.665916	1.829104	1.291935
26	1	0	4.956008	0.631174	-0.484870

Structure 5/PyH$^+$

E(RM062X) = -648.147713777

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.922430	-0.149686	-0.262165
2	7	0	1.615542	1.166080	-0.613274
3	6	0	0.772778	1.580466	0.274770
4	8	0	0.483103	0.657437	1.217852
5	6	0	1.234184	-0.505766	0.887353
6	6	0	2.813832	-1.013790	-1.087582
7	6	0	0.132433	2.915060	0.399882
8	8	0	1.095758	-1.527741	1.590636
9	1	0	2.423534	-1.153498	-2.103623
10	1	0	2.906530	-1.999832	-0.626133
11	1	0	3.822399	-0.597805	-1.186632

12	1	0	0.488274	3.439466	1.291804
13	1	0	-0.953826	2.816240	0.484005
14	1	0	0.370767	3.515255	-0.478120
15	6	0	-0.752548	-1.379908	-0.864952
16	6	0	-1.138418	-0.298355	-1.636157
17	6	0	-2.123911	0.552293	-1.156474
18	6	0	-2.735532	0.295470	0.072743
19	6	0	-2.322860	-0.795373	0.803164
20	7	0	-1.364448	-1.598078	0.311426
21	1	0	-2.420615	1.417414	-1.738185
22	1	0	0.005940	-2.093196	-1.154612
23	1	0	-0.644252	-0.118872	-2.581481
24	1	0	-3.509097	0.940372	0.466287
25	1	0	-2.716443	-1.057645	1.775587
26	1	0	-0.976101	-2.323945	0.912645

Structure 5/PyAc^{+}

E(RM062X) = -800.777529375

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.658130	0.865359	0.346768
2	7	0	-1.146834	1.745098	-0.599205
3	6	0	0.043903	2.058426	-0.193003
4	8	0	0.386658	1.476335	0.978722
5	6	0	-0.717636	0.675907	1.366844
6	6	0	-3.068638	0.384105	0.339055
7	6	0	0.983371	3.048788	-0.777213
8	8	0	-0.633101	-0.017652	2.383115
9	1	0	-3.756778	1.114371	0.781066
10	1	0	-3.156434	-0.541180	0.913681
11	1	0	-3.414899	0.192080	-0.680540
12	1	0	2.009310	2.674572	-0.764037
13	1	0	0.964058	3.979267	-0.200719
14	1	0	0.689861	3.270622	-1.803295
15	6	0	-0.935356	-1.633751	-0.702668
16	7	0	0.451409	-1.198354	-0.401509
17	8	0	-1.458238	-2.378764	0.073259
18	6	0	-1.473591	-1.248282	-2.043382
19	6	0	1.167816	-0.438799	-1.271861
20	6	0	1.003812	-1.649150	0.755149
21	1	0	-1.452577	-0.170560	-2.205665
22	1	0	-0.877565	-1.736698	-2.820611
23	1	0	-2.496632	-1.613112	-2.101863
24	6	0	2.478496	-0.117988	-0.994422
25	1	0	0.679961	-0.136107	-2.185251
26	6	0	2.304594	-1.333252	1.070071
27	1	0	0.362081	-2.256430	1.373481
28	6	0	3.057184	-0.561017	0.189830
29	1	0	3.032688	0.473159	-1.710967
30	1	0	2.720078	-1.701847	1.998309
31	1	0	4.087327	-0.316769	0.419637

