Electronic Supplementary Information

Frontier Orbitals and Transition States in the Oxidation and Degradation of L-Ascorbic Acid: A DFT Study

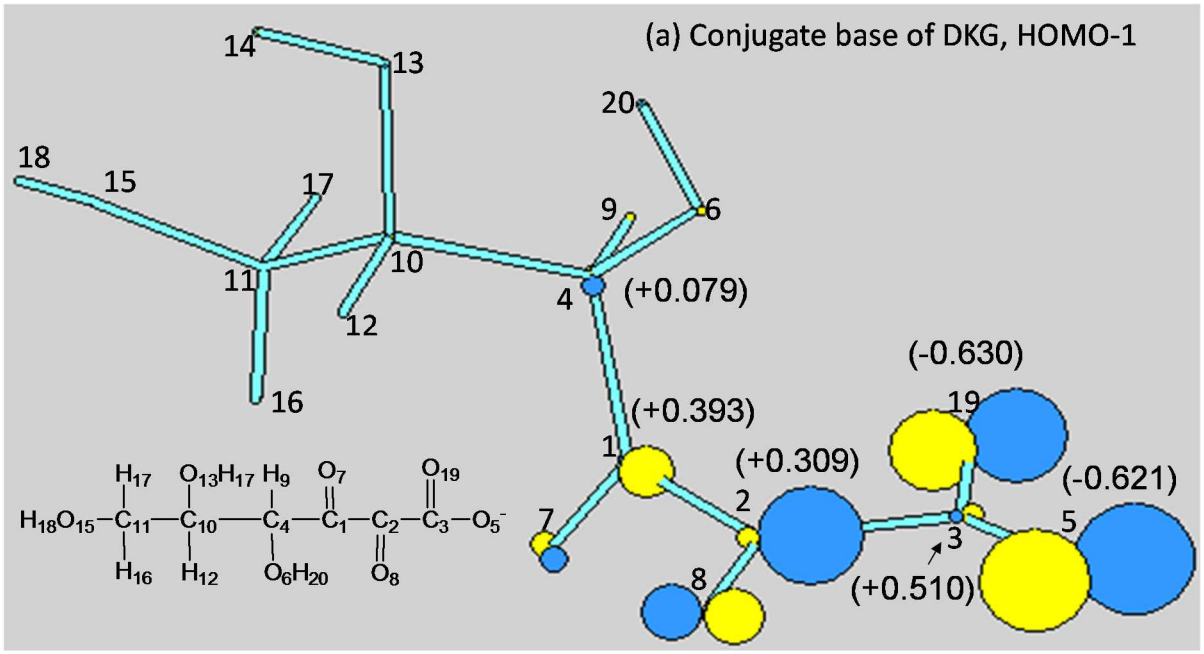
Shinichi Yamabe,[a]* Noriko Tsuchida,[b] Shoko Yamazaki[c] and Shigeyoshi Sakaki[a]

[a]*Fukui Institute for Fundamental Chemistry, Kyoto University, Takano-Nishihiraki-cho 34-4, Sakyou-ku, Kyoto 606-8103, Japan*

[b]*Department of Liberal Arts, Faculty of Medicine, Saitama Medical University, 38 Morohongo, Moroyama-machi, Iruma-gun, Saitama 350-0495 Japan*

[c]*Department of Chemistry, Nara University of Education, Takabatake-cho, Nara 630-8528, Japan*

email:yamabes@fukui.kyoto-u.ac.jp



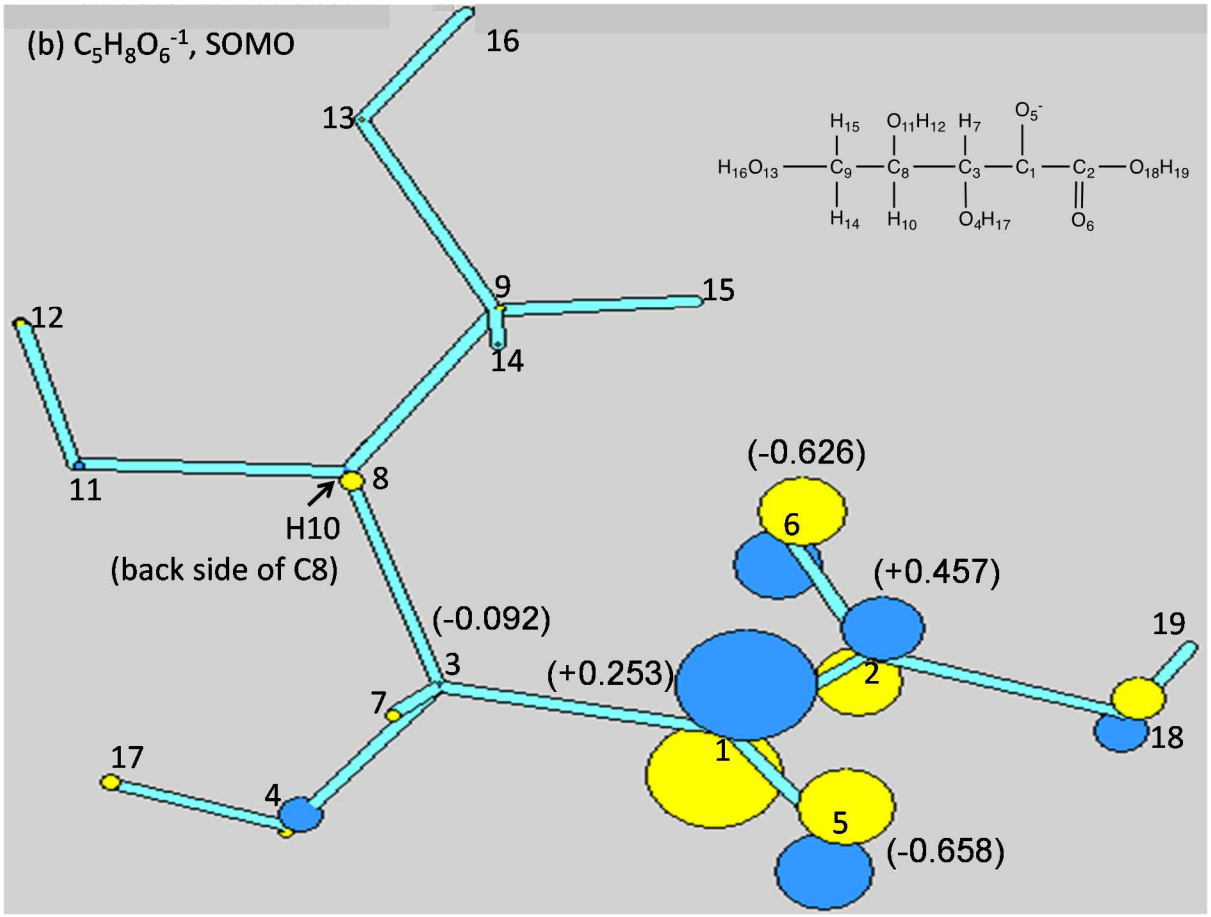


Figure S1. Frontier orbitals, HOMO-1 and SOMO. (a) HOMO-1 of the conjugate base of DKG, and (b) SOMO of (HO)CH_2-CH(OH)-CH(OH)-C·(-O^-)-COOH. Values in parentheses are Mulliken electronic charges. In Figure S1(a), the largest lobe of HOMO-1 is at the either

carboxylate oxygen atom, O(5) or O(19). The OH· radical might add to it. To check the possibility of whether the carboxylate oxygen is bound to OH· a model adduct geometry of Me-C(=O)O-OH·⁻ was optimized. However, the optimization leads to a different geometry, Me-C(=O)-O⁻·····H-O·. Thus, while the addition is apparently likely according to the (HOMO-1) extension, the adduct is unstable (thermodynamically unlikely).

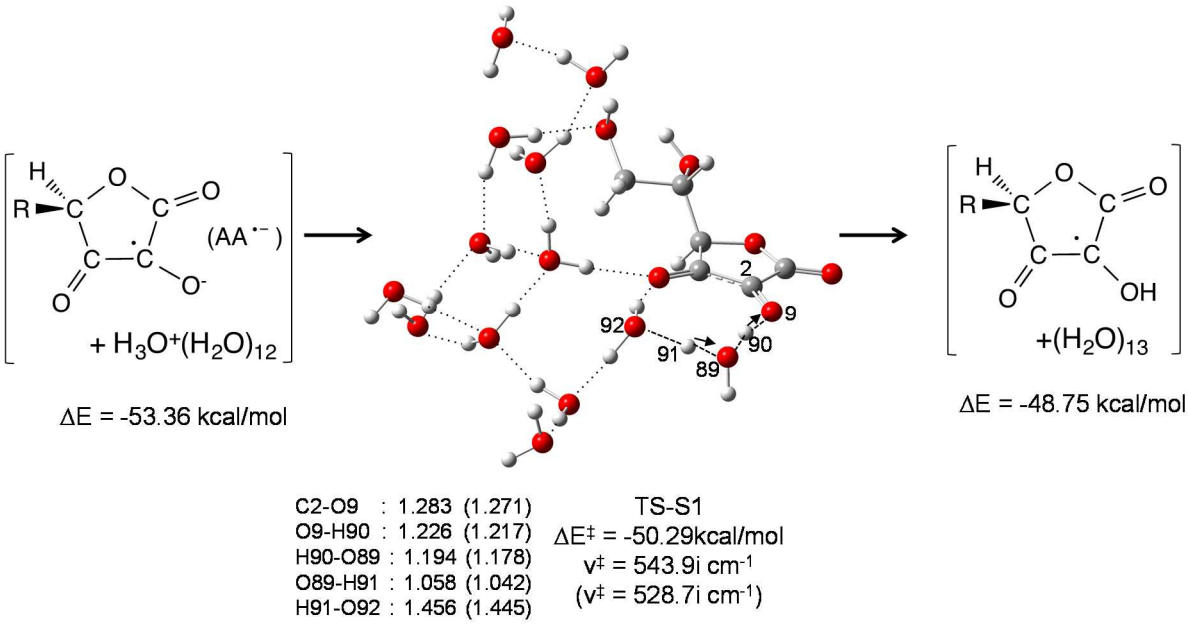


Figure S2. A proton-shift TS from the ascorbate anion radical (AA·⁻) to the neutral radical. ΔE = -53.36 kcal/mol is taken from Figure 1. The apparent instability of ΔE = -48.75 kcal/mol relative to ΔE = -50.29 kcal/mol (TS) comes from splice of electronic and zero-point vibrational energies. The electronic energies are -1677.786533 a.u. (TS-S1) and -1677.787476 a.u. (product), which is in the correct stability order.

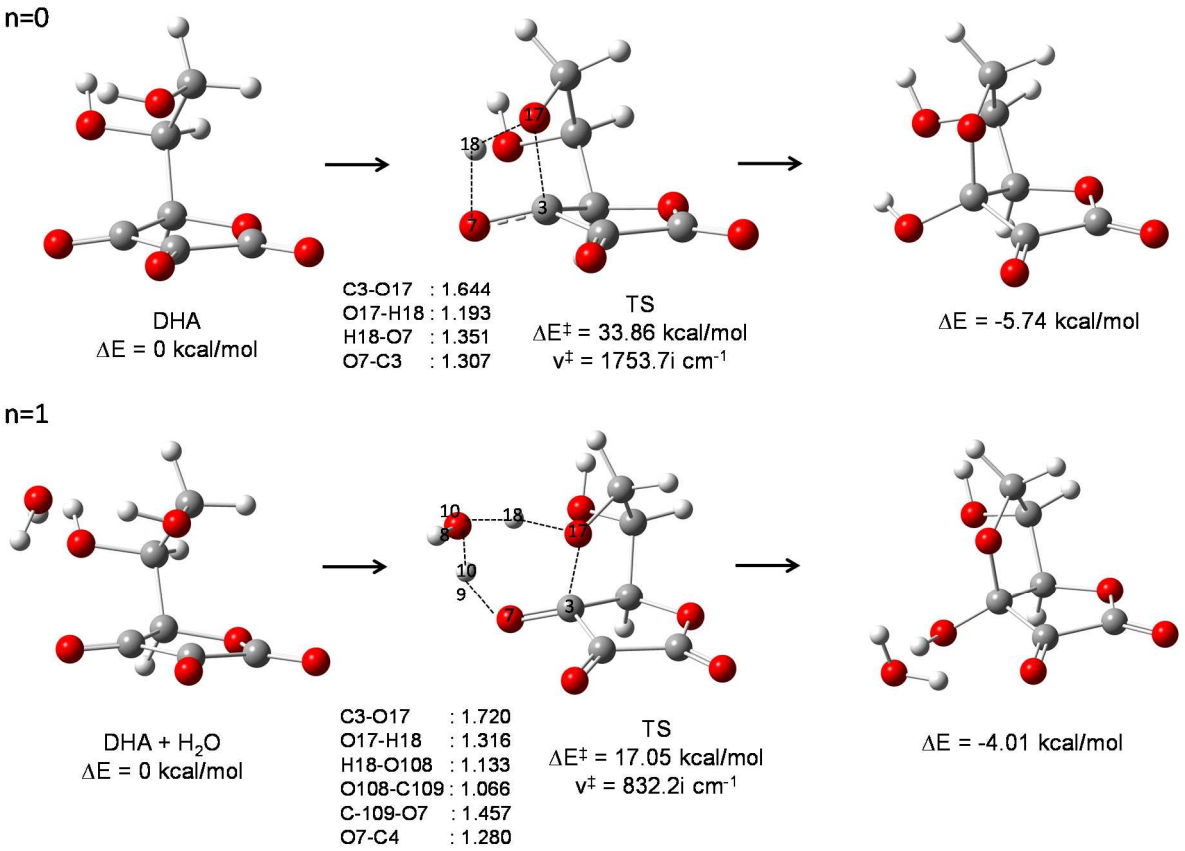


Figure S3 (continued)

