Electronic Supplementary Information

How is the anionic tetrahedral intermediate involved in isomerization of aspartyl peptides to iso-aspartyl ones? A DFT study on the tetra-peptide

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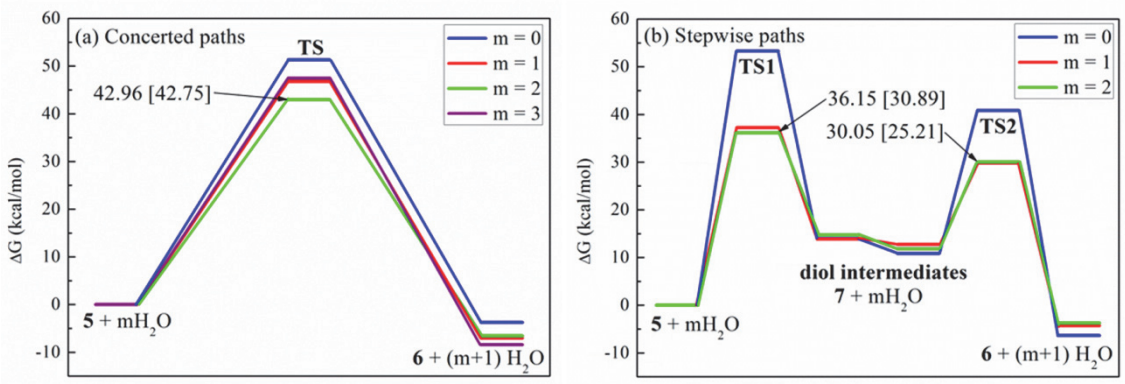

Fig. S1 Changes of Gibbs free energies in the concerted (a) and stepwise (b) paths in the reaction of Scheme 5. In (b), the m = 3 TS1 was sought, which however leads to the m = 2 + 1 TS1. Here, +1 means that one water molecule stays at a catalyst one. For m = 2, B3LYP/6-31G(d) and [B3PW91/6-31+G(d,p)] activation free energies are shown in kcal/mol. 1 kcal = 4.184 kJ.

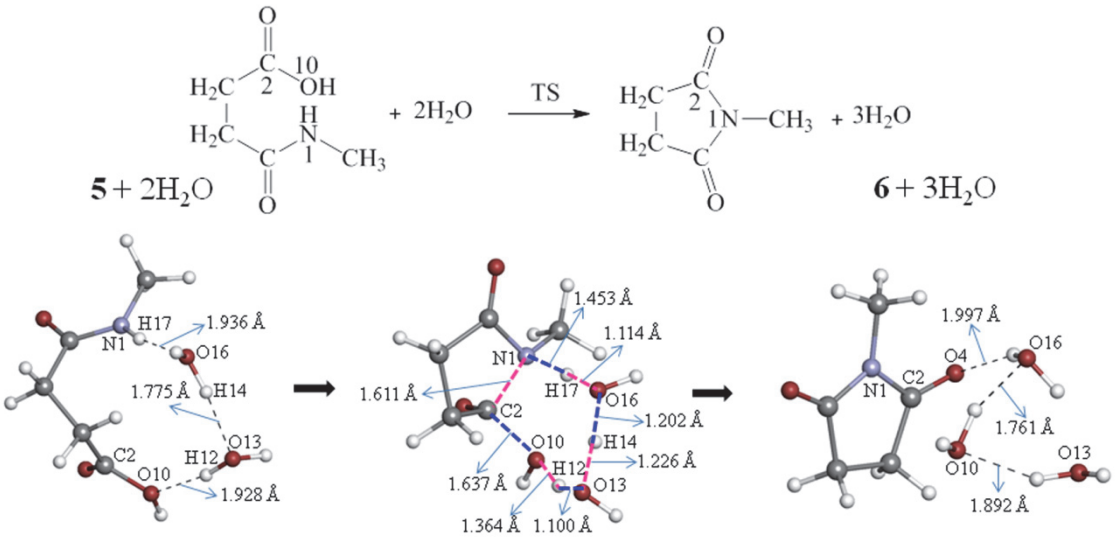

Fig. S2 Geometric changes in the concerted reaction of Scheme 5 (m = 2). At TS, red and blue broken lines stand for covalent bonds formed and cleaved, respectively.

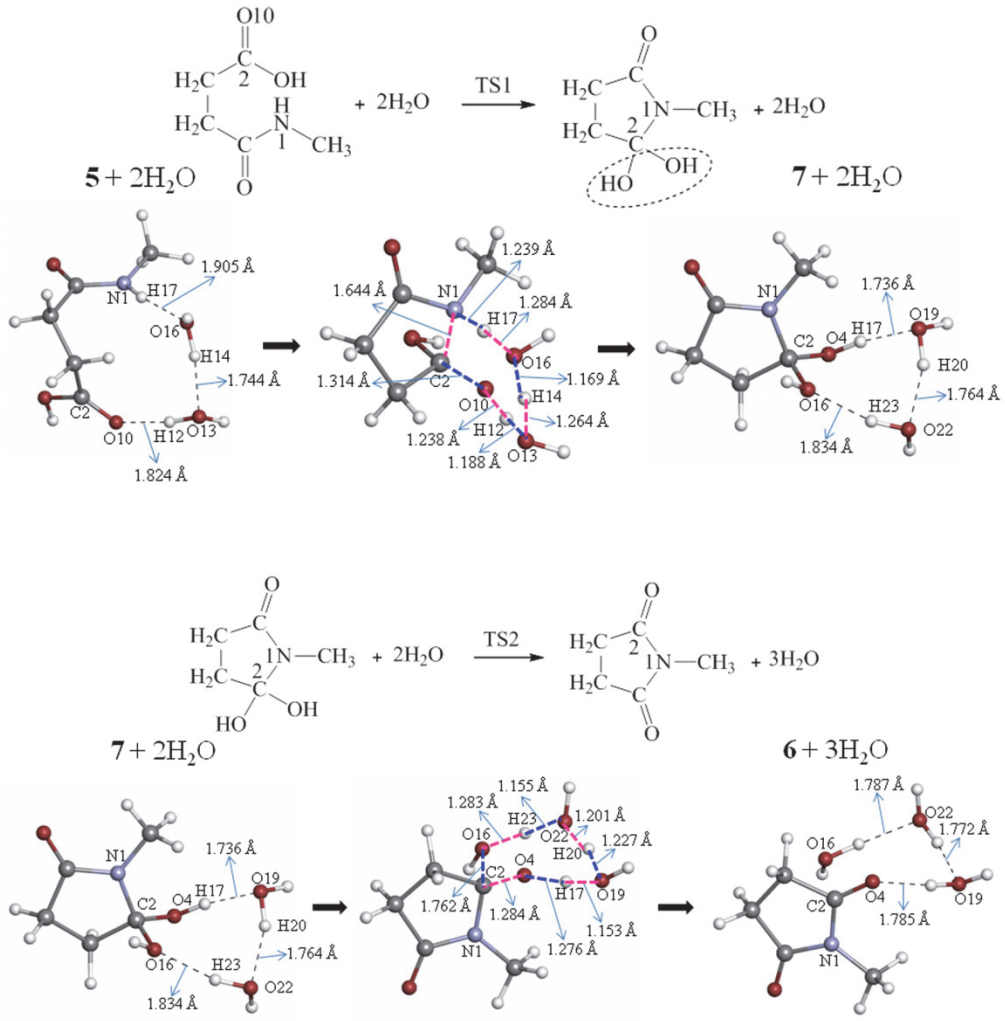

Fig. S3 Geometric changes in the stepwise reaction of Scheme 5 (m = 2).

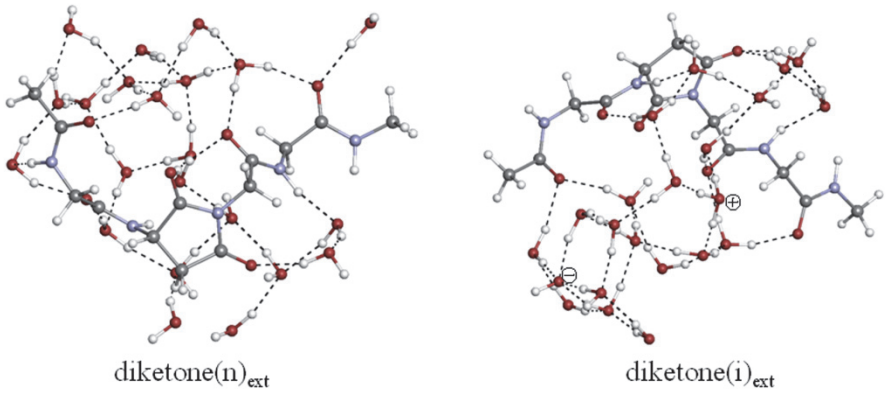

Fig. S4 Two geometries of the succinimide derivative, Ac-Gly-Asu-Gly-Gly-NHMe (**2**), solvated by $(H_2O)_{14+8}$ and $H_3O^+(OH^-)(H_2O)_{12+8}$, respectively. The former is defined as diketone(n)$_{ext}$, and the latter as diketone(i)$_{ext}$. Diketone(i)$_{ext}$ is 5.77 kcal/mol less stable than diketone(n)$_{ext}$ in Gibbs free energies.

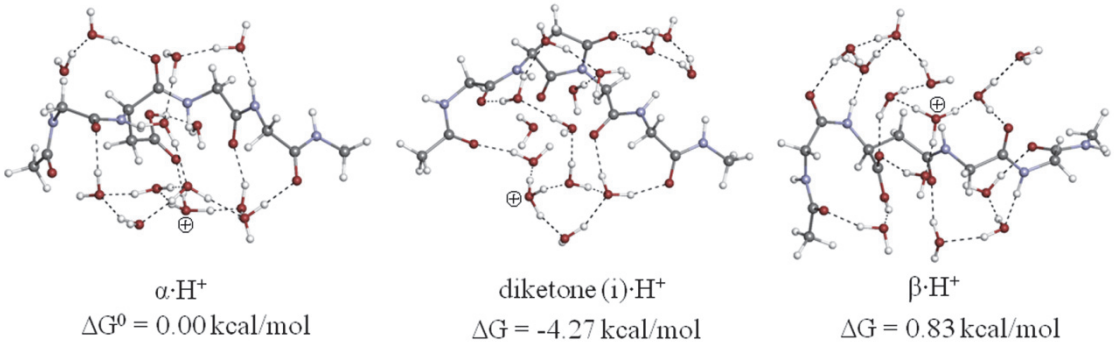

Fig. S5 Geometries of $\alpha \cdot H^+$, diketone(i)H^+ and $\beta \cdot H^+$ with the molecular formula $C_{13}H_{48}N_5O_{20}^{(+1)}$. Relative stability is expressed by ΔG (negative values, more stable).

Cartesian coordinates of the optimized geometries for Figs. 1, 2, 3, 5, S4 and S5.

[Thermal correction to Gibbs free energy and B3LYP/ 6-311++G(d,p) scrf=(pcm,solvent=water)// B3LYP/ 6-31G(d) electronic energy, "E(RB3LYP)" in a.u.(=Hartree, 1 a.u. = 627.5095 kcal/mol) for Fig. 4 are also shown].

α form, reactant in Fig. 1

vucw3aa.extrev.log E(RB3LYP) = -2303.098674 a.u.
Thermal correction to Gibbs Free Energy= 0.609501 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.608715	0.947901	0.380956
2	6	0	-1.204198	3.418472	-0.546568
3	6	0	-0.678288	0.767743	0.718583
4	8	0	-1.784381	3.548919	0.634546
5	8	0	-1.027735	0.452510	1.871421
6	6	0	-1.621644	2.168101	-1.289490
7	6	0	-1.742654	0.911473	-0.396710
8	1	0	-2.601489	2.342603	-1.751367
9	7	0	-1.722365	-0.273715	-1.246483
10	6	0	1.672204	0.737547	1.365447
11	1	0	-0.909796	2.004244	-2.098232
12	1	0	0.897256	3.611301	-2.397492
13	6	0	2.787802	-0.057901	0.701152
14	1	0	2.077241	1.699755	1.698447
15	1	0	1.250516	0.212857	2.223849
16	8	0	0.961654	0.535834	-2.339990
17	1	0	0.858148	0.935612	-0.628617
18	1	0	1.670022	-0.114576	-2.572535
19	8	0	-0.395553	4.219137	-1.013174
20	1	0	-1.332688	4.280413	1.199494
21	1	0	-2.689030	0.961676	0.137882
22	8	0	1.663058	3.124718	-2.759530
23	1	0	1.257588	1.420752	-2.680408
24	1	0	2.342037	3.218977	-2.056526
25	8	0	3.558734	0.517239	-0.101743
26	7	0	2.813755	-1.362801	0.965061
27	6	0	3.712018	-2.279489	0.296922
28	1	0	2.190248	-1.742890	1.698311
29	6	0	5.182395	-2.089584	0.709141
30	1	0	3.403616	-3.292115	0.579636
31	1	0	3.598316	-2.190183	-0.789764
32	6	0	-2.437491	-1.420513	-1.082823
33	1	0	-0.935498	-0.329112	-1.897046
34	8	0	-2.151216	-2.424250	-1.746560
35	6	0	-3.597663	-1.426261	-0.069486
36	1	0	-3.272015	-1.031592	0.895572
37	7	0	-4.760325	-0.670374	-0.505700
38	1	0	-3.878633	-2.467322	0.064852
39	1	0	-2.556806	0.468153	2.902019

40	8	0	-3.444106	0.225906	3.236210
41	1	0	-3.367200	-0.734206	3.370966
42	1	0	-1.347496	-1.411563	2.252206
43	8	0	-1.495829	-2.252854	2.723072
44	1	0	-1.723561	-2.927573	2.028569
45	1	0	-3.359599	-3.994044	-1.589297
46	8	0	-3.927499	-4.570896	-1.039811
47	1	0	-4.767546	-4.068190	-1.042932
48	8	0	1.209241	-2.494505	2.944541
49	1	0	1.439801	-2.350520	3.873467
50	1	0	0.213428	-2.509716	2.923245
51	1	0	4.811596	0.094143	-1.355197
52	8	0	5.299553	-0.273409	-2.124064
53	1	0	5.832101	-0.983679	-1.724073
54	1	0	-4.399531	1.120718	1.997759
55	8	0	-4.662863	1.638219	1.197270
56	1	0	-4.090122	2.421605	1.215165
57	8	0	3.343679	3.220155	-0.474671
58	1	0	3.442156	2.248689	-0.295121
59	1	0	4.245288	3.552851	-0.603827
60	8	0	2.939908	-1.306206	-2.969444
61	1	0	2.902276	-1.548076	-3.906796
62	1	0	3.841608	-0.917107	-2.823805
63	8	0	-0.473445	5.158137	2.179288
64	1	0	0.436051	5.170764	1.762532
65	1	0	-0.742830	6.088715	2.212517
66	1	0	-1.420302	-3.758215	-0.064498
67	8	0	-1.851966	-4.109727	0.731820
68	1	0	-2.712706	-4.421598	0.358195
69	1	0	1.038182	5.152542	-0.133368
70	8	0	1.673331	5.261238	0.600423
71	1	0	2.293720	4.514499	0.465557
72	8	0	5.525886	-1.483546	1.707018
73	7	0	6.079361	-2.652551	-0.179528
74	1	0	5.702962	-3.335335	-0.828009
75	6	0	7.481210	-2.818374	0.200622
76	1	0	7.793610	-1.926742	0.744966
77	1	0	7.633247	-3.690896	0.848402
78	1	0	8.090955	-2.928228	-0.699606
79	6	0	-5.848693	-1.287036	-1.046532
80	1	0	-4.858647	0.270160	-0.118781
81	8	0	-5.887949	-2.486746	-1.326145
82	6	0	-7.035556	-0.378075	-1.316820
83	1	0	-7.146701	-0.251256	-2.399292
84	1	0	-7.941739	-0.867873	-0.950346
85	1	0	-6.938674	0.606764	-0.851269

TS1(n) from the alpha substrate to an ion pair in Fig. 1

zuck6.chk E(RB3LYP) = -2303.057909 a.u.
Thermal correction to Gibbs Free Energy= 0.612116 a.u.

1	7	0	0.671219	-1.276473	-0.031775

2	6	0	0.017324	-3.125095	-0.052874
3	6	0	-0.418977	-0.540285	0.152023
4	8	0	-0.556855	-3.193102	-1.276271
5	8	0	-0.586313	0.667248	-0.160451
6	6	0	-1.006840	-2.778072	1.025738
7	6	0	-1.580261	-1.396335	0.692488
8	1	0	-1.787033	-3.545945	1.044789
9	7	0	-2.330714	-0.788418	1.771849
10	6	0	1.704166	-0.815342	-0.954245
11	1	0	-0.502688	-2.773334	1.997503
12	1	0	1.848707	-3.662780	1.290542
13	6	0	2.662969	0.176909	-0.293037
14	1	0	2.283036	-1.686325	-1.272287
15	1	0	1.260055	-0.357810	-1.848585
16	8	0	1.808618	-1.188885	2.822951
17	1	0	1.420062	-0.899403	1.975195
18	1	0	2.486255	-0.498939	3.077309
19	8	0	1.013768	-3.891393	0.189395
20	1	0	0.124367	-3.416663	-1.986615
21	1	0	-2.249072	-1.504838	-0.164198
22	8	0	2.630396	-3.428676	2.003390
23	1	0	2.357983	-2.515093	2.441136
24	1	0	3.444072	-3.244820	1.440857
25	8	0	3.782911	-0.195787	0.132751
26	7	0	2.201964	1.422356	-0.164694
27	6	0	2.876497	2.496418	0.552849
28	1	0	1.288066	1.639931	-0.564196
29	6	0	3.936990	3.237325	-0.279364
30	1	0	2.102581	3.207736	0.857073
31	1	0	3.348721	2.104836	1.451790
32	6	0	-3.282047	0.187117	1.649157
33	1	0	-1.949080	-0.857351	2.710002
34	8	0	-3.667454	0.794718	2.648800
35	6	0	-3.833175	0.499350	0.244288
36	1	0	-3.003961	0.679975	-0.437507
37	7	0	-4.664191	-0.543944	-0.334350
38	1	0	-4.407508	1.418817	0.338512
39	1	0	-0.970443	0.872474	-1.931525
40	8	0	-1.404051	1.143971	-2.768054
41	1	0	-1.948855	1.888382	-2.431588
42	1	0	-1.667827	2.435927	-0.219763
43	8	0	-1.963771	3.116990	-0.849354
44	1	0	-2.762350	3.545233	-0.433650
45	1	0	-5.027862	2.073510	2.422467
46	8	0	-5.700352	2.608518	1.946807
47	1	0	-6.195257	1.913951	1.463159
48	8	0	0.578093	3.193686	-1.886211
49	1	0	0.218019	2.605522	-2.576176
50	1	0	-0.244727	3.520076	-1.455303
51	1	0	5.208737	0.616301	1.058060
52	8	0	5.687829	1.106731	1.755825
53	1	0	5.677135	2.019290	1.388241
54	1	0	-2.400520	-0.538172	-2.738300
55	8	0	-2.830141	-1.370116	-2.438313
56	1	0	-2.103462	-2.000240	-2.288882

57	8	0	4.509360	-2.758773	0.247246
58	1	0	4.284195	-1.790446	0.124551
59	1	0	5.455997	-2.794980	0.456341
60	8	0	3.646903	0.669068	3.444573
61	1	0	3.842521	0.912370	4.360167
62	1	0	4.481052	0.832646	2.919020
63	8	0	1.201406	-3.488625	-3.241470
64	1	0	2.043266	-3.798565	-2.806125
65	1	0	0.980521	-4.174977	-3.889248
66	1	0	-4.826825	4.514928	-0.325716
67	8	0	-4.188685	4.166175	0.313507
68	1	0	-4.741737	3.623308	0.944136
69	1	0	2.360692	-4.452059	-0.957912
70	8	0	3.084732	-4.422270	-1.620246
71	1	0	3.762996	-3.866654	-1.189107
72	8	0	5.103096	3.336956	0.122191
73	7	0	3.478731	3.769546	-1.430142
74	1	0	2.489629	3.657356	-1.662371
75	6	0	4.329702	4.512664	-2.344639
76	1	0	5.349462	4.484612	-1.959412
77	1	0	4.305934	4.064642	-3.344330
78	1	0	4.003729	5.556432	-2.420954
79	6	0	-6.017100	-0.539033	-0.182250
80	1	0	-4.237714	-1.070063	-1.098877
81	8	0	-6.617552	0.257196	0.543112
82	6	0	-6.762661	-1.612552	-0.955866
83	1	0	-7.195387	-2.324375	-0.244767
84	1	0	-7.591590	-1.146513	-1.495953
85	1	0	-6.127987	-2.156818	-1.660762

The former diol(n) in Fig. 1
zuck2.for.chk

E(RB3LYP) = -2303.081621 a.u.
Thermal correction to Gibbs Free Energy= 0.611940 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.453894	-1.285641	-0.138959
2	6	0	0.120812	-2.772933	-0.122871
3	6	0	-0.594785	-0.540848	0.253727
4	8	0	-0.374448	-3.144343	-1.368004
5	8	0	-0.671888	0.696236	0.158907
6	6	0	-1.013889	-2.804797	0.922931
7	6	0	-1.730081	-1.470914	0.700592
8	1	0	-1.647626	-3.678578	0.767707
9	7	0	-2.546873	-0.970984	1.778956
10	6	0	1.500411	-0.750559	-1.010099
11	1	0	-0.569090	-2.853563	1.922945
12	1	0	1.636396	-3.242016	1.070745
13	6	0	2.531341	0.136151	-0.295485
14	1	0	2.032112	-1.592812	-1.450944
15	1	0	1.040362	-0.181604	-1.826982