TS 5/PyAc^{+}→6a
Imaginary Freq: -120.3649

E(RM062X) = -800.774160143

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.860403	-0.389478	-0.934333
2	7	0	-1.024274	1.001808	-0.939715
3	6	0	-2.110645	1.223412	-0.289537
4	8	0	-2.816900	0.100906	0.033187
5	6	0	-2.075625	-0.975190	-0.450562
6	6	0	0.038373	-1.067334	-1.916600
7	6	0	-2.707302	2.524045	0.094801
8	8	0	-2.495576	-2.113664	-0.370660
9	1	0	0.933442	-0.463968	-2.091558
10	1	0	-0.456107	-1.211002	-2.883817
11	1	0	0.348191	-2.054596	-1.561326
12	1	0	-2.826340	2.578916	1.179366
13	1	0	-3.693942	2.646678	-0.359748
14	1	0	-2.055431	3.331401	-0.236451
15	6	0	0.009008	-0.455326	1.135863
16	7	0	1.387439	-0.079679	0.567687
17	8	0	-0.540527	0.447159	1.746979
18	6	0	-0.102958	-1.910493	1.503444
19	6	0	2.300189	-1.001796	0.206424
20	6	0	1.640739	1.235188	0.428942
21	1	0	0.008651	-2.592237	0.661149
22	1	0	0.648973	-2.143923	2.264614
23	1	0	-1.091642	-2.054808	1.935057
24	6	0	3.513416	-0.620295	-0.330406
25	1	0	2.043587	-2.038878	0.360839
26	6	0	2.835008	1.668273	-0.110794
27	1	0	0.852759	1.892780	0.766132
28	6	0	3.786702	0.732221	-0.498162
29	1	0	4.227895	-1.383880	-0.606819
30	1	0	3.010570	2.730632	-0.215499
31	1	0	4.732265	1.053404	-0.918273

TS 5/PyAc^{+}→6b

Imaginary Freq: -116.7879
E(RM062X) = -800.773485678

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.240037	1.089555	-0.749054
2	7	0	-2.458859	1.433202	-0.160380
3	6	0	-3.026610	0.310256	0.140748
4	8	0	-2.302130	-0.770906	-0.199640
5	6	0	-1.133094	-0.279780	-0.789981
6	6	0	-0.303350	2.102536	-1.309924
7	6	0	-4.334805	0.090664	0.807315
8	8	0	-0.260530	-1.104407	-1.214422
9	1	0	-0.752449	2.638981	-2.152453
10	1	0	0.607150	1.614323	-1.665615
11	1	0	-0.019014	2.849411	-0.561974
12	1	0	-4.987182	-0.529479	0.187750

13	1	0	-4.814643	1.053671	0.978118
14	1	0	-4.200974	-0.415754	1.766877
15	6	0	0.832975	-1.816136	0.295552
16	7	0	1.591999	-0.481394	0.364404
17	8	0	0.110047	-2.029278	1.236467
18	6	0	1.504110	-2.875723	-0.527992
19	6	0	2.631186	-0.193321	-0.443569
20	6	0	1.125300	0.420588	1.244699
21	1	0	1.711471	-2.562414	-1.547514
22	1	0	2.431437	-3.178670	-0.032831
23	1	0	0.824855	-3.726282	-0.550991
24	6	0	3.258212	1.030277	-0.369082
25	1	0	2.946043	-0.961134	-1.133978
26	6	0	1.716045	1.667168	1.355144
27	1	0	0.299632	0.090168	1.858620
28	6	0	2.794683	1.978521	0.542469
29	1	0	4.098462	1.232420	-1.019523
30	1	0	1.321473	2.374167	2.072808
31	1	0	3.274976	2.947044	0.615350

Structure 6a

E(RM062X) = -552.550729199

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.436406	0.166310	-0.505605
2	7	0	-0.718527	-0.642860	-0.882667
3	6	0	-1.695489	-0.257983	-0.174885
4	8	0	-1.433978	0.756086	0.732622
5	6	0	-0.108753	1.071054	0.599847
6	6	0	0.942075	1.015094	-1.667870
7	6	0	-3.090687	-0.746163	-0.178983
8	8	0	0.425741	1.912208	1.247706
9	1	0	1.296242	0.361520	-2.466131
10	1	0	1.762796	1.648747	-1.333249
11	1	0	0.133219	1.640189	-2.050030
12	1	0	-3.767687	0.076463	-0.419403
13	1	0	-3.352634	-1.120217	0.813316
14	1	0	-3.196071	-1.540353	-0.914909
15	6	0	1.573404	-0.699814	0.097250
16	8	0	2.713209	-0.326427	0.001993
17	6	0	1.167648	-1.961388	0.797721
18	1	0	2.029269	-2.396608	1.300273
19	1	0	0.371067	-1.761194	1.520649
20	1	0	0.766083	-2.666136	0.064731