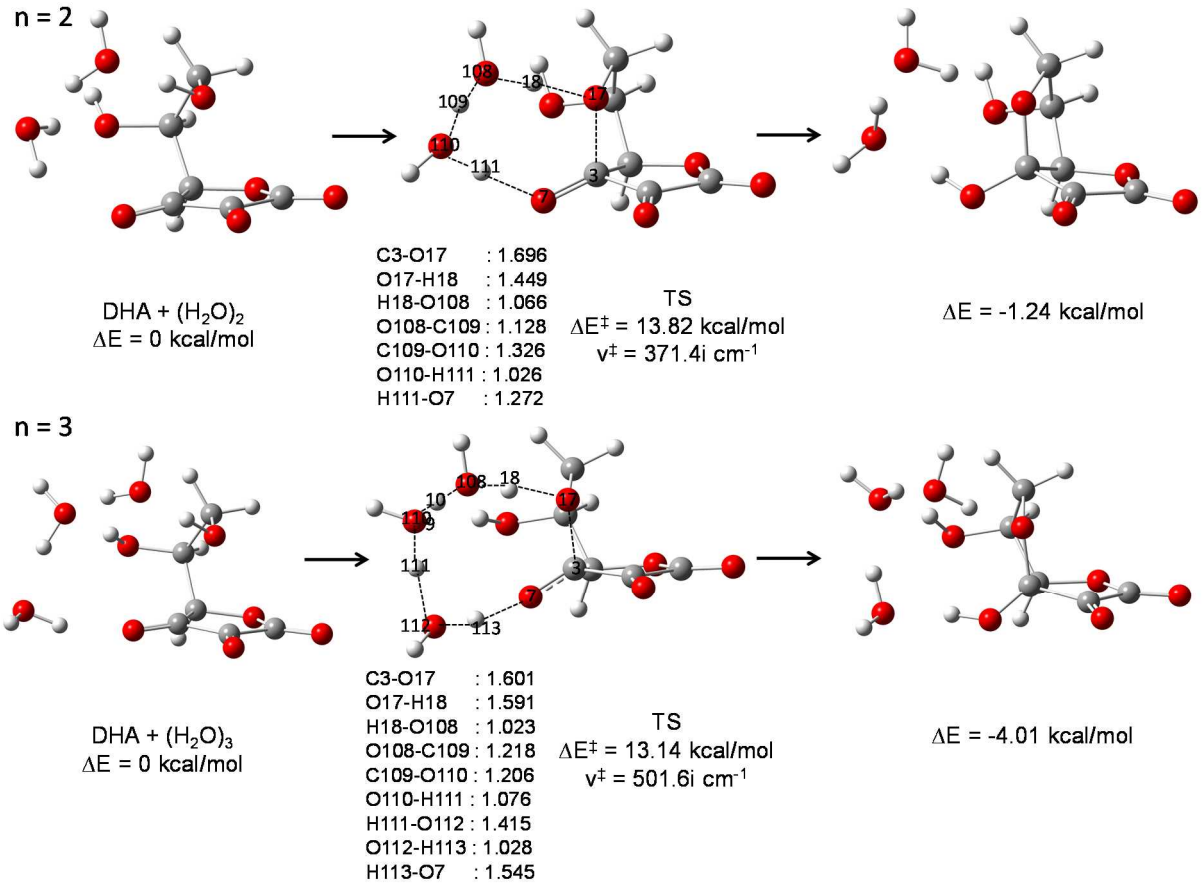


Figure S3. Geometric changes of ring-closure reactions of DHA + $(H_2O)_n$, n=0, 1, 2 and 3. The activation energy (in kcal/mol) was obtained by the difference of the sum of electronic and vibrational energies between TS and DHA + $(H_2O)_n$, $\Delta E^{\ddagger}$. $\Delta E^{\ddagger}$ = +33.86 for n=0, $\Delta E^{\ddagger}$ = +17.05 for n=1, $\Delta E^{\ddagger}$ = +13.82 for n=2 and $\Delta E^{\ddagger}$ = +13.14 for n=3. Thus, n=0 and n=1 reactions are ruled out by the large energies. While that of n=2 is slightly larger than that of n=3, the small difference indicates that the n=2 reaction is more likely by the smaller entropy loss in formation of the water cluster.

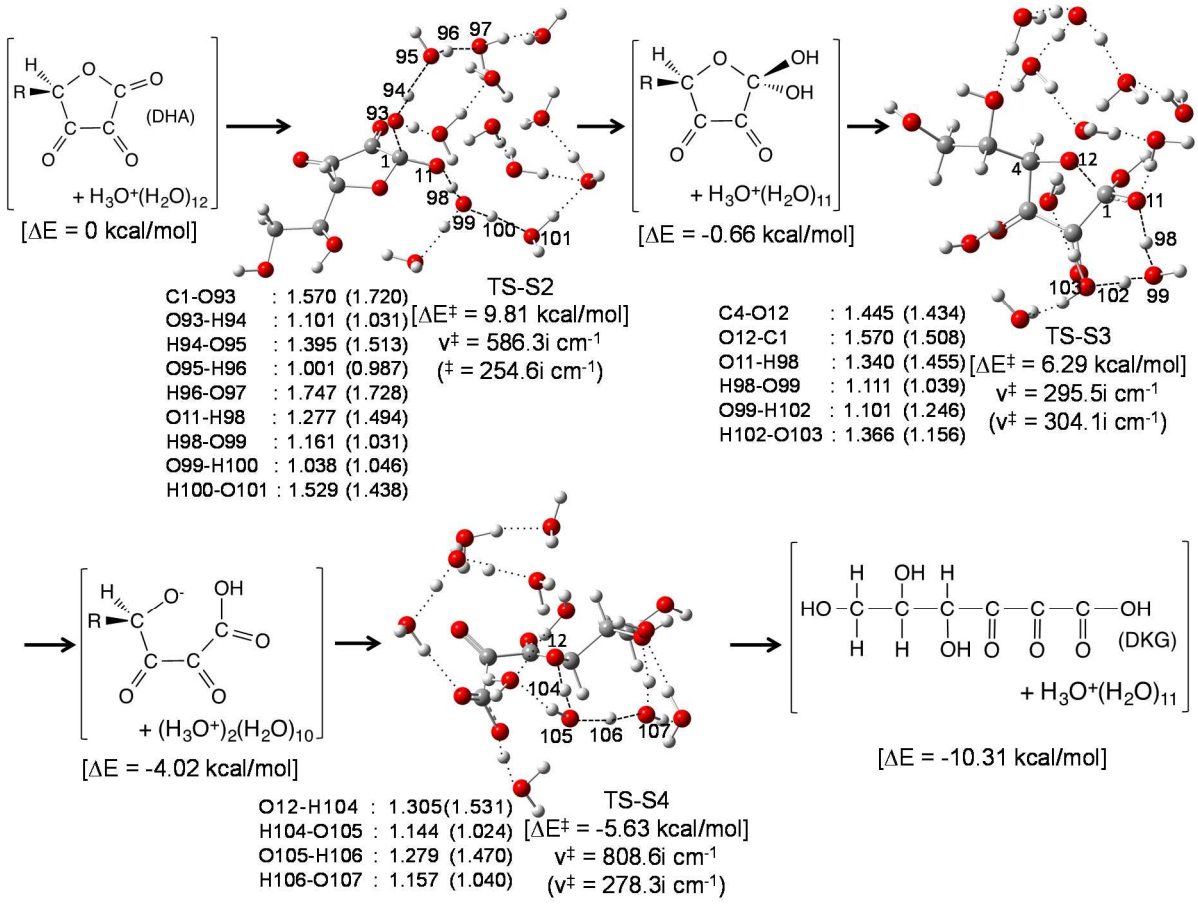


Figure S4. The acid catalyzed ring opening (ester hydrolysis) of DHA to DKG. Relative energies in square brackets are also shown in Figure 4.

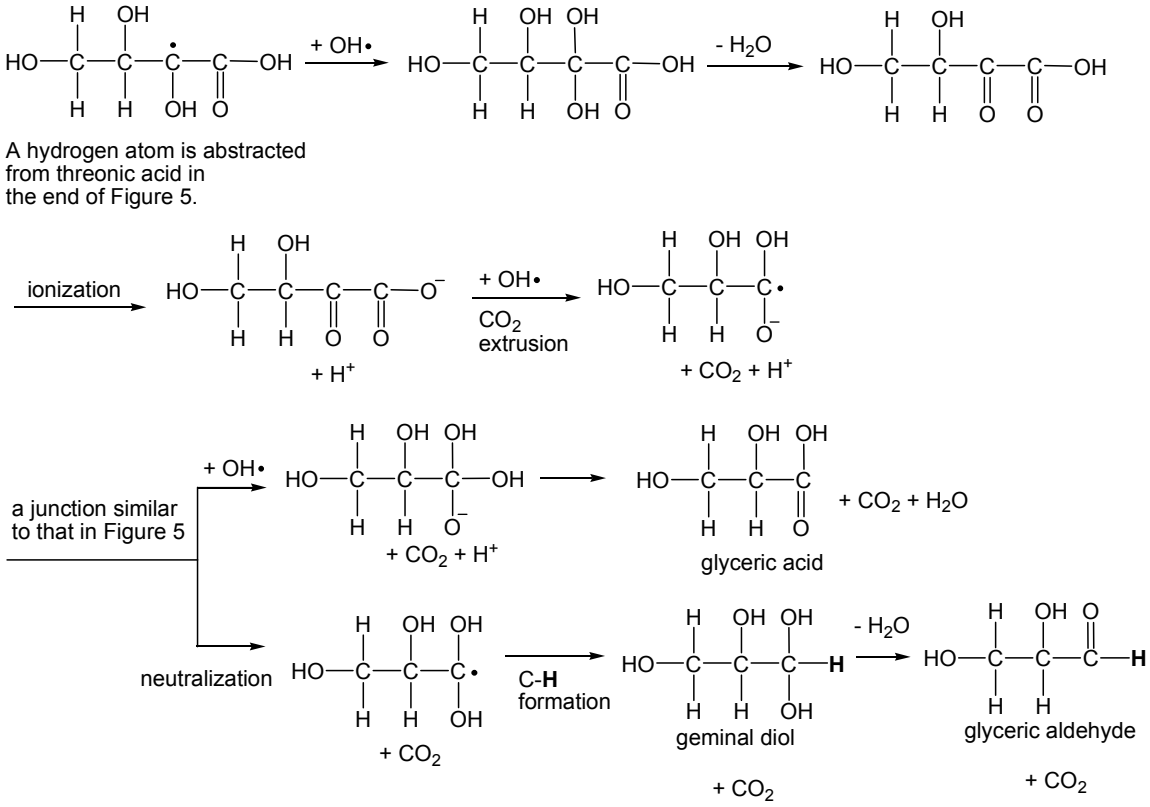


Figure S5. Degradation from the C-H cleaved radical of threonic acid to glyceric aldehyde and acid.

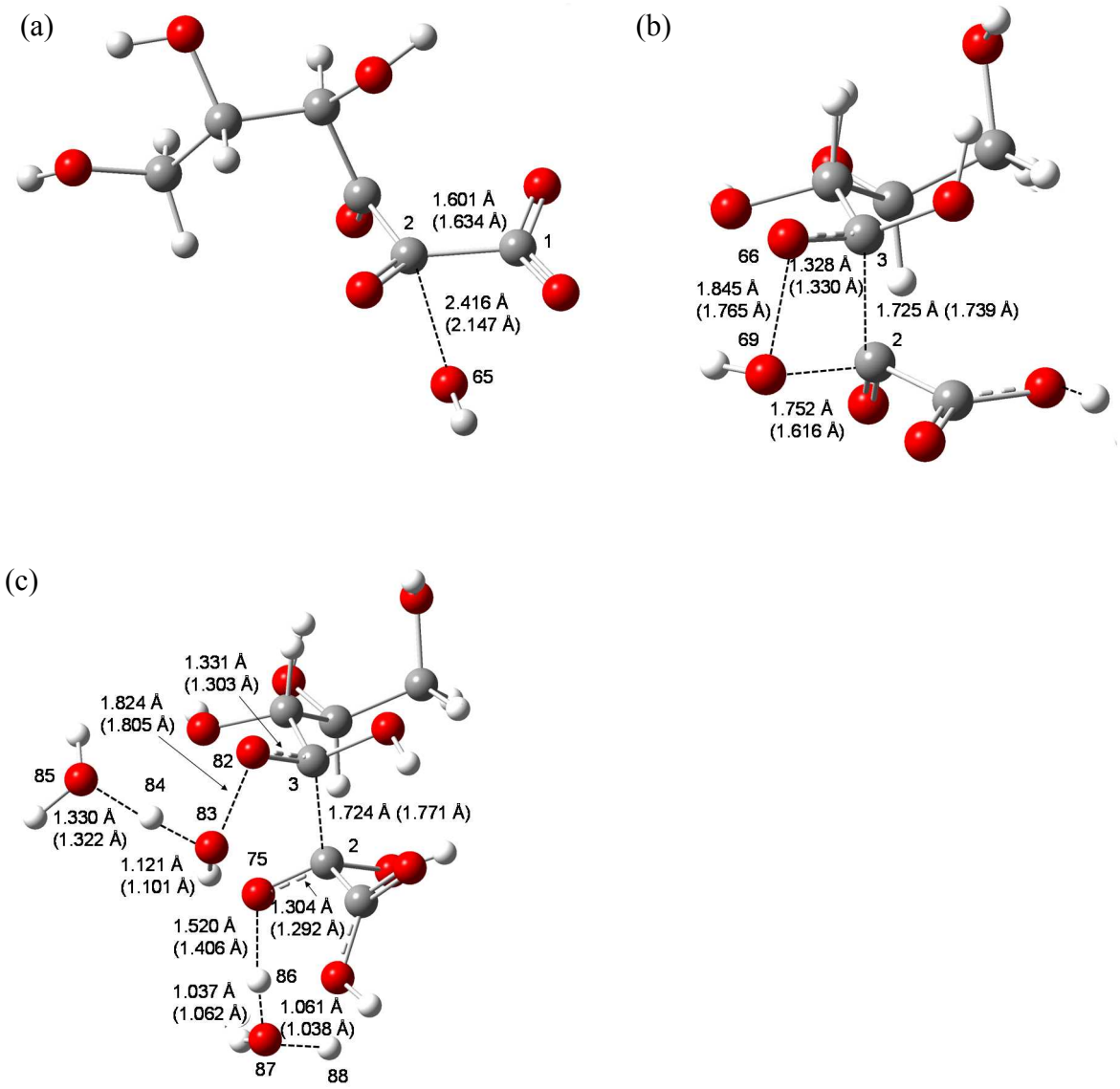


Figure S6. TS geometries showing bond interchanges for the degradation. They are central parts of (a) TS13 in Figure 4, (b) TS19 in Figure 6 and (c) TS21 in Figure 7, respectively.