16	8	0	2.136318	-0.273221	3.125637
17	1	0	1.636285	0.334984	2.562238
18	1	0	2.986964	0.203523	3.311526
19	8	0	1.228058	-3.520287	0.176279
20	1	0	0.400400	-3.319314	-1.980886
21	1	0	-2.354283	-1.569247	-0.191867
22	8	0	2.501352	-2.856400	2.323351
23	1	0	2.369273	-1.917084	2.615921
24	1	0	3.391291	-2.888360	1.914773
25	8	0	3.636875	-0.325252	0.045528
26	7	0	2.173418	1.414653	-0.109753
27	6	0	3.034532	2.435187	0.479335
28	1	0	1.280396	1.740487	-0.482348
29	6	0	4.000639	3.086729	-0.529574
30	1	0	2.379885	3.206022	0.897721
31	1	0	3.622061	2.013864	1.291697
32	6	0	-3.524688	-0.019254	1.659502
33	1	0	-2.231872	-1.117459	2.732455
34	8	0	-4.009926	0.496026	2.665514
35	6	0	-3.979537	0.378104	0.240307
36	1	0	-3.112823	0.623262	-0.371382
37	7	0	-4.749790	-0.637896	-0.457960
38	1	0	-4.579890	1.278394	0.352822
39	1	0	-1.032231	0.969725	-1.677494
40	8	0	-1.443652	1.218400	-2.528560
41	1	0	-2.037407	1.933533	-2.209907
42	1	0	-1.817550	2.465349	0.057986
43	8	0	-2.108944	3.120849	-0.599337
44	1	0	-2.935660	3.529031	-0.216621
45	1	0	-5.355956	1.810593	2.407252
46	8	0	-5.986900	2.370387	1.905268
47	1	0	-6.442535	1.704291	1.348462
48	8	0	0.451295	3.230996	-1.628694
49	1	0	0.071553	2.683773	-2.342704
50	1	0	-0.360375	3.556580	-1.176951
51	1	0	5.234511	0.367074	0.768420
52	8	0	5.932112	0.845003	1.259472
53	1	0	5.935333	1.713307	0.798086
54	1	0	-2.307614	-0.561733	-2.675859
55	8	0	-2.698257	-1.422170	-2.413022
56	1	0	-1.947123	-2.035161	-2.299174
57	8	0	4.572034	-2.869533	0.399697
58	1	0	4.229201	-1.981809	0.135669
59	1	0	5.526136	-2.750716	0.528340
60	8	0	4.406142	1.188082	3.440619
61	1	0	4.889063	1.203596	4.279180
62	1	0	5.085308	1.038349	2.725659
63	8	0	1.778757	-3.414174	-2.964323
64	1	0	2.448982	-3.935175	-2.431487
65	1	0	1.670472	-3.900638	-3.795392
66	1	0	-5.030167	4.448264	-0.179458
67	8	0	-4.420736	4.057119	0.462819
68	1	0	-4.996118	3.464994	1.025288
69	1	0	2.533165	-4.781765	-0.662338
70	8	0	3.303798	-4.784784	-1.260754

71	1	0	3.920421	-4.177379	-0.795811
72	8	0	5.223420	3.056140	-0.352662
73	7	0	3.401980	3.693652	-1.575796
74	1	0	2.383201	3.676702	-1.637869
75	6	0	4.151005	4.357595	-2.630440
76	1	0	5.212390	4.281299	-2.392971
77	1	0	3.962638	3.883580	-3.600725
78	1	0	3.871380	5.414949	-2.696655
79	6	0	-6.111751	-0.647573	-0.419351
80	1	0	-4.256513	-1.150475	-1.189124
81	8	0	-6.775877	0.118041	0.282176
82	6	0	-6.780975	-1.694636	-1.291599
83	1	0	-7.255277	-2.441055	-0.645473
84	1	0	-7.573698	-1.214626	-1.872040
85	1	0	-6.088238	-2.201896	-1.968974

TS2(n) in Fig. 1-2 from the fomer diol(n) to diketeone(n) vucw3.ext3.chk

E(RB3LYP) = -2303.054474 a.u.

Thermal correction to Gibbs Free Energy= 0.607186 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.394738	0.284194	-0.696746
2	6	0	0.504852	-0.728023	0.378971
3	6	0	-0.848660	0.402485	-1.209739
4	8	0	1.685646	-1.220467	0.525113
5	8	0	-1.201450	1.213135	-2.077274
6	6	0	-0.751708	-1.589605	0.124555
7	6	0	-1.763749	-0.600044	-0.477514
8	1	0	-0.489808	-2.333211	-0.632767
9	7	0	-2.506531	0.104102	0.573904
10	6	0	1.513083	1.117397	-1.090525
11	1	0	-1.105983	-2.096547	1.024290
12	1	0	-2.460985	-1.060329	-1.174768
13	6	0	2.773283	0.309526	-1.403115
14	1	0	1.218416	1.636435	-2.005741
15	1	0	1.674999	1.885183	-0.339850
16	8	0	0.078617	0.062020	1.716200
17	1	0	2.665373	-1.788511	1.909209
18	1	0	0.365644	1.035493	1.707193
19	8	0	2.930489	-2.228032	2.750674
20	1	0	1.612611	-1.601375	3.505534
21	1	0	2.691574	-3.164050	2.578489
22	8	0	0.668722	-1.266603	3.665652
23	1	0	0.400892	-0.551600	2.682651
24	1	0	0.115384	-2.092129	3.559275
25	8	0	2.757880	-0.529471	-2.322020
26	7	0	3.917477	0.653509	-0.763314
27	6	0	3.952741	1.308230	0.545653
28	1	0	4.730568	0.035465	-0.941714
29	6	0	3.609615	2.805564	0.566584

30	1	0	3.280931	0.815520	1.254421
31	1	0	4.972008	1.189523	0.928164
32	6	0	-3.573421	0.939710	0.481317
33	1	0	-1.952104	0.256116	1.413769
34	8	0	-3.837784	1.705615	1.423776
35	6	0	-4.450780	0.990304	-0.770156
36	1	0	-3.944766	1.637232	-1.493763
37	7	0	-4.719149	-0.272095	-1.431110
38	1	0	-5.379594	1.473478	-0.452703
39	1	0	-2.435000	0.552741	-3.304098
40	8	0	-3.160514	0.106773	-3.793850
41	1	0	-3.469603	0.764337	-4.434406
42	1	0	-0.492301	3.263017	-1.496814
43	8	0	0.064866	3.909711	-1.031917
44	1	0	0.058737	3.599346	-0.105691
45	1	0	-5.953524	1.829685	1.631125
46	8	0	-6.840544	1.589901	1.311639
47	1	0	-6.736923	0.641800	1.107783
48	8	0	6.116496	-1.124874	-0.864710
49	1	0	5.653372	-1.861844	-1.349987
50	1	0	6.244664	-1.474926	0.030067
51	1	0	3.943717	-2.020456	-2.454708
52	8	0	4.457696	-2.804573	-2.172264
53	1	0	3.840247	-3.241899	-1.546643
54	1	0	2.073294	-2.674624	-0.219430
55	8	0	2.202542	-3.585861	-0.607073
56	1	0	1.653508	-3.523546	-1.425754
57	8	0	1.678481	-4.623064	1.790530
58	1	0	1.780891	-4.376392	0.824512
59	1	0	2.022997	-5.525096	1.870636
60	8	0	-0.558064	-3.553376	2.981200
61	1	0	0.172768	-4.061752	2.550423
62	1	0	-0.972586	-4.155894	3.616004
63	8	0	0.401639	2.646688	1.611264
64	1	0	-0.337469	2.896613	2.230291
65	1	0	1.250999	3.048929	1.894117
66	1	0	-1.959636	2.450795	3.876215
67	8	0	-1.866147	2.882230	3.014749
68	1	0	-2.601320	2.518456	2.465629
69	1	0	1.408617	-1.707444	-2.684571
70	8	0	0.849774	-2.517274	-2.741446
71	1	0	0.929908	-2.814300	-3.660283
72	8	0	3.103528	3.309798	1.576208
73	7	0	3.907522	3.500688	-0.546924
74	1	0	4.242189	2.973100	-1.342920
75	6	0	3.476260	4.882431	-0.739222
76	1	0	3.584198	5.417831	0.205517
77	1	0	4.110069	5.351097	-1.495635
78	1	0	2.426665	4.918012	-1.054628
79	6	0	-5.546808	-1.195755	-0.872824
80	1	0	-4.363990	-0.366211	-2.384716
81	8	0	-6.033152	-1.059365	0.250965
82	6	0	-5.834196	-2.422692	-1.721611
83	1	0	-5.637256	-3.319011	-1.126220
84	1	0	-6.898550	-2.431233	-1.979186

85	1	0	-5.245061	-2.461077	-2.642573

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diketone(n) in Fig. 1 and 2
vucw3.ext3for.chk E(RB3LYP) = -2303.088221 a.u.
Thermal correction to Gibbs Free Energy= 0.605549 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.417440	-0.138637	-0.601801
2	6	0	-0.440809	1.082655	0.060607
3	6	0	0.829922	-0.434705	-1.124092
4	8	0	-1.457031	1.506354	0.595485
5	8	0	1.083282	-1.404389	-1.826341
6	6	0	0.907221	1.746518	-0.101964
7	6	0	1.825921	0.611016	-0.586852
8	1	0	0.792419	2.511313	-0.878648
9	7	0	2.554693	0.012094	0.527416
10	6	0	-1.553038	-1.044010	-0.555945
11	1	0	1.221396	2.238945	0.819880
12	1	0	2.518019	0.912688	-1.370579
13	6	0	-2.811690	-0.447219	-1.167524
14	1	0	-1.276856	-1.973153	-1.069523
15	1	0	-1.697017	-1.314008	0.489200
16	8	0	0.676986	-0.012860	2.663660
17	1	0	-2.469052	2.061632	2.215476
18	1	0	0.010054	-0.703378	2.482979
19	8	0	-2.790764	2.654387	2.915078
20	1	0	-1.224913	2.272679	3.844858
21	1	0	-2.595792	3.539971	2.544357
22	8	0	-0.263991	2.108225	3.980808
23	1	0	0.262576	0.719606	3.210870
24	1	0	0.155314	2.823168	3.453227
25	8	0	-2.750830	0.328319	-2.142400
26	7	0	-3.987499	-0.852805	-0.647729
27	6	0	-4.149871	-1.529229	0.641882
28	1	0	-4.840768	-0.391496	-1.017305
29	6	0	-3.608523	-2.969884	0.728932
30	1	0	-3.682808	-0.968496	1.457447
31	1	0	-5.226076	-1.555251	0.841395
32	6	0	3.596441	-0.868607	0.477523
33	1	0	2.031702	0.003260	1.416200
34	8	0	3.897938	-1.527841	1.479495
35	6	0	4.398859	-1.095238	-0.809405
36	1	0	3.833207	-1.797209	-1.429911
37	7	0	4.685483	0.070742	-1.627206
38	1	0	5.324389	-1.580506	-0.484981
39	1	0	2.302650	-1.016147	-3.286059
40	8	0	2.980552	-0.605139	-3.858097
41	1	0	3.273798	-1.314845	-4.448803
42	1	0	0.451083	-3.394334	-1.221535
43	8	0	-0.222669	-3.888828	-0.728292
44	1	0	-0.135888	-3.551305	0.191179

45	1	0	6.018719	-1.761266	1.576130
46	8	0	6.882690	-1.620442	1.150757
47	1	0	6.828334	-0.685971	0.878454
48	8	0	-6.355367	0.480444	-1.397367
49	1	0	-5.940894	1.257486	-1.859747
50	1	0	-6.813894	0.865319	-0.635425
51	1	0	-4.085929	1.597658	-2.637210
52	8	0	-4.746027	2.316185	-2.558354
53	1	0	-4.325183	2.923482	-1.915922
54	1	0	-2.681226	2.772734	-0.269043
55	8	0	-2.816170	3.576126	-0.808020
56	1	0	-2.171018	3.422484	-1.544850
57	8	0	-1.927357	4.940778	1.385823
58	1	0	-2.214894	4.597034	0.499766
59	1	0	-2.347522	5.808085	1.485212
60	8	0	0.627489	4.113717	2.195017
61	1	0	-0.221482	4.504854	1.889121
62	1	0	1.115837	4.841265	2.607796
63	8	0	-0.260585	-2.582814	1.814765
64	1	0	0.522923	-2.753628	2.414429
65	1	0	-1.043885	-3.032559	2.183607
66	1	0	1.651297	-1.490790	3.536009
67	8	0	1.915284	-2.419743	3.372950
68	1	0	2.692161	-2.303598	2.787229
69	1	0	-1.570557	1.605742	-2.615147
70	8	0	-1.122097	2.481354	-2.675994
71	1	0	-1.184808	2.738257	-3.608540
72	8	0	-3.075183	-3.364156	1.767036
73	7	0	-3.805413	-3.735787	-0.362966
74	1	0	-4.171830	-3.287664	-1.192202
75	6	0	-3.290421	-5.098762	-0.466352
76	1	0	-3.364916	-5.571745	0.514502
77	1	0	-3.901118	-5.654414	-1.182427
78	1	0	-2.242446	-5.094081	-0.784256
79	6	0	5.609438	0.994233	-1.238962
80	1	0	4.307177	0.059804	-2.573936
81	8	0	6.159186	0.961644	-0.138899
82	6	0	5.916330	2.085840	-2.251021
83	1	0	5.809832	3.059615	-1.764088
84	1	0	6.961663	1.992117	-2.563390
85	1	0	5.276091	2.051165	-3.137639

TS3(n) in Fig. 1-3 from diketone(n) to diol(n) latter
wuck1.chk E(RB3LYP) = -2303.058315 a.u.
Thermal correction to Gibbs Free Energy= 0.603312 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.870908	-0.254150	-0.059113
2	6	0	-0.532237	-0.650951	-0.350167
3	6	0	1.502212	0.243738	-1.166667
4	8	0	-0.689290	-1.930654	-0.511579

5	8	0	2.714252	0.429754	-1.240803
6	6	0	-0.892026	0.265074	-1.591772
7	6	0	0.478967	0.456109	-2.267914
8	1	0	-1.583365	-0.312362	-2.208326
9	1	0	0.601533	1.432545	-2.741694
10	6	0	1.616346	-0.980596	0.965596
11	7	0	-1.467140	1.570387	-1.291489
12	8	0	-1.352294	-0.175076	0.843825
13	6	0	2.765893	-0.133649	1.507039
14	1	0	0.923944	-1.186586	1.788317
15	1	0	1.982105	-1.939402	0.587680
16	8	0	-0.060039	1.880359	1.905059
17	1	0	0.859060	1.601675	1.662801
18	1	0	0.037927	1.975867	2.882253
19	1	0	-0.933168	0.612874	1.323458
20	1	0	-2.049998	-2.864691	-0.509691
21	1	0	0.659644	-0.326605	-3.012104
22	8	0	-2.829011	-3.399176	-0.169746
23	1	0	-2.829994	-2.514504	1.139422
24	1	0	-2.419618	-4.188814	0.250283
25	8	0	2.563089	1.034634	1.933371
26	7	0	3.961408	-0.717048	1.527343
27	6	0	5.171213	0.037088	1.836630
28	1	0	4.071281	-1.659089	1.091978
29	1	0	4.975707	0.712201	2.673777
30	1	0	5.960024	-0.665617	2.107926
31	6	0	5.626539	0.803789	0.580080
32	6	0	-2.764421	1.860559	-1.113345
33	1	0	-0.803470	2.343984	-1.087050
34	8	0	-3.176251	3.016520	-0.891491
35	6	0	-3.783199	0.723182	-1.179781
36	1	0	-3.541119	-0.040776	-0.438849
37	7	0	-5.092512	1.278898	-0.886038
38	1	0	-3.778330	0.213912	-2.150455
39	1	0	2.884277	-2.883549	-2.302564
40	8	0	3.841865	-3.041220	-2.145902
41	1	0	4.299217	-2.197028	-2.392370
42	1	0	5.622412	-0.358472	-1.900633
43	8	0	4.981252	-0.564403	-2.608662
44	1	0	4.185280	-0.065970	-2.343130
45	1	0	-2.275461	4.584485	-0.883854
46	8	0	-1.692930	5.369291	-0.756386
47	1	0	-2.002893	5.761899	0.073315
48	8	0	4.013179	-3.235005	0.451603
49	1	0	3.976042	-3.191419	-0.561457
50	1	0	4.728601	-3.854956	0.653997
51	1	0	1.898465	1.472061	3.709200
52	8	0	1.206874	1.793268	4.324518
53	1	0	1.543545	2.643579	4.645680
54	1	0	0.436678	-2.538300	-1.736395
55	8	0	1.052342	-2.702363	-2.496148
56	1	0	0.713101	-3.495809	-2.935308
57	8	0	-2.604155	-1.932299	1.951738
58	1	0	-1.917113	-1.030367	1.456430
59	1	0	-3.490654	-1.585460	2.284033

60	8	0	-1.595208	-4.842407	1.845911
61	1	0	-1.594522	-3.966782	2.271249
62	1	0	-2.147659	-5.392498	2.421660
63	8	0	0.322287	3.541872	-0.380367
64	1	0	-0.235232	4.346842	-0.511737
65	1	0	0.137750	3.259190	0.536863
66	8	0	-5.053258	-1.120686	2.579312
67	1	0	-5.464813	-0.972528	1.691749
68	1	0	-5.580795	-1.822807	2.988836
69	8	0	-4.590856	-2.186623	-2.078607
70	1	0	-4.079296	-2.847174	-1.576633
71	1	0	-5.168006	-1.796166	-1.398690
72	8	0	6.441130	0.309570	-0.201654
73	7	0	5.033783	2.010498	0.414265
74	1	0	4.209697	2.181028	0.982113
75	6	0	5.162328	2.764760	-0.825871
76	1	0	6.116117	2.505913	-1.286939
77	1	0	4.349167	2.520158	-1.518091
78	1	0	5.141592	3.836339	-0.607831
79	6	0	-6.051385	0.610181	-0.232474
80	1	0	-5.135043	2.290301	-0.967760
81	8	0	-5.947319	-0.601510	0.057442
82	6	0	-7.292241	1.390693	0.147709
83	1	0	-8.167405	0.890643	-0.278068
84	1	0	-7.401255	1.371559	1.237222
85	1	0	-7.272288	2.429943	-0.191244

The latter diol(n) in Fig. 1-4 wuck1.for.chk

E(RB3LYP) = -2303.086199 a.u.

Thermal correction to Gibbs Free Energy= 0.608892 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.907515	0.249953	0.192629
2	6	0	0.511208	0.585867	0.163360
3	6	0	-1.421668	0.003184	-1.054708
4	8	0	0.595171	1.985129	0.114804
5	8	0	-2.617220	-0.125158	-1.288975
6	6	0	1.007107	-0.037197	-1.197856
7	6	0	-0.276222	-0.043579	-2.052681
8	1	0	1.770802	0.623778	-1.613622
9	1	0	-0.360921	-0.918481	-2.701035
10	6	0	-1.741364	0.685032	1.310117
11	7	0	1.538295	-1.384335	-1.074296
12	8	0	1.178686	0.129761	1.298511
13	6	0	-2.908323	-0.276464	1.527956
14	1	0	-1.108352	0.669895	2.202697
15	1	0	-2.107903	1.704719	1.159491
16	8	0	-0.032723	-2.279541	1.723576
17	1	0	-0.937050	-1.967158	1.479303
18	1	0	-0.197904	-2.588071	2.644506
19	1	0	0.883130	-0.807010	1.485627

20	1	0	1.547492	2.319645	0.057997
21	1	0	-0.343893	0.853176	-2.678942
22	8	0	2.857328	3.282905	0.221228
23	1	0	3.072919	2.937722	1.140972
24	1	0	2.340580	4.106347	0.342826
25	8	0	-2.709222	-1.508724	1.673993
26	7	0	-4.115863	0.282496	1.578703
27	6	0	-5.327387	-0.530495	1.589051
28	1	0	-4.202418	1.297532	1.360784
29	1	0	-5.181815	-1.387380	2.251681
30	1	0	-6.154823	0.079306	1.953823
31	6	0	-5.656924	-0.969503	0.149683
32	6	0	2.818518	-1.737779	-0.850801
33	1	0	0.855434	-2.168815	-1.098391
34	8	0	3.187412	-2.926277	-0.822785
35	6	0	3.848959	-0.642818	-0.604173
36	1	0	3.641383	-0.183398	0.371326
37	7	0	5.166188	-1.251547	-0.617311
38	1	0	3.799548	0.166274	-1.343979
39	1	0	-2.869621	3.401621	-1.664921
40	8	0	-3.831669	3.436306	-1.465940
41	1	0	-4.239003	2.665902	-1.939135
42	1	0	-5.516838	0.741998	-1.987695
43	8	0	-4.832493	1.118930	-2.575228
44	1	0	-4.044362	0.580858	-2.376567
45	1	0	2.295059	-4.438303	-1.274765
46	8	0	1.695542	-5.209275	-1.403864
47	1	0	1.906970	-5.800691	-0.666147
48	8	0	-4.035039	2.994909	1.092246
49	1	0	-3.977945	3.178274	0.093535
50	1	0	-4.754541	3.560441	1.409108
51	1	0	-2.184582	-2.368046	3.372465
52	8	0	-1.533721	-2.795462	3.964946
53	1	0	-1.843396	-3.710185	4.047281
54	1	0	-0.488792	2.868042	-1.180774
55	8	0	-1.015197	3.442779	-1.769643
56	1	0	-0.707182	4.330849	-1.523524
57	8	0	3.132125	2.033020	2.523171
58	1	0	2.517268	1.298392	2.339882
59	1	0	4.039846	1.638382	2.551985
60	8	0	0.490157	4.795863	0.495674
61	1	0	0.150347	3.930517	0.787740
62	1	0	0.179937	5.431036	1.158902
63	8	0	-0.334759	-3.460525	-0.818550
64	1	0	0.228179	-4.227934	-1.085374
65	1	0	-0.200043	-3.382043	0.147227
66	8	0	5.718830	1.153722	2.373322
67	1	0	5.937168	1.108672	1.414413
68	1	0	6.287169	1.854494	2.726320
69	8	0	4.292779	2.164206	-1.967744
70	1	0	3.859244	2.721060	-1.290944
71	1	0	5.099697	1.854728	-1.517063
72	8	0	-6.410490	-0.297147	-0.557041
73	7	0	-5.030771	-2.100916	-0.251624
74	1	0	-4.260891	-2.416775	0.329493