Structure 6b

E(RM062X) = -552.540993754

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.769355	1.206156	-0.043410
2	7	0	2.071078	0.748921	0.181018
3	6	0	2.036646	-0.526898	-0.019293
4	8	0	0.810202	-0.979305	-0.366795
5	6	0	0.029460	0.133042	-0.374935
6	6	0	0.378347	2.633931	0.095764
7	6	0	3.135589	-1.516103	0.072618
8	8	0	-1.257877	-0.026571	-0.750401
9	1	0	0.979619	3.261933	-0.565654
10	1	0	0.538497	2.975455	1.121085
11	1	0	-0.674504	2.771892	-0.154299
12	1	0	3.294764	-2.001274	-0.892921
13	1	0	2.897194	-2.286967	0.808214
14	1	0	4.047681	-1.002671	0.371718
15	6	0	-2.155240	-0.417201	0.229470
16	8	0	-1.816068	-0.589473	1.359889
17	6	0	-3.517405	-0.573529	-0.355010
18	1	0	-3.823018	0.361980	-0.826876
19	1	0	-3.488262	-1.345152	-1.127379
20	1	0	-4.220086	-0.851233	0.426209

TS 6a→7

Imaginary Freq: -134.9406
E(RM062X) = -781.606608834

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.366345	0.104006	-0.086755
2	7	0	0.697460	1.095640	-0.919617
3	6	0	-0.172495	1.801489	-0.252109
4	8	0	-0.260023	1.473326	1.000159
5	6	0	0.531683	0.225916	1.205433
6	6	0	2.811850	0.501428	0.198925
7	6	0	-0.926742	2.948585	-0.784043
8	8	0	0.840646	-0.072534	2.310587
9	1	0	3.387855	0.502252	-0.728724
10	1	0	3.244660	-0.221312	0.889702
11	1	0	2.851191	1.496549	0.645858
12	1	0	-0.454664	3.866713	-0.422959
13	1	0	-1.948343	2.901351	-0.412063
14	1	0	-0.913877	2.934937	-1.872444
15	6	0	1.293885	-1.328474	-0.658731
16	8	0	1.918542	-2.191676	-0.099105
17	6	0	0.525557	-1.545422	-1.928102
18	1	0	0.359814	-2.611674	-2.074039
19	1	0	-0.419070	-1.000490	-1.927055
20	1	0	1.130577	-1.165104	-2.760018
21	1	0	0.894443	1.257404	-1.901735
22	6	0	-2.000326	-0.696928	0.113372
23	8	0	-2.169465	0.252732	-0.659086
24	8	0	-0.901966	-0.966385	0.727322
25	6	0	-3.133080	-1.661002	0.405014
26	1	0	-3.474119	-1.502088	1.431394
27	1	0	-3.964205	-1.499033	-0.279637
28	1	0	-2.778408	-2.690272	0.332009

TS 6a→7(isomer)