Detailed definition of all species in Scheme 1.

AAH_2 is *R*-(3,4)-dihydroxy-5-((*S*)-1,2-dihydroxyethyl)furan-2(5*H*)-one). $AA^{\cdot -}$ is the anion radical (ascorbate free radical). DHA is dehydroascorbic acid. DKG is diketogulonic acid (4,5,6-trihydroxy-2,3-dioxohexanoic acid). BH is a bicyclic hemiketal (2,6-dioxa-4,4,5,8-tetrahydroxybicyclo[3.3.0]octan-3-one). THDH is 4,5,5,6-tetrahydroxy-2,3-dioxohexanoic acid. L-xylonic and L-lyxonic acids are 2,3,4,5-tetrahydroxypentanoic acids with *R* and *S* configurations at C3 (the atom numbering in Scheme 1), respectively.

Explanation for each step in Scheme 5.

We start by considering the reaction steps in Scheme 5**(A)**.

step [a]: the electrolytic dissociation of AAH_2, TS1 in Fig.1.

step [b]: the electrophilic addition of $OH\cdot$ to AAH^-, TS2.

step [c]: dehydration form the adduct leading to the anion radical $AA^{\cdot -}$, TS3.

step [d]: the electrophilic addition of $OH\cdot$ to $AA^{\cdot -}$ (the radical-radical recombination).

step [e]: dehydration of the adduct leading to DHA, TS4 in Fig. 3.

step [f]: ring closure with aid of two water molecules after the rotation of the side chain (-R), TS5 and TS6.

step [g]: hydration leading to BH, TS7. Ring opening of the hemiketal gives an unstable species, and BH is the intermediate of the reversible process.

step [h]: the opening of the lactone ring of DHA (ester hydrolysis) leading to DKG, TS10 and TS11 in Fig. 4 and Scheme 4.

We then consider the steps in Scheme 5**(B)**.

step [i]: the electrolytic dissociation of DKG, TS12 in Figure 4.

step [j]: the electrophilic $OH\cdot$ addition to the carboxylate along with the CO_2 elimination (degradation), TS13.

step [k]: the $OH\cdot$ addition to the anion radical (radical-radical recombination).

step [l]: the dehydration leading to L-threo-2-pentulosonic acid, R-CH(OH)-C(=O)-COOH.

step [m]: similar to the step [i].

step [n]: similar to the step [j].

step [o]: similar to the step [k].

step [p]: similar to the step [l].

step [q]: protonation leading to the neutral radical R-CH(OH)-C·(OH)-COOH, TS14 in Figure 6.

step [r]: the hydrogen abstraction by the radical TS15 in Figure 6. (The planarity at the radical center, C3, may afford stereochemical isomers, L-xylonic and L-lyxonic acids.)

Finally we examine the steps in Scheme 5**(C)**.

step [s]: the electrophile DKG subject to the nucleophilic addition of H_2O_2 via HO_2^- + H^+, TS16 in Figure 7.

step [t]: neutralization of the adduct, TS18 in Figure 7.

step [u]: the C2-C3 cleavage leading to two carboxylic acids, TS19 in Figure 7 and TS21 in Figure 8.

Cartesian coordinates of the optimized geometries
and energies by B3LYP/ 6-31G* SCRF=(PCM, solvent=water)

==== Precursor in Figure 1, AAH2 + OH(.) + (H2O)12====

vitacoh2k.for.txt
Stoichiometry C6H33O19(2)

Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.482930	-0.938012	0.183250
2	6	0	-3.799801	-1.189943	0.329012
3	6	0	-4.215741	-2.163767	-0.665760
4	6	0	-1.966623	-1.788895	-0.965516
5	8	0	-5.331961	-2.615217	-0.845478
6	8	0	-3.135057	-2.513549	-1.423537
7	8	0	-1.759084	-0.110920	0.948592
8	1	0	-0.901840	0.260471	0.541907
9	8	0	-4.678525	-0.642256	1.214445
10	1	0	-5.557639	-1.012853	1.008850
11	1	0	-1.631591	-1.169479	-1.806680
12	6	0	-0.855883	-2.794748	-0.629503
13	6	0	0.444071	-2.065616	-0.272672
14	1	0	-1.187055	-3.423775	0.211673
15	8	0	-0.638961	-3.583891	-1.789349
16	1	0	0.250972	-3.963569	-1.663121
17	8	0	1.553485	-2.965905	-0.354028
18	1	0	0.387823	-1.619390	0.721849
19	1	0	0.615782	-1.271866	-1.005524
20	1	0	1.860091	-3.133276	0.574916
21	8	0	0.444060	1.027129	0.221041
22	1	0	0.284341	2.015553	0.323743
23	1	0	1.141932	0.743007	0.882628
24	8	0	2.496080	0.054064	1.656611
25	1	0	2.359378	-0.817034	2.087286
26	1	0	2.990856	-0.205418	0.843627
27	8	0	-0.052098	3.623165	0.114642
28	1	0	0.469452	3.801502	-0.720277
29	1	0	-1.016799	3.623429	-0.134358
30	8	0	3.485588	-0.976430	-0.743227
31	1	0	2.889674	-1.762252	-0.771872
32	1	0	3.108417	-0.314326	-1.371646
33	8	0	2.566390	-2.731676	2.114028
34	1	0	3.545940	-2.874131	1.976930
35	1	0	2.323984	-3.276363	2.879801
36	8	0	1.519622	3.833064	-2.076533
37	1	0	2.328378	4.303846	-1.764174
38	1	0	1.797680	2.895304	-2.157963
39	8	0	5.207736	-3.188039	1.644596
40	1	0	5.715757	-2.586759	2.223172
41	1	0	6.241411	-2.404886	-0.250449
42	8	0	5.947703	-1.609238	0.221906
43	1	0	5.081602	-1.374328	-0.200657
44	8	0	1.981644	0.986040	-2.017902
45	1	0	1.335154	0.975249	-1.258841
46	1	0	1.480134	0.664464	-2.785461
47	8	0	-2.741525	3.976627	0.014542
48	1	0	-3.084386	3.272919	0.619409
49	1	0	-2.481978	4.705621	0.620906
50	8	0	3.787823	5.170847	-1.147474
51	1	0	3.981398	5.876165	-1.786222
52	1	0	3.504032	5.650537	-0.352276
53	8	0	-3.497493	1.996504	1.816226
54	1	0	-4.266878	1.447794	1.580962
55	1	0	-2.761673	1.363557	1.696676
56	8	0	-1.154259	5.724340	1.573523
57	1	0	-0.516527	5.087949	1.174261
58	1	0	-1.035731	6.530946	1.047061

SCF Done: E(UB3LYP) = -1677.70831166 A.U. after 1 cycles
Zero-point correction= 0.466478 (a.u.)
Thermal correction to Energy= 0.510468

Thermal correction to Enthalpy= 0.511412
Thermal correction to Gibbs Free Energy= 0.384874
Sum of electronic and zero-point Energies= -1677.241834
Sum of electronic and thermal Energies= -1677.197843
Sum of electronic and thermal Enthalpies= -1677.196899
Sum of electronic and thermal Free Energies= -1677.323438

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.324	152.830	266.322

====TS1, ionization TS, AAH2 -> AAH(-) + H(+) ====
vitacoh2k.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.020543	-1.551203	0.156998
2	6	0	-3.239259	-2.144435	0.285811
3	6	0	-3.386224	-3.198251	-0.683847
4	6	0	-1.306827	-2.275500	-0.985295
5	8	0	-4.350008	-3.927503	-0.868932
6	8	0	-2.242254	-3.283680	-1.436436
7	8	0	-1.516905	-0.569735	0.861453
8	1	0	-0.645652	0.263181	0.453763
9	8	0	-4.247590	-1.831550	1.164787
10	1	0	-5.002649	-2.402862	0.931028
11	1	0	-1.134971	-1.599893	-1.832959
12	6	0	0.023167	-2.949951	-0.629366
13	6	0	1.066305	-1.900010	-0.240501
14	1	0	-0.144593	-3.649769	0.204634
15	8	0	0.473626	-3.649156	-1.782434
16	1	0	1.426282	-3.789175	-1.627578
17	8	0	2.384915	-2.458430	-0.287268
18	1	0	0.856881	-1.493484	0.749616
19	1	0	1.033912	-1.086090	-0.970886
20	1	0	2.709053	-2.504811	0.648029
21	8	0	0.130945	1.086955	0.238648
22	1	0	-0.305320	2.094943	0.313980
23	1	0	0.911511	0.984089	0.883821
24	8	0	2.348822	0.763400	1.613572
25	1	0	2.472374	-0.095079	2.076507
26	1	0	2.921859	0.640817	0.818032
27	8	0	-0.816385	3.360685	0.245999
28	1	0	-0.431444	3.704590	-0.611634
29	1	0	-1.811237	3.261311	0.112918
30	8	0	3.653351	-0.001271	-0.717319
31	1	0	3.318368	-0.930197	-0.726496
32	1	0	3.117422	0.497174	-1.378614
33	8	0	3.226522	-1.838774	2.188288
34	1	0	4.209643	-1.700504	2.073689
35	1	0	3.126065	-2.385273	2.983981
36	8	0	0.470910	4.048255	-2.028306
37	1	0	1.147170	4.710015	-1.747820
38	1	0	0.979350	3.220729	-2.164171
39	8	0	5.898274	-1.534340	1.776150
40	1	0	6.198290	-0.788615	2.331428
41	1	0	6.698354	-0.563663	-0.145753
42	8	0	6.182227	0.133301	0.290507
43	1	0	5.294222	0.096854	-0.148358
44	8	0	1.645358	1.401632	-2.066524
45	1	0	1.005693	1.209764	-1.337343
46	1	0	1.274592	0.967195	-2.852792
47	8	0	-3.442322	2.982143	0.013257
48	1	0	-3.590296	2.226179	0.638628
49	1	0	-3.840050	3.759797	0.468657
50	8	0	2.365953	5.920334	-1.200205
51	1	0	2.404969	6.601632	-1.890949
52	1	0	1.974760	6.382605	-0.441084
53	8	0	-3.641560	0.926591	1.833315
54	1	0	-4.291395	0.234051	1.615445
55	1	0	-2.796874	0.458166	1.635658
56	8	0	-4.448123	5.251721	1.325282

57	1	0	-3.643541	5.743674	1.556846
58	1	0	-4.868519	5.804110	0.646293

SCF Done: E(UB3LYP) = -1677.69812896 A.U. after 1 cycles

1	2	3
A	A	A
Frequencies -- -650.9103	11.0745	16.4517

Zero-point correction= 0.459160 (a.u.)
Thermal correction to Energy= 0.503092
Thermal correction to Enthalpy= 0.504036
Thermal correction to Gibbs Free Energy= 0.376756
Sum of electronic and zero-point Energies= -1677.238969
Sum of electronic and thermal Energies= -1677.195037
Sum of electronic and thermal Enthalpies= -1677.194093
Sum of electronic and thermal Free Energies= -1677.321373

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	315.695	151.582	267.883

==== AAH(-) + OH(.) + H3O(+)(H2O)11 ====
vitacoh2k.rev.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.847953	-1.804485	0.125048
2	6	0	-3.011778	-2.518710	0.265843
3	6	0	-3.041456	-3.623752	-0.639391
4	6	0	-1.079201	-2.494087	-1.010018
5	8	0	-3.918989	-4.467874	-0.793300
6	8	0	-1.883293	-3.635278	-1.389236
7	8	0	-1.424933	-0.765355	0.753828
8	1	0	-0.388154	0.491829	0.486426
9	8	0	-4.055292	-2.264552	1.136721
10	1	0	-4.754023	-2.906120	0.912829
11	1	0	-1.027801	-1.833222	-1.885765
12	6	0	0.342368	-2.950075	-0.678057
13	6	0	1.237093	-1.743527	-0.368896
14	1	0	0.308351	-3.627877	0.190282
15	8	0	0.861633	-3.630475	-1.815126
16	1	0	1.829586	-3.589978	-1.698435
17	8	0	2.620546	-2.110433	-0.466549
18	1	0	1.013906	-1.333073	0.616095
19	1	0	1.060690	-0.966934	-1.120162
20	1	0	2.961379	-2.215957	0.459035
21	8	0	0.188463	1.310265	0.468115
22	1	0	-0.690943	2.629757	0.542877
23	1	0	0.943982	1.151354	1.107818
24	8	0	2.465259	0.890531	1.813815
25	1	0	2.642373	-0.010634	2.160063
26	1	0	2.985451	0.883810	0.975382
27	8	0	-1.249335	3.457257	0.334430
28	1	0	-0.856011	3.806021	-0.561056
29	1	0	-2.273535	3.122801	0.203289
30	8	0	3.661161	0.468663	-0.673160
31	1	0	3.381027	-0.474918	-0.759233
32	1	0	3.061838	0.994580	-1.254420
33	8	0	3.505770	-1.715067	2.037481
34	1	0	4.467953	-1.486198	1.897297
35	1	0	3.489972	-2.370432	2.753035
36	8	0	-0.092466	4.185537	-1.840822
37	1	0	0.436407	5.000462	-1.644989
38	1	0	0.570822	3.465304	-1.952869
39	8	0	6.124630	-1.149308	1.548591
40	1	0	6.392421	-0.439118	2.163597
41	1	0	6.753440	0.062505	-0.297783
42	8	0	6.217570	0.675303	0.231068
43	1	0	5.311126	0.621166	-0.168062
44	8	0	1.507240	1.837874	-1.827792
45	1	0	0.966487	1.564318	-1.033312
46	1	0	1.138553	1.336432	-2.574229
47	8	0	-3.584300	2.635475	0.084345