75	6	0	-5.052907	-2.541256	-1.640353
76	1	0	-5.974265	-2.180970	-2.099259
77	1	0	-4.195447	-2.141240	-2.192849
78	1	0	-5.028638	-3.633837	-1.679156
79	6	0	6.298373	-0.552281	-0.462713
80	1	0	5.163120	-2.262153	-0.711805
81	8	0	6.302595	0.685074	-0.295682
82	6	0	7.594955	-1.334776	-0.487778
83	1	0	8.253261	-0.899635	-1.245555
84	1	0	8.092696	-1.223879	0.481180
85	1	0	7.456345	-2.398798	-0.698531

diol(later,n) -> beta product TS4(n) in Fig. 1
luckw3a.chk E(RB3LYP) = -2303.046419 a.u.
Thermal correction to Gibbs Free Energy= 0.613077 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.506352	-0.350308	0.324886
2	6	0	0.900119	0.369613	0.757586
3	6	0	-0.947893	0.351023	-0.839790
4	8	0	0.432370	1.550532	1.395370
5	8	0	-2.115725	0.432849	-1.165005
6	6	0	1.459830	0.801916	-0.657374
7	6	0	0.231453	0.935306	-1.578182
8	1	0	1.907019	1.779691	-0.498329
9	1	0	0.358705	0.388713	-2.520149
10	6	0	-1.490860	-0.434952	1.444894
11	7	0	2.451634	-0.090503	-1.227383
12	1	0	-5.953155	-0.009477	1.449260
13	6	0	-2.842596	-1.013537	1.035904
14	1	0	-1.048284	-1.074682	2.214539
15	1	0	-1.612195	0.564861	1.863805
16	8	0	0.165687	-2.672250	-0.435887
17	1	0	-0.173486	-1.567562	-0.065901
18	1	0	-0.434952	-3.348189	-0.002557
19	8	0	1.658491	-0.388865	1.503188
20	1	0	1.025940	1.705249	2.187108
21	1	0	0.002846	1.977438	-1.819406
22	8	0	2.350152	-2.918745	0.814541
23	1	0	1.107391	-2.839196	-0.008125
24	1	0	2.009184	-3.424152	1.618378
25	8	0	-2.960606	-2.167303	0.556174
26	7	0	-3.889642	-0.223137	1.284505
27	6	0	-5.237191	-0.591667	0.867500
28	1	0	-3.717612	0.768260	1.548217
29	1	0	-5.390077	-1.657789	1.053417
30	1	0	2.327601	-1.960502	1.078993
31	6	0	-5.439676	-0.242564	-0.617417
32	6	0	3.786917	-0.045294	-1.035912
33	1	0	2.104620	-0.808376	-1.892708
34	8	0	4.565958	-0.824447	-1.606800

35	6	0	4.378003	1.021702	-0.099361
36	1	0	5.421425	0.738549	0.065724
37	7	0	4.291143	2.364676	-0.659661
38	1	0	3.858617	1.034396	0.858035
39	1	0	-1.806945	4.005872	-0.171221
40	8	0	-2.772606	3.989363	0.000234
41	1	0	-3.190354	3.584757	-0.801225
42	1	0	-4.688006	2.132928	-1.778245
43	8	0	-3.854831	2.536908	-2.094653
44	1	0	-3.212402	1.809055	-2.017972
45	1	0	4.931381	-2.768017	-0.912942
46	8	0	4.542516	-3.658261	-0.847435
47	1	0	3.812220	-3.528360	-0.206953
48	8	0	-3.212938	2.348392	2.019157
49	1	0	-3.042550	2.972253	1.244671
50	1	0	-3.783814	2.848260	2.620365
51	1	0	-2.055728	-3.502931	1.068393
52	8	0	-1.341146	-4.196800	1.124320
53	1	0	-1.744519	-5.026784	0.826277
54	1	0	0.208430	3.117134	0.496693
55	8	0	0.096226	3.892440	-0.101185
56	1	0	0.357622	4.652570	0.441289
57	8	0	1.058120	-4.045032	2.846320
58	1	0	0.913255	-3.235457	3.391437
59	1	0	0.184255	-4.225407	2.449240
60	1	0	4.081837	-2.141301	-3.183416
61	8	0	3.640673	-2.990643	-3.369812
62	1	0	3.868113	-3.488485	-2.545894
63	8	0	1.217651	-1.889280	-3.003504
64	1	0	2.033047	-2.406373	-3.261553
65	1	0	0.739132	-2.463739	-2.381128
66	1	0	1.015260	-1.012619	2.989064
67	8	0	0.604952	-1.510813	3.743565
68	1	0	0.819825	-1.008970	4.543780
69	8	0	2.387402	1.699706	3.218635
70	1	0	2.549357	0.825130	2.811442
71	1	0	2.928052	2.316525	2.682197
72	8	0	-5.925375	0.837210	-0.960953
73	7	0	-5.016322	-1.191616	-1.484898
74	1	0	-4.422319	-1.919442	-1.100551
75	6	0	-4.979538	-0.938894	-2.918887
76	1	0	-5.922068	-0.480419	-3.224754
77	1	0	-4.162031	-0.261393	-3.192589
78	1	0	-4.852134	-1.888043	-3.444253
79	6	0	3.808859	3.441883	0.021713
80	1	0	4.652058	2.506111	-1.593371
81	8	0	3.402042	3.375985	1.183609
82	6	0	3.726844	4.737095	-0.760871
83	1	0	4.075891	5.558276	-0.130137
84	1	0	4.297830	4.726408	-1.693952
85	1	0	2.670739	4.914081	-0.994991

The beta product in Fig. 1
luckw3.extrev.chk E(RB3LYP) = -2303.099373 a.u.
Thermal correction to Gibbs Free Energy= 0.610951 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.954647	-0.721713	0.408616
2	6	0	1.648311	0.742363	0.624436
3	6	0	-0.881942	0.202616	-0.568616
4	8	0	0.979201	1.785939	1.081025
5	8	0	-1.681388	1.149553	-0.672044
6	6	0	1.630821	0.672847	-0.915976
7	6	0	0.316024	0.040056	-1.488638
8	1	0	1.655517	1.715790	-1.236770
9	1	0	0.488200	-1.020817	-1.671355
10	6	0	-1.912133	-0.616674	1.502392
11	7	0	2.763199	-0.068154	-1.445505
12	1	0	2.684774	-1.917735	1.210991
13	6	0	-3.261580	-1.214514	1.111248
14	1	0	-1.505610	-1.164178	2.356845
15	1	0	-2.020661	0.433260	1.781870
16	8	0	0.472355	-3.073672	-0.366121
17	1	0	-0.401916	-1.584019	0.284236
18	1	0	-0.118242	-3.727151	0.067687
19	8	0	2.254969	-0.036072	1.360092
20	1	0	1.244685	1.987966	2.042931
21	1	0	0.092568	0.516516	-2.445140
22	8	0	2.696178	-2.892867	1.154351
23	1	0	1.325513	-3.105419	0.142987
24	1	0	2.206774	-3.211566	1.966005
25	8	0	-3.358509	-2.408781	0.745185
26	7	0	-4.303177	-0.377878	1.164016
27	6	0	-5.624059	-0.772858	0.686251
28	1	0	-4.132594	0.625880	1.374114
29	1	0	-5.803951	-1.816329	0.958351
30	1	0	-6.374649	-0.133479	1.152380
31	6	0	-5.699499	-0.561110	-0.833861
32	6	0	4.086340	0.176530	-1.277081
33	1	0	2.547350	-0.998585	-1.873553
34	8	0	4.942985	-0.651509	-1.612979
35	6	0	4.598010	1.478220	-0.638054
36	1	0	5.657823	1.529287	-0.904240
37	7	0	3.910738	2.708015	-1.001756
38	1	0	4.533676	1.395535	0.450835
39	1	0	-2.492244	4.149071	-0.338009
40	8	0	-3.447062	4.005327	-0.166897
41	1	0	-3.755848	3.493912	-0.954165
42	1	0	-4.846550	1.684251	-1.918252
43	8	0	-3.998452	2.121763	-2.134847
44	1	0	-3.316718	1.582582	-1.693531
45	1	0	5.319093	-2.316364	-0.349400
46	8	0	5.204927	-3.256517	-0.123683
47	1	0	4.374163	-3.278083	0.397357

48	8	0	-3.658552	2.245621	1.823220
49	1	0	-3.544473	2.888950	1.057561
50	1	0	-4.241848	2.710956	2.440673
51	1	0	-2.090940	-3.538829	1.181001
52	8	0	-1.337707	-4.150767	1.400237
53	1	0	-1.735202	-5.027583	1.509935
54	1	0	-0.955471	2.842230	-0.945778
55	8	0	-0.617923	3.714541	-0.645928
56	1	0	-0.315251	3.496050	0.250413
57	8	0	0.951168	-3.525396	3.105206
58	1	0	0.779204	-2.624739	3.456346
59	1	0	0.133375	-3.767173	2.623402
60	1	0	4.860004	-2.476182	-2.858832
61	8	0	4.543662	-3.394724	-2.797030
62	1	0	4.775953	-3.608655	-1.859795
63	8	0	2.006689	-2.472698	-2.653110
64	1	0	2.869984	-2.957269	-2.762894
65	1	0	1.471170	-2.994334	-2.024349
66	1	0	1.338271	-0.459681	2.969067
67	8	0	0.693758	-0.795790	3.625027
68	1	0	0.967166	-0.432867	4.480443
69	8	0	2.059864	2.746261	3.226846
70	1	0	2.703645	2.148568	3.638612
71	1	0	2.612990	3.273195	2.601686
72	8	0	-6.213909	0.450040	-1.318690
73	7	0	-5.098618	-1.518332	-1.575244
74	1	0	-4.575699	-2.234243	-1.081234
75	6	0	-4.931867	-1.357579	-3.015451
76	1	0	-5.904121	-1.369460	-3.517665
77	1	0	-4.441193	-0.405893	-3.246680
78	1	0	-4.325177	-2.183216	-3.392114
79	6	0	3.487776	3.621148	-0.081750
80	1	0	3.857061	2.953831	-1.981287
81	8	0	3.639755	3.426247	1.129990
82	6	0	2.773290	4.834596	-0.634612
83	1	0	1.703185	4.608355	-0.738434
84	1	0	2.888174	5.665660	0.063780
85	1	0	3.152560	5.132589	-1.617458

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alpha form, in Fig. 3, reactant common to that in Fig. 1
vucw3aa.extrev.log E(RB3LYP) = -2303.09867400

The first step, TS1(i) in Fig. 3
vuc2p4.chk E(RB3LYP) = -2303.073231 a.u.
Thermal correction to Gibbs Free Energy= 0.604839 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.253523	-0.594107	-0.308773
2	6	0	-0.602542	-0.869900	2.801589
3	6	0	-0.958545	-1.119030	-0.207069

4	8	0	-0.742073	-2.166779	2.564458
5	8	0	-1.385127	-2.124545	-0.860855
6	6	0	-1.612834	0.010211	2.105117
7	6	0	-2.022099	-0.416215	0.678174
8	1	0	-2.519539	0.038334	2.723624
9	7	0	-2.530775	0.782315	0.000446
10	6	0	1.056625	-1.244320	-1.336193
11	1	0	-1.214146	1.024743	2.109901
12	1	0	0.397588	0.948694	0.014301
13	6	0	2.426181	-0.606480	-1.501395
14	1	0	1.195898	-2.310382	-1.126901
15	1	0	0.552826	-1.204875	-2.315340
16	8	0	0.279456	1.952848	0.304850
17	8	0	0.270552	-0.412683	3.537997
18	1	0	0.857147	2.671684	-0.382888
19	1	0	0.615169	2.057552	1.257645
20	1	0	0.093551	-2.631185	2.914093
21	1	0	-2.834706	-1.130976	0.758436
22	8	0	1.076079	2.184745	2.807465
23	1	0	0.756196	1.368544	3.251488
24	1	0	2.053305	2.073116	2.783175
25	8	0	2.656880	0.572715	-1.203823
26	7	0	3.369122	-1.435127	-1.999077
27	6	0	4.717710	-0.968558	-2.197562
28	1	0	3.126482	-2.417822	-2.194419
29	6	0	5.365374	-0.492627	-0.884404
30	1	0	5.309227	-1.802450	-2.589276
31	1	0	4.746989	-0.160661	-2.940249
32	6	0	-3.454056	0.868766	-0.989598
33	1	0	-1.948948	1.613589	0.097984
34	8	0	-3.588764	1.928507	-1.625804
35	6	0	-4.309746	-0.350690	-1.359633
36	1	0	-3.653858	-1.092470	-1.825414
37	7	0	-4.987912	-1.000930	-0.249371
38	1	0	-5.034311	0.008019	-2.095144
39	1	0	-0.630226	-3.379326	-1.878153
40	8	0	-0.259978	-4.088098	-2.459983
41	1	0	-0.746499	-4.006350	-3.293045
42	8	0	3.652572	1.442509	2.240819
43	1	0	3.364115	0.517491	2.017911
44	1	0	4.407026	1.341779	2.840277
45	1	0	-5.445267	2.107773	-2.519232
46	8	0	-6.365559	1.817136	-2.646183
47	1	0	-6.613798	1.558405	-1.739231
48	8	0	2.471102	-4.082307	-2.527668
49	1	0	1.480442	-4.091809	-2.593560
50	1	0	2.667394	-4.763400	-1.867382
51	1	0	3.886247	2.478051	0.672106
52	8	0	3.959755	2.818405	-0.245749
53	1	0	3.747068	2.019013	-0.770307
54	1	0	-3.160814	-3.611937	1.229361
55	8	0	-3.508823	-3.426845	0.343472
56	1	0	-2.721998	-3.081547	-0.144919
57	8	0	1.488026	3.545605	-1.068990
58	1	0	2.429542	3.531207	-0.744628

59	1	0	1.041666	4.420227	-0.868088
60	8	0	-0.115070	5.568262	-0.446087
61	1	0	-0.973107	5.085926	-0.566946
62	1	0	-0.074203	5.725386	0.509533
63	8	0	1.641668	-2.948519	3.370157
64	1	0	2.136221	-2.425116	2.694060
65	1	0	1.627486	-2.334140	4.123957
66	8	0	2.712082	-1.064477	1.582099
67	1	0	3.445054	-1.249533	0.945516
68	1	0	1.918509	-0.841173	1.048245
69	8	0	-2.437602	4.116752	-0.422613
70	1	0	-3.245779	4.576360	-0.150945
71	1	0	-2.761062	3.400820	-1.022741
72	8	0	5.071929	-0.976397	0.212888
73	7	0	6.324124	0.446724	-1.038087
74	1	0	6.406163	0.892675	-1.941580
75	6	0	6.981943	1.095354	0.088600
76	1	0	6.432779	1.997794	0.379369
77	1	0	7.003500	0.393152	0.922693
78	1	0	8.005884	1.360348	-0.187769
79	6	0	-6.051168	-0.422989	0.368632
80	1	0	-4.677765	-1.938406	0.017262
81	8	0	-6.467201	0.700933	0.081015
82	6	0	-6.709231	-1.257750	1.455538
83	1	0	-6.791778	-0.654533	2.364530
84	1	0	-7.726956	-1.508256	1.138431
85	1	0	-6.170198	-2.183212	1.677787

Int1(i), linear form anion in Fig. 3

E(RB3LYP) = -2303.078549 a.u.

Thermal correction to Gibbs Free Energy= 0.609247 a.u.

1	7	0	-0.129167	-0.927726	-0.202400
2	6	0	-0.733216	-0.253906	2.691207
3	6	0	-1.340289	-1.391396	-0.021950
4	8	0	-0.762717	-1.558596	2.884076
5	8	0	-1.787344	-2.538460	-0.373595
6	6	0	-1.893513	0.316522	1.910675
7	6	0	-2.360367	-0.419080	0.619976
8	1	0	-2.744627	0.380903	2.601288
9	7	0	-2.723477	0.637295	-0.337259
10	6	0	0.772042	-1.835487	-0.868320
11	1	0	-1.621077	1.343783	1.667316
12	1	0	0.074016	0.745848	-0.357813
13	6	0	2.144435	-1.217229	-1.070598
14	1	0	0.912504	-2.771417	-0.302452
15	1	0	0.394618	-2.156601	-1.849938
16	8	0	-0.020143	1.754436	-0.431365
17	8	0	0.143939	0.471106	3.176511
18	1	0	0.949466	2.348614	-1.649500
19	1	0	0.410808	2.099324	0.383384
20	1	0	0.106756	-1.823136	3.334535
21	1	0	-3.247521	-1.004319	0.841820
22	8	0	1.049021	2.764998	1.959647

23	1	0	0.638852	2.063197	2.520387
24	1	0	2.017757	2.583072	1.971157
25	8	0	2.467796	-0.128131	-0.541651
26	7	0	3.005395	-1.918950	-1.818115
27	6	0	4.359172	-1.447161	-2.024639
28	1	0	2.709998	-2.847748	-2.163347
29	6	0	5.093460	-1.154881	-0.704478
30	1	0	4.911595	-2.235660	-2.545074
31	1	0	4.367054	-0.560098	-2.670578
32	6	0	-3.629761	0.628613	-1.343098
33	1	0	-1.981553	1.331035	-0.463190
34	8	0	-3.614740	1.513532	-2.213886
35	6	0	-4.654662	-0.505541	-1.470392
36	1	0	-4.127068	-1.383532	-1.859595
37	7	0	-5.340778	-0.911591	-0.260783
38	1	0	-5.368958	-0.158338	-2.220865
39	1	0	-1.030649	-3.841239	-1.273946
40	8	0	-0.687581	-4.573135	-1.852507
41	1	0	-1.318802	-4.617335	-2.585400
42	8	0	3.749179	2.052667	1.917748
43	1	0	3.666725	1.067109	2.054324
44	1	0	4.249863	2.382742	2.679496
45	8	0	1.960530	-4.454338	-2.523043
46	1	0	0.982707	-4.478787	-2.345656
47	1	0	2.315388	-5.148863	-1.948239
48	1	0	3.955579	2.433024	-0.065052
49	8	0	3.851707	2.221218	-1.013844
50	1	0	3.394788	1.351160	-0.974301
51	1	0	-4.028518	-3.644495	1.509452
52	8	0	-4.186464	-3.402441	0.585153
53	1	0	-3.287305	-3.160036	0.238452
54	8	0	1.454491	3.013624	-2.206254
55	1	0	2.369944	2.989509	-1.837777
56	1	0	0.621031	4.120155	-1.899445
57	8	0	-0.146083	4.823507	-1.625663
58	1	0	-1.059607	4.425221	-1.904838
59	1	0	-0.143714	4.914147	-0.613124
60	8	0	1.619826	-1.777393	4.040753
61	1	0	2.254215	-1.573595	3.315266
62	1	0	1.420413	-0.881885	4.368200
63	8	0	3.263058	-0.619106	2.039280
64	1	0	3.991824	-1.146474	1.634461
65	1	0	2.663031	-0.481898	1.269974
66	8	0	-2.449492	3.947103	-2.331063
67	1	0	-2.672555	4.155686	-3.249849
68	1	0	-2.789635	3.018800	-2.192112
69	8	0	5.006500	-1.914144	0.266040
70	7	0	5.891037	-0.060118	-0.728747
71	1	0	5.646009	0.677833	-1.380338
72	6	0	6.652371	0.349158	0.442793
73	1	0	6.052028	0.983809	1.106247
74	1	0	6.962250	-0.543728	0.987300
75	1	0	7.537221	0.905513	0.122532
76	6	0	-6.283789	-0.105995	0.307787
77	1	0	-5.141382	-1.843726	0.111537

78	8	0	-6.546626	1.011272	-0.124414
79	6	0	-6.995171	-0.697985	1.517745
80	1	0	-6.941897	0.016031	2.345168
81	1	0	-8.054127	-0.834143	1.274134
82	1	0	-6.580436	-1.658653	1.837696
83	8	0	-0.094481	5.028595	0.985517
84	1	0	0.306451	4.242124	1.434778
85	1	0	0.388191	5.800373	1.314882

Ring closure in the anion state, TS2(i) in Fig. 3
vuc2p3.chk E(RB3LYP) = -2303.066481 a.u.
Thermal correction to Gibbs Free Energy= 0.607690 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.201654	-1.389368	0.355653
2	6	0	-0.291466	-0.636104	2.232940
3	6	0	-1.435694	-1.583029	-0.032924
4	8	0	-0.217567	-1.806453	2.905800
5	8	0	-1.900564	-2.393858	-0.897463
6	6	0	-1.746438	-0.173531	2.031701
7	6	0	-2.390719	-0.615810	0.691749
8	1	0	-2.326557	-0.570786	2.869711
9	7	0	-2.645507	0.553967	-0.159592
10	6	0	0.872281	-2.231366	-0.080216
11	1	0	-1.766639	0.916094	2.108139
12	1	0	0.464101	0.781846	-0.436983
13	6	0	1.983520	-1.443155	-0.766495
14	1	0	1.337138	-2.701849	0.803245
15	1	0	0.545592	-3.046858	-0.731391
16	8	0	0.008626	1.652438	-0.502884
17	8	0	0.649975	0.204277	2.361881
18	1	0	0.716616	2.495086	-1.816256
19	1	0	0.366218	2.144026	0.276186
20	1	0	0.700599	-1.915337	3.278376
21	1	0	-3.336328	-1.123660	0.862743
22	8	0	0.985141	2.792440	1.808539
23	1	0	0.715713	1.909632	2.185224
24	1	0	1.968086	2.748107	1.746983
25	8	0	2.108945	-0.211583	-0.607611
26	7	0	2.858149	-2.164011	-1.481819
27	6	0	4.083809	-1.560894	-1.949789
28	1	0	2.659317	-3.158939	-1.667333
29	6	0	4.921447	-1.013256	-0.777189
30	1	0	4.668249	-2.333390	-2.459287
31	1	0	3.883438	-0.763678	-2.676981
32	6	0	-3.581523	0.740184	-1.118431
33	1	0	-1.827752	1.164483	-0.268431
34	8	0	-3.508160	1.706146	-1.897490
35	6	0	-4.725734	-0.256144	-1.345572
36	1	0	-4.313773	-1.091025	-1.922244
37	7	0	-5.383926	-0.812398	-0.181821