Imaginary Freq: -113.3318
E(RM062X) = -781.601325886

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.992114	-0.426172	-0.471304
2	7	0	0.526123	0.875368	-0.927686
3	6	0	-0.133290	1.519605	-0.006244
4	8	0	-0.159553	0.889293	1.139789
5	6	0	0.349553	-0.456850	0.928847
6	6	0	0.620529	-1.567683	-1.396915
7	6	0	-0.647835	2.893092	-0.111691
8	8	0	0.598173	-1.151421	1.850845
9	1	0	-0.422423	-1.481254	-1.688634
10	1	0	0.768261	-2.514056	-0.877335
11	1	0	1.265823	-1.549081	-2.276751
12	1	0	0.095726	3.564780	0.329128
13	1	0	-1.580120	2.969704	0.442723
14	1	0	-0.800124	3.155586	-1.156933
15	6	0	2.531710	-0.402394	-0.198264
16	8	0	3.153379	-1.420976	-0.330201
17	6	0	3.140202	0.897015	0.242567
18	1	0	4.155618	0.720991	0.592121
19	1	0	3.158870	1.592755	-0.601547
20	1	0	2.549541	1.361622	1.037407
21	1	0	0.590345	1.201313	-1.886756
22	6	0	-2.531188	-0.441988	-0.101401
23	8	0	-2.406161	0.687812	-0.613799
24	8	0	-1.581228	-1.143425	0.363514
25	6	0	-3.914948	-1.069021	-0.011123
26	1	0	-4.676104	-0.401648	-0.413577
27	1	0	-3.924014	-2.010288	-0.565678
28	1	0	-4.142218	-1.301890	1.031610

TS1 6b→7

Imaginary Freq: -213.3289
E(RM062X) = -781.586930050

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.706820	1.442073	0.636967
2	7	0	-0.365422	1.887117	-0.147792
3	6	0	-0.841673	0.865787	-0.868384
4	8	0	0.029208	-0.137578	-0.782849
5	6	0	0.917770	0.192193	0.215917
6	6	0	1.391042	2.284268	1.647209
7	6	0	-1.710838	0.990012	-2.058878
8	8	0	1.798754	-0.757539	0.572629
9	1	0	0.693674	2.588298	2.430940
10	1	0	1.799892	3.183401	1.180674
11	1	0	2.207898	1.724956	2.103147

12	1	0	-2.187976	0.030231	-2.244453
13	1	0	-1.095987	1.281883	-2.914742
14	1	0	-2.464795	1.754871	-1.877279
15	6	0	2.943708	-0.873181	-0.210186
16	8	0	3.150756	-0.135607	-1.122695
17	6	0	3.780036	-2.006331	0.272892
18	1	0	3.997498	-1.875574	1.334255
19	1	0	3.218683	-2.936165	0.157710
20	1	0	4.701220	-2.051323	-0.302243
21	1	0	-0.855880	2.763764	-0.023892
22	6	0	-2.812096	-0.906034	0.302008
23	8	0	-2.675991	-1.662891	-0.664109
24	6	0	-3.725993	-1.296815	1.456520
25	8	0	-2.241500	0.232537	0.444680
26	1	0	-3.149310	-1.325393	2.384090
27	1	0	-4.506016	-0.542047	1.579735
28	1	0	-4.183418	-2.269935	1.280976

INT 6b→7

E(RM062X) = -781.600670297

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642684	1.480135	-0.465369
2	7	0	0.489148	1.840508	0.321169
3	6	0	1.099535	0.587351	0.715551
4	8	0	0.059843	-0.354296	0.633200
5	6	0	-0.869799	0.196401	-0.229566
6	6	0	-1.403646	2.477234	-1.257355
7	6	0	1.733622	0.622702	2.081673
8	8	0	-1.840044	-0.642719	-0.662741
9	1	0	-0.767045	2.944642	-2.013513
10	1	0	-1.788173	3.266916	-0.605927
11	1	0	-2.245188	1.999527	-1.760485
12	1	0	2.147552	-0.348055	2.343876
13	1	0	0.972947	0.909429	2.807234
14	1	0	2.525491	1.374368	2.083049
15	6	0	-2.938037	-0.814781	0.156773
16	8	0	-3.064506	-0.221086	1.184616
17	6	0	-3.871169	-1.815902	-0.437451
18	1	0	-4.126171	-1.524348	-1.457640
19	1	0	-3.369652	-2.785110	-0.482392
20	1	0	-4.768497	-1.887676	0.171900
21	1	0	1.146608	2.469271	-0.130443
22	6	0	2.727628	-0.895094	-0.352653
23	8	0	2.590563	-1.759670	0.471641
24	6	0	3.619912	-0.977334	-1.555678
25	8	0	2.082258	0.290543	-0.323572
26	1	0	3.007648	-0.944931	-2.459620
27	1	0	4.294828	-0.120068	-1.577213
28	1	0	4.188528	-1.903971	-1.527719