48	1	0	-3.651709	1.821677	0.669906
49	1	0	-4.194909	3.303990	0.488388
50	8	0	1.353160	6.455079	-1.258718
51	1	0	1.094904	7.134881	-1.902432
52	1	0	1.015418	6.793630	-0.413407
53	8	0	-3.580011	0.530881	1.741448
54	1	0	-4.207843	-0.186490	1.537871
55	1	0	-2.716234	0.096761	1.502912
56	8	0	-5.244595	4.517300	1.215259
57	1	0	-4.678043	5.239957	1.531427
58	1	0	-5.759081	4.920957	0.497260

SCF Done: E(UB3LYP) = -1677.70608651 A.U. after 1 cycles
Zero-point correction= 0.463480 (a.u.)
Thermal correction to Energy= 0.507257
Thermal correction to Enthalpy= 0.508201
Thermal correction to Gibbs Free Energy= 0.380957
Sum of electronic and zero-point Energies= -1677.242607
Sum of electronic and thermal Energies= -1677.198830
Sum of electronic and thermal Enthalpies= -1677.197886
Sum of electronic and thermal Free Energies= -1677.325130

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	318.308	151.165	267.808

==== TS2 in Figure 1 OH(.) addition to AAH(-) ====
vitacoh2f.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.464063	-1.483490	0.345791
2	6	0	-2.816323	-1.877386	0.305686
3	6	0	-2.936599	-2.980764	-0.658187
4	6	0	-0.804775	-2.120661	-0.878421
5	8	0	-3.877258	-3.716836	-0.875945
6	8	0	-1.764817	-3.088671	-1.362121
7	8	0	-0.867112	-0.702030	1.150215
8	1	0	0.294543	0.530358	0.872922
9	8	0	-3.739807	-1.721592	1.316386
10	1	0	-4.451008	-1.250614	0.821467
11	1	0	-0.685194	-1.365940	-1.667711
12	6	0	0.550174	-2.795565	-0.657099
13	6	0	1.603804	-1.758485	-0.241034
14	1	0	0.450519	-3.569571	0.120526
15	8	0	0.939427	-3.383493	-1.891968
16	1	0	1.907425	-3.483077	-1.818012
17	8	0	2.920599	-2.257544	-0.508031
18	1	0	1.495552	-1.491039	0.810475
19	1	0	1.472526	-0.856245	-0.846527
20	1	0	3.362447	-2.421947	0.363490
21	8	0	0.896149	1.317010	0.798605
22	1	0	-0.017334	2.625553	0.849972
23	1	0	1.711570	1.112896	1.348678
24	8	0	3.265157	0.707688	1.844931
25	1	0	3.397402	-0.210597	2.163040
26	1	0	3.687259	0.673067	0.953236
27	8	0	-0.661104	3.371776	0.591761
28	1	0	-0.291419	3.726583	-0.330898
29	1	0	-1.595523	2.903728	0.461306
30	8	0	4.194305	0.234557	-0.756775
31	1	0	3.790189	-0.659356	-0.860464
32	1	0	3.610240	0.851881	-1.253863
33	8	0	4.180141	-1.965460	1.849241
34	1	0	5.059558	-1.638678	1.510603
35	1	0	4.377249	-2.625620	2.532417
36	8	0	0.390675	4.118847	-1.587201
37	1	0	0.910801	4.945546	-1.407186
38	1	0	1.061001	3.411733	-1.741107
39	8	0	-3.813732	-0.549106	-0.877081
40	1	0	-3.370165	0.272637	-0.578467
41	1	0	6.780506	-1.456363	0.090304

42	8	0	6.326530	-0.812223	0.657009
43	1	0	5.794968	-0.269537	0.033707
44	8	0	2.000614	1.795993	-1.647322
45	1	0	1.545703	1.548360	-0.796123
46	1	0	1.542400	1.287188	-2.337442
47	8	0	-2.844734	2.096453	0.382721
48	1	0	-2.906274	1.615484	1.259889
49	1	0	-3.646796	2.679107	0.325296
50	8	0	1.804405	6.395586	-1.027549
51	1	0	1.342824	7.146002	-1.436346
52	1	0	1.708600	6.552817	-0.073908
53	8	0	-2.735724	0.626847	2.635617
54	1	0	-3.374480	-0.094383	2.471609
55	1	0	-1.916400	0.193749	2.291160
56	8	0	-5.052968	3.710583	0.205809
57	1	0	-4.752000	4.592006	-0.069435
58	1	0	-5.575950	3.395296	-0.549458

SCF Done: E(UB3LYP) = -1677.72073719 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-185.9360	13.3411	22.8950

Zero-point correction= 0.465463 (a.u.)
Thermal correction to Energy= 0.508090
Thermal correction to Enthalpy= 0.509034
Thermal correction to Gibbs Free Energy= 0.386463
Sum of electronic and zero-point Energies= -1677.255274
Sum of electronic and thermal Energies= -1677.212647
Sum of electronic and thermal Enthalpies= -1677.211703
Sum of electronic and thermal Free Energies= -1677.334274

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	318.831	148.181	257.973

==== adduct of OH(.) to AAH(-) in Figure 1 ====
vitacoh2f.rev.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.266310	-1.573657	0.297843
2	6	0	-2.717272	-1.801295	0.030549
3	6	0	-2.655645	-2.989596	-0.931798
4	6	0	-0.521428	-2.101779	-0.907825
5	8	0	-3.564231	-3.742644	-1.213550
6	8	0	-1.421434	-3.110784	-1.468332
7	8	0	-0.768012	-0.731413	1.171703
8	1	0	0.189449	0.512564	0.886232
9	8	0	-3.448796	-2.133635	1.207942
10	1	0	-4.359570	-2.308906	0.908755
11	1	0	-0.390454	-1.349097	-1.704937
12	6	0	0.851286	-2.726081	-0.657791
13	6	0	1.807521	-1.650267	-0.122444
14	1	0	0.752204	-3.548607	0.067729
15	8	0	1.348251	-3.217209	-1.898397
16	1	0	2.314842	-3.259165	-1.773663
17	8	0	3.168889	-2.027400	-0.375503
18	1	0	1.636944	-1.470801	0.939647
19	1	0	1.622972	-0.716393	-0.661614
20	1	0	3.631734	-2.095106	0.497148
21	8	0	0.733993	1.362275	0.787910
22	1	0	-0.264400	2.543414	0.852676
23	1	0	1.556463	1.255858	1.349162
24	8	0	3.167281	1.040497	1.860558
25	1	0	3.410327	0.157438	2.209788
26	1	0	3.579379	1.021512	0.964531
27	8	0	-0.998431	3.227610	0.619270
28	1	0	-0.733349	3.565550	-0.343576
29	1	0	-1.881088	2.679313	0.580802
30	8	0	4.126138	0.587722	-0.742710
31	1	0	3.836347	-0.353233	-0.808007

32	1	0	3.465778	1.111253	-1.251778
33	8	0	4.416196	-1.500473	1.949502
34	1	0	5.241615	-1.076256	1.584705
35	1	0	4.705946	-2.110457	2.646087
36	8	0	-0.170703	3.945893	-1.666799
37	1	0	0.234662	4.848652	-1.584598
38	1	0	0.585360	3.328279	-1.808389
39	8	0	-3.405336	-0.772265	-0.685366
40	1	0	-3.212039	0.095562	-0.256144
41	1	0	6.903949	-0.726178	0.125395
42	8	0	6.382217	-0.124492	0.680244
43	1	0	5.775956	0.324622	0.050417
44	8	0	1.758295	1.869327	-1.669882
45	1	0	1.345853	1.609044	-0.798340
46	1	0	1.360410	1.271762	-2.325502
47	8	0	-3.078280	1.724989	0.628792
48	1	0	-3.038313	1.245495	1.514760
49	1	0	-3.944932	2.211275	0.602905
50	8	0	0.935961	6.436562	-1.396573
51	1	0	0.320495	7.079252	-1.785649
52	1	0	0.929729	6.649767	-0.449130
53	8	0	-2.745463	0.155175	2.738600
54	1	0	-3.334475	-0.583879	2.484921
55	1	0	-1.899221	-0.160891	2.308633
56	8	0	-5.452245	3.078557	0.549592
57	1	0	-5.254542	4.003296	0.328018
58	1	0	-5.951261	2.754750	-0.218205

SCF Done: E(UB3LYP) = -1677.74179701 A.U. after 1 cycles
Zero-point correction= 0.467939 (a.u.)
Thermal correction to Energy= 0.510007
Thermal correction to Enthalpy= 0.510951
Thermal correction to Gibbs Free Energy= 0.389949
Sum of electronic and zero-point Energies= -1677.273858
Sum of electronic and thermal Energies= -1677.231790
Sum of electronic and thermal Enthalpies= -1677.230846
Sum of electronic and thermal Free Energies= -1677.351848

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.034	147.346	254.670

==== TS3 leading to AA(., -) anion radical ====
vitacoh2p.txt
Stoichiometry C6H33O19(2)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.439446	-0.654415	-0.521081
2	6	0	2.729501	-0.037077	-0.357747
3	6	0	3.452162	-0.873883	0.641286
4	6	0	1.304031	-1.725442	0.556064
5	8	0	4.625082	-0.833574	0.965550
6	8	0	2.588673	-1.744449	1.229594
7	8	0	0.517165	-0.347664	-1.349009
8	1	0	-1.273559	-0.585539	-1.204435
9	8	0	3.490752	0.433497	-1.385399
10	1	0	3.127760	1.299707	-1.695845
11	1	0	0.546820	-1.460525	1.304835
12	6	0	1.016408	-3.147894	0.054191
13	6	0	-0.296303	-3.189062	-0.724252
14	1	0	1.850597	-3.462336	-0.594382
15	8	0	0.924395	-3.997747	1.190529
16	1	0	0.408877	-4.768896	0.890845
17	8	0	-0.756064	-4.535742	-0.926997
18	1	0	-0.201875	-2.659645	-1.674327
19	1	0	-1.075920	-2.716240	-0.126167
20	1	0	-0.219512	-4.940180	-1.630301
21	8	0	-2.234672	-0.688167	-0.987667
22	1	0	-3.121008	0.670694	-0.942968
23	1	0	-2.553700	-1.519924	-1.428634
24	8	0	-3.056698	-3.109028	-2.041670
25	1	0	-2.944845	-3.119677	-3.005936
26	1	0	-2.432549	-3.793174	-1.718950
27	8	0	-3.548443	1.546224	-0.657912

28	1	0	-3.908757	1.367133	0.353716
29	1	0	-2.747290	2.198941	-0.574035
30	8	0	2.498821	1.525016	0.599508
31	1	0	1.618868	1.454051	1.034633
32	8	0	-0.175836	1.585144	1.639051
33	1	0	-0.184782	2.131958	2.441562
34	1	0	-0.601825	2.147189	0.936260
35	1	0	3.997624	1.926852	1.545469
36	8	0	-4.213550	1.059964	1.685977
37	1	0	-5.036793	0.504048	1.713088
38	1	0	-3.457015	0.448532	1.920576
39	8	0	4.913086	1.940222	1.907718
40	1	0	5.216010	1.058975	1.630357
41	1	0	2.426989	2.610860	-0.600412
42	8	0	2.474909	2.954817	-1.552660
43	1	0	3.146276	3.654589	-1.572836
44	8	0	-2.017682	-0.498758	1.822854
45	1	0	-2.107647	-0.711190	0.866062
46	1	0	-1.330224	0.212174	1.834675
47	8	0	-1.408535	2.922383	-0.391258
48	1	0	-0.852384	2.695629	-1.207974
49	1	0	-1.488476	3.913166	-0.350421
50	8	0	-6.485353	-0.468490	1.713631
51	1	0	-7.246522	0.134205	1.741352
52	1	0	-6.556079	-0.895410	0.844149
53	8	0	0.044022	2.163124	-2.454005
54	1	0	0.892904	2.640499	-2.307462
55	1	0	0.263777	1.243991	-2.166550
56	8	0	-1.656775	5.634451	-0.282835
57	1	0	-2.548262	5.856317	-0.598042
58	1	0	-1.665320	5.900070	0.651344

SCF Done: E(UB3LYP) = -1677.72817738 A.U. after 1 cycles
NFock= 1 Conv=0.30D-08 -V/T= 2.0086

	1	2	3
	A	A	A
Frequencies --	-285.9664	16.8265	21.8383

Zero-point correction= 0.464747 (a.u.)
Thermal correction to Energy= 0.507202
Thermal correction to Enthalpy= 0.508146
Thermal correction to Gibbs Free Energy= 0.386621
Sum of electronic and zero-point Energies= -1677.263430
Sum of electronic and thermal Energies= -1677.220975
Sum of electronic and thermal Enthalpies= -1677.220031
Sum of electronic and thermal Free Energies= -1677.341556

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	318.274	148.206	255.771
Electronic	0.000	0.000	1.377

==== AA(., -) very stable anion radical, the last of Fig. 1 ====
vitacoh2p.rev.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.647341	-0.665190	-0.352371
2	6	0	2.862350	0.078366	-0.179653
3	6	0	3.692586	-0.665062	0.808927
4	6	0	1.740699	-1.889595	0.558053
5	8	0	4.793303	-0.385507	1.237534
6	8	0	3.021832	-1.780703	1.225846
7	8	0	0.647579	-0.399965	-1.071376
8	1	0	-1.129168	-0.975422	-1.011431
9	8	0	3.241338	1.172717	-0.698673
10	1	0	2.390584	2.503699	-1.362353
11	1	0	0.962615	-1.842185	1.330463
12	6	0	1.662214	-3.257072	-0.132195
13	6	0	0.336190	-3.402810	-0.879346
14	1	0	2.506821	-3.345922	-0.834426
15	8	0	1.750754	-4.250181	0.879973