38	1	0	-5.443245	0.283143	-1.968579
39	1	0	-1.121672	-3.556474	-1.954673
40	8	0	-0.713382	-4.164415	-2.625532
41	1	0	-0.842915	-3.704278	-3.468185
42	8	0	3.729672	2.350376	1.573674
43	1	0	3.679522	1.401708	1.901782
44	1	0	4.315051	2.812428	2.192762
45	8	0	1.935563	-4.726200	-2.212292
46	1	0	0.975968	-4.560519	-2.409678
47	1	0	1.928894	-5.468586	-1.590314
48	1	0	3.716534	2.384448	-0.355166
49	8	0	3.530480	2.134081	-1.283825
50	1	0	3.073766	1.270771	-1.179315
51	1	0	-4.119189	-4.030881	0.618032
52	8	0	-4.330872	-3.469411	-0.141769
53	1	0	-3.452131	-3.155890	-0.470852
54	8	0	1.214260	3.209686	-2.300266
55	1	0	2.146840	3.054344	-2.003186
56	1	0	0.494297	4.342395	-1.801061
57	8	0	-0.208554	5.063596	-1.437554
58	1	0	-1.159547	4.701594	-1.654624
59	1	0	-0.143666	5.128241	-0.422934
60	8	0	2.267549	-2.114985	4.046377
61	1	0	2.832676	-1.455907	3.580892
62	1	0	2.148278	-1.746813	4.935170
63	8	0	3.314525	-0.177988	2.335157
64	1	0	3.733046	-0.708633	1.620895
65	1	0	2.333499	-0.136844	2.154388
66	8	0	-2.554771	4.194028	-1.900441
67	1	0	-2.937281	4.447178	-2.753097
68	1	0	-2.786324	3.226973	-1.797887
69	8	0	4.863935	-1.510955	0.349354
70	7	0	5.764349	-0.004341	-1.101943
71	1	0	5.523100	0.555704	-1.910227
72	6	0	6.588328	0.642811	-0.090368
73	1	0	6.016658	1.393525	0.468867
74	1	0	6.948623	-0.116454	0.604952
75	1	0	7.439794	1.126025	-0.576100
76	6	0	-6.237640	-0.055320	0.566188
77	1	0	-5.260700	-1.812813	-0.014671
78	8	0	-6.424487	1.137413	0.350035
79	6	0	-6.946687	-0.797144	1.691736
80	1	0	-6.779307	-0.260530	2.630585
81	1	0	-8.024501	-0.786002	1.498805
82	1	0	-6.618315	-1.834969	1.804328
83	8	0	-0.125410	5.156350	1.167494
84	1	0	0.216974	4.304256	1.542656
85	1	0	0.411248	5.858841	1.561940

After nucleophilic addition of H-O(40) anion to C(2)=O,
the anionic tetrahedral intermediate, Int2(i), in Fig. 3
duc2q.for.log E(RB3LYP) = -2303.077901 a.u.
Thermal correction to Gibbs Free Energy= 0.616676 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.639920	-1.808927	-1.404585
2	6	0	0.661481	-1.680074	-1.757424
3	6	0	-0.919924	-2.949283	-0.467682
4	8	0	0.869650	4.758386	-1.665052
5	8	0	-2.093787	-3.511495	-0.596148
6	6	0	1.455698	-2.885921	-1.193206
7	6	0	0.333367	-3.831850	-0.728103
8	1	0	2.043737	-3.312346	-2.013289
9	1	0	0.601587	-4.427794	0.146177
10	6	0	-1.647347	-0.861891	-1.850158
11	7	0	2.345318	-2.534793	-0.081631
12	1	0	1.215615	1.353254	3.801946
13	6	0	-1.837570	0.278234	-0.848793
14	1	0	-1.282742	-0.416966	-2.779747
15	1	0	-2.578076	-1.396348	-2.047358
16	8	0	0.801942	-0.001683	1.102096
17	1	0	0.456548	0.503268	0.337679
18	1	0	0.248866	-0.814143	1.108267
19	8	0	1.133341	-0.775666	-2.445294
20	1	0	0.980568	3.884567	-2.094330
21	1	0	0.060342	-4.512593	-1.537948
22	8	0	0.457241	1.574148	3.150162
23	1	0	0.557049	0.909020	2.391715
24	1	0	0.603111	2.609006	2.673693
25	8	0	-0.953388	1.152868	-0.724848
26	7	0	-2.954136	0.238365	-0.115443
27	6	0	-3.278863	1.208469	0.921186
28	1	0	-3.674017	-0.481868	-0.272739
29	6	0	-4.288620	2.256055	0.422714
30	1	0	-3.698105	0.664273	1.774356
31	1	0	-2.373105	1.719517	1.242227
32	6	0	3.466442	-1.774171	-0.084228
33	1	0	2.056230	-2.841485	0.848873
34	8	0	4.066576	-1.504305	0.964836
35	6	0	4.051043	-1.298312	-1.416162
36	7	0	4.965094	-0.203584	-1.155907
37	1	0	4.572743	-2.150074	-1.880350
38	1	0	3.281580	-0.957282	-2.110616
39	1	0	0.046009	4.657296	-1.146461
40	8	0	-0.755156	-2.361462	0.924069
41	1	0	-1.662484	-2.307216	1.299990
42	1	0	-3.656345	-3.584805	2.114725
43	8	0	-3.494092	-2.864871	1.485982
44	1	0	-3.075175	-3.289625	0.667896
45	1	0	3.204501	1.371716	4.582449
46	8	0	2.412188	0.821223	4.672077
47	1	0	2.674080	-0.075368	4.299066
48	8	0	-5.249157	-1.345956	-0.023372
49	1	0	-4.865350	-1.909432	0.686437
50	1	0	-5.170797	-1.919342	-0.823363
51	1	0	-2.167394	3.914352	0.252733

52	8	0	-1.194110	3.805095	0.145222
53	1	0	-1.101888	2.897688	-0.221523
54	8	0	-4.294773	-2.933354	-2.033094
55	1	0	-3.445901	-3.240558	-1.616605
56	1	0	-4.609209	-3.663079	-2.585418
57	8	0	0.730094	3.732014	2.059897
58	1	0	1.495838	3.674782	1.398964
59	1	0	-0.070039	3.871153	1.484918
60	1	0	3.477613	-1.469684	2.722813
61	8	0	3.078623	-1.530793	3.618108
62	1	0	2.317693	-2.126639	3.475771
63	8	0	1.162883	-3.348019	2.558465
64	1	0	0.323974	-3.085019	2.106278
65	1	0	1.040626	-4.253688	2.878357
66	1	0	2.131366	4.264887	-0.447556
67	8	0	2.532440	3.565588	0.132738
68	1	0	2.298289	2.772249	-0.400274
69	8	0	1.658152	2.036188	-2.020497
70	1	0	1.115684	1.230161	-2.106808
71	1	0	2.493859	1.815617	-2.488057
72	8	0	-3.988911	3.452030	0.334190
73	7	0	-5.499186	1.751399	0.099934
74	1	0	-5.626936	0.740224	0.132415
75	6	0	-6.567140	2.567316	-0.456357
76	1	0	-6.268532	3.613294	-0.381652
77	1	0	-6.745572	2.319816	-1.509553
78	1	0	-7.494908	2.413126	0.104207
79	6	0	4.862018	0.990338	-1.800129
80	1	0	5.401650	-0.233126	-0.241617
81	8	0	4.163856	1.137557	-2.808931
82	6	0	5.637135	2.142780	-1.193476
83	1	0	6.118196	2.709077	-1.994945
84	1	0	4.921910	2.809083	-0.694004
85	1	0	6.391883	1.823754	-0.468260

The direct conversion from the ion pair Int2(i) to the second ion-pair Int3(i) TS3'(i)
vuc2p7.chk E(RB3LYP) = -2303.008740 a.u.
Thermal correction to Gibbs Free Energy= 0.617934 a.u.

1	7	0	0.648805	1.290172	0.090718
2	6	0	-0.666093	1.083456	-0.358233
3	6	0	0.831142	2.710474	0.455359
4	8	0	-0.511844	1.729207	-1.985103
5	8	0	1.947883	3.031832	0.991054
6	6	0	-1.542973	2.160658	0.397138
7	6	0	-0.511525	3.048427	1.120954
8	1	0	-2.122963	2.728814	-0.331621
9	1	0	-0.434279	2.763329	2.174595
10	6	0	1.748976	0.609372	-0.574186
11	7	0	-2.449155	1.511530	1.336232
12	1	0	-2.605150	-3.493075	0.504867
13	6	0	2.524482	-0.373399	0.303579
14	1	0	1.361473	0.025971	-1.415225

15	1	0	2.435830	1.349941	-0.988173
16	8	0	-0.611589	-1.523741	1.715944
17	1	0	-0.940932	-0.990805	0.941740
18	1	0	0.364611	-1.498402	1.558640
19	8	0	-1.143525	-0.109735	-0.516187
20	1	0	-1.348571	1.649071	-2.491697
21	1	0	-0.729938	4.114164	1.053057
22	8	0	-1.654478	-3.774801	0.490956
23	1	0	-1.204085	-3.089787	1.040180
24	1	0	-0.882448	-3.907767	-0.754819
25	8	0	1.974114	-1.327870	0.897744
26	7	0	3.852058	-0.194985	0.314082
27	6	0	4.750624	-1.120112	0.967094
28	1	0	4.223924	0.714167	-0.011948
29	6	0	5.309616	-2.165558	-0.015320
30	1	0	5.553250	-0.552244	1.448677
31	1	0	4.194572	-1.658720	1.742372
32	6	0	-3.612857	0.916258	1.035061
33	1	0	-2.027848	1.202051	2.230703
34	8	0	-4.157551	0.094399	1.802299
35	6	0	-4.372691	1.334260	-0.232930
36	7	0	-5.573114	0.533601	-0.360535
37	1	0	-4.619326	2.402523	-0.150146
38	1	0	-3.773283	1.211731	-1.134801
39	1	0	-0.013158	2.725893	-1.723020
40	8	0	0.640877	3.539517	-0.984806
41	1	0	1.547528	3.737858	-1.322378
42	1	0	3.582179	2.650478	0.432052
43	8	0	4.458041	2.494517	-0.008363
44	1	0	4.355153	2.999407	-0.839246
45	1	0	-4.237152	-1.817040	1.000969
46	8	0	-4.143547	-2.780356	1.119958
47	1	0	-3.954056	-2.830778	2.080661
48	1	0	2.549644	4.650384	0.971433
49	8	0	3.166880	5.393893	0.722367
50	1	0	4.015173	5.100336	1.092294
51	1	0	2.909835	-3.627625	-0.819312
52	8	0	2.070145	-3.808218	-0.350703
53	1	0	1.998777	-3.021888	0.232976
54	8	0	3.238548	4.351169	-1.720847
55	1	0	3.254945	4.907702	-0.885421
56	1	0	3.306255	4.970553	-2.462813
57	8	0	-0.201625	-3.937208	-1.561701
58	1	0	-0.289309	-3.045064	-2.074595
59	1	0	0.746122	-3.942042	-1.150211
60	1	0	-3.358711	-1.011239	3.072892
61	8	0	-2.934966	-1.772771	3.524686
62	1	0	-2.111357	-1.900573	3.016376
63	8	0	-1.102298	0.515590	3.663017
64	1	0	-1.730073	-0.046141	4.154528
65	1	0	-0.644909	-0.141740	3.098853
66	1	0	-0.446749	-1.048210	-1.773717
67	8	0	-0.265369	-1.597720	-2.582823
68	1	0	-0.944887	-1.272293	-3.204590
69	8	0	-2.522502	0.178608	-2.907205

70	1	0	-2.297782	-0.092448	-1.990769
71	1	0	-3.497005	0.069220	-2.964370
72	8	0	4.607142	-2.686230	-0.881277
73	7	0	6.613324	-2.485711	0.175013
74	1	0	7.137202	-1.978164	0.873990
75	6	0	7.305672	-3.502032	-0.602756
76	1	0	6.581756	-3.940450	-1.289904
77	1	0	8.126575	-3.061665	-1.179403
78	1	0	7.707092	-4.284737	0.050026
79	6	0	-5.857573	-0.248254	-1.442083
80	1	0	-6.000057	0.281041	0.522801
81	8	0	-5.246275	-0.182418	-2.509904
82	6	0	-6.986985	-1.238989	-1.228437
83	1	0	-7.386029	-1.539267	-2.198162
84	1	0	-6.588407	-2.127214	-0.721496
85	1	0	-7.790232	-0.826179	-0.609715

O(40)-H(41)- anion elimination, TS3(i), from int2(i) to diketone(i) in Fig. 3
duc2q.chk E(RB3LYP) = -2303.074492 a.u.
Thermal correction to Gibbs Free Energy= 0.613721 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.724724	-1.921835	-1.563739
2	6	0	0.634995	-1.754454	-1.750451
3	6	0	-1.041024	-3.030491	-0.762198
4	8	0	1.080897	4.853118	-1.696236
5	8	0	-2.200056	-3.462088	-0.635625
6	6	0	1.378743	-2.955935	-1.113194
7	6	0	0.225805	-3.871679	-0.650062
8	1	0	1.966869	-3.424645	-1.910893
9	1	0	0.355746	-4.247577	0.362886
10	6	0	-1.689649	-0.923229	-2.009663
11	7	0	2.252915	-2.596636	-0.001831
12	1	0	1.263498	1.361094	3.777609
13	6	0	-1.802735	0.241435	-1.015960
14	1	0	-1.317537	-0.511763	-2.950464
15	1	0	-2.648079	-1.415448	-2.181991
16	8	0	0.780197	0.111651	1.112484
17	1	0	0.485648	0.601914	0.323828
18	1	0	0.164368	-0.705677	1.151449
19	8	0	1.132755	-0.830993	-2.366571
20	1	0	1.180985	3.979300	-2.126769
21	1	0	0.105553	-4.725990	-1.325919
22	8	0	0.504152	1.610829	3.127114
23	1	0	0.599165	0.961239	2.313551
24	1	0	0.661174	2.591263	2.722413
25	8	0	-0.909322	1.110233	-0.977062
26	7	0	-2.877169	0.238303	-0.221668
27	6	0	-3.112401	1.229461	0.821704
28	1	0	-3.610981	-0.475811	-0.303027
29	6	0	-4.136680	2.292091	0.384626

30	1	0	-3.478710	0.702292	1.708863
31	1	0	-2.177360	1.726043	1.072476
32	6	0	3.410485	-1.889910	-0.026957
33	1	0	1.913008	-2.828383	0.938809
34	8	0	4.012621	-1.595921	1.011696
35	6	0	4.035106	-1.508677	-1.373554
36	7	0	4.954388	-0.406680	-1.168594
37	1	0	4.561401	-2.392918	-1.765551
38	1	0	3.292981	-1.196243	-2.108085
39	1	0	0.252214	4.751223	-1.185927
40	8	0	-0.684647	-2.020678	1.136491
41	1	0	-1.565005	-1.888179	1.525487
42	1	0	-3.708557	-3.454787	2.343240
43	8	0	-3.585765	-2.783696	1.655651
44	1	0	-3.074231	-3.218915	0.937498
45	1	0	3.232519	1.327867	4.518371
46	8	0	2.420766	0.814101	4.645434
47	1	0	2.640715	-0.110067	4.300121
48	8	0	-5.258926	-1.214005	0.127168
49	1	0	-4.884708	-1.800722	0.822854
50	1	0	-5.301371	-1.791003	-0.668730
51	1	0	-2.010373	3.916159	0.103993
52	8	0	-1.037312	3.808478	-0.005940
53	1	0	-0.949214	2.917285	-0.402782
54	8	0	-4.559621	-2.826008	-1.970541
55	1	0	-3.740709	-3.178735	-1.556728
56	1	0	-4.941156	-3.554195	-2.481903
57	8	0	0.829100	3.829349	2.039069
58	1	0	1.616103	3.763535	1.422411
59	1	0	0.065935	3.936013	1.420143
60	1	0	3.434499	-1.522395	2.800481
61	8	0	3.005464	-1.575325	3.680414
62	1	0	2.212123	-2.124025	3.488794
63	8	0	1.022702	-3.169154	2.581046
64	1	0	0.206940	-2.721448	2.114339
65	1	0	0.720570	-3.988848	2.997543
66	1	0	2.333313	4.304683	-0.455642
67	8	0	2.702567	3.589161	0.122455
68	1	0	2.393294	2.806067	-0.383097
69	8	0	1.642953	2.071099	-1.983669
70	1	0	0.958046	1.379844	-2.005500
71	1	0	2.421726	1.688314	-2.443998
72	8	0	-3.818882	3.478579	0.246502
73	7	0	-5.381776	1.813485	0.175143
74	1	0	-5.532688	0.807056	0.247233
75	6	0	-6.474884	2.649636	-0.294545
76	1	0	-6.136141	3.685989	-0.288830
77	1	0	-6.772166	2.374923	-1.313669
78	1	0	-7.343448	2.548128	0.364682
79	6	0	4.796400	0.781819	-1.816485
80	1	0	5.414801	-0.409843	-0.265649
81	8	0	4.045465	0.904602	-2.789983
82	6	0	5.587876	1.950804	-1.267272
83	1	0	6.044397	2.492028	-2.100173
84	1	0	4.890960	2.635322	-0.766102

85	1	0	6.365375	1.651692	-0.557938

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diketone(i) C13H47N5O20 with H3O+ and OH- in Fig. 2 and 3
duc2q.rev.chk E(RB3LYP) = -2303.090307 a.u.
Thermal correction to Gibbs Free Energy = 0.614248 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.723502	-1.877271	-1.684518
2	6	0	0.667565	-1.716577	-1.718069
3	6	0	-1.113483	-3.079846	-1.121295
4	8	0	1.241605	4.906747	-1.731192
5	8	0	-2.267812	-3.478928	-1.042285
6	6	0	1.324250	-2.952519	-1.058672
7	6	0	0.119093	-3.818327	-0.638795
8	1	0	1.917329	-3.446909	-1.836805
9	1	0	0.056183	-3.904130	0.453006
10	6	0	-1.635240	-0.850616	-2.202859
11	7	0	2.166356	-2.631522	0.083552
12	1	0	1.373411	1.316694	3.714437
13	6	0	-1.735559	0.314879	-1.206346
14	1	0	-1.209596	-0.465508	-3.131617
15	1	0	-2.601479	-1.317532	-2.401677
16	8	0	0.485109	-0.044676	1.110751
17	1	0	0.201026	0.479571	0.339489
18	1	0	-0.328416	-0.600584	1.419898
19	8	0	1.225541	-0.775793	-2.232929
20	1	0	1.334066	4.047245	-2.189586
21	1	0	0.131857	-4.826572	-1.061330
22	8	0	0.624666	1.592110	3.064536
23	1	0	0.625723	0.913817	2.283215
24	1	0	0.800080	2.571495	2.621347
25	8	0	-0.827139	1.174408	-1.174223
26	7	0	-2.773249	0.292000	-0.376738
27	6	0	-2.940876	1.229283	0.728940
28	1	0	-3.512799	-0.430069	-0.415991
29	6	0	-3.994134	2.303410	0.411297
30	1	0	-3.234267	0.644156	1.605061
31	1	0	-1.995253	1.721643	0.942261
32	6	0	3.360332	-1.984525	0.088522
33	1	0	1.717768	-2.730554	1.002867
34	8	0	3.916509	-1.663621	1.143799
35	6	0	4.083369	-1.710136	-1.236725
36	7	0	5.003828	-0.605052	-1.055353
37	1	0	4.623517	-2.625188	-1.523247
38	1	0	3.402600	-1.439104	-2.042812
39	1	0	0.405979	4.803278	-1.233161
40	8	0	-1.380188	-1.509268	2.095641
41	1	0	-1.550526	-1.055813	2.937088
42	1	0	-3.289941	-3.464226	0.879896
43	8	0	-3.609232	-2.847571	1.557978
44	1	0	-2.778247	-2.323511	1.797164

45	1	0	3.329865	1.117315	4.490977
46	8	0	2.462331	0.708860	4.630317
47	1	0	2.572235	-0.251239	4.338031
48	8	0	-5.063085	-1.132856	0.110240
49	1	0	-4.645970	-1.793725	0.740361
50	1	0	-5.251570	-1.645401	-0.704335
51	1	0	-1.884245	3.933602	0.070572
52	8	0	-0.914955	3.828521	-0.080351
53	1	0	-0.847926	2.957653	-0.523907
54	8	0	-4.682724	-2.575241	-2.218271
55	1	0	-3.908887	-3.040380	-1.841935
56	1	0	-5.177646	-3.242710	-2.716073
57	8	0	0.961323	3.766336	1.943492
58	1	0	1.749934	3.702947	1.325020
59	1	0	0.195427	3.884997	1.327261
60	1	0	3.241373	-1.725076	2.889053
61	8	0	2.734516	-1.763458	3.727541
62	1	0	1.882623	-2.166610	3.441133
63	8	0	0.571671	-3.033987	2.493472
64	1	0	-0.297716	-2.431153	2.403757
65	1	0	0.333183	-3.811441	3.020570
66	1	0	2.499202	4.307562	-0.498603
67	8	0	2.834754	3.552350	0.047329
68	1	0	2.499083	2.808322	-0.503279
69	8	0	1.773636	2.109888	-2.072237
70	1	0	1.049138	1.460114	-2.034278
71	1	0	2.530978	1.642635	-2.486639
72	8	0	-3.680847	3.493731	0.282696
73	7	0	-5.251233	1.831508	0.289755
74	1	0	-5.393621	0.820740	0.345829
75	6	0	-6.378818	2.680314	-0.058963
76	1	0	-6.028779	3.712193	-0.099522
77	1	0	-6.791773	2.401258	-1.035538
78	1	0	-7.170004	2.595658	0.693810
79	6	0	4.846553	0.571171	-1.731615
80	1	0	5.460968	-0.581611	-0.151640
81	8	0	4.096810	0.670395	-2.707287
82	6	0	5.646802	1.748032	-1.213389
83	1	0	6.123220	2.250463	-2.059580
84	1	0	4.956346	2.463510	-0.747835
85	1	0	6.411097	1.463710	-0.483929

C(2)....O(4)H(20) dissociation TS4(i) from diketeone(i) to Int3(i) in Fig. 3
duc2p7.chk E(RB3LYP) = -2303.074948 a.u.
Thermal correction to Gibbs Free Energy = 0.613213 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.271898	1.241686	-0.680292
2	6	0	0.995973	0.787246	-0.341319
3	6	0	-0.228426	2.330008	-1.549844
4	8	0	1.368436	2.426304	1.194565