TS2 6b→7

Imaginary Freq: -402.3539

E(RM062X) = -781.566309839

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.602698	1.048503	-0.811410
2	7	0	0.516328	1.789199	-0.295632
3	6	0	1.437778	1.015705	0.282340
4	8	0	0.115553	-0.429912	0.817157
5	6	0	-0.748705	-0.067831	-0.050771
6	6	0	-1.534985	1.677043	-1.785096
7	6	0	2.172610	1.492031	1.488404
8	8	0	-1.861245	-0.889113	-0.234895
9	1	0	-1.049185	1.878266	-2.744554
10	1	0	-1.933381	2.627269	-1.409230
11	1	0	-2.379633	1.011719	-1.973837
12	1	0	2.078240	0.759989	2.287414
13	1	0	1.750498	2.441526	1.816057
14	1	0	3.232539	1.612182	1.257927
15	6	0	-2.989891	-0.572053	0.450433
16	8	0	-3.060167	0.362746	1.199121
17	6	0	-4.087802	-1.539545	0.136161
18	1	0	-4.277265	-1.541601	-0.938936
19	1	0	-3.777930	-2.546417	0.422837
20	1	0	-4.989766	-1.260195	0.675213
21	1	0	0.275603	2.617433	0.245443
22	6	0	2.721418	-0.954653	-0.140744
23	8	0	3.034924	-1.122030	0.997471
24	6	0	3.003614	-1.853096	-1.298440
25	8	0	2.027492	0.153659	-0.583324
26	1	0	2.055624	-2.248221	-1.671957
27	1	0	3.471319	-1.287366	-2.105867
28	1	0	3.648561	-2.668405	-0.980588

INT2 6b→7

E(RM062X) = -781.591423081

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.499687	1.138566	0.436296
2	7	0	-0.741875	1.664780	0.034320
3	6	0	-1.904162	1.090128	0.011082
4	8	0	0.126740	-0.954926	-0.622183
5	6	0	0.792721	-0.153123	0.024466
6	6	0	1.447242	2.149833	1.006934
7	6	0	-3.096521	1.730441	-0.596411
8	8	0	2.083456	-0.604245	0.475222
9	1	0	1.092225	2.557798	1.958708
10	1	0	1.589675	2.993656	0.319133
11	1	0	2.425072	1.704471	1.184162
12	1	0	-3.278075	1.315031	-1.589657
13	1	0	-2.936047	2.805615	-0.684559
14	1	0	-3.973383	1.532672	0.021894
15	6	0	3.119502	-0.423806	-0.361730
16	8	0	3.038004	0.186541	-1.396789

17	6	0	4.362816	-1.076467	0.164827
18	1	0	4.554802	-0.744554	1.186711
19	1	0	4.213047	-2.158127	0.187633
20	1	0	5.208200	-0.834202	-0.475041
21	1	0	-0.735663	2.633798	-0.290175
22	6	0	-2.493587	-1.201703	0.029475
23	8	0	-2.931519	-1.157725	-1.078029
24	6	0	-2.435610	-2.368968	0.953256
25	8	0	-1.996833	-0.073769	0.668647
26	1	0	-1.434330	-2.453408	1.375886
27	1	0	-3.143067	-2.210046	1.771256
28	1	0	-2.700648	-3.272578	0.409702