16	1	0	1.336950	-5.044499	0.494496
17	8	0	0.065424	-4.773026	-1.214172
18	1	0	0.314693	-2.771007	-1.770211
19	1	0	-0.477806	-3.112009	-0.214319
20	1	0	0.606444	-5.015214	-1.985214
21	8	0	-2.042742	-1.236254	-0.751825
22	1	0	-3.146726	-0.056333	-0.843939
23	1	0	-2.241077	-2.101664	-1.202685
24	8	0	-2.526082	-3.677499	-1.936050
25	1	0	-2.534341	-3.565592	-2.900362
26	1	0	-1.761521	-4.268556	-1.767095
27	8	0	-3.740234	0.748315	-0.664653
28	1	0	-3.996826	0.668062	0.391510
29	1	0	-3.103651	1.559075	-0.752121
30	8	0	1.455614	3.970607	1.077400
31	1	0	0.832315	3.244287	1.296913
32	8	0	-0.625811	2.049226	1.551348
33	1	0	-1.093611	2.513248	2.265861
34	1	0	-1.126695	2.298447	0.726412
35	1	0	3.174148	3.359945	1.384066
36	8	0	-4.157319	0.517385	1.772215
37	1	0	-4.853671	-0.169859	1.947060
38	1	0	-3.284639	0.104932	2.034510
39	8	0	4.099341	3.025486	1.396352
40	1	0	4.076906	2.316097	0.728665
41	1	0	1.546935	3.907057	0.101420
42	8	0	1.894875	3.323957	-1.625407
43	1	0	2.519105	3.846169	-2.154403
44	8	0	-1.678757	-0.533268	1.993199
45	1	0	-1.756920	-0.943024	1.104662
46	1	0	-1.186684	0.307750	1.833710
47	8	0	-1.959278	2.586265	-0.755208
48	1	0	-1.306369	2.339804	-1.488672
49	1	0	-2.242853	3.527009	-0.912562
50	8	0	-6.088566	-1.372913	2.202300
51	1	0	-6.937087	-0.908632	2.290976
52	1	0	-6.183659	-1.879992	1.379415
53	8	0	-0.188148	1.837710	-2.567858
54	1	0	0.530304	2.499263	-2.425740
55	1	0	0.178730	1.032784	-2.137477
56	8	0	-2.736879	5.161497	-1.174863
57	1	0	-3.698050	5.209860	-1.043564
58	1	0	-2.373436	5.699814	-0.452694

SCF Done: E(UB3LYP) = -1677.78502617 A.U. after 1 cycles

Zero-point correction= 0.465612 (a.u.)
Thermal correction to Energy= 0.509582
Thermal correction to Enthalpy= 0.510526
Thermal correction to Gibbs Free Energy= 0.383753
Sum of electronic and zero-point Energies= -1677.319414
Sum of electronic and thermal Energies= -1677.275445
Sum of electronic and thermal Enthalpies= -1677.274500
Sum of electronic and thermal Free Energies= -1677.401273

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	319.767	151.366	266.816

==== precursor, AAH.(-) + HO. + H3O(+)(H2O)11 in Figure 3 ====
trione9bx.for.txt

Stoichiometry C6H32O19
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.546805	-1.038175	-0.966385
2	6	0	0.395955	-0.633408	-0.031039
3	6	0	0.755249	-1.401926	1.254105
4	6	0	2.657532	-1.619116	-0.089524
5	8	0	0.070754	-1.562366	2.247354
6	8	0	2.026245	-1.848321	1.204811
7	8	0	1.603867	-0.883300	-2.167361
8	8	0	-0.856268	-1.119265	-0.478384

9	1	0	-1.216058	-0.537352	-1.198963
10	1	0	2.979763	-2.596808	-0.461284
11	6	0	3.869196	-0.700515	0.084284
12	6	0	4.629451	-0.510706	-1.230616
13	1	0	3.517618	0.283780	0.432023
14	8	0	4.722254	-1.297981	1.047630
15	1	0	5.579531	-0.848778	0.927774
16	8	0	5.801541	0.245078	-0.878016
17	1	0	4.032524	0.036843	-1.965380
18	1	0	4.913669	-1.485967	-1.642875
19	1	0	6.496649	0.054474	-1.527563
20	8	0	0.475229	0.702305	0.180636
21	1	0	-2.060392	-1.556672	0.651208
22	8	0	-2.844373	-1.932116	1.139482
23	1	0	-2.535822	-2.077307	2.048896
24	1	0	-4.133580	-0.956938	0.818164
25	8	0	-4.837367	-0.443458	0.302197
26	1	0	-4.437221	0.502753	0.127663
27	1	0	-4.832170	-0.918385	-0.663198
28	8	0	-3.666721	1.715004	-0.354465
29	1	0	-4.210100	2.534568	-0.512930
30	1	0	-2.934106	1.943912	0.302932
31	8	0	-4.569920	-1.538710	-1.936632
32	1	0	-3.803863	-1.005825	-2.265190
33	1	0	-4.186853	-2.423259	-1.675004
34	8	0	-1.593019	2.111692	1.206244
35	1	0	-1.639183	1.653588	2.082115
36	1	0	-0.932672	1.552607	0.711874
37	8	0	-5.166203	3.937137	-0.778841
38	1	0	-5.368104	3.990944	-1.727448
39	1	0	-6.031118	3.790553	-0.361823
40	8	0	-3.510369	-3.780520	-0.837036
41	1	0	-3.222229	-3.323225	-0.013814
42	1	0	-4.254096	-4.337889	-0.556560
43	8	0	-2.441108	0.211804	-2.231571
44	1	0	-2.154711	0.637361	-3.055580
45	1	0	-2.851940	0.924742	-1.671595
46	1	0	1.587291	1.966354	-0.487068
47	8	0	2.177627	2.755737	-0.450675
48	1	0	2.231791	2.921187	0.507366
49	1	0	1.030881	1.546956	1.655569
50	8	0	1.136392	2.278728	2.315782
51	1	0	0.387223	2.852610	2.068536
52	1	0	3.748995	2.698927	-1.381861
53	8	0	4.567807	2.668004	-1.924993
54	1	0	5.125744	2.018931	-1.459402
55	1	0	-0.134085	1.311095	3.467790
56	8	0	-0.978150	0.821830	3.579007
57	1	0	-0.764247	-0.060961	3.219331

SCF Done: E(RB3LYP) = -1677.17489736 A.U. after 1 cycles

Zero-point correction= 0.457154 (a.u.)
Thermal correction to Energy= 0.498989
Thermal correction to Enthalpy= 0.499933
Thermal correction to Gibbs Free Energy= 0.380497
Sum of electronic and zero-point Energies= -1676.717744
Sum of electronic and thermal Energies= -1676.675909
Sum of electronic and thermal Enthalpies= -1676.674964
Sum of electronic and thermal Free Energies= -1676.794401

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.120	146.713	251.375

==== TS4, H2O elimination to form DHA in Figure 3 ====
trione9bx.txt

Stoichiometry C6H32O19
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.444306	-0.480755	-0.930552
2	6	0	0.270008	0.177696	-0.160692
3	6	0	0.734538	0.009136	1.313321

4	6	0	2.305587	-1.227692	0.088461
5	8	0	0.221928	0.481352	2.310146
6	8	0	1.813599	-0.781986	1.393196
7	8	0	1.617293	-0.442587	-2.126735
8	8	0	-0.783158	-0.963123	-0.232748
9	1	0	-1.402909	-0.805387	-1.023399
10	1	0	2.091725	-2.300399	0.015459
11	6	0	3.817078	-1.015649	0.064746
12	6	0	4.453743	-1.226684	-1.308188
13	1	0	4.022727	0.013603	0.380259
14	8	0	4.367308	-1.942189	0.997968
15	1	0	5.329817	-1.902644	0.856051
16	8	0	5.856338	-1.007325	-1.084818
17	1	0	4.057471	-0.523479	-2.045665
18	1	0	4.276114	-2.251267	-1.658253
19	1	0	6.343248	-1.295397	-1.873015
20	8	0	-0.165287	1.322414	-0.572280
21	1	0	-1.469082	-1.082278	0.737459
22	8	0	-2.143929	-1.341663	1.736854
23	1	0	-1.841914	-0.774919	2.469856
24	1	0	-3.201401	-1.165539	1.539722
25	8	0	-4.532669	-1.092845	1.126986
26	1	0	-4.581431	-0.277833	0.552741
27	1	0	-4.558111	-1.842820	0.461102
28	8	0	-4.298101	0.887562	-0.660233
29	1	0	-5.070135	1.321465	-1.104503
30	1	0	-3.695396	1.618988	-0.321554
31	8	0	-4.134595	-2.980205	-0.750847
32	1	0	-3.639378	-2.378260	-1.347897
33	1	0	-3.434409	-3.469044	-0.253190
34	8	0	-2.473261	2.658479	0.037136
35	1	0	-2.242068	2.841699	0.979611
36	1	0	-1.701703	2.113301	-0.251398
37	8	0	-6.449890	2.073010	-1.894139
38	1	0	-6.454811	1.771113	-2.817183
39	1	0	-7.250784	1.676092	-1.514337
40	8	0	-2.221742	-4.082408	0.959759
41	1	0	-2.058343	-3.261219	1.466277
42	1	0	-2.731266	-4.640115	1.569411
43	8	0	-2.738642	-0.810703	-1.968809
44	1	0	-2.588962	-0.610686	-2.906804
45	1	0	-3.350307	-0.096700	-1.610444
46	1	0	2.754570	2.128489	-1.467756
47	8	0	3.035220	2.063617	-0.541425
48	1	0	2.466734	2.719614	-0.073887
49	1	0	0.474165	2.725192	0.099199
50	8	0	0.921238	3.499187	0.549011
51	1	0	0.726304	4.263223	-0.018921
52	1	0	4.920624	2.024231	-0.415789
53	8	0	5.877412	1.849367	-0.301719
54	1	0	5.988181	0.945321	-0.650369
55	1	0	-0.407972	3.443969	1.935220
56	8	0	-1.151931	3.051598	2.443328
57	1	0	-0.859882	2.122965	2.524391

SCF Done: E(RB3LYP) = -1677.15477943 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-693.0874	18.8825	24.4319

Zero-point correction= 0.450610 (a.u.)
Thermal correction to Energy= 0.492903
Thermal correction to Enthalpy= 0.493847
Thermal correction to Gibbs Free Energy= 0.373616
Sum of electronic and zero-point Energies= -1676.704169
Sum of electronic and thermal Energies= -1676.661877
Sum of electronic and thermal Enthalpies= -1676.660933
Sum of electronic and thermal Free Energies= -1676.781163

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	309.301	147.841	253.046

==== DHA + (H2O)13 in Figure 3 ====
trione9bx.rev.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.593874	-0.591657	-1.300858
2	6	0	0.541420	0.408373	-0.834558
3	6	0	0.439655	0.197842	0.677407
4	6	0	2.032558	-1.368555	-0.063336
5	8	0	-0.249598	0.796899	1.472257
6	8	0	1.266105	-0.794191	1.046901
7	8	0	1.993434	-0.730881	-2.433210
8	8	0	-0.736086	-1.625221	-0.896417
9	1	0	-1.537152	-1.269100	-1.358288
10	1	0	1.714318	-2.409658	-0.163864
11	6	0	3.512102	-1.319716	0.315700
12	6	0	4.463918	-1.637963	-0.836632
13	1	0	3.741764	-0.309033	0.672714
14	8	0	3.688346	-2.265140	1.366167
15	1	0	4.650443	-2.314212	1.506879
16	8	0	5.772117	-1.507938	-0.257481
17	1	0	4.334294	-0.941682	-1.670466
18	1	0	4.299537	-2.661135	-1.196367
19	1	0	6.422620	-1.870988	-0.879239
20	8	0	-0.020193	1.249635	-1.502734
21	1	0	-1.079445	-1.873964	-0.000241
22	8	0	-1.872359	-2.182926	1.533504
23	1	0	-1.317185	-2.112194	2.325854
24	1	0	-2.626554	-1.516444	1.646908
25	8	0	-4.005523	-0.641194	1.642850
26	1	0	-3.845578	0.171334	1.104813
27	1	0	-4.509738	-1.223007	1.013093
28	8	0	-3.728692	1.344240	-0.256647
29	1	0	-4.610874	1.737449	-0.468593
30	1	0	-3.065257	2.092733	-0.311124
31	8	0	-4.981652	-2.290412	-0.319761
32	1	0	-4.404008	-1.853251	-0.985434
33	1	0	-4.469225	-3.087390	-0.038181
34	8	0	-1.876765	3.255609	-0.570909
35	1	0	-1.497353	3.504794	0.311120
36	1	0	-1.201064	2.650896	-0.936528
37	8	0	-6.221730	2.387452	-0.847913
38	1	0	-6.611548	1.798218	-1.514207
39	1	0	-6.773200	2.245752	-0.061196
40	8	0	-3.388524	-4.326821	0.730218
41	1	0	-2.757604	-3.675000	1.122099
42	1	0	-3.901776	-4.645620	1.489577
43	8	0	-3.167868	-0.734480	-1.822499
44	1	0	-3.300953	-0.531279	-2.761787
45	1	0	-3.361630	0.114609	-1.324156
46	1	0	2.885119	2.032233	-1.429600
47	8	0	2.904229	1.744889	-0.501672
48	1	0	2.600297	2.537767	0.004820
49	1	0	2.038454	4.764733	0.255758
50	8	0	2.016198	4.010544	0.869312
51	1	0	2.646210	4.247618	1.571182
52	1	0	4.790190	1.559333	-0.067862
53	8	0	5.698814	1.407111	0.260400
54	1	0	5.876759	0.475046	0.034226
55	1	0	0.276892	3.859312	1.561861
56	8	0	-0.631516	3.618367	1.846169
57	1	0	-0.577809	2.647851	1.931580

SCF Done: E(RB3LYP) = -1677.16668791 A.U. after 1 cycles

Zero-point correction= 0.454172 (a.u.)
Thermal correction to Energy= 0.499264
Thermal correction to Enthalpy= 0.500208
Thermal correction to Gibbs Free Energy= 0.371583
Sum of electronic and zero-point Energies= -1676.712516
Sum of electronic and thermal Energies= -1676.667424
Sum of electronic and thermal Enthalpies= -1676.666480
Sum of electronic and thermal Free Energies= -1676.795105