5	8	0	-1.192216	3.009465	-1.852550
6	6	0	2.014650	1.401091	-1.314669
7	6	0	1.204532	2.501597	-2.024745
8	1	0	2.858827	1.827623	-0.778484
9	1	0	1.247377	2.429959	-3.115926
10	6	0	-1.447839	0.851189	0.084528
11	7	0	2.504835	0.365248	-2.218739
12	1	0	2.270263	-3.021296	1.482996
13	6	0	-2.427232	-0.019829	-0.707901
14	1	0	-1.090049	0.258050	0.926740
15	1	0	-1.943068	1.741904	0.467250
16	8	0	0.316625	-2.514876	-0.957992
17	1	0	0.760884	-1.712610	-0.610387
18	1	0	-0.627110	-2.243194	-0.932347
19	8	0	1.169741	-0.235754	0.339008
20	1	0	2.108932	2.025644	1.682729
21	1	0	1.544552	3.498676	-1.727815
22	8	0	1.354189	-3.367182	1.532668
23	1	0	0.980370	-3.274050	0.626006
24	1	0	0.429716	-2.627904	2.541268
25	8	0	-2.235699	-1.243805	-0.883672
26	7	0	-3.525198	0.600217	-1.151879
27	6	0	-4.527456	-0.124544	-1.896597
28	1	0	-3.672515	1.614501	-0.941705
29	6	0	-5.337147	-1.098184	-1.025232
30	1	0	-5.224219	0.608994	-2.315858
31	1	0	-4.059679	-0.665883	-2.726522
32	6	0	3.506998	-0.511585	-1.926790
33	1	0	1.836594	-0.040585	-2.890656
34	8	0	3.721752	-1.504763	-2.628638
35	6	0	4.409393	-0.235625	-0.710927
36	7	0	5.221532	-1.409219	-0.436634
37	1	0	5.035872	0.645474	-0.888675
38	1	0	3.821543	-0.023111	0.179412
39	1	0	0.320942	2.414023	2.137734
40	8	0	-0.458595	2.299827	2.886805
41	1	0	-0.261421	2.967648	3.562689
42	1	0	-3.546556	3.297179	0.436090
43	8	0	-3.765216	3.270822	-0.530605
44	1	0	-2.936415	3.522556	-0.978892
45	1	0	2.064905	3.748052	0.620842
46	8	0	2.598053	4.475799	0.147412
47	1	0	2.648535	5.216778	0.768380
48	8	0	-4.179901	0.189467	2.227614
49	1	0	-4.713154	-0.017634	1.417421
50	1	0	-4.796756	0.065482	2.966172
51	1	0	-3.092161	-1.265135	2.128519
52	8	0	-2.507952	-2.024468	1.893977
53	1	0	-2.415727	-1.972635	0.922077
54	1	0	-2.153758	2.750815	2.384810
55	8	0	-3.097845	2.881204	2.122320
56	1	0	-3.503436	2.000881	2.257141
57	8	0	-0.259777	-2.196753	3.174610
58	1	0	0.053495	-1.222196	3.513129
59	1	0	-1.149802	-2.125438	2.681079

60	1	0	1.991071	-1.900078	-3.641030
61	8	0	1.047507	-1.645199	-3.638393
62	1	0	0.711601	-2.091918	-2.832063
63	1	0	4.102977	3.653845	-0.267769
64	8	0	4.802501	3.085082	-0.678716
65	1	0	4.881989	3.451810	-1.572030
66	1	0	0.061997	0.823226	3.617912
67	8	0	0.513678	0.018617	4.004378
68	1	0	1.447456	0.078035	3.678555
69	8	0	2.783645	0.099120	2.525911
70	1	0	2.211418	-0.087051	1.749184
71	1	0	3.447108	-0.613656	2.456280
72	8	0	-5.553900	-0.899226	0.173775
73	7	0	-5.861054	-2.148529	-1.693208
74	1	0	-5.563168	-2.302926	-2.646532
75	6	0	-6.686372	-3.166410	-1.058748
76	1	0	-7.053257	-2.763303	-0.114809
77	1	0	-7.534250	-3.415053	-1.703768
78	1	0	-6.110026	-4.076378	-0.855286
79	6	0	4.861398	-2.346500	0.470125
80	1	0	5.796540	-1.726560	-1.206036
81	8	0	3.969743	-2.162118	1.317006
82	6	0	5.625389	-3.653680	0.427361
83	1	0	6.003234	-3.876332	1.429244
84	1	0	4.931407	-4.455033	0.152095
85	1	0	6.458075	-3.648161	-0.281202

Int3(i), the anion intermediate with 5-membered ring
duc2p7.rev.chk E(RB3LYP) = -2303.079933 a.u.
Thermal correction to Gibbs Free Energy= 0.618096 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.254809	1.387807	-0.566956
2	6	0	1.099919	1.051189	-0.094186
3	6	0	-0.270735	2.384864	-1.498411
4	8	0	1.369015	2.073199	1.035390
5	8	0	-1.261135	3.008894	-1.871417
6	6	0	2.010396	1.522790	-1.290319
7	6	0	1.156805	2.598321	-1.990373
8	1	0	2.938061	1.948082	-0.906209
9	1	0	1.189151	2.530822	-3.081981
10	6	0	-1.421000	0.925058	0.165786
11	7	0	2.349435	0.432111	-2.189210
12	1	0	2.301599	-2.920678	1.419595
13	6	0	-2.389075	0.072357	-0.664720
14	1	0	-1.042800	0.277700	0.959468
15	1	0	-1.959343	1.762835	0.609351
16	8	0	0.396304	-2.287063	-0.973611
17	1	0	0.782104	-1.439156	-0.614629
18	1	0	-0.563809	-2.092387	-0.928866
19	8	0	1.230276	-0.161162	0.367290

20	1	0	2.078731	1.644694	1.568427
21	1	0	1.474826	3.608011	-1.711541
22	8	0	1.406827	-3.319826	1.371154
23	1	0	1.049515	-3.088275	0.472457
24	1	0	0.468247	-2.781789	2.391790
25	8	0	-2.201823	-1.149058	-0.864911
26	7	0	-3.490177	0.690901	-1.104106
27	6	0	-4.469752	-0.028899	-1.883343
28	1	0	-3.643773	1.701195	-0.894114
29	6	0	-5.211441	-1.099460	-1.069423
30	1	0	-5.211034	0.696957	-2.233723
31	1	0	-3.995452	-0.483112	-2.760927
32	6	0	3.348869	-0.465129	-2.000343
33	1	0	1.642606	0.090866	-2.856674
34	8	0	3.532457	-1.418935	-2.767223
35	6	0	4.292546	-0.281508	-0.799325
36	7	0	5.034511	-1.516630	-0.598367
37	1	0	4.969495	0.565973	-0.957980
38	1	0	3.725606	-0.080691	0.105919
39	1	0	0.124785	2.186513	2.285446
40	8	0	-0.498447	2.157081	3.061529
41	1	0	-0.172217	2.831958	3.677545
42	1	0	-3.538972	3.371510	0.494839
43	8	0	-3.731149	3.364831	-0.472487
44	1	0	-2.875211	3.541125	-0.912547
45	1	0	2.172755	3.673621	0.635498
46	8	0	2.736200	4.427818	0.344618
47	1	0	2.744361	5.053530	1.083582
48	8	0	-4.191046	0.134274	2.226878
49	1	0	-4.692195	-0.081791	1.396389
50	1	0	-4.822430	-0.039917	2.942824
51	1	0	-3.051091	-1.311692	2.105035
52	8	0	-2.471457	-2.058951	1.828611
53	1	0	-2.365724	-1.938919	0.862008
54	1	0	-2.301231	2.698828	2.559255
55	8	0	-3.218158	2.850005	2.250735
56	1	0	-3.624704	1.958945	2.296147
57	8	0	-0.246482	-2.438472	3.082127
58	1	0	0.059150	-1.540197	3.517658
59	1	0	-1.134336	-2.284683	2.593856
60	1	0	1.776988	-1.700392	-3.773540
61	8	0	0.834735	-1.453232	-3.697414
62	1	0	0.588639	-1.880435	-2.847435
63	1	0	4.308867	3.624861	-0.138218
64	8	0	5.014443	3.076267	-0.548482
65	1	0	5.109063	3.462326	-1.432174
66	1	0	0.046616	0.528521	3.824740
67	8	0	0.545385	-0.260134	4.137478
68	1	0	1.447187	-0.142716	3.739648
69	8	0	2.667758	0.074361	2.511825
70	1	0	2.101100	-0.210283	1.731456
71	1	0	3.445478	-0.509563	2.415930
72	8	0	-5.473531	-0.961891	0.130329
73	7	0	-5.633268	-2.163797	-1.784742
74	1	0	-5.287246	-2.267757	-2.728557

75	6	0	-6.373013	-3.272760	-1.199709
76	1	0	-6.822701	-2.926418	-0.269094
77	1	0	-7.159539	-3.598314	-1.886656
78	1	0	-5.713574	-4.120495	-0.979796
79	6	0	4.759704	-2.381668	0.402718
80	1	0	5.409642	-1.916528	-1.450300
81	8	0	4.046609	-2.094477	1.381997
82	6	0	5.385569	-3.757108	0.294365
83	1	0	5.938228	-3.968236	1.214458
84	1	0	4.582803	-4.498158	0.216870
85	1	0	6.054919	-3.865561	-0.563202

Ring opening at the latter stage, TS5(i)
vuc2p8.chk E(RB3LYP) = -2303.056924 a.u.
Thermal correction to Gibbs Free Energy= 0.618350 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.335433	-0.557217	-0.911391
2	6	0	1.741899	0.018834	-0.883663
3	6	0	-0.473601	-0.839032	-2.214353
4	8	0	1.661871	1.272990	-1.508672
5	8	0	-1.474672	-0.704269	-2.944295
6	6	0	2.033261	-1.112923	-1.903526
7	6	0	0.838226	-1.316046	-2.846189
8	1	0	2.894150	-0.764616	-2.485242
9	1	0	0.754941	-2.366631	-3.144740
10	6	0	-1.432771	0.175482	-0.286542
11	7	0	2.403336	-2.341337	-1.223340
12	1	0	2.014053	-0.019436	2.060191
13	6	0	-2.549707	-0.709299	0.291053
14	1	0	-1.026865	0.731589	0.567266
15	1	0	-1.888622	0.888949	-0.979700
16	8	0	0.174157	-2.101549	1.549450
17	1	0	0.297680	-1.654053	0.678691
18	1	0	-0.795214	-1.980769	1.679705
19	8	0	2.140896	-0.020452	0.279028
20	1	0	2.151737	1.897859	-0.869863
21	1	0	0.969471	-0.743780	-3.769787
22	8	0	1.584324	-0.229325	2.916019
23	1	0	1.060301	-1.031940	2.640848
24	1	0	0.670629	0.924458	3.123190
25	8	0	-2.425242	-1.286985	1.401403
26	7	0	-3.675500	-0.796785	-0.426920
27	6	0	-4.791784	-1.601835	0.003511
28	1	0	-3.773193	-0.276162	-1.330900
29	6	0	-6.021836	-0.758744	0.357121
30	1	0	-5.044198	-2.332048	-0.775456
31	1	0	-4.483965	-2.149737	0.900589
32	6	0	3.502266	-2.514573	-0.452374
33	1	0	1.667007	-3.037459	-1.020167
34	8	0	3.647768	-3.496933	0.287630

35	6	0	4.666978	-1.508718	-0.516143
36	7	0	5.183224	-1.362546	0.835984
37	1	0	5.438901	-1.935064	-1.170612
38	1	0	4.407839	-0.522857	-0.891930
39	1	0	0.129076	2.382591	-1.445756
40	8	0	-0.397755	3.173915	-1.191427
41	1	0	-0.058189	3.895597	-1.743763
42	1	0	-3.727475	1.488271	-2.507717
43	8	0	-3.930937	0.565358	-2.791937
44	1	0	-3.064441	0.194121	-3.069829
45	1	0	3.074866	1.449226	-2.791670
46	8	0	4.000476	1.438768	-3.112785
47	1	0	3.963943	1.689914	-4.047754
48	8	0	-3.980966	2.208727	1.161591
49	1	0	-4.640714	1.481516	0.997089
50	1	0	-4.510959	2.935703	1.525509
51	1	0	-2.930843	1.510091	2.457693
52	8	0	-2.365318	0.975177	3.065863
53	1	0	-2.380213	0.075782	2.667754
54	1	0	-2.296596	3.070313	-1.474401
55	8	0	-3.267140	2.978276	-1.539452
56	1	0	-3.542475	2.744079	-0.628785
57	8	0	0.053375	1.767558	3.242993
58	1	0	0.262205	2.463187	2.508033
59	1	0	-0.941934	1.474769	3.186138
60	1	0	1.871405	-4.483421	0.338062
61	8	0	0.934555	-4.397874	0.072082
62	1	0	0.572499	-3.784714	0.747422
63	1	0	4.989861	2.413538	-1.891201
64	8	0	5.279447	2.893028	-1.083093
65	1	0	5.571248	2.183427	-0.478546
66	1	0	0.109291	3.435485	0.587537
67	8	0	0.612967	3.505042	1.428486
68	1	0	1.550622	3.426401	1.138649
69	8	0	2.985371	2.766120	0.219974
70	1	0	3.358174	2.013094	0.728202
71	1	0	3.804861	3.088574	-0.265903
72	8	0	-5.944580	0.384464	0.819973
73	7	0	-7.205633	-1.385737	0.175738
74	1	0	-7.198937	-2.300723	-0.253117
75	6	0	-8.491217	-0.789512	0.505747
76	1	0	-8.298871	0.156927	1.010793
77	1	0	-9.079379	-0.599553	-0.398953
78	1	0	-9.059832	-1.447617	1.171044
79	6	0	5.158228	-0.203562	1.532663
80	1	0	5.179190	-2.234351	1.355501
81	8	0	4.969105	0.908518	1.013588
82	6	0	5.351468	-0.337390	3.030361
83	1	0	5.943996	0.504816	3.394507
84	1	0	4.363280	-0.293241	3.505541
85	1	0	5.831656	-1.277284	3.317995

Conjugated base of the beta product, Int4(i) in Fig. 3
vuc2p8.for.chk E(RB3LYP) = -2303.074757 a.u.

Thermal correction to Gibbs Free Energy= 0.615596 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.714519	0.638779	-0.794899
2	6	0	-2.248935	-0.256802	-0.770472
3	6	0	0.326495	0.013937	-1.882454
4	8	0	-2.241307	-1.533925	-1.166339
5	8	0	0.749272	-1.107018	-2.343902
6	6	0	-2.192487	0.722725	-1.950185
7	6	0	-0.804239	0.690873	-2.674108
8	1	0	-2.944151	0.361374	-2.663256
9	1	0	-0.528236	1.723602	-2.908544
10	6	0	1.727377	-0.026391	0.021990
11	7	0	-2.535586	2.066661	-1.521885
12	1	0	-1.769792	1.004103	1.873072
13	6	0	2.942950	0.876408	0.227420
14	1	0	1.316596	-0.219838	1.016979
15	1	0	2.055962	-0.975449	-0.402606
16	8	0	0.345901	2.741928	0.872322
17	1	0	0.344454	2.041072	0.140473
18	1	0	1.289453	2.747075	1.133362
19	8	0	-2.368708	0.059203	0.400291
20	1	0	-2.468926	-2.098420	-0.341442
21	1	0	-0.904952	0.147768	-3.614742
22	8	0	-1.153161	1.309395	2.567421
23	1	0	-0.555202	1.932851	2.060883
24	1	0	-0.432678	0.123948	3.006635
25	8	0	2.995510	1.709688	1.161807
26	7	0	3.937683	0.716407	-0.660854
27	6	0	5.146758	1.495824	-0.592712
28	1	0	3.842318	-0.015140	-1.403157
29	6	0	6.350772	0.674756	-0.112980
30	1	0	5.358979	1.947020	-1.569966
31	1	0	4.981592	2.302421	0.130376
32	6	0	-3.661966	2.423692	-0.859684
33	1	0	-1.788614	2.780570	-1.453674
34	8	0	-3.782248	3.514564	-0.289923
35	6	0	-4.882222	1.485918	-0.858043
36	7	0	-5.474817	1.503174	0.469271
37	1	0	-5.596094	1.888658	-1.588878
38	1	0	-4.686779	0.449508	-1.125525
39	1	0	0.624807	-2.376843	-1.318780
40	8	0	0.627011	-3.149968	-0.668578
41	1	0	0.232680	-3.893594	-1.149124
42	1	0	3.660781	-2.086846	-1.916771
43	8	0	3.581363	-1.301781	-2.514821
44	1	0	2.610819	-1.236844	-2.660090
45	1	0	-3.609971	-2.011414	-2.377269
46	8	0	-4.534019	-2.113262	-2.679912
47	1	0	-4.484778	-2.599648	-3.516627
48	8	0	4.250702	-1.753353	1.775633
49	1	0	4.902594	-1.142063	1.341922

50	1	0	4.800310	-2.355337	2.301859
51	1	0	3.173335	-0.761467	2.864429
52	8	0	2.585709	-0.102257	3.305423
53	1	0	2.688515	0.697064	2.741348
54	1	0	2.489480	-3.370212	-0.526572
55	8	0	3.464519	-3.269285	-0.566717
56	1	0	3.698283	-2.802885	0.261952
57	8	0	0.089625	-0.743317	3.328482
58	1	0	-0.121221	-1.543461	2.708602
59	1	0	1.102405	-0.537510	3.333353
60	1	0	-1.919043	4.497546	-0.483774
61	8	0	-1.045580	4.365249	-0.899741
62	1	0	-0.477072	4.022020	-0.174896
63	1	0	-5.237074	-3.013415	-1.215402
64	8	0	-5.440898	-3.327868	-0.304995
65	1	0	-5.817000	-2.531277	0.115716
66	1	0	-0.057223	-2.873252	0.966370
67	8	0	-0.476353	-2.775282	1.855721
68	1	0	-1.435064	-2.903699	1.703402
69	8	0	-3.168994	-2.735544	0.934165
70	1	0	-3.570528	-1.905871	1.263453
71	1	0	-3.966798	-3.200326	0.532827
72	8	0	6.248174	-0.266200	0.679908
73	7	0	7.546267	1.095506	-0.586674
74	1	0	7.552643	1.843772	-1.265719
75	6	0	8.817520	0.496342	-0.210282
76	1	0	8.614749	-0.266987	0.540817
77	1	0	9.300543	0.028563	-1.075281
78	1	0	9.490849	1.250380	0.211259
79	6	0	-5.575190	0.408246	1.258181
80	1	0	-5.516949	2.423358	0.892104
81	8	0	-5.332648	-0.738666	0.853807
82	6	0	-6.010273	0.661662	2.688603
83	1	0	-6.809486	-0.038984	2.945375
84	1	0	-5.165536	0.458454	3.356046
85	1	0	-6.355763	1.684416	2.862706

The last step, formation of the beta product from the ion pair, TS6(i) in Fig. 3
duc2py.chk E(RB3LYP) = -2303.072530 a.u.
Thermal correction to Gibbs Free Energy= 0.609395 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.760740	-0.607172	-0.738168
2	6	0	2.277415	0.255785	-0.698163
3	6	0	-0.317190	0.000970	-1.823910
4	8	0	2.255611	1.538610	-1.053370
5	8	0	-0.709926	1.119768	-2.283930
6	6	0	2.218383	-0.693331	-1.905413
7	6	0	0.805708	-0.714820	-2.588627
8	1	0	2.929641	-0.279257	-2.630505
9	1	0	0.529888	-1.761220	-2.750375

10	6	0	-1.800852	0.043563	0.057798
11	7	0	2.620854	-2.035826	-1.529161
12	1	0	1.745466	-1.170103	1.738333
13	6	0	-3.018841	-0.874045	0.178004
14	1	0	-1.430209	0.210958	1.073202
15	1	0	-2.095831	1.000951	-0.366735
16	8	0	-0.338270	-2.645530	0.646864
17	1	0	-0.434878	-1.769684	-0.102327
18	1	0	-1.266608	-2.742055	0.946343
19	8	0	2.409347	-0.098927	0.462361
20	1	0	2.504801	2.093953	-0.217097
21	1	0	0.874133	-0.231674	-3.563966
22	8	0	1.077050	-1.565578	2.342498
23	1	0	0.396897	-2.099218	1.649803
24	1	0	0.561090	-0.714250	2.789032
25	8	0	-3.057333	-1.799540	1.016322
26	7	0	-4.019334	-0.621611	-0.684475
27	6	0	-5.227514	-1.405299	-0.689605
28	1	0	-3.909812	0.152784	-1.377046
29	6	0	-6.436571	-0.627694	-0.151882
30	1	0	-5.434792	-1.772518	-1.702647
31	1	0	-5.064228	-2.270771	-0.037511
32	6	0	3.759056	-2.377820	-0.876474
33	1	0	1.899090	-2.777978	-1.481632
34	8	0	3.899820	-3.475085	-0.326680
35	6	0	4.957480	-1.413889	-0.870141
36	7	0	5.570043	-1.444260	0.447421
37	1	0	5.668759	-1.784429	-1.620426
38	1	0	4.733993	-0.377198	-1.114980
39	1	0	-0.594885	2.444001	-1.233096
40	8	0	-0.610461	3.201063	-0.580334
41	1	0	-0.214325	3.953876	-1.044427
42	1	0	-3.636077	2.228351	-1.830046
43	8	0	-3.583526	1.462303	-2.458058
44	1	0	-2.620161	1.366275	-2.611694
45	1	0	3.554771	2.044812	-2.326385
46	8	0	4.461525	2.131273	-2.681529
47	1	0	4.373539	2.621847	-3.512706
48	8	0	-4.288845	1.718162	1.787128
49	1	0	-4.964588	1.140975	1.347153
50	1	0	-4.808240	2.304619	2.359461
51	1	0	-3.257943	0.602956	2.905727
52	8	0	-2.726073	-0.095247	3.346769
53	1	0	-2.841070	-0.865950	2.755848
54	1	0	-2.466994	3.424459	-0.386695
55	8	0	-3.441481	3.329293	-0.445248
56	1	0	-3.694195	2.827045	0.358083
57	8	0	-0.061970	0.395157	3.340116
58	1	0	0.117680	1.239432	2.840503
59	1	0	-1.051103	0.282158	3.403999
60	1	0	1.931322	-4.508060	-0.543062
61	8	0	1.093869	-4.320140	-1.006060
62	1	0	0.506168	-3.928445	-0.318810
63	1	0	5.226770	3.038566	-1.244984
64	8	0	5.455570	3.358817	-0.343226

65	1	0	5.850384	2.568300	0.071205
66	1	0	0.085089	2.843283	1.102880
67	8	0	0.495613	2.677675	1.978898
68	1	0	1.444612	2.855696	1.844477
69	8	0	3.232551	2.746734	0.990159
70	1	0	3.668497	1.942940	1.338851
71	1	0	4.005162	3.218170	0.552235
72	8	0	-6.335710	0.286069	0.671158
73	7	0	-7.633089	-1.056785	-0.617350
74	1	0	-7.638701	-1.786325	-1.316571
75	6	0	-8.908548	-0.504512	-0.187398
76	1	0	-8.703384	0.250376	0.571575
77	1	0	-9.434016	-0.035861	-1.026737
78	1	0	-9.545066	-1.285927	0.241772
79	6	0	5.666478	-0.360625	1.252084
80	1	0	5.640652	-2.370671	0.852145
81	8	0	5.395650	0.787611	0.869844
82	6	0	6.138587	-0.625744	2.668216
83	1	0	6.964213	0.053460	2.898781
84	1	0	5.321929	-0.397309	3.361496
85	1	0	6.462781	-1.656899	2.833309

The beta product form in Fig. 3 common to that in the last of Fig. 1
luckw3.extrev.chk E(RB3LYP) = -2303.099373 a.u.