TS3 6b→7

Imaginary Freq: -64.3431
E(RM062X) = -781.588133898

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.019694	-0.489085	0.633008
2	7	0	1.237815	-1.231870	0.508572
3	6	0	2.286683	-0.809042	-0.126170
4	8	0	-0.339657	-0.600439	-1.706903
5	6	0	-0.663723	-0.318677	-0.557481
6	6	0	-0.465314	-0.278629	2.029679
7	6	0	3.443211	-1.676704	-0.439392
8	8	0	-1.890197	0.421259	-0.396562
9	1	0	0.263046	0.298561	2.611653
10	1	0	-0.633045	-1.227156	2.555193
11	1	0	-1.405839	0.272662	2.034039
12	1	0	3.541629	-1.743733	-1.526088
13	1	0	3.309736	-2.674324	-0.025056
14	1	0	4.350443	-1.215622	-0.044920
15	6	0	-3.001937	-0.284999	-0.132732
16	8	0	-3.010019	-1.480123	0.017443
17	6	0	-4.205246	0.606767	-0.053827
18	1	0	-4.039015	1.388248	0.690101
19	1	0	-4.355620	1.093050	-1.020050
20	1	0	-5.083610	0.021020	0.207345
21	1	0	1.287221	-2.183474	0.870714
22	6	0	1.633908	1.475696	0.147496
23	8	0	1.929865	1.677981	1.279690
24	6	0	0.887479	2.336561	-0.805877
25	8	0	2.348001	0.424085	-0.564098
26	1	0	1.617447	2.991939	-1.293037
27	1	0	0.393667	1.739844	-1.570965
28	1	0	0.176759	2.948645	-0.253720

Structure 7

E(RM062X) = -781.640508579

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.997465	-0.394160	0.610149
2	7	0	0.959769	1.042879	0.809441
3	6	0	0.333729	1.910653	-0.025693
4	8	0	-0.233963	1.526440	-1.040507
5	6	0	-0.297468	-0.902386	-0.028295
6	6	0	1.138061	-1.078319	1.973196
7	6	0	0.383877	3.361489	0.368177
8	8	0	-0.339423	-1.713916	-0.904069
9	1	0	2.076967	-0.768853	2.436158
10	1	0	1.153029	-2.161053	1.856862
11	1	0	0.306484	-0.790793	2.616739
12	1	0	-0.637762	3.741410	0.419103
13	1	0	0.907890	3.912173	-0.415669
14	1	0	0.882758	3.525973	1.322560
15	1	0	1.383854	1.398842	1.656126
16	8	0	-1.381721	-0.445649	0.647807
17	6	0	-2.672682	-0.453751	0.122107
18	8	0	-3.560497	-0.394024	0.915005
19	6	0	-2.823796	-0.463424	-1.364744
20	1	0	-2.031043	0.110076	-1.842845
21	1	0	-2.773199	-1.493137	-1.722307
22	1	0	-3.802109	-0.048966	-1.600809
23	6	0	2.168223	-0.815035	-0.328830
24	8	0	2.853638	-1.760288	-0.031337
25	6	0	2.398460	-0.004560	-1.571695
26	1	0	1.479110	0.057423	-2.156361
27	1	0	2.681416	1.016624	-1.301856
28	1	0	3.194723	-0.463423	-2.155228

TS 5/PyAc^{+}→12

Imaginary Freq: -22.8096
E(RM062X) = -800.765956119

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.682386	0.721487	-0.935834
2	7	0	3.009553	0.829583	-0.505079
3	6	0	3.341642	-0.349992	-0.097578
4	8	0	2.355433	-1.264156	-0.214405
5	6	0	1.244081	-0.582185	-0.779270
6	6	0	0.936241	1.852437	-1.552365
7	6	0	4.644090	-0.798584	0.458815
8	8	0	0.181995	-1.210152	-0.971913
9	1	0	-0.051039	1.509536	-1.872430
10	1	0	1.453039	2.248565	-2.433657
11	1	0	0.789812	2.689846	-0.859186
12	1	0	5.086025	-1.580568	-0.164929
13	1	0	4.523785	-1.204908	1.466752
14	1	0	5.328129	0.048706	0.497876
15	6	0	-2.026721	1.313993	0.477166
16	6	0	-0.983821	1.906392	1.132340
17	6	0	-0.037377	1.099616	1.783133
18	6	0	-0.207835	-0.272587	1.802449
19	6	0	-1.248887	-0.834112	1.090606
20	7	0	-2.153259	-0.042257	0.463183