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.293	154.944	270.715

==== rotation TS, TS5, in DHA in Figure 3 ====
rot1.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.310258	-1.550948	0.411209
2	6	0	-4.102897	-2.294470	-0.670698
3	6	0	-4.950103	-1.226852	-1.364737
4	6	0	-3.640819	-0.069670	0.246828
5	8	0	-5.742290	-1.379048	-2.259329
6	8	0	-4.680177	-0.034106	-0.792843
7	8	0	-2.638561	-2.074687	1.265431
8	8	0	-4.089024	-3.474235	-0.915676
9	1	0	-4.108950	0.290776	1.166581
10	6	0	-2.518131	0.929570	-0.162163
11	6	0	-1.099002	0.369324	-0.335611
12	1	0	-2.819037	1.290648	-1.156982
13	8	0	-2.567175	1.995609	0.774914
14	1	0	-1.767510	2.597052	0.681398
15	8	0	-0.486900	-0.131985	0.845775
16	1	0	-0.493940	1.166825	-0.787781
17	1	0	-1.120605	-0.456382	-1.055429
18	1	0	-0.493815	0.549082	1.565329
19	8	0	-0.273643	1.608470	2.978475
20	1	0	-1.181654	1.605047	3.387530
21	1	0	0.340041	1.271740	3.650052
22	8	0	2.187125	0.156414	0.193076
23	1	0	1.276186	-0.087466	0.491401
24	1	0	2.123114	1.126279	-0.032443
25	8	0	3.663344	-3.069291	2.656434
26	1	0	3.904063	-2.145664	2.348427
27	1	0	4.270727	-3.238327	3.394030
28	8	0	1.770833	2.728908	-0.514376
29	1	0	2.543203	3.345637	-0.457800
30	1	0	1.522705	2.662667	-1.480268
31	8	0	-0.392143	3.518687	0.981228
32	1	0	-0.170190	3.057415	1.818822
33	1	0	0.374633	3.306604	0.389819
34	1	0	-2.950471	1.811971	2.511794
35	8	0	-2.905744	1.618745	3.478661
36	1	0	-3.223293	2.429434	3.907980
37	1	0	3.923680	-4.648167	-0.022426
38	8	0	4.692849	-4.361161	0.494626
39	1	0	4.295224	-3.967403	1.319020
40	1	0	2.674333	-0.675549	-1.173412
41	8	0	3.083933	-1.148239	-1.957858
42	1	0	2.540358	-1.942764	-2.085780
43	1	0	2.843239	-0.090550	-3.346537
44	8	0	2.660114	0.538328	-4.090842
45	1	0	2.141661	0.016027	-4.723154
46	8	0	3.909844	4.458785	-0.316919
47	1	0	3.674371	5.104650	0.369084
48	1	0	4.648012	3.962900	0.073471
49	8	0	0.958677	2.373781	-3.044272
50	1	0	1.087840	3.177426	-3.572168
51	1	0	1.577311	1.705020	-3.448858
52	1	0	5.223903	-2.835386	-0.270038
53	8	0	5.433524	-1.917911	-0.578055
54	1	0	4.678775	-1.686502	-1.164622
55	8	0	4.405856	-0.690304	1.655373
56	1	0	4.883654	-1.062608	0.867086
57	1	0	3.586154	-0.316224	1.256321

SCF Done: E(RB3LYP) = -1677.16729906 A.U. after 1 cycles

1	2	3
A	A	A
Frequencies -- -35.7796	8.0088	12.7700

Zero-point correction= 0.454837 (a.u.)
Thermal correction to Energy= 0.498102
Thermal correction to Enthalpy= 0.499046
Thermal correction to Gibbs Free Energy= 0.370604

Sum of electronic and zero-point Energies= -1676.712462
Sum of electronic and thermal Energies= -1676.669197
Sum of electronic and thermal Enthalpies= -1676.668253
Sum of electronic and thermal Free Energies= -1676.796695

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	312.564	148.994	270.330

==== After rotation of the R group in DHA in Figure 3 ====

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.837477	-0.962578	0.479266
2	6	0	-3.320554	-2.341743	0.069775
3	6	0	-3.267702	-2.315697	-1.461657
4	6	0	-3.952046	-0.154132	-0.806257
5	8	0	-2.945711	-3.206612	-2.204744
6	8	0	-3.698167	-1.104252	-1.889289
7	8	0	-4.178264	-0.635639	1.593038
8	8	0	-3.068049	-3.286766	0.773797
9	1	0	-4.971999	0.219896	-0.925751
10	6	0	-2.941376	1.005101	-0.941575
11	6	0	-1.511365	0.466618	-0.949738
12	1	0	-3.126598	1.491123	-1.912022
13	8	0	-3.195135	1.900875	0.125932
14	1	0	-2.401379	2.496392	0.243877
15	8	0	-1.275592	-0.454294	0.123760
16	1	0	-0.809803	1.304768	-0.906409
17	1	0	-1.326382	-0.079942	-1.877006
18	1	0	-1.287085	0.042851	0.989690
19	8	0	-1.158357	0.995049	2.427133
20	1	0	-2.055578	1.240856	2.789117
21	1	0	-0.651176	0.616095	3.162478
22	8	0	1.544872	-0.213588	-0.115028
23	1	0	0.628087	-0.536853	0.026540
24	1	0	1.457080	0.775079	-0.250608
25	8	0	4.216898	-2.161025	3.170029
26	1	0	3.968939	-1.322959	2.698393
27	1	0	4.901493	-1.886200	3.800532
28	8	0	1.402184	2.463898	-0.336721
29	1	0	2.140212	2.679076	0.298222
30	1	0	1.712341	2.750241	-1.242616
31	8	0	-0.964451	3.269987	0.842730
32	1	0	-0.849807	2.627205	1.576051
33	1	0	-0.143306	3.129820	0.309684
34	1	0	-3.826123	1.739446	1.983422
35	8	0	-3.637848	1.886895	2.934694
36	1	0	-3.548696	2.850544	3.017261
37	1	0	4.884690	-3.902999	0.649666
38	8	0	5.527049	-3.297838	1.052873
39	1	0	5.065720	-2.965144	1.868616
40	1	0	2.466048	-0.818488	-1.402742
41	8	0	3.155810	-1.054573	-2.085420
42	1	0	2.932218	-1.951253	-2.382982
43	1	0	2.941672	0.115551	-3.388514
44	8	0	2.792279	0.807273	-4.081386
45	1	0	1.969358	0.534756	-4.517137
46	8	0	3.422869	2.742355	1.459187
47	1	0	3.019322	3.021821	2.296316
48	1	0	3.599727	1.772512	1.584184
49	8	0	2.217492	3.147208	-2.815933
50	1	0	3.073792	3.596393	-2.737356
51	1	0	2.431454	2.291492	-3.278581
52	1	0	5.464780	-1.809118	0.086182
53	8	0	5.340976	-0.908053	-0.308526
54	1	0	4.669197	-1.031711	-1.017188
55	8	0	3.684371	0.014473	1.593884
56	1	0	4.363213	-0.240670	0.897835
57	1	0	2.825907	-0.178970	1.141877

SCF Done: E(RB3LYP) = -1677.19232519 A.U. after 1 cycles

Zero-point correction= 0.457544 (a.u.)
Thermal correction to Energy= 0.500256
Thermal correction to Enthalpy= 0.501200
Thermal correction to Gibbs Free Energy= 0.376264
Sum of electronic and zero-point Energies= -1676.734781
Sum of electronic and thermal Energies= -1676.692069
Sum of electronic and thermal Enthalpies= -1676.691125
Sum of electronic and thermal Free Energies= -1676.816061

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.915	148.960	262.949

==== ring closure TS, TS6, in Figure 3 ====
trione24ext.txt
Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.961169	-0.148241	-0.374075
2	6	0	-2.903423	0.510516	0.620698
3	6	0	-3.620991	-0.630549	1.356268
4	6	0	-2.253292	-1.657070	-0.263919
5	8	0	-4.415893	-0.541518	2.258937
6	8	0	-3.243193	-1.803957	0.806483
7	8	0	-1.630689	0.428472	-1.442460
8	8	0	-3.119017	1.686896	0.794399
9	1	0	-2.680528	-2.054897	-1.185746
10	6	0	-0.987057	-2.399216	0.162189
11	6	0	-0.418900	-1.518425	1.279687
12	1	0	-1.224092	-3.410359	0.519010
13	8	0	-0.148227	-2.425904	-0.983082
14	1	0	0.675392	-2.949467	-0.768322
15	8	0	-0.587748	-0.169709	0.843203
16	1	0	-0.960779	-1.694530	2.217766
17	1	0	0.641175	-1.726095	1.464765
18	1	0	0.715253	0.192556	0.000483
19	1	0	-0.286664	0.016345	-2.508319
20	8	0	0.650292	0.117590	-2.825535
21	1	0	0.698859	1.061469	-3.150997
22	8	0	1.559602	0.353751	-0.561085
23	1	0	1.239504	0.180929	-1.616689
24	1	0	2.292048	-0.316760	-0.258948
25	8	0	0.747865	2.776917	-3.212799
26	1	0	1.340177	3.017195	-2.431966
27	1	0	1.123615	3.212970	-3.993784
28	8	0	3.298280	-1.322461	0.286140
29	1	0	4.230940	-1.108691	0.010104
30	1	0	3.252309	-1.236053	1.288792
31	8	0	2.126197	-3.707465	-0.345907
32	1	0	2.506847	-4.067611	-1.162890
33	1	0	2.681049	-2.913617	-0.136288
34	1	0	-1.066502	-2.987534	-2.493847
35	8	0	-1.721936	-3.208406	-3.190539
36	1	0	-2.019746	-4.097166	-2.942168
37	1	0	-1.746309	2.286470	-1.544470
38	8	0	-1.602857	3.238042	-1.750260
39	1	0	-0.875356	3.209085	-2.409837
40	1	0	-0.340749	1.179184	1.891389
41	8	0	-0.099454	2.016995	2.368761
42	1	0	-0.801221	2.149727	3.026797
43	1	0	1.453857	1.668267	3.164190
44	8	0	2.319371	1.427360	3.579770
45	1	0	2.127805	1.402710	4.530705
46	8	0	5.840519	-0.730050	-0.469973
47	1	0	6.186975	-1.480265	-0.980395
48	1	0	5.803489	-0.003973	-1.114118
49	8	0	2.887598	-1.132325	2.888217
50	1	0	3.656890	-1.380172	3.424793
51	1	0	2.689364	-0.187462	3.140330
52	1	0	-0.720671	3.780203	-0.324763
53	8	0	-0.079475	4.052003	0.384172
54	1	0	-0.163796	3.366800	1.083769

55	8	0	2.090441	3.204367	-0.969171
56	1	0	1.347423	3.591586	-0.420080
57	1	0	2.119024	2.272273	-0.678505

SCF Done: E(RB3LYP) = -1677.17907343 A.U. after 1 cycles

1	2	3
A	A	A
Frequencies -- -158.7874	21.1394	23.0621

Zero-point correction= 0.452286 (a.u.)
Thermal correction to Energy= 0.494138
Thermal correction to Enthalpy= 0.495082
Thermal correction to Gibbs Free Energy= 0.375231
Sum of electronic and zero-point Energies= -1676.726787
Sum of electronic and thermal Energies= -1676.684935
Sum of electronic and thermal Enthalpies= -1676.683991
Sum of electronic and thermal Free Energies= -1676.803842

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	310.076	146.021	252.248

==== Five membered formed, and the bicyclic intermediate is formed in Figure 3 ==== trione24ext.rev.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.873060	-0.147620	-0.042478
2	6	0	-3.043586	0.272032	0.855140
3	6	0	-3.802377	-1.008251	1.232680
4	6	0	-2.163365	-1.645347	-0.332458
5	8	0	-4.737821	-1.112650	1.983644
6	8	0	-3.239347	-2.042018	0.574010
7	8	0	-1.766362	0.720242	-1.082437
8	8	0	-3.338089	1.384044	1.213445
9	1	0	-2.486354	-1.844489	-1.354614
10	6	0	-0.881227	-2.387573	0.045359
11	6	0	-0.363963	-1.527401	1.198969
12	1	0	-1.083865	-3.418754	0.358980
13	8	0	-0.046006	-2.318092	-1.094376
14	1	0	0.805745	-2.814718	-0.912468
15	8	0	-0.668485	-0.163101	0.789618
16	1	0	-0.888255	-1.757474	2.133043
17	1	0	0.710934	-1.594950	1.373031
18	1	0	1.054138	0.382650	-0.222292
19	1	0	-1.083652	0.442284	-1.797350
20	8	0	0.030424	0.344628	-2.907694
21	1	0	0.120993	1.299844	-3.153085
22	8	0	1.802994	0.498876	-0.836533
23	1	0	0.805805	0.194058	-2.314752
24	1	0	2.498470	-0.148757	-0.533208
25	8	0	0.251967	3.079226	-3.061061
26	1	0	1.022194	3.204518	-2.417485
27	1	0	0.466912	3.600160	-3.850657
28	8	0	3.547288	-1.336221	0.090619
29	1	0	4.512651	-1.186778	-0.074438
30	1	0	3.405176	-1.300044	1.078461
31	8	0	2.246086	-3.594002	-0.597538
32	1	0	2.569771	-3.923355	-1.451206
33	1	0	2.840791	-2.825992	-0.377970
34	1	0	-0.955018	-2.789700	-2.658754
35	8	0	-1.631124	-2.978035	-3.344327
36	1	0	-1.945966	-3.864381	-3.108232
37	1	0	-1.882632	2.664295	-0.960771
38	8	0	-1.704658	3.604633	-1.163054
39	1	0	-1.112306	3.544472	-1.948968
40	1	0	-0.251805	1.244882	1.927116
41	8	0	0.099577	1.992133	2.459992
42	1	0	-0.585015	2.176195	3.124136
43	1	0	1.624165	1.483868	3.254821
44	8	0	2.468409	1.170914	3.661471
45	1	0	2.252911	1.057964	4.600865