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Diketone(i)EXT in Fig. 5, the ion pair intermediate diketone(i) in the further extended model, octa-peptide and (H2O)13+8+11 with the molecular formula C21H97N9O43
diketi4a.chk E(B3LYP) = -4588.508638 a.u.
Thermal correction to Gibbs Free Energy= 1.259849 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.717717	2.808488	-2.054407
2	6	0	0.548711	2.202369	-2.496323
3	6	0	1.584292	4.178832	-1.882401
4	8	0	1.394604	-2.997716	0.174593
5	8	0	2.472700	4.898958	-1.445303
6	6	0	-0.560732	3.271873	-2.565215
7	6	0	0.202958	4.593320	-2.344944
8	1	0	-1.030133	3.222341	-3.550750
9	1	0	-0.264640	5.245960	-1.604125
10	6	0	2.939610	2.080611	-1.740329
11	7	0	-1.553820	3.076145	-1.510379
12	8	0	-3.202192	1.405556	4.215825
13	6	0	2.944671	1.648494	-0.270110
14	1	0	2.980322	1.176869	-2.355167
15	1	0	3.793753	2.709524	-1.989471
16	8	0	0.846785	1.994506	3.628301
17	1	0	0.465481	1.747139	2.745923
18	1	0	0.809332	2.977840	3.585251
19	8	0	0.438204	1.020495	-2.760802

20	1	0	0.941367	-2.377479	-0.459587
21	1	0	0.308052	5.159690	-3.275701
22	8	0	-0.945426	0.540065	4.783624
23	1	0	-0.243146	1.216563	4.447665
24	1	0	-0.757738	-0.321868	4.269716
25	8	0	1.943126	1.083150	0.209876
26	7	0	4.068607	1.915826	0.399424
27	6	0	4.321949	1.502737	1.779639
28	1	0	4.867396	2.319991	-0.119149
29	6	0	5.273276	0.301362	1.737776
30	1	0	4.780132	2.338863	2.314012
31	1	0	3.382672	1.248917	2.268742
32	6	0	-2.621588	2.245163	-1.495460
33	1	0	-1.465487	3.703052	-0.691951
34	8	0	-3.467091	2.295179	-0.589845
35	6	0	-2.785933	1.208413	-2.610676
36	7	0	-4.077355	0.568214	-2.454405
37	1	0	-2.692173	1.677105	-3.598361
38	1	0	-1.991156	0.461444	-2.531020
39	1	0	1.534071	-2.431962	0.971450
40	8	0	0.680667	4.645890	2.723546
41	1	0	0.427847	5.355688	3.336326
42	1	0	2.655164	5.417593	0.395205
43	8	0	2.856862	5.638256	1.328590
44	1	0	1.529313	4.953452	2.318036
45	1	0	-3.790758	0.652961	3.917971
46	1	0	-1.940682	0.907357	4.516659
47	1	0	-3.125065	2.008214	3.429122
48	8	0	5.702271	5.625624	1.106727
49	1	0	4.758040	5.536129	1.357253
50	1	0	5.673292	5.617184	0.115612
51	1	0	3.017892	-1.115781	2.160467
52	8	0	2.045056	-1.052182	2.036427
53	1	0	1.934245	-0.284241	1.430576
54	8	0	5.470030	5.299806	-1.634725
55	1	0	4.507972	5.159806	-1.701501
56	1	0	5.850657	4.394449	-1.662426
57	8	0	-0.339672	-1.569199	3.316309
58	1	0	-0.867311	-1.443636	2.483574
59	1	0	0.586708	-1.384021	3.028303
60	1	0	-3.247049	2.755761	1.208253
61	8	0	-2.733829	2.986810	2.014123
62	1	0	-1.859070	2.568958	1.807405
63	8	0	-1.287094	4.957351	0.677834
64	1	0	-0.508832	4.854918	1.271676
65	1	0	-1.997912	4.542940	1.213673
66	1	0	-1.051417	-1.100308	0.067188
67	8	0	-1.482512	-0.844962	0.922599
68	1	0	-2.470815	-0.906589	0.774148
69	8	0	-0.063471	-1.352929	-1.342461
70	1	0	0.355423	-0.546935	-1.698386
71	1	0	-0.374688	-1.884495	-2.144418
72	8	0	4.857221	-0.879604	1.724234
73	7	0	6.562736	0.629771	1.606009
74	1	0	6.820402	1.620712	1.654579

75	6	0	7.577636	-0.329811	1.211925
76	1	0	7.565622	-1.203598	1.863661
77	6	0	7.445404	-0.738795	-0.264161
78	1	0	8.552661	0.152452	1.324244
79	6	0	-4.311696	-0.733627	-2.678721
80	1	0	-4.743529	1.066190	-1.871853
81	8	0	-3.496972	-1.515753	-3.196242
82	6	0	-5.713981	-1.232931	-2.303966
83	1	0	-5.638782	-2.317810	-2.180996
84	7	0	-6.221350	-0.612883	-1.089578
85	1	0	-6.376429	-1.040529	-3.151357
86	8	0	-4.124930	-1.204536	0.666158
87	1	0	-3.961521	-2.212143	0.710566
88	1	0	-4.358179	-0.934040	1.592403
89	8	0	-4.656980	-0.636631	3.283067
90	1	0	-4.282633	-1.533898	3.516060
91	1	0	-5.649072	-0.686160	3.286737
92	1	0	2.729106	6.601057	1.380275
93	8	0	-3.327256	-3.667168	0.768803
94	1	0	-3.935515	-4.384289	1.013701
95	1	0	-3.223560	-3.181803	2.467885
96	8	0	-3.292538	-2.877554	3.411302
97	1	0	-3.166647	-3.684101	3.963659
98	1	0	-3.685772	-3.859623	-0.883672
99	8	0	-3.901776	-4.096327	-1.836993
100	1	0	-3.724991	-3.277250	-2.341047
101	1	0	-0.365475	-3.475380	3.426454
102	8	0	-0.288489	-4.454028	3.370771
103	1	0	-0.503977	-4.654394	2.427333
104	1	0	-2.368424	-4.951665	-2.081172
105	8	0	-1.399643	-5.155429	-2.135460
106	1	0	-1.113630	-5.087278	-1.193721
107	8	0	-0.881893	-4.689995	0.630072
108	1	0	-1.785964	-4.230379	0.690428
109	1	0	-0.197676	-4.000792	0.472837
110	8	0	7.168677	0.096607	-1.147965
111	7	0	7.723978	-2.025084	-0.520852
112	6	0	7.887874	-2.532041	-1.881161
113	1	0	7.684847	-2.684413	0.266604
114	6	0	6.955150	-3.710150	-2.173511
115	1	0	7.732545	-1.700166	-2.567322
116	1	0	8.912122	-2.900913	-2.003213
117	8	0	7.182988	-4.820463	-1.661898
118	7	0	5.933985	-3.468142	-3.010122
119	1	0	5.645981	-2.494846	-3.150475
120	6	0	4.962354	-4.505547	-3.332707
121	1	0	5.484470	-5.417574	-3.631142
122	1	0	4.318179	-4.737183	-2.476783
123	1	0	4.343122	-4.157628	-4.161276
124	1	0	-5.605130	-0.767936	-0.273159
125	6	0	-7.472073	-0.168272	-0.841568
126	6	0	-8.447269	-0.048962	-2.030251
127	8	0	-7.846669	0.145907	0.296782
128	7	0	-9.641195	0.696016	-1.705824
129	1	0	-7.958278	0.450893	-2.871020

130	1	0	-8.707059	-1.056022	-2.373569
131	6	0	-10.700560	0.248495	-0.983243
132	1	0	-9.607616	1.712930	-1.801748
133	6	0	-10.784917	-1.230580	-0.671149
134	8	0	-11.591952	1.031824	-0.611391
135	1	0	-10.707269	-1.839867	-1.578041
136	1	0	-9.973552	-1.522497	0.003129
137	1	0	-11.742363	-1.428849	-0.188180
138	1	0	5.517557	-0.386684	-2.167973
139	8	0	4.754754	-0.827095	-2.592878
140	1	0	4.371536	-1.379341	-1.871474
141	1	0	6.760165	1.879267	-1.167080
142	8	0	6.396423	2.774593	-0.977836
143	1	0	6.885366	3.076403	-0.170815
144	8	0	7.173000	3.469187	1.512484
145	1	0	8.069442	3.764710	1.736909
146	1	0	6.602355	4.301566	1.485759
147	1	0	5.823596	-5.201152	-0.423407
148	8	0	5.159996	-5.043682	0.281569
149	1	0	4.695145	-4.231944	-0.031904
150	1	0	6.215691	-4.127157	1.368627
151	8	0	6.747287	-3.434628	1.841721
152	1	0	6.090413	-2.737482	2.019843
153	1	0	0.192393	1.649311	0.678718
154	8	0	-0.515051	1.567887	1.346507
155	1	0	-0.920349	0.662257	1.190601
156	1	0	-7.427562	-0.383057	1.989906
157	8	0	-7.351872	-0.646085	2.936684
158	1	0	-7.723389	0.108693	3.420145
159	8	0	-2.508425	-5.170439	4.744582
160	1	0	-1.641834	-4.992065	4.282092
161	1	0	-2.895687	-5.903154	4.239902
162	1	0	-11.123291	2.752925	-1.063071
163	8	0	-10.562725	3.477974	-1.428461
164	1	0	-10.099155	3.821168	-0.647932
165	1	0	4.291851	-2.019633	0.255584
166	8	0	4.018557	-2.583133	-0.495401
167	1	0	3.053998	-2.770528	-0.335344
168	1	0	-1.045071	-3.672523	-2.953422
169	8	0	-0.897911	-2.780839	-3.380462
170	1	0	-1.786880	-2.392347	-3.488323

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Extended models of diketone(n) and diketone(i), which are shown as diketone(n)ext and diketone(i)ext, respectively, in Fig. S4.

An aminosuccinyl-residue intermediate, "diketone(n)ext", the extended model in the left of Fig. S4 with the molecular formula C13H63N5O28.

diketi2.chk E(RB3LYP) = -2914.923522 a.u.
Thermal correction to Gibbs Free Energy= 0.789057 a.u.
Standard orientation:

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

1	7	0	-1.410389	-1.762736	-2.294465
2	6	0	-0.062835	-1.796105	-2.664488
3	6	0	-1.816315	-2.912442	-1.630286
4	8	0	0.774997	4.443186	-2.674881
5	8	0	-2.941476	-3.081228	-1.176562
6	6	0	0.565455	-3.052502	-2.026116
7	6	0	-0.657357	-3.885724	-1.605223
8	1	0	1.193882	-3.563383	-2.754624
9	1	0	-0.568444	-4.362288	-0.622183
10	6	0	-2.279020	-0.617145	-2.556598
11	7	0	1.360778	-2.672348	-0.861552
12	1	0	0.795091	0.537935	3.559055
13	6	0	-2.113138	0.437024	-1.455972
14	1	0	-1.964569	-0.170589	-3.501630
15	1	0	-3.306260	-0.972220	-2.647543
16	8	0	0.162468	-0.539483	0.626373
17	1	0	0.003350	0.148047	-0.047625
18	1	0	-1.318327	-0.983847	1.482476
19	8	0	0.493098	-0.942118	-3.321098
20	1	0	1.118966	3.529725	-2.724740
21	1	0	-0.868444	-4.672695	-2.338323
22	8	0	0.048062	0.792398	2.940172
23	1	0	0.349280	-0.037644	1.470497
24	1	0	0.248596	1.702550	2.605465
25	8	0	-1.065259	1.122515	-1.410502
26	7	0	-3.105792	0.526394	-0.571808
27	6	0	-3.124405	1.450291	0.557168
28	1	0	-3.914472	-0.110183	-0.595853
29	6	0	-4.107573	2.604638	0.314309
30	1	0	-3.412142	0.888371	1.449179
31	1	0	-2.131181	1.860858	0.716156
32	6	0	2.661560	-2.297236	-0.803141
33	1	0	0.837263	-2.351600	-0.045483
34	8	0	3.155608	-1.965416	0.286001
35	6	0	3.512723	-2.319294	-2.078300
36	7	0	4.588752	-1.349863	-2.015033
37	1	0	3.923951	-3.329873	-2.198066
38	1	0	2.911769	-2.083943	-2.956313
39	1	0	0.176680	4.411354	-1.904425
40	8	0	-1.853188	-1.081163	2.310801
41	1	0	-1.498661	-0.331951	2.842502
42	1	0	-3.590515	-3.025170	0.787338
43	8	0	-3.980255	-2.685541	1.616434
44	1	0	-3.311377	-2.034154	1.938619
45	1	0	2.833400	0.548678	4.167490
46	8	0	2.097833	-0.047926	4.436174
47	1	0	2.249753	-0.893312	3.939780
48	8	0	-5.484551	-0.755270	0.152202
49	1	0	-5.124051	-1.431065	0.772515
50	1	0	-5.725904	-1.265186	-0.659283
51	1	0	-1.856511	3.961859	-0.186582
52	8	0	-0.905144	3.776896	-0.367167
53	1	0	-0.922241	2.880011	-0.767524
54	8	0	-5.481721	-2.176566	-2.173441

55	1	0	-4.705115	-2.708337	-1.912938
56	1	0	-6.157113	-2.821509	-2.437334
57	8	0	0.805034	3.107819	1.690910
58	1	0	1.489859	2.759834	1.055813
59	1	0	0.124074	3.505432	1.093594
60	1	0	2.442671	-2.241093	2.088710
61	8	0	2.308471	-2.412545	3.043258
62	1	0	1.408226	-2.793441	3.124052
63	8	0	-0.413868	-3.258865	3.200432
64	1	0	-0.874533	-2.438268	2.896503
65	1	0	-1.157482	-3.779724	3.591066
66	1	0	2.292410	1.990248	-0.932278
67	8	0	2.684000	2.322558	-0.081334
68	1	0	3.291549	1.629796	0.273736
69	8	0	1.589761	1.667980	-2.474258
70	1	0	0.746980	1.178586	-2.418326
71	1	0	2.218632	1.086376	-2.960971
72	8	0	-3.682671	3.769031	0.165133
73	7	0	-5.395223	2.244478	0.279236
74	1	0	-5.605572	1.247759	0.368188
75	6	0	-6.508015	3.145510	0.002993
76	1	0	-6.151921	4.175121	-0.018007
77	1	0	-6.963279	2.902520	-0.963245
78	1	0	-7.266831	3.043159	0.784400
79	6	0	4.547246	-0.188890	-2.709685
80	1	0	5.261870	-1.427407	-1.243872
81	8	0	3.640891	0.088695	-3.514359
82	6	0	5.705426	0.759811	-2.476295
83	1	0	6.180226	0.974204	-3.438988
84	1	0	5.324514	1.705775	-2.078852
85	1	0	6.453337	0.362208	-1.786654
86	8	0	4.905408	1.185432	1.065351
87	1	0	5.266014	2.023976	0.689562
88	1	0	4.678578	1.397116	2.006106
89	8	0	4.027870	1.809625	3.594417
90	1	0	3.517115	2.671872	3.558844
91	1	0	4.729433	1.953388	4.249707
92	8	0	2.579150	4.080481	3.493663
93	1	0	1.864623	3.876318	2.835050
94	1	0	2.114383	4.125203	4.344453
95	1	0	-3.307189	-4.083703	2.837917
96	8	0	-2.758319	-4.737996	3.322580
97	1	0	-2.275858	-5.195232	2.599439
98	1	0	-0.476131	-4.484164	1.866097
99	8	0	-0.829968	-5.241754	1.336807
100	1	0	-0.200502	-5.964335	1.491763
101	1	0	5.732850	-0.406469	0.754628
102	8	0	5.931992	-1.351503	0.552263
103	1	0	5.054982	-1.760113	0.692438
104	1	0	-4.479121	5.449083	-0.048025
105	8	0	-4.952090	6.295663	-0.184255
106	1	0	-5.045196	6.341786	-1.148441
107	8	0	5.119225	3.594695	-0.274786
108	1	0	5.177827	4.356217	0.324017
109	1	0	4.154530	3.391604	-0.326516

An aminosuccinyl-residue intermediate, "diketone(i)ext", the extended model in the right of Fig. S4 with the molecular formula C13H63N5O28.

diketi2c.chk E(RB3LYP) = -2914.915641 a.u.

Thermal correction to Gibbs Free Energy= 0.790373 a.u.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.907825	-1.835717	-1.492790
2	6	0	-1.640308	-2.387759	-1.665133
3	6	0	-3.725450	-2.601828	-0.680262
4	8	0	1.248366	2.964740	-2.915511
5	8	0	-4.891995	-2.327422	-0.423182
6	6	0	-1.533072	-3.650845	-0.786395
7	6	0	-2.945715	-3.805396	-0.191703
8	1	0	-1.273877	-4.496251	-1.428647
9	1	0	-2.942747	-3.806788	0.902503
10	6	0	-3.275186	-0.533741	-2.050830
11	7	0	-0.521004	-3.468549	0.248297
12	1	0	1.063658	0.968396	3.631410
13	6	0	-2.782852	0.568506	-1.105906
14	1	0	-2.758414	-0.423847	-3.005814
15	1	0	-4.352656	-0.508353	-2.215636
16	8	0	-0.906686	-0.139932	1.629468
17	1	0	-1.010505	0.181990	0.710803
18	1	0	-1.817590	-0.266689	1.986252
19	8	0	-0.779882	-1.911251	-2.376652
20	1	0	1.337027	2.002648	-2.780511
21	1	0	-3.446611	-4.718180	-0.524717
22	8	0	0.338601	1.558572	3.130355
23	1	0	-0.187583	0.907231	2.542044
24	1	0	0.808086	2.231668	2.454420
25	8	0	-1.550760	0.768426	-0.984099
26	7	0	-3.716639	1.216360	-0.413166
27	6	0	-3.439121	2.266211	0.562971
28	1	0	-4.716978	0.988991	-0.500533
29	6	0	-3.826867	3.647899	0.012809
30	1	0	-4.007971	2.044452	1.470691
31	1	0	-2.381141	2.268568	0.812479
32	6	0	0.825099	-3.546245	0.091516
33	1	0	-0.851706	-3.161371	1.169716
34	8	0	1.606950	-3.286546	1.011362
35	6	0	1.359385	-4.007304	-1.275364
36	7	0	2.800425	-4.067384	-1.293966
37	1	0	0.956116	-4.998928	-1.508624
38	1	0	1.023199	-3.320420	-2.052942
39	1	0	0.687308	3.246351	-2.166767
40	8	0	-3.244745	-0.706186	2.944310
41	1	0	-3.310281	-0.221966	3.782908
42	1	0	-5.604115	-1.607910	1.179189
43	8	0	-5.751750	-0.909846	1.851098
44	1	0	-4.168110	-0.760571	2.585042

45	1	0	2.877782	0.132868	4.008323
46	8	0	1.948091	0.047482	4.333456
47	1	0	1.644884	-0.869050	4.070768
48	8	0	-6.473478	1.147548	0.041295
49	1	0	-6.400378	0.526100	0.798928
50	1	0	-6.801953	0.584350	-0.700934
51	1	0	-1.266897	3.899010	-0.484394
52	8	0	-0.443274	3.360740	-0.582123
53	1	0	-0.776736	2.450122	-0.731543
54	8	0	-6.740330	-0.694621	-1.952594
55	1	0	-6.305624	-1.436825	-1.491110
56	1	0	-7.557227	-1.063149	-2.324487
57	8	0	1.396030	3.081091	1.437631
58	1	0	1.983632	2.457417	0.922988
59	1	0	0.680393	3.294975	0.784668
60	1	0	1.319688	-2.665806	2.739302
61	8	0	1.044422	-2.409470	3.646302
62	1	0	0.065547	-2.453067	3.581534
63	8	0	-1.645313	-2.932925	2.939288
64	1	0	-2.307229	-2.205624	3.042941
65	1	0	-1.992902	-3.685905	3.443315
66	1	0	2.115832	0.938961	-0.741903
67	8	0	2.738998	1.350934	-0.094347
68	1	0	3.284417	0.594405	0.271226
69	8	0	1.241486	0.173206	-2.061193
70	1	0	0.308805	-0.064518	-1.906447
71	1	0	1.727136	-0.672451	-2.167073
72	8	0	-2.968950	4.505335	-0.256972
73	7	0	-5.142238	3.844358	-0.159365
74	1	0	-5.779286	3.065123	0.008046
75	6	0	-5.665326	5.075461	-0.738098
76	1	0	-5.372046	5.938552	-0.133177
77	1	0	-5.289147	5.223302	-1.756100
78	1	0	-6.753677	5.010698	-0.763621
79	6	0	3.585182	-3.018786	-1.636823
80	1	0	3.236483	-4.827049	-0.788677
81	8	0	3.128321	-1.974937	-2.137872
82	6	0	5.060568	-3.193239	-1.362390
83	1	0	5.638645	-2.669013	-2.124588
84	1	0	5.266652	-2.709953	-0.400209
85	1	0	5.358988	-4.243584	-1.313300
86	8	0	4.348711	-0.654455	0.744101
87	1	0	5.146001	-0.150700	0.392604
88	1	0	4.414053	-0.558822	1.719897
89	8	0	4.551120	0.155153	3.410193
90	1	0	5.056858	0.940704	3.046287
91	1	0	5.176900	-0.316379	3.982099
92	1	0	-6.391328	-1.283838	2.480147
93	8	0	6.141015	1.021234	-0.216376
94	1	0	7.090777	0.853166	-0.323791
95	1	0	6.046316	1.661181	1.197602
96	8	0	5.924136	2.069466	2.142887
97	1	0	6.822013	2.168260	2.498051
98	1	0	5.639692	0.229735	-1.742669
99	8	0	5.399711	-0.199057	-2.607795

100	1	0	4.568174	-0.682470	-2.423512
101	1	0	5.235820	3.781148	1.656494
102	8	0	4.878336	4.545803	1.160716
103	1	0	4.772805	4.155810	0.264646
104	1	0	4.989074	1.297058	-3.605133
105	8	0	4.782160	2.206746	-3.915775
106	1	0	4.689117	2.669590	-3.055773
107	8	0	4.677271	3.010910	-1.198538
108	1	0	5.385156	2.356722	-0.912889
109	1	0	3.868139	2.512955	-0.926686

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Geometries of alphaH+, diketone(i)H+ and betaH+ with the molecular formula C13H48N5O20(+1) in Fig. S5.