21	1	0	0.803274	1.555166	2.293304
22	1	0	-2.781408	1.885764	-0.040627
23	1	0	-0.902288	2.984331	1.127965
24	1	0	0.494084	-0.926222	2.302206
25	1	0	-1.428604	-1.895621	1.036184
26	6	0	-3.236285	-0.710628	-0.280054
27	8	0	-3.357725	-1.888783	-0.143023
28	6	0	-4.083930	0.153885	-1.152942
29	1	0	-3.466166	0.689105	-1.877381
30	1	0	-4.787663	-0.492667	-1.671198
31	1	0	-4.634173	0.884068	-0.555663

TS 5/PyH$^+$→12′

Imaginary Freq: -221.7209
E(RM062X) = -648.138433262

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.683330	0.039975	0.923607
2	7	0	1.614552	-0.981181	0.674020
3	6	0	2.459811	-0.488432	-0.161569
4	8	0	2.239755	0.816254	-0.477363
5	6	0	1.127084	1.225418	0.288302
6	6	0	-0.267678	-0.008127	2.066393
7	6	0	3.636428	-1.148244	-0.780069
8	8	0	0.723799	2.376041	0.233827
9	1	0	-1.130837	0.636674	1.867278
10	1	0	0.190518	0.326706	3.003205
11	1	0	-0.626325	-1.029602	2.216512
12	1	0	4.555732	-0.625264	-0.503543
13	1	0	3.560868	-1.138147	-1.870049
14	1	0	3.692097	-2.179268	-0.433315
15	6	0	-2.724267	-1.370807	0.057057
16	6	0	-1.426636	-1.497138	-0.334123
17	6	0	-0.712957	-0.367784	-0.834336
18	6	0	-1.475550	0.812388	-1.080643
19	6	0	-2.771684	0.885341	-0.664244
20	7	0	-3.374764	-0.185998	-0.090825
21	1	0	0.196285	-0.543080	-1.400852
22	1	0	-3.303510	-2.183103	0.475046
23	1	0	-0.930439	-2.452080	-0.218144
24	1	0	-1.026930	1.672771	-1.556153
25	1	0	-3.386647	1.767056	-0.787017
26	1	0	-4.345048	-0.116319	0.190706

Structure 8

E(RM062X) = -629.008504224

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.573901	-0.174485	0.525674

2	7	0	0.870377	-0.412322	0.729199
3	6	0	1.967236	0.014532	0.077039
4	8	0	1.940720	0.890268	-0.800413
5	6	0	-1.026819	1.270203	0.187998
6	6	0	-1.256611	-0.594609	1.823614
7	6	0	3.267963	-0.618970	0.472278
8	8	0	-2.182406	1.560860	0.372501
9	1	0	-0.993346	-1.625970	2.063841
10	1	0	-2.336405	-0.527742	1.717956
11	1	0	-0.933307	0.060346	2.634876
12	1	0	3.971846	0.171982	0.734259
13	1	0	3.664062	-1.145064	-0.399149
14	1	0	3.169049	-1.316697	1.302251
15	1	0	1.044368	-1.122814	1.430236
16	8	0	-0.170262	2.122150	-0.322838
17	6	0	-1.040094	-1.101555	-0.647698
18	8	0	-1.644532	-2.111287	-0.399766
19	6	0	-0.689104	-0.678865	-2.045179
20	1	0	-1.255867	0.222337	-2.302642
21	1	0	0.370871	-0.429812	-2.127306
22	1	0	-0.944615	-1.473624	-2.743778
23	1	0	0.710516	1.679874	-0.573167