46	8	0	6.220464	-0.902639	-0.388492
47	1	0	6.553760	-1.662109	-0.893783
48	1	0	6.273597	-0.163378	-1.016154
49	8	0	2.807728	-1.324179	2.654488
50	1	0	3.402824	-1.796586	3.257120
51	1	0	2.717102	-0.408688	3.037326
52	1	0	-0.482653	4.024060	0.048481
53	8	0	0.302167	4.170445	0.637620
54	1	0	0.236270	3.453197	1.304397
55	8	0	2.103033	3.242664	-1.183199
56	1	0	1.526679	3.619888	-0.462315
57	1	0	2.136139	2.277827	-0.982131

SCF Done: E(RB3LYP) = -1677.19618818 A.U. after 1 cycles

Zero-point correction= 0.456447 (a.u.)
Thermal correction to Energy= 0.499310
Thermal correction to Enthalpy= 0.500255
Thermal correction to Gibbs Free Energy= 0.378462
Sum of electronic and zero-point Energies= -1676.739741
Sum of electronic and thermal Energies= -1676.696878
Sum of electronic and thermal Enthalpies= -1676.695934
Sum of electronic and thermal Free Energies= -1676.817726

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.322	149.636	256.334

===== H2O addition TS (TS7) to the bicyclic intermediate in Figure 3 ==== trione3bext.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.157508	-0.711061	0.182641
2	6	0	0.792521	-0.209858	-0.455808
3	6	0	1.255581	0.813230	-1.522156
4	6	0	3.217232	-0.231921	-0.847016
5	8	0	0.579319	1.610007	-2.142802
6	8	0	2.555822	0.623698	-1.812654
7	8	0	2.451723	-0.201242	1.433455
8	8	0	0.027092	-1.116802	-0.999621
9	1	0	4.006984	0.354832	-0.377425
10	6	0	3.776221	-1.508981	-1.484090
11	6	0	2.726136	-2.558746	-1.087490
12	1	0	3.874890	-1.408209	-2.572320
13	8	0	5.039164	-1.730970	-0.863103
14	1	0	5.384799	-2.576911	-1.190473
15	8	0	2.225067	-2.127393	0.184696
16	1	0	1.913289	-2.592758	-1.821605
17	1	0	3.147830	-3.560027	-0.963293
18	1	0	1.939625	-0.688630	2.135490
19	8	0	0.018092	0.576866	0.624961
20	1	0	-1.046835	0.895342	0.213864
21	1	0	0.490134	1.465850	0.888286
22	1	0	-1.409317	-0.689522	-1.882541
23	8	0	-2.340071	-0.401888	-2.096582
24	1	0	-2.896334	-1.087373	-1.642144
25	8	0	-2.169031	1.290571	-0.187657
26	1	0	-2.337316	0.710532	-1.032045
27	1	0	-1.979037	2.231770	-0.477295
28	8	0	-3.605491	-2.144792	-0.426134
29	1	0	-3.800202	-1.519359	0.322486
30	1	0	-4.429231	-2.665808	-0.588272
31	8	0	0.940897	2.932104	1.031122
32	1	0	0.280523	3.399043	0.467100
33	1	0	0.775108	3.238765	1.958638
34	8	0	-0.992829	3.562780	-0.854227
35	1	0	-0.473904	3.137226	-1.565305
36	1	0	-1.358061	4.410748	-1.223853
37	8	0	1.257577	-1.478929	3.537024
38	1	0	1.345433	-0.841012	4.263392
39	1	0	0.288493	-1.487557	3.334930

40	8	0	0.473102	3.737209	3.620773
41	1	0	0.108628	2.969350	4.090552
42	1	0	1.337248	3.878893	4.040896
43	1	0	-0.593364	-2.450203	-0.025255
44	8	0	-1.168449	-3.034185	0.536323
45	1	0	-2.069080	-2.888753	0.157456
46	1	0	-1.244708	-1.987657	1.834949
47	8	0	-1.256229	-1.217678	2.487471
48	1	0	-0.814569	-0.509748	1.972553
49	8	0	-2.008400	5.876739	-1.860008
50	1	0	-2.971380	5.849212	-1.736146
51	1	0	-1.718178	6.605491	-1.287180
52	8	0	-3.767189	-0.315872	1.595884
53	1	0	-2.977154	-0.636212	2.092318
54	1	0	-3.413585	0.442269	1.088562
55	8	0	-5.905583	-3.619594	-0.885493
56	1	0	-6.083161	-3.571167	-1.839044
57	1	0	-5.665417	-4.549443	-0.741190

SCF Done: E(RB3LYP) = -1677.17296485 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-621.7462	13.3412	20.7480

Zero-point correction= 0.454466 (a.u.)
Thermal correction to Energy= 0.495383
Thermal correction to Enthalpy= 0.496328
Thermal correction to Gibbs Free Energy= 0.376955
Sum of electronic and zero-point Energies= -1676.718498
Sum of electronic and thermal Energies= -1676.677581
Sum of electronic and thermal Enthalpies= -1676.676637
Sum of electronic and thermal Free Energies= -1676.796010

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	310.858	143.213	251.240

==== bicyclic hemiketal intermediate in Figure 3 ====
trione3bext.for.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.124864	-0.828257	0.231391
2	6	0	0.803004	-0.190476	-0.357773
3	6	0	1.329535	0.730137	-1.486660
4	6	0	3.211072	-0.450971	-0.810888
5	8	0	0.710757	1.575586	-2.097913
6	8	0	2.597658	0.415540	-1.797553
7	8	0	2.462729	-0.320197	1.466331
8	8	0	0.029443	-1.179740	-0.946244
9	1	0	4.034237	0.101850	-0.358095
10	6	0	3.694409	-1.777956	-1.404361
11	6	0	2.579194	-2.751343	-0.991358
12	1	0	3.810285	-1.716838	-2.493635
13	8	0	4.933908	-2.054183	-0.759598
14	1	0	5.234943	-2.927791	-1.056843
15	8	0	2.072335	-2.246119	0.253445
16	1	0	1.783805	-2.773860	-1.744650
17	1	0	2.942771	-3.767704	-0.818110
18	1	0	1.844135	-0.658927	2.172236
19	8	0	0.042282	0.525552	0.585022
20	1	0	-1.596885	1.196261	0.077379
21	1	0	0.512303	1.395028	0.861278
22	1	0	-0.762948	-0.787218	-1.450120
23	8	0	-2.169003	-0.371801	-2.153027
24	1	0	-2.780257	-1.012510	-1.704821
25	8	0	-2.430984	1.598995	-0.252337
26	1	0	-2.363847	0.473968	-1.683813
27	1	0	-2.143373	2.521934	-0.451462
28	8	0	-3.618046	-1.997756	-0.507367
29	1	0	-3.850431	-1.326567	0.192897

30	1	0	-4.451759	-2.479973	-0.729131
31	8	0	1.014171	2.869157	1.085582
32	1	0	0.390615	3.370290	0.506273
33	1	0	0.779692	3.109537	2.015696
34	8	0	-0.789984	3.688552	-0.830397
35	1	0	-0.344748	3.117593	-1.486573
36	1	0	-0.882106	4.581208	-1.252920
37	8	0	1.011340	-1.192270	3.599081
38	1	0	1.085168	-0.457519	4.229121
39	1	0	0.054737	-1.199019	3.342069
40	8	0	0.361830	3.395813	3.723057
41	1	0	0.065632	2.541007	4.076187
42	1	0	1.195555	3.564495	4.191674
43	1	0	-0.713139	-2.618915	0.134991
44	8	0	-1.392180	-3.064550	0.683873
45	1	0	-2.237845	-2.839774	0.218851
46	1	0	-1.467107	-1.854461	1.888566
47	8	0	-1.453888	-1.006009	2.423130
48	1	0	-0.961841	-0.399221	1.825465
49	8	0	-1.048456	6.151156	-2.002848
50	1	0	-1.998749	6.324662	-2.103425
51	1	0	-0.755793	6.816847	-1.359048
52	8	0	-3.927487	-0.091621	1.409029
53	1	0	-3.153850	-0.379618	1.947650
54	1	0	-3.577203	0.674222	0.902069
55	8	0	-5.948620	-3.356974	-1.133184
56	1	0	-5.987858	-3.410657	-2.102017
57	1	0	-5.819050	-4.278175	-0.854495

SCF Done: E(RB3LYP) = -1677.20146922 A.U. after 1 cycles

Zero-point correction= 0.460171 (a.u.)
Thermal correction to Energy= 0.501714
Thermal correction to Enthalpy= 0.502658
Thermal correction to Gibbs Free Energy= 0.383723
Sum of electronic and zero-point Energies= -1676.741298
Sum of electronic and thermal Energies= -1676.699755
Sum of electronic and thermal Enthalpies= -1676.698811
Sum of electronic and thermal Free Energies= -1676.817746

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	314.830	146.042	250.321

=== Ion-pair formation TS, TS8, in Figure 3 ====
trione10a.txt

Stoichiometry C6H32O19
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.762120	-0.699676	-0.651113
2	6	0	1.376836	-1.009476	-1.320193
3	6	0	0.366941	-0.061199	-0.575441
4	6	0	2.466780	0.470708	0.331840
5	8	0	-0.639067	0.350314	-1.265037
6	8	0	1.178307	0.980005	-0.039886
7	8	0	3.240735	-1.882539	-0.043159
8	8	0	1.383622	-0.590717	-2.647025
9	1	0	2.474626	0.143197	1.373843
10	6	0	3.554816	1.495909	0.021495
11	6	0	3.848606	1.187638	-1.449722
12	1	0	3.215823	2.527558	0.177797
13	8	0	4.643649	1.156763	0.873077
14	1	0	5.399409	1.716043	0.631460
15	8	0	3.738389	-0.243266	-1.551957
16	1	0	3.113706	1.667970	-2.106414
17	1	0	4.856799	1.467056	-1.764810
18	1	0	4.208196	-1.790215	0.025193
19	8	0	-0.092653	-0.825814	0.728757
20	1	0	-0.869683	-0.148409	1.288777
21	1	0	-0.596483	-1.652839	0.431854
22	8	0	-1.762576	0.569683	1.853500
23	1	0	-1.965869	1.297132	1.179363
24	1	0	-2.616840	-0.011704	1.875688

25	8	0	-2.016276	2.343699	-0.099979
26	1	0	-1.492525	1.721659	-0.676997
27	1	0	-1.335670	3.005633	0.211626
28	8	0	-3.061421	-1.005201	-1.121626
29	1	0	-2.242670	-0.464214	-1.231915
30	1	0	-3.720454	-0.628302	-1.770343
31	8	0	-3.841955	-0.913629	1.533783
32	1	0	-3.716131	-0.928515	0.550669
33	1	0	-3.609495	-1.835685	1.817189
34	8	0	0.140294	3.561732	0.940849
35	1	0	-0.018542	3.291781	1.880830
36	1	0	0.661988	2.817825	0.582820
37	1	0	1.137499	-1.628573	2.207885
38	8	0	1.950504	-1.956289	2.630678
39	1	0	2.507587	-2.153313	1.856154
40	8	0	-4.790214	0.330764	-2.692000
41	1	0	-5.685896	0.088618	-2.407738
42	1	0	-4.641052	1.230010	-2.290603
43	8	0	-1.490432	-2.926055	-0.172787
44	1	0	-2.161386	-2.445704	-0.725384
45	1	0	-0.762512	-3.181970	-0.772302
46	1	0	-3.504351	2.695534	-1.006637
47	8	0	-4.341963	2.766967	-1.528232
48	1	0	-5.032337	2.865964	-0.853786
49	8	0	-2.957860	-3.469713	2.112678
50	1	0	-2.369057	-3.521770	1.327531
51	1	0	-2.345734	-3.374976	2.860042
52	8	0	1.026787	-2.369205	-1.205793
53	1	0	1.832487	-2.853296	-0.940100
54	1	0	0.483574	-0.223170	-2.787884
55	8	0	-0.474563	2.519536	3.440005
56	1	0	-1.154484	3.084628	3.840611
57	1	0	-0.973579	1.742350	3.107611

SCF Done: E(RB3LYP) = -1677.17047571 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-612.5830	25.4591	28.5669

Zero-point correction= 0.458332 (a.u.)
Thermal correction to Energy= 0.496980
Thermal correction to Enthalpy= 0.497924
Thermal correction to Gibbs Free Energy= 0.388394
Sum of electronic and zero-point Energies= -1676.712144
Sum of electronic and thermal Energies= -1676.673496
Sum of electronic and thermal Enthalpies= -1676.672551
Sum of electronic and thermal Free Energies= -1676.782081

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	311.860	141.205	230.525

==== The ion-pair intermediate in Figure 3 ====
trione10a.rev.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.768682	-0.748697	-0.570206
2	6	0	1.366593	-1.127994	-1.161441
3	6	0	0.350422	-0.188490	-0.397048
4	6	0	2.492656	0.505411	0.309376
5	8	0	-0.669986	0.179903	-1.150139
6	8	0	1.178608	0.945346	-0.036810
7	8	0	3.282630	-1.865422	0.131371
8	8	0	1.290750	-0.780708	-2.503329
9	1	0	2.570988	0.277646	1.375578
10	6	0	3.536437	1.519774	-0.154446
11	6	0	3.785318	1.062704	-1.594990
12	1	0	3.167429	2.551566	-0.097338
13	8	0	4.671807	1.314938	0.681151
14	1	0	5.393926	1.870024	0.344971