Protonated alpha reactant(substrate) in Fig. S5
alphah+.chk E(RB3LYP) = -2303.542014 a.u.
Thermal correction to Gibbs Free Energy= 0.620044 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.254728	-1.786191	0.182728
2	6	0	1.369201	-1.781903	-2.303356
3	6	0	0.965660	-1.848929	0.744150
4	8	0	1.913998	-2.971114	-2.174242
5	8	0	1.187280	-2.460762	1.801098
6	6	0	1.980557	-0.711672	-1.432192
7	6	0	2.073629	-0.986365	0.098364
8	1	0	3.003058	-0.540508	-1.785341
9	7	0	1.960364	0.287464	0.808860
10	6	0	-1.475410	-2.252194	0.825528
11	1	0	1.418502	0.208160	-1.583180
12	1	0	-0.310646	0.054141	-3.301380
13	6	0	-2.555998	-1.211690	0.518632
14	1	0	-1.783617	-3.225607	0.420896
15	1	0	-1.312403	-2.361947	1.897351
16	8	0	0.106148	1.982236	-1.175750
17	1	0	-0.425388	-1.196208	-0.625560
18	1	0	-0.640019	2.324637	-0.603530
19	8	0	0.431331	-1.545908	-3.079435
20	1	0	1.431376	-3.620592	-2.782184
21	1	0	3.020406	-1.476014	0.319216
22	8	0	-0.697772	0.973289	-3.323985
23	1	0	-0.307314	1.494581	-2.498155
24	1	0	-1.762607	0.925573	-3.154689
25	8	0	-2.514207	-0.599553	-0.559096
26	7	0	-3.495224	-1.011518	1.458849
27	6	0	-4.370085	0.149789	1.351970
28	1	0	-3.342781	-1.417922	2.401633
29	6	0	-5.438467	0.067061	0.257095
30	1	0	-4.872653	0.271734	2.316803
31	1	0	-3.783612	1.053054	1.161093

32	6	0	2.850635	1.066156	1.465739
33	1	0	1.005466	0.649214	0.890967
34	8	0	2.438381	2.077351	2.067929
35	6	0	4.335439	0.718849	1.491380
36	1	0	4.474871	-0.161763	2.127351
37	7	0	4.918871	0.428250	0.192773
38	1	0	4.825621	1.577140	1.958117
39	1	0	2.904543	-2.569792	2.448801
40	8	0	3.860392	-2.479783	2.664936
41	1	0	4.003478	-2.977858	3.483031
42	1	0	0.271398	-1.418095	3.374536
43	8	0	-0.349347	-0.855748	3.870217
44	1	0	-0.398636	-0.013607	3.362948
45	1	0	0.857524	2.610735	-1.009259
46	8	0	2.002552	3.694928	-0.206980
47	1	0	2.113933	3.309997	0.690752
48	8	0	-2.850537	-1.810189	4.001302
49	1	0	-2.911869	-2.621413	4.525237
50	1	0	-1.916220	-1.479271	4.096963
51	1	0	-4.696309	2.342362	-0.743036
52	8	0	-3.975745	2.919719	-1.123634
53	1	0	-4.421275	3.718257	-1.449149
54	1	0	4.879711	-2.586257	1.211939
55	8	0	5.229830	-2.371972	0.315142
56	1	0	5.741777	-3.141752	0.029042
57	8	0	-3.126639	0.883475	-2.783103
58	1	0	-3.158424	0.252055	-2.032403
59	1	0	-3.433408	1.733355	-2.378542
60	8	0	-1.684398	3.098132	0.467616
61	1	0	-1.267387	4.003331	0.441941
62	1	0	-2.548873	3.155737	-0.001920
63	8	0	0.371237	-4.301935	-3.845438
64	1	0	-0.040838	-3.452083	-4.087634
65	1	0	0.731663	-4.668046	-4.668704
66	1	0	0.498533	1.887620	2.397841
67	8	0	-0.310152	1.376281	2.182860
68	1	0	-0.939406	2.006051	1.764886
69	8	0	-0.211575	5.326553	0.143571
70	1	0	-0.076855	5.997347	0.829172
71	1	0	0.683337	4.975007	-0.062911
72	8	0	-5.770869	1.080936	-0.374476
73	7	0	-6.015163	-1.133496	0.080180
74	1	0	-5.671755	-1.901508	0.641906
75	6	0	-7.085179	-1.385241	-0.877045
76	1	0	-7.251631	-0.468998	-1.443075
77	1	0	-6.802990	-2.190825	-1.562017
78	1	0	-8.009821	-1.661407	-0.359827
79	6	0	4.980352	1.374934	-0.776937
80	1	0	5.330560	-0.498734	0.068435
81	8	0	4.442318	2.479994	-0.646469
82	6	0	5.762781	1.007890	-2.023167
83	1	0	5.189087	1.295362	-2.908728
84	1	0	6.691403	1.588889	-2.036993
85	1	0	6.016661	-0.054697	-2.075516
86	1	0	2.898512	3.571442	-0.588327

The protonated beta product in Fig. S5
luckw3.extrev.chk E(RB3LYP) = -2303.540943 a.u.
Thermal correction to Gibbs Free Energy= 0.620303 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.860242	-0.127664	-0.075655
2	6	0	-2.087343	-0.902426	0.170564
3	6	0	0.403424	-0.941253	-1.054950
4	8	0	-1.732731	-2.114515	0.528493
5	8	0	0.767206	-2.114373	-1.221881
6	6	0	-2.133674	-0.746717	-1.351529
7	6	0	-0.716080	-0.328816	-1.886932
8	1	0	-2.370925	-1.735964	-1.752800
9	1	0	-0.646396	0.759568	-1.863879
10	6	0	1.722181	-0.572271	1.014057
11	7	0	-3.085997	0.266928	-1.779178
12	1	0	-2.527252	1.874864	0.970001
13	6	0	3.087417	0.114605	0.977658
14	1	0	1.231767	-0.334250	1.966313
15	1	0	1.828284	-1.652467	0.943044
16	8	0	-0.032328	2.750041	-0.433039
17	1	0	0.597942	0.857317	-0.124209
18	1	0	0.616128	3.197210	0.157984
19	8	0	-2.328069	0.006969	0.968753
20	1	0	-1.785860	-2.231369	1.535315
21	1	0	-0.624444	-0.656351	-2.923983
22	8	0	-2.216674	2.801722	1.062196
23	1	0	-1.442045	2.830704	0.421514
24	1	0	-1.397451	2.849902	2.376404
25	8	0	3.180709	1.359649	1.001824
26	7	0	4.132459	-0.715030	0.939023
27	6	0	5.482537	-0.246383	0.741357
28	1	0	3.955457	-1.742636	0.887623
29	1	0	5.520361	0.818534	0.990365
30	1	0	6.161093	-0.783566	1.414075
31	6	0	5.926589	-0.436139	-0.725317
32	6	0	-4.352176	0.536183	-1.360834
33	1	0	-2.736767	0.944694	-2.478749
34	8	0	-4.906068	1.593280	-1.684759
35	6	0	-5.159426	-0.415434	-0.469747
36	1	0	-6.206284	-0.157042	-0.656283
37	7	0	-4.938323	-1.843048	-0.646643
38	1	0	-4.948566	-0.191417	0.579478
39	1	0	2.742590	-3.728554	0.957224
40	8	0	3.641582	-3.426308	0.709419
41	1	0	3.639844	-3.455940	-0.283266
42	1	0	4.028863	-2.206888	-2.002476
43	8	0	3.462484	-3.004093	-1.973534
44	1	0	2.552225	-2.657326	-1.952200
45	1	0	-4.070770	3.239586	-1.529376

46	8	0	-3.530044	4.000392	-1.217345
47	1	0	-3.336336	3.792028	-0.282527
48	1	0	-0.216812	3.320497	-1.223089
49	8	0	-1.222035	4.076453	-2.456924
50	1	0	-1.040235	4.955493	-2.823596
51	1	0	2.091913	2.465709	1.580712
52	8	0	1.440543	3.199761	1.796695
53	1	0	1.969629	3.985814	2.091561
54	1	0	0.689296	-3.462311	0.086332
55	8	0	0.826787	-4.028322	0.874943
56	1	0	0.812163	-4.935077	0.530675
57	8	0	-0.689971	2.716019	3.127279
58	1	0	-0.756425	1.724590	3.379420
59	1	0	0.235190	2.887448	2.680464
60	8	0	2.823126	5.409575	2.576956
61	1	0	2.886792	5.620541	3.521089
62	1	0	3.717946	5.536893	2.226287
63	8	0	-2.009233	1.855344	-3.863312
64	1	0	-1.649989	2.716013	-3.545127
65	1	0	-2.694995	2.084803	-4.508725
66	1	0	-1.506554	-0.049485	2.579086
67	8	0	-0.908837	0.163139	3.332340
68	1	0	-1.225212	-0.399911	4.057320
69	8	0	-2.363366	-2.415722	3.055793
70	1	0	-2.133974	-3.288503	3.413703
71	1	0	-3.307753	-2.474647	2.768556
72	8	0	5.121681	-0.682852	-1.621817
73	7	0	7.255072	-0.279792	-0.931032
74	1	0	7.849138	-0.098742	-0.133051
75	6	0	7.881905	-0.398258	-2.240947
76	1	0	7.095562	-0.607972	-2.965948
77	1	0	8.387872	0.533417	-2.515414
78	1	0	8.608847	-1.217109	-2.250676
79	6	0	-4.766815	-2.696443	0.404946
80	1	0	-5.177208	-2.245274	-1.543761
81	8	0	-4.635844	-2.280534	1.561196
82	6	0	-4.688423	-4.169375	0.066156
83	1	0	-3.652899	-4.502171	0.197745
84	1	0	-5.312744	-4.728553	0.767965
85	1	0	-5.000165	-4.402059	-0.955789
86	1	0	-2.127063	4.131594	-2.004051

Protonated diketone(i) in Fig. S5
diketoh+.chk E(RB3LYP) = -2303.550755 a.u.
Thermal correction to Gibbs Free Energy= 0.621985 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.449382	-1.889474	-1.878783
2	6	0	0.919903	-1.634962	-2.042337
3	6	0	-0.698034	-2.914166	-0.990394
4	8	0	0.571782	5.458487	-0.665481

5	8	0	-1.823504	-3.265234	-0.636590
6	6	0	1.707687	-2.626933	-1.158747
7	6	0	0.615245	-3.554261	-0.588726
8	1	0	2.424200	-3.164653	-1.783825
9	1	0	0.671074	-3.649579	0.499876
10	6	0	-1.474376	-0.971141	-2.375679
11	7	0	2.405383	-1.919581	-0.096188
12	1	0	0.486712	0.951842	4.382630
13	6	0	-1.737749	0.137243	-1.342089
14	1	0	-1.076845	-0.506034	-3.280301
15	1	0	-2.374063	-1.540753	-2.616776
16	8	0	-0.007288	-0.958335	0.888988
17	1	0	-0.157431	-0.024138	0.670596
18	1	0	-0.472193	-1.146880	1.738309
19	8	0	1.373117	-0.748477	-2.729681
20	1	0	0.675146	5.596887	-1.619632
21	1	0	0.658287	-4.562240	-1.016056
22	8	0	0.123504	0.756780	3.478647
23	1	0	0.908091	0.276744	3.100557
24	1	0	0.186929	2.282119	2.591028
25	8	0	-0.857858	0.989867	-1.101942
26	7	0	-2.919541	0.086112	-0.722049
27	6	0	-3.333038	0.997116	0.340776
28	1	0	-3.599006	-0.659310	-0.903661
29	6	0	-4.362778	2.028619	-0.157357
30	1	0	-3.762169	0.395127	1.147151
31	1	0	-2.465076	1.531892	0.719153
32	6	0	3.604074	-1.276636	-0.158549
33	1	0	1.782235	-1.592658	0.647617
34	8	0	4.004579	-0.593265	0.785946
35	6	0	4.461259	-1.448843	-1.423218
36	7	0	5.601817	-0.565383	-1.426677
37	1	0	4.807824	-2.486551	-1.495771
38	1	0	3.855686	-1.226578	-2.304890
39	1	0	-0.278514	4.966416	-0.549927
40	8	0	-1.170862	-1.600750	3.266179
41	1	0	-0.980208	-0.678864	3.575766
42	1	0	-2.745322	-2.846520	1.016445
43	8	0	-3.380751	-2.536136	1.696092
44	1	0	-2.105553	-1.691920	2.994388
45	1	0	2.356063	1.454470	5.822046
46	8	0	1.831666	0.685020	5.553637
47	1	0	2.376691	0.216047	4.885854
48	8	0	-5.191255	-1.475943	-0.280414
49	1	0	-4.793583	-1.906906	0.504263
50	1	0	-5.152349	-2.152843	-0.992273
51	1	0	-2.354956	3.667449	-0.118261
52	8	0	-1.364740	3.618007	-0.062290
53	1	0	-1.143763	2.807137	-0.566969
54	8	0	-4.198451	-3.136077	-2.206210
55	1	0	-3.407045	-3.445492	-1.725259
56	1	0	-4.502431	-3.878195	-2.750513
57	8	0	0.317500	3.114713	2.072035
58	1	0	1.435359	3.311996	1.111747
59	1	0	-0.490702	3.291542	1.540934

60	1	0	3.075240	-0.548065	2.392396
61	8	0	2.446223	-0.627059	3.146891
62	1	0	2.150726	-1.568666	3.154351
63	8	0	1.142607	-3.079418	3.029813
64	1	0	0.258269	-2.711212	3.254527
65	1	0	1.342929	-3.725236	3.724691
66	1	0	1.609443	4.430295	-0.073572
67	8	0	2.063151	3.597069	0.321918
68	1	0	2.000050	2.887925	-0.433547
69	8	0	1.811618	2.068848	-1.687995
70	1	0	1.083644	1.424172	-1.741140
71	1	0	2.639578	1.620874	-1.969851
72	8	0	-4.053338	3.218156	-0.308943
73	7	0	-5.583794	1.525601	-0.408451
74	1	0	-5.717456	0.520138	-0.306444
75	6	0	-6.681927	2.331234	-0.927542
76	1	0	-6.390480	3.380375	-0.878701
77	1	0	-6.903530	2.067984	-1.967914
78	1	0	-7.579813	2.174093	-0.322693
79	6	0	5.439308	0.758239	-1.725190
80	1	0	6.406408	-0.830144	-0.875506
81	8	0	4.376338	1.197629	-2.163554
82	6	0	6.646959	1.645721	-1.516349
83	1	0	6.771923	2.282670	-2.395652
84	1	0	6.459208	2.299995	-0.658030
85	1	0	7.570532	1.087418	-1.339975
86	1	0	-3.672654	-3.341515	2.153888

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Cartesian coordinates of the optimized TS geometries and Gibbs free energies in a.u. in Fig. S1, S2 and S3 calculated by B3PW91/6-31+G(d,p)

==== concerted paths ====

m=0 sucw1TSg.high3.log G = -476.074021 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.327679	0.678156	0.238808
2	6	0	1.124521	-0.057763	-0.331226
3	6	0	-1.347242	-0.289414	0.091450
4	8	0	1.892324	0.642681	-0.942741
5	8	0	-2.522935	-0.028005	-0.033895
6	6	0	0.651445	-1.466998	-0.633327
7	6	0	-0.702071	-1.661591	0.057857
8	1	0	0.548206	-1.530066	-1.722168
9	1	0	-0.567613	-2.006395	1.090210
10	8	0	1.471983	-0.153080	1.401295
11	1	0	2.251141	0.408663	1.519236
12	1	0	0.372784	0.481146	1.209784
13	6	0	-0.586615	2.063440	-0.134672
14	1	0	1.412874	-2.182291	-0.316636

15	1	0	-1.363851	-2.363940	-0.451520
16	1	0	-0.914330	2.643922	0.730872
17	1	0	0.347040	2.477568	-0.528468
18	1	0	-1.363697	2.105492	-0.900732

m=1 sucw2TSg.high3.log G = -552.473775 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.238270	0.570786	0.229347
2	6	0	-0.661831	-0.778206	0.432528
3	6	0	1.520055	0.100462	-0.207351
4	8	0	-0.782986	-1.149544	1.598344
5	8	0	2.538282	0.744671	-0.107659
6	6	0	-0.110342	-1.639567	-0.710619
7	6	0	1.379095	-1.299370	-0.762222
8	1	0	-0.311040	-2.688271	-0.486152
9	1	0	1.821251	-1.351964	-1.761064
10	1	0	-0.371928	1.192011	-0.718088
11	8	0	-1.266855	1.521960	-1.466331
12	1	0	-1.540710	2.442234	-1.387012
13	8	0	-2.131417	-0.246250	-0.167834
14	1	0	-2.656816	-0.129797	0.636224
15	1	0	-1.923551	0.755683	-0.877447
16	6	0	0.258071	1.467008	1.392374
17	1	0	-0.601996	-1.383947	-1.652285
18	1	0	1.975405	-1.949750	-0.111854
19	1	0	1.169938	2.065849	1.364038
20	1	0	-0.615679	2.123495	1.366203
21	1	0	0.220748	0.860298	2.301594

Cartesian coordinates of the optimized alpha (reactant) and two rate-determining TS geometries with Gibbs free energies in a.u. calculated by B3PW91/6-311++G(d,p) scrf=(pcm, solvent=water)//B3PW91/6-31+G(d,p).

alpha form (1)

alpha1.higha.chk E(RB3PW91) = -2302.182653 a.u.
Thermal correction to Gibbs Free Energy= 0.599859 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.551500	0.650694	-0.415762
2	6	0	0.754819	3.515421	0.298668
3	6	0	0.742460	0.701485	-0.754112
4	8	0	1.145620	3.546150	-0.953905
5	8	0	1.159220	0.390894	-1.887439
6	6	0	1.383652	2.409022	1.110766
7	6	0	1.742312	1.123666	0.342705

8	1	0	2.306548	2.801813	1.554757
9	7	0	1.910619	0.047573	1.306831
10	6	0	-1.573627	0.280521	-1.387190
11	1	0	0.710973	2.188525	1.940484
12	1	0	-1.224751	3.681834	2.249671
13	6	0	-2.720573	-0.405464	-0.665732
14	1	0	-1.964435	1.175584	-1.885942
15	1	0	-1.128497	-0.365528	-2.146042
16	8	0	-0.949497	0.585211	2.384939
17	1	0	-0.810241	0.713991	0.585398
18	1	0	-1.560044	-0.088955	2.752192
19	8	0	-0.044601	4.306748	0.800123
20	1	0	0.598586	4.188866	-1.526896
21	1	0	2.684429	1.293683	-0.177531
22	8	0	-1.910462	3.126853	2.659453
23	1	0	-1.331953	1.459925	2.635447
24	1	0	-2.645811	3.138602	2.018524
25	8	0	-3.479606	0.262872	0.072793
26	7	0	-2.813136	-1.720242	-0.828512
27	6	0	-3.782715	-2.526142	-0.133941
28	1	0	-2.207299	-2.194889	-1.523503
29	6	0	-5.214088	-2.339556	-0.654810
30	1	0	-3.499595	-3.573294	-0.284776
31	1	0	-3.734948	-2.326846	0.942847
32	6	0	2.766086	-1.008845	1.249304
33	1	0	1.177569	-0.035097	2.011253
34	8	0	2.689979	-1.908062	2.088285
35	6	0	3.827344	-1.046672	0.142647
36	1	0	3.494467	-0.527563	-0.758369
37	7	0	5.093967	-0.483788	0.564629
38	1	0	3.981277	-2.096047	-0.110379
39	1	0	2.637203	1.077495	-2.639925
40	8	0	3.517549	1.390558	-2.944142
41	1	0	3.822287	0.754861	-3.599369
42	1	0	1.373068	-1.580088	-2.398927
43	8	0	1.256873	-2.499427	-2.683017
44	1	0	1.868732	-3.071274	-2.161643
45	1	0	3.372936	-3.614890	1.629048
46	8	0	3.890533	-4.258351	1.106741
47	1	0	4.773438	-3.841250	1.083410
48	8	0	-1.294807	-3.126455	-2.635124
49	1	0	-1.579962	-3.233027	-3.547795
50	1	0	-0.312017	-2.946457	-2.660741
51	1	0	-4.613115	-0.078476	1.365390
52	8	0	-5.117815	-0.221460	2.196695
53	1	0	-5.873898	-0.764416	1.946739
54	1	0	4.512077	1.906102	-1.607242
55	8	0	4.928029	2.105628	-0.736227
56	1	0	5.117101	3.048406	-0.732295
57	8	0	-3.758965	2.959456	0.469421
58	1	0	-3.634786	2.006914	0.245056
59	1	0	-4.697180	3.064828	0.662458
60	8	0	-2.864689	-1.187562	3.426941
61	1	0	-2.856782	-1.241177	4.387841
62	1	0	-3.749295	-0.849250	3.165531