Structure 9

E(RM062X) = -440.441744686

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.673501	0.720702	-0.419096
2	7	0	0.671474	0.798618	0.118874
3	6	0	1.622020	-0.101889	-0.227899
4	8	0	1.361069	-1.057396	-0.948178
5	6	0	-1.488911	1.913337	0.075763
6	6	0	2.999493	0.128608	0.338550
7	1	0	-1.565732	1.906267	1.166369
8	1	0	-2.493973	1.880426	-0.346136
9	1	0	-1.012989	2.845665	-0.235494
10	1	0	3.066706	1.041900	0.929578
11	1	0	3.712549	0.175995	-0.486337
12	1	0	3.266689	-0.726788	0.962284
13	1	0	0.925033	1.592123	0.691241
14	6	0	-1.396039	-0.565307	-0.009265
15	8	0	-2.249866	-1.020616	-0.734375
16	6	0	-1.058358	-1.168836	1.326534
17	1	0	-0.957525	-0.393321	2.089557
18	1	0	-1.826562	-1.886148	1.611456
19	1	0	-0.095842	-1.682665	1.250158
20	1	0	-0.636515	0.720634	-1.511899

Structure 12

E(RM062X) = -800.809546291

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.356698	0.041584	0.356459
2	7	0	2.217662	-1.139588	0.265923
3	6	0	3.384129	-0.736594	-0.011858
4	8	0	3.545270	0.633839	-0.142912
5	6	0	2.317798	1.193451	0.099053
6	6	0	0.739531	0.167323	1.744019
7	6	0	4.616835	-1.530098	-0.212387
8	8	0	2.145671	2.372762	0.092776
9	1	0	0.146183	1.081234	1.810129
10	1	0	1.522145	0.197150	2.505257
11	1	0	0.095514	-0.692935	1.935971
12	1	0	5.382995	-1.204812	0.494732
13	1	0	4.999659	-1.370306	-1.222816
14	1	0	4.398959	-2.585460	-0.062492
15	6	0	-1.856030	-1.248253	-0.369909
16	6	0	-0.552339	-1.266829	-0.646705
17	6	0	0.281342	-0.022318	-0.786019
18	6	0	-0.608331	1.191333	-0.803749
19	6	0	-1.910133	1.145067	-0.523965
20	7	0	-2.582524	-0.053857	-0.228867
21	1	0	0.855233	-0.072599	-1.720304
22	1	0	-2.420424	-2.162995	-0.265242
23	1	0	-0.067083	-2.227981	-0.762339
24	1	0	-0.173249	2.152998	-1.045906
25	1	0	-2.541595	2.021607	-0.524801
26	6	0	-3.932012	-0.008360	0.115267
27	8	0	-4.512341	1.056116	0.193185
28	6	0	-4.618343	-1.320207	0.387781
29	1	0	-4.121801	-1.865399	1.192950
30	1	0	-5.643926	-1.102617	0.676415
31	1	0	-4.622250	-1.952108	-0.503259

Structure 12′

E(RM062X) = -648.163066399

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.395212	0.043985	0.375172
2	7	0	1.340089	-1.073231	0.314651
3	6	0	2.453531	-0.606237	-0.062478
4	8	0	2.502136	0.760294	-0.285246
5	6	0	1.253455	1.245510	0.015535
6	6	0	-0.190225	0.200350	1.771808
7	6	0	3.730054	-1.320839	-0.289603
8	8	0	1.001210	2.409892	-0.031107
9	1	0	-0.831207	1.082857	1.812207
10	1	0	0.608211	0.309418	2.509100
11	1	0	-0.778669	-0.684923	2.019674
12	1	0	4.497363	-0.924965	0.379515
13	1	0	4.065288	-1.167496	-1.317547
14	1	0	3.588496	-2.383064	-0.101111
15	6	0	-2.700765	-1.475910	-0.018151
16	6	0	-1.451138	-1.458817	-0.500134
17	6	0	-0.705752	-0.166910	-0.734152

18	6	0	-1.686376	0.978740	-0.798869
19	6	0	-2.927103	0.873700	-0.304424
20	7	0	-3.409614	-0.311182	0.224932
21	1	0	-0.145497	-0.233031	-1.674995
22	1	0	-3.232095	-2.396187	0.192220
23	1	0	-0.947046	-2.396730	-0.694371
24	1	0	-1.369565	1.922271	-1.224177
25	1	0	-3.626978	1.700441	-0.308501
26	1	0	-4.393756	-0.380617	0.433512