63	8	0	-0.398444	4.916905	-2.490255
64	1	0	-1.238033	5.042383	-1.969225
65	1	0	-0.169441	5.766195	-2.880664
66	1	0	2.960729	-5.108827	-1.755959
67	8	0	2.908711	-4.227139	-1.376453
68	1	0	3.250155	-4.296300	-0.442708
69	1	0	-1.614168	5.075830	-0.015303
70	8	0	-2.313115	5.142404	-0.689829
71	1	0	-2.922144	4.411276	-0.476683
72	8	0	-5.468836	-1.814094	-1.725894
73	7	0	-6.172928	-2.820421	0.194452
74	1	0	-5.865741	-3.384354	0.975129
75	6	0	-7.559277	-2.940868	-0.223585
76	1	0	-7.797649	-2.099239	-0.875252
77	1	0	-7.742143	-3.868386	-0.779280
78	1	0	-8.210518	-2.914659	0.653215
79	6	0	6.147654	-1.253145	0.938415
80	1	0	5.245776	0.500399	0.353820
81	8	0	6.096869	-2.481579	1.037493
82	6	0	7.423843	-0.503741	1.248329
83	1	0	7.643840	-0.619099	2.313770
84	1	0	8.243187	-0.965995	0.692454
85	1	0	7.373197	0.560670	1.006977

TS4(n), the rate-determining step in the neutral (without ionization) reaction. mu = 777.37 icm-1
ts4n.highb.chk E(RB3PW91) = -2302.136162 a.u.
Thermal correction to Gibbs Free Energy= 0.606017 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.707251	0.158903	0.072633
2	6	0	-0.731522	-0.662721	-0.000474
3	6	0	1.316503	-0.002284	-1.199212
4	8	0	-0.353706	-1.982218	0.280264
5	8	0	2.517160	-0.034869	-1.371825
6	6	0	-1.031306	-0.576851	-1.558117
7	6	0	0.247349	-0.089923	-2.252959
8	1	0	-1.227912	-1.606710	-1.865449
9	1	0	0.108776	0.912077	-2.681611
10	6	0	1.516273	-0.214367	1.250824
11	7	0	-2.169833	0.245729	-1.890722
12	1	0	5.916735	-0.498668	1.981822
13	6	0	2.854524	0.504992	1.347216
14	1	0	0.922780	0.046631	2.133563
15	1	0	1.661108	-1.296433	1.252432
16	8	0	-0.039194	2.561217	0.200533
17	1	0	0.327106	1.400464	0.151034
18	1	0	0.434368	3.009063	0.948760
19	8	0	-1.606246	-0.146269	0.803126
20	1	0	-0.959553	-2.377005	0.982687
21	1	0	0.585823	-0.744329	-3.058584
22	8	0	-2.433580	2.363382	1.092001

23	1	0	-1.023714	2.572517	0.477508
24	1	0	-2.188313	2.418338	2.054178
25	8	0	2.937279	1.757397	1.358028
26	7	0	3.918292	-0.281786	1.477903
27	6	0	5.262680	0.261046	1.552977
28	1	0	3.808635	-1.313627	1.431364
29	1	0	5.260492	1.147938	2.194037
30	1	0	-2.368618	1.395991	0.879227
31	6	0	5.794760	0.592514	0.151584
32	6	0	-3.452849	-0.113492	-1.698799
33	1	0	-1.985100	1.204738	-2.221673
34	8	0	-4.412862	0.625798	-1.956792
35	6	0	-3.712221	-1.524357	-1.177801
36	1	0	-3.058835	-1.756267	-0.337352
37	7	0	-5.077156	-1.635061	-0.732347
38	1	0	-3.498466	-2.243618	-1.982877
39	1	0	2.598355	-3.868855	-1.357739
40	8	0	3.525039	-3.875637	-1.046811
41	1	0	4.014690	-3.213601	-1.584363
42	1	0	5.498771	-1.382339	-1.806541
43	8	0	4.759027	-1.745098	-2.323320
44	1	0	4.055216	-1.086420	-2.232492
45	1	0	-4.982817	4.359891	0.515314
46	8	0	-4.165856	4.261258	0.017465
47	1	0	-3.647011	3.559639	0.461567
48	8	0	3.494005	-2.995683	1.397694
49	1	0	3.531965	-3.386315	0.469081
50	1	0	3.869216	-3.649431	1.994836
51	1	0	1.931500	2.758473	2.182822
52	8	0	1.155689	3.312632	2.472510
53	1	0	1.489667	4.180910	2.722065
54	1	0	0.362855	-3.220785	-0.873206
55	8	0	0.756244	-3.756239	-1.592054
56	1	0	0.347432	-4.626040	-1.532812
57	8	0	-1.409520	2.280555	3.582546
58	1	0	-1.418918	1.313595	3.735606
59	1	0	-0.483927	2.552818	3.475778
60	1	0	-4.325012	2.449722	-2.499710
61	8	0	-4.059488	3.379397	-2.634690
62	1	0	-4.206968	3.803772	-1.765323
63	8	0	-1.448002	2.859906	-2.799730
64	1	0	-2.383203	3.202534	-2.836140
65	1	0	-0.986111	3.419713	-2.165998
66	1	0	-1.809069	-0.409868	2.398664
67	8	0	-1.927472	-0.490246	3.390294
68	1	0	-2.877097	-0.453573	3.553279
69	8	0	-1.941333	-3.103683	2.039368
70	1	0	-1.928095	-2.511088	2.808692
71	1	0	-2.865265	-3.099653	1.715545
72	8	0	6.474190	-0.217313	-0.482133
73	7	0	5.446242	1.812314	-0.308783
74	1	0	4.725204	2.299136	0.212286
75	6	0	5.762016	2.253178	-1.653421
76	1	0	6.673257	1.749634	-1.978996
77	1	0	4.958270	2.011132	-2.358306

78	1	0	5.925811	3.333586	-1.655352
79	6	0	-5.419053	-2.264213	0.414299
80	1	0	-5.731732	-1.007255	-1.183790
81	8	0	-4.606093	-2.880688	1.114525
82	6	0	-6.878585	-2.201383	0.797344
83	1	0	-6.960753	-1.787654	1.805865
84	1	0	-7.484368	-1.604897	0.111029
85	1	0	-7.274390	-3.220229	0.829739

TS5(i), the rate-determining step in the ion-pair containing (withionization) reaction. mu = 104.45 icm-1

ts5i.highf.chk E(RB3PW91) = -2302.145010 a.u.
Thermal correction to Gibbs Free Energy= 0.612040 a.u.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.409158	-0.040392	0.965846
2	6	0	-1.695733	0.262378	0.515394
3	6	0	0.322154	0.290449	2.230753
4	8	0	-1.779441	1.582501	0.776748
5	8	0	1.100860	1.028834	2.921894
6	6	0	-2.006955	-0.550398	1.786882
7	6	0	-0.946455	-0.259619	2.865297
8	1	0	-2.960560	-0.152637	2.152212
9	1	0	-0.712579	-1.174117	3.421356
10	6	0	1.488055	0.495821	0.171196
11	7	0	-2.200303	-1.950754	1.495540
12	1	0	-1.617775	0.610722	-2.043689
13	6	0	2.367665	-0.610324	-0.395045
14	1	0	1.066476	1.024165	-0.690182
15	1	0	2.116266	1.194777	0.734822
16	8	0	-0.348655	-2.446746	-1.624805
17	1	0	-0.906998	-1.757755	-1.223077
18	1	0	0.526445	-2.030014	-1.704738
19	8	0	-1.858034	-0.173513	-0.639751
20	1	0	-2.011904	2.106621	-0.057403
21	1	0	-1.315120	0.466066	3.594851
22	8	0	-1.489782	1.156951	-2.876520
23	1	0	-1.707718	0.591899	-3.626223
24	1	0	-0.141662	2.030384	-2.925751
25	8	0	2.186992	-1.055132	-1.554437
26	7	0	3.333568	-1.067090	0.406924
27	6	0	4.186668	-2.153784	0.016818
28	1	0	3.500624	-0.594250	1.322113
29	6	0	5.597156	-1.710040	-0.368974
30	1	0	4.230613	-2.893843	0.824230
31	1	0	3.742009	-2.632916	-0.863215
32	6	0	-3.317341	-2.436604	0.904588
33	1	0	-1.384628	-2.576014	1.426868
34	8	0	-3.418166	-3.604918	0.517449
35	6	0	-4.512392	-1.491651	0.765263
36	7	0	-5.454099	-2.049879	-0.170309

37	1	0	-4.970105	-1.346687	1.755331
38	1	0	-4.219262	-0.508489	0.395713
39	1	0	1.265850	2.540757	2.222490
40	8	0	1.418497	3.409667	1.744956
41	1	0	1.312632	4.101646	2.407252
42	1	0	4.128486	1.216808	2.354095
43	8	0	3.801514	0.368850	2.720067
44	1	0	2.883144	0.572869	2.997135
45	1	0	-3.144594	2.209016	1.982019
46	8	0	-4.053909	2.340659	2.305470
47	1	0	-4.021291	3.043377	2.962339
48	8	0	4.747378	1.767402	-1.384963
49	1	0	5.098843	0.872044	-1.134135
50	1	0	5.497300	2.241494	-1.762473
51	1	0	3.438043	1.486092	-2.511290
52	8	0	2.639984	1.198597	-3.019720
53	1	0	2.422699	0.303444	-2.660820
54	1	0	3.340415	3.167060	1.375798
55	8	0	4.238595	2.796390	1.316332
56	1	0	4.376275	2.557706	0.383616
57	8	0	0.665970	2.625735	-2.845229
58	1	0	0.568471	3.167605	-1.977162
59	1	0	1.572891	2.022545	-2.902679
60	1	0	-1.393906	-4.475690	0.533017
61	8	0	-0.504727	-4.103667	0.635518
62	1	0	-0.338773	-3.651817	-0.219526
63	1	0	-4.958633	2.518603	0.640580
64	8	0	-5.066005	2.556268	-0.328014
65	1	0	-5.464156	1.703872	-0.587964
66	1	0	0.571264	3.736710	0.156618
67	8	0	0.202830	3.962282	-0.728387
68	1	0	-0.765719	3.983258	-0.656708
69	8	0	-2.610538	3.084980	-1.159804
70	1	0	-2.485702	2.648179	-2.019323
71	1	0	-3.582799	2.973573	-0.935149
72	8	0	5.854972	-0.585723	-0.811342
73	7	0	6.540561	-2.664007	-0.236902
74	1	0	6.266194	-3.549231	0.163208
75	6	0	7.926732	-2.483888	-0.623580
76	1	0	8.024654	-1.496036	-1.073762
77	1	0	8.585433	-2.544033	0.248443
78	1	0	8.224466	-3.242932	-1.353345
79	6	0	-6.164573	-1.273264	-1.018637
80	1	0	-5.368526	-3.048883	-0.321022
81	8	0	-6.144236	-0.037537	-0.971806
82	6	0	-7.017699	-1.999032	-2.032356
83	1	0	-8.063416	-1.722564	-1.871702
84	1	0	-6.739266	-1.657387	-3.032823
85	1	0	-6.923076	-3.086433	-1.982491

The result of ADMP step 4500 (i.e., 450 femtoseconds starting from TS4(n) in Figure 1)
luckw3a.log
Symmetry turned off by external request.
Stoichiometry C13H47N5O20
Full point group C1 NOp 1
Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.903015	-0.790742	0.665783
2	6	0	1.947012	0.645838	0.746483
3	6	0	-0.671205	0.043936	-0.360164
4	8	0	1.626356	1.841735	1.262859
5	8	0	-1.426580	1.031939	-0.506967
6	6	0	1.847830	0.665933	-0.780149
7	6	0	0.599752	-0.196616	-1.157148
8	1	0	1.708495	1.671705	-1.128683
9	1	0	0.903231	-1.236311	-1.037295
10	6	0	-2.025301	-0.599887	1.590529
11	7	0	2.977748	-0.053260	-1.409713
12	1	0	-6.444752	-0.257961	1.284355
13	6	0	-3.306668	-1.131784	0.950105
14	1	0	-1.826352	-1.192782	2.489259
15	1	0	-2.159652	0.491519	1.732466
16	8	0	0.037519	-3.163781	-0.761294
17	1	0	-0.420263	-1.704919	0.539287
18	1	0	-0.627199	-3.803235	-0.462788
19	8	0	2.244286	-0.351876	1.420940
20	1	0	2.005712	2.098647	2.188661
21	1	0	0.376109	0.033807	-2.221125
22	8	0	2.284559	-3.324942	0.862283
23	1	0	0.847703	-3.437596	-0.251592
24	1	0	1.657975	-3.434561	1.630635
25	8	0	-3.375230	-2.291834	0.494762
26	7	0	-4.354068	-0.294834	1.022025
27	6	0	-5.716897	-0.763461	0.642535
28	1	0	-4.278598	0.674772	1.451835
29	1	0	-5.784260	-1.855701	0.777230
30	1	0	2.378230	-2.333517	0.864817
31	6	0	-5.857494	-0.280976	-0.787802
32	6	0	4.316218	0.186296	-1.564303
33	1	0	2.738763	-0.917613	-1.947576
34	8	0	5.042332	-0.717860	-1.995939
35	6	0	5.055806	1.472650	-1.261815
36	1	0	5.785466	1.706744	-2.048351
37	7	0	4.193517	2.649048	-1.069216
38	1	0	5.599486	1.356852	-0.305264
39	1	0	-2.583788	4.114955	0.534108
40	8	0	-3.563743	3.964750	0.518669
41	1	0	-3.760908	3.568831	-0.344079
42	1	0	-4.834141	2.074528	-1.473237
43	8	0	-3.974526	2.493628	-1.697547
44	1	0	-3.295817	1.902198	-1.331834
45	1	0	4.811328	-2.547441	-0.607643

46	8	0	4.636665	-3.497655	-0.610913
47	1	0	3.785059	-3.597337	-0.193423
48	8	0	-4.380049	2.110751	2.125606
49	1	0	-4.024823	2.869382	1.533975
50	1	0	-4.211479	2.396584	3.034110
51	1	0	-2.394004	-3.615854	0.711551
52	8	0	-1.779829	-4.339084	0.981015
53	1	0	-2.321187	-5.151811	0.967229
54	1	0	-0.903814	2.868961	-0.252699
55	8	0	-0.773452	3.694734	0.260388
56	1	0	-0.245602	3.405691	0.971781
57	8	0	0.212514	-3.491444	2.699254
58	1	0	0.134921	-2.532964	2.948668
59	1	0	-0.575438	-3.743433	2.145319
60	1	0	4.638130	-2.591393	-3.423215
61	8	0	4.196711	-3.477408	-3.287337
62	1	0	4.194176	-3.614585	-2.283852
63	8	0	1.956104	-2.165950	-2.906943
64	1	0	2.712879	-2.746266	-3.180831
65	1	0	1.291354	-2.769314	-2.549295
66	1	0	1.244527	-0.653599	2.986078
67	8	0	0.561801	-0.863567	3.655575
68	1	0	0.957667	-1.356400	4.352091
69	8	0	2.914092	2.995686	3.186551
70	1	0	3.208157	2.762131	4.094235
71	1	0	3.742958	3.146078	2.607729
72	8	0	-6.230025	0.887602	-0.952188
73	7	0	-5.404240	-1.081820	-1.786832
74	1	0	-4.987574	-1.995755	-1.624841
75	6	0	-5.377201	-0.528508	-3.119067
76	1	0	-6.176008	0.200824	-3.318175
77	1	0	-4.483891	0.086633	-3.350145
78	1	0	-5.466616	-1.256680	-3.887739
79	6	0	4.070666	3.336263	0.088011
80	1	0	3.704042	2.987665	-1.893711
81	8	0	4.691507	3.006998	1.112691
82	6	0	3.061804	4.481650	0.113496
83	1	0	2.776650	4.708395	1.173276
84	1	0	3.651515	5.356977	-0.255369
85	1	0	2.137687	4.407901	-0.517681

Standard basis: 6-31G(d) (6D, 7F)
664 basis functions
160 alpha electrons 160 beta electrons
nuclear repulsion energy 5515.4551046180 Hartrees.
NAtoms= 85 NActive= 85
SCF Done: E(RB3LYP) = -2302.00143821 A.U. after 1 cycles
Convg = 0.2000D+01 -V/T = 2.0090
ADMP step 4500
Summary information for step 4500
Time (fs) 450.000000
EKinC = 0.0650329; EKinPA = 0.0019471; EKinPB = 0.0019471
EKin = 0.0689270; EPot=-2302.0014382; ETot=-2301.9325112
ETot-EKinP = -2301.9364053

The result of ADMP step 4500 (i.e., 450 femtoseconds starting from TS5(i) in Figure 3)
vuc2p8.log
Symmetry turned off by external request.
Stoichiometry C13H47N5O20

Full point group C1 NOp 1
Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.240133	-0.322893	-1.223964
2	6	0	1.201059	-0.147149	-0.883174
3	6	0	-0.486546	-0.700390	-2.501157
4	8	0	1.456032	1.350556	-1.307827
5	8	0	-1.574556	-0.689407	-3.095451
6	6	0	1.895953	-0.999884	-1.999122
7	6	0	0.859524	-1.031993	-3.122152
8	1	0	2.760135	-0.468654	-2.313934
9	1	0	0.759942	-1.970797	-3.737127
10	6	0	-1.225780	0.219053	-0.323404
11	7	0	2.245892	-2.320587	-1.508183
12	1	0	1.776928	0.365076	1.988586
13	6	0	-2.266527	-0.738332	0.274231
14	1	0	-0.648112	0.575855	0.547168
15	1	0	-1.811055	0.998521	-0.855940
16	8	0	0.643867	-2.209354	1.872255
17	1	0	1.010722	-1.494160	1.291315
18	1	0	-0.325059	-1.961007	1.837039
19	8	0	1.564818	-0.282953	0.359594
20	1	0	1.855625	1.630585	-0.467104
21	1	0	1.037082	-0.292689	-3.838902
22	8	0	1.686442	0.280570	2.971268
23	1	0	1.364340	-0.640141	3.026215
24	1	0	0.630575	1.445247	3.391974
25	8	0	-2.134703	-1.267523	1.417215
26	7	0	-3.388252	-0.880452	-0.455744
27	6	0	-4.459302	-1.718366	-0.023260
28	1	0	-3.532083	-0.424504	-1.393736
29	6	0	-5.675409	-0.838753	0.312002
30	1	0	-4.665588	-2.524853	-0.753653
31	1	0	-4.095332	-2.196160	0.880244
32	6	0	3.358732	-2.581650	-0.732641
33	1	0	1.497464	-3.007454	-1.364498
34	8	0	3.495709	-3.677615	-0.170085
35	6	0	4.481571	-1.520153	-0.665467
36	7	0	5.137001	-1.578900	0.651421
37	1	0	5.236691	-1.625284	-1.470566
38	1	0	4.158865	-0.501235	-0.735186
39	1	0	0.060201	2.496054	-1.003359
40	8	0	-0.408644	3.309290	-0.696214
41	1	0	-0.047035	3.994512	-1.251674
42	1	0	-3.927713	1.444422	-2.453745
43	8	0	-4.118273	0.548507	-2.832180
44	1	0	-3.302676	0.448025	-3.368893

45	1	0	2.560459	1.562328	-2.497602
46	8	0	3.437001	1.425839	-2.946442
47	1	0	3.418123	2.111053	-3.666983
48	8	0	-4.016226	2.371110	1.328051
49	1	0	-4.600078	1.560315	1.281159
50	1	0	-4.499355	3.060342	1.774207
51	1	0	-2.973725	1.613485	2.406424
52	8	0	-2.352387	1.097600	3.015907
53	1	0	-2.244761	0.249528	2.546854
54	1	0	-2.527594	3.231653	-1.435344
55	8	0	-3.471698	2.954297	-1.416149
56	1	0	-3.633895	2.766536	-0.463820
57	8	0	-0.117570	2.104725	3.548128
58	1	0	0.102516	2.915781	2.888632
59	1	0	-1.106574	1.645408	3.265953
60	1	0	1.807734	-4.550073	0.098515
61	8	0	0.846819	-4.421985	0.059473
62	1	0	0.702146	-3.685943	0.734984
63	1	0	4.536602	2.209717	-1.627914
64	8	0	4.763169	2.885650	-0.976285
65	1	0	5.422053	2.411209	-0.448589
66	1	0	0.103564	3.697971	0.999539
67	8	0	0.574591	3.887598	1.839860
68	1	0	1.491795	3.658416	1.595508
69	8	0	2.844873	2.630587	1.008884
70	1	0	3.333313	1.854188	1.347311
71	1	0	3.464704	2.998469	0.295892
72	8	0	-5.558176	0.233673	0.902269
73	7	0	-6.869103	-1.303421	-0.114376
74	1	0	-6.916160	-2.079889	-0.768289
75	6	0	-8.030939	-0.455898	0.167247
76	1	0	-7.846903	0.224357	0.950171
77	1	0	-8.429791	0.066124	-0.737696
78	1	0	-8.790497	-1.132380	0.506779
79	6	0	5.263489	-0.448125	1.382007
80	1	0	5.217975	-2.497905	1.064189
81	8	0	5.093219	0.691587	0.905360
82	6	0	5.570230	-0.695868	2.841289
83	1	0	6.252235	0.099064	3.299299
84	1	0	4.629166	-0.700787	3.408974
85	1	0	6.095196	-1.620286	2.997351

Rotational constants (GHZ): 0.1233462 0.0548249 0.0514614
Standard basis: 6-31G(d) (6D, 7F)
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned off.
664 basis functions
160 alpha electrons 160 beta electrons
nuclear repulsion energy 5674.3970890666 Hartrees.
NAtoms= 85 NActive= 85
SCF Done: E(RB3LYP) = -2302.00945535 A.U. after 1 cycles
Convg = 0.2000D+01 -V/T = 2.0089

Summary information for step 4500

```
 Time (fs)   450.000000
 EKinC     =      0.0605922; EKinPA = 0.0018104; EKinPB = 0.0018104
 EKin      =      0.0642130; EPot=-2302.0094554; ETot   =-2301.9452423
 ETot-EKinP =  -2301.9488632
=====================================================================
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(15) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr. J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision B.01, Gaussian, Inc.: Wallingford CT, 2010.