15	8	0	3.713885	-0.372426	-1.541756
16	1	0	3.011829	1.450930	-2.267887
17	1	0	4.772378	1.333466	-1.977956
18	1	0	4.250183	-1.757796	0.160412
19	8	0	-0.030716	-0.774081	0.874517
20	1	0	-1.251666	0.295191	1.739558
21	1	0	-0.530284	-1.604315	0.671587
22	8	0	-2.039310	0.839187	1.998142
23	1	0	-2.138902	1.458188	1.212427
24	1	0	-3.212043	-0.194706	1.699390
25	8	0	-2.014729	2.302465	-0.250228
26	1	0	-1.485104	1.570373	-0.686997
27	1	0	-1.317258	2.962870	0.018351
28	8	0	-2.981842	-1.138402	-1.055770
29	1	0	-2.113953	-0.629064	-1.111488
30	1	0	-3.586525	-0.740110	-1.756927
31	8	0	-3.842283	-0.896976	1.293952
32	1	0	-3.546995	-0.963197	0.268125
33	1	0	-3.599090	-1.803760	1.716475
34	8	0	0.158866	3.537797	0.762305
35	1	0	-0.079072	3.415601	1.715451
36	1	0	0.627185	2.708738	0.534940
37	1	0	1.200927	-1.370118	2.301419
38	8	0	1.973469	-1.691871	2.804240
39	1	0	2.568470	-1.964380	2.083511
40	8	0	-4.539068	0.130111	-2.793341
41	1	0	-5.461781	-0.055936	-2.557174
42	1	0	-4.396946	1.079042	-2.517199
43	8	0	-1.410892	-3.091010	0.027490
44	1	0	-2.021508	-2.661248	-0.612675
45	1	0	-0.560508	-3.217238	-0.446938
46	1	0	-3.332445	2.635154	-1.350017
47	8	0	-4.096842	2.686237	-1.980709
48	1	0	-4.850452	2.931357	-1.420960
49	8	0	-3.069635	-3.211860	2.187479
50	1	0	-2.377333	-3.403959	1.510578
51	1	0	-2.582187	-3.101927	3.020524
52	8	0	1.082302	-2.505508	-0.979846
53	1	0	1.886920	-2.919379	-0.611395
54	1	0	0.399195	-0.359707	-2.568600
55	8	0	-0.726686	2.933336	3.332966
56	1	0	-1.400217	3.595288	3.557201
57	1	0	-1.248437	2.146704	3.052089

SCF Done: E(RB3LYP) = -1677.18339234 A.U. after 1 cycles

Zero-point correction= 0.463255 (a.u.)
Thermal correction to Energy= 0.501118
Thermal correction to Enthalpy= 0.502062
Thermal correction to Gibbs Free Energy= 0.394690
Sum of electronic and zero-point Energies= -1676.720137
Sum of electronic and thermal Energies= -1676.682274
Sum of electronic and thermal Enthalpies= -1676.681330
Sum of electronic and thermal Free Energies= -1676.788702

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	314.456	139.272	225.984

==== Ring opening TS, TS9, in Figure 3 ====
trione10k.txt

Stoichiometry C6H32O19
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.765068	-0.761520	-0.523228
2	6	0	1.404799	-1.078848	-1.250926
3	6	0	0.289401	-0.187806	-0.612854
4	6	0	2.568546	0.574926	0.255587
5	8	0	-0.624986	0.223080	-1.386469
6	8	0	1.343607	1.109562	-0.251006
7	8	0	3.092636	-1.865369	0.299604
8	8	0	1.503954	-0.716901	-2.588207
9	1	0	2.519231	0.412445	1.333988

10	6	0	3.769771	1.425967	-0.164531
11	6	0	4.083082	0.848918	-1.547006
12	1	0	3.531814	2.496155	-0.198215
13	8	0	4.784909	1.134021	0.789058
14	1	0	5.599901	1.579702	0.506801
15	8	0	3.829097	-0.561522	-1.417506
16	1	0	3.424318	1.277623	-2.310560
17	1	0	5.125372	0.971773	-1.849970
18	1	0	4.065100	-1.889440	0.356746
19	8	0	-0.063443	-0.596670	0.687146
20	1	0	-1.386970	0.410641	1.608289
21	1	0	-0.607359	-1.437118	0.574895
22	8	0	-2.129935	0.965213	1.930981
23	1	0	-2.286799	1.923932	0.468424
24	1	0	-2.916146	0.334753	1.938271
25	8	0	-2.057080	2.380887	-0.386604
26	1	0	-1.581540	1.667307	-0.879802
27	1	0	-0.566844	3.075197	0.325779
28	8	0	-3.109836	-1.089399	-1.060686
29	1	0	-2.322399	-0.521048	-1.209608
30	1	0	-3.765448	-0.819231	-1.763840
31	8	0	-4.070003	-0.791325	1.547284
32	1	0	-3.839781	-0.861811	0.588901
33	1	0	-3.747686	-1.646333	1.925755
34	8	0	0.310450	3.065361	0.795034
35	1	0	0.079685	2.962548	1.768363
36	1	0	0.896645	1.974397	0.309448
37	1	0	1.022011	-1.045259	2.348040
38	8	0	1.768828	-1.333050	2.902809
39	1	0	2.349790	-1.741585	2.236903
40	8	0	-4.837465	0.002851	-2.806181
41	1	0	-5.732871	-0.227298	-2.511156
42	1	0	-4.706795	0.937158	-2.486791
43	8	0	-1.452081	-2.821589	0.107974
44	1	0	-2.142963	-2.432581	-0.488452
45	1	0	-0.708888	-3.099176	-0.465616
46	1	0	-3.581293	2.523257	-1.325143
47	8	0	-4.418301	2.531904	-1.853384
48	1	0	-5.112631	2.692514	-1.194974
49	8	0	-2.928063	-3.183651	2.427961
50	1	0	-2.325186	-3.277630	1.657694
51	1	0	-2.340130	-2.919370	3.153516
52	8	0	1.054461	-2.443300	-1.113042
53	1	0	1.787094	-2.872635	-0.626975
54	1	0	0.626691	-0.331262	-2.801739
55	8	0	-0.542687	2.670348	3.307515
56	1	0	-1.019910	3.473144	3.572821
57	1	0	-1.252519	2.035806	3.037704

SCF Done: E(RB3LYP) = -1677.16822871 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-274.8946	24.6651	30.1961

Zero-point correction= 0.459322 (a.u.)
Thermal correction to Energy= 0.497875
Thermal correction to Enthalpy= 0.498819
Thermal correction to Gibbs Free Energy= 0.389841
Sum of electronic and zero-point Energies= -1676.708907
Sum of electronic and thermal Energies= -1676.670354
Sum of electronic and thermal Enthalpies= -1676.669410
Sum of electronic and thermal Free Energies= -1676.778388

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	312.421	141.427	229.364

==== The last species in Figure 3, a carboxylic acid ====
trione10k.rev.txt

Stoichiometry C6H32O19

Standard orientation:

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

1	6	0	2.414507	-0.124993	-0.753460
2	6	0	1.421848	0.619802	-1.713470
3	6	0	0.049413	0.866417	-1.042292
4	6	0	2.722152	0.578583	0.606483
5	8	0	-0.252579	1.964041	-0.618832
6	8	0	2.593335	1.989149	0.554035
7	8	0	1.937159	-1.441807	-0.534432
8	8	0	1.975147	1.844140	-2.087185
9	1	0	2.088844	0.161669	1.393113
10	6	0	4.189433	0.165922	0.799265
11	6	0	4.721795	0.287248	-0.624643
12	1	0	4.712108	0.801319	1.521208
13	8	0	4.142487	-1.202569	1.226822
14	1	0	5.042501	-1.567490	1.201731
15	8	0	3.647201	-0.208433	-1.450643
16	1	0	4.940357	1.331739	-0.876747
17	1	0	5.607959	-0.323597	-0.817599
18	1	0	2.667033	-1.875910	-0.041020
19	8	0	-0.779322	-0.170053	-0.890579
20	1	0	-1.525900	-0.403329	0.985280
21	1	0	-0.581813	-0.995368	-1.425629
22	8	0	-2.071163	-0.249785	1.779632
23	1	0	-2.317515	1.504154	1.579769
24	1	0	-2.802837	-0.944290	1.692989
25	8	0	-2.197588	2.446681	1.301932
26	1	0	-1.674078	2.353620	0.476205
27	1	0	-0.271763	2.525936	2.061165
28	8	0	-3.560377	-0.857898	-1.339035
29	1	0	-2.850246	-0.254322	-1.057528
30	1	0	-4.305238	-0.239510	-1.592989
31	8	0	-3.814918	-2.114910	1.144053
32	1	0	-3.938636	-1.718637	0.249094
33	1	0	-3.136000	-2.824969	0.974118
34	8	0	0.626717	2.326766	2.394967
35	1	0	0.525684	1.448685	2.829610
36	1	0	1.848993	2.228041	1.175760
37	1	0	0.389561	-1.891142	2.353725
38	8	0	0.456599	-2.580554	1.657515
39	1	0	0.797903	-2.098966	0.879448
40	8	0	-5.441061	1.015945	-1.720289
41	1	0	-6.280977	0.657935	-1.391807
42	1	0	-5.165881	1.671829	-1.023796
43	8	0	-1.419693	-2.436417	-1.974919
44	1	0	-2.318517	-2.031048	-2.042379
45	1	0	-1.208739	-2.787604	-2.854823
46	1	0	-3.834466	2.733697	0.598324
47	8	0	-4.735923	2.840208	0.202790
48	1	0	-5.340155	2.698020	0.948253
49	8	0	-1.759249	-3.797757	0.526204
50	1	0	-1.609228	-3.509978	-0.398721
51	1	0	-1.004799	-3.387761	1.017845
52	8	0	1.168570	-0.154761	-2.847059
53	1	0	2.031378	-0.474025	-3.168713
54	1	0	2.203487	2.294191	-1.241428
55	8	0	0.108232	-0.300152	3.316508
56	1	0	0.026787	-0.428363	4.275631
57	1	0	-0.819291	-0.307066	2.956728

SCF Done: E(RB3LYP) = -1677.20202510 A.U. after 1 cycles

Zero-point correction= 0.463069 (a.u.)
Thermal correction to Energy= 0.502708
Thermal correction to Enthalpy= 0.503652
Thermal correction to Gibbs Free Energy= 0.392212
Sum of electronic and zero-point Energies= -1676.738956
Sum of electronic and thermal Energies= -1676.699317
Sum of electronic and thermal Enthalpies= -1676.698373
Sum of electronic and thermal Free Energies= -1676.809813

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	315.454	144.312	234.545

==== The first species DHA + (H2O)13 in Figure 4 is the same as that in Figure 3 ==== trione9bx.rev.txt

==== H2O addition to DHA to form the tetrahedral intermediate in Figure 3 ==== trione5zzext.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.300768	-1.836373	-0.928576
2	6	0	0.792827	-1.889373	-1.250027
3	6	0	0.248669	-0.530016	-0.823091
4	6	0	2.557672	-0.453856	-0.345971
5	8	0	-0.780122	0.011515	-1.298435
6	8	0	1.350252	0.294942	-0.633569
7	8	0	3.085630	-2.740840	-1.100109
8	8	0	0.194852	-2.819403	-1.737115
9	1	0	2.667665	-0.553234	0.743817
10	6	0	3.737309	0.324482	-0.920389
11	6	0	5.087940	-0.342728	-0.656097
12	1	0	3.597781	0.444982	-2.004775
13	8	0	3.728006	1.603001	-0.285584
14	1	0	4.620318	1.967477	-0.441812
15	8	0	6.061960	0.616650	-1.077882
16	1	0	5.177045	-1.279726	-1.216403
17	1	0	5.189286	-0.560038	0.415064
18	1	0	6.893006	0.429817	-0.615395
19	8	0	-0.006831	-1.072715	0.857814
20	1	0	-0.585754	0.003066	1.455758
21	1	0	-0.718016	-1.764082	0.819932
22	8	0	-1.085621	0.895841	1.894997
23	1	0	-1.065625	1.606705	1.136985
24	1	0	-2.089022	0.623990	2.026198
25	8	0	-0.875417	2.482122	-0.112996
26	1	0	-0.794622	1.727009	-0.749216
27	1	0	0.058958	2.838730	0.015402
28	8	0	-3.311791	-0.751716	-0.704202
29	1	0	-2.408944	-0.514391	-1.046211
30	1	0	-3.868398	-0.988530	-1.496590
31	8	0	-3.517836	0.136188	1.995586
32	1	0	-3.639113	-0.123269	1.055909
33	1	0	-3.554886	-0.728165	2.491873
34	8	0	1.570310	3.298650	0.559952
35	1	0	1.495047	3.002021	1.499758
36	1	0	2.236274	2.693604	0.170512
37	1	0	1.241705	-1.365873	2.199553
38	8	0	1.994276	-1.367328	2.830496
39	1	0	2.383259	-2.248795	2.718608
40	8	0	-4.940600	-0.848608	-2.875048
41	1	0	-5.791919	-1.247317	-2.631613
42	1	0	-5.064898	0.112413	-2.705972
43	8	0	-2.170844	-2.804116	0.681906
44	1	0	-2.718088	-2.216648	0.098752
45	1	0	-2.023193	-3.622688	0.181158
46	1	0	-4.145972	1.038533	-1.066059
47	8	0	-4.668251	1.641833	-1.636319
48	1	0	-5.446734	1.867636	-1.100144
49	8	0	-3.439915	-2.355365	3.084491
50	1	0	-2.991851	-2.732984	2.291038
51	1	0	-2.751267	-2.352345	3.768604
52	1	0	-2.212213	3.585329	-0.925941
53	8	0	-2.953363	4.008133	-1.404270
54	1	0	-3.562150	3.261478	-1.563298
55	8	0	1.078148	2.344006	3.137735
56	1	0	0.724530	3.091194	3.646466
57	1	0	0.293930	1.788957	2.953355

SCF Done: E(RB3LYP) = -1677.14592281   A.U. after   1 cycles

	1	2	3
	A	A	A
Frequencies --	-395.2983	21.9851	22.1597

Zero-point correction= 0.452364 (a.u.)
Thermal correction to Energy= 0.494851
Thermal correction to Enthalpy= 0.495796
Thermal correction to Gibbs Free Energy= 0.375441

Sum of electronic and zero-point Energies= -1676.693559
Sum of electronic and thermal Energies= -1676.651071
Sum of electronic and thermal Enthalpies= -1676.650127
Sum of electronic and thermal Free Energies= -1676.770481

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	310.524	147.957	253.307

==== a tetrahedral intermediate in Figure 4 ====
trione5zzext.rev.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.490871	-1.907848	-0.868407
2	6	0	0.957600	-2.049551	-1.028041
3	6	0	0.367018	-0.768919	-0.417472
4	6	0	2.712168	-0.574420	-0.172902
5	8	0	-0.622050	-0.233820	-1.201271
6	8	0	1.450234	0.120068	-0.337678
7	8	0	3.301718	-2.730886	-1.223578
8	8	0	0.376537	-2.989901	-1.510746
9	1	0	2.888770	-0.753677	0.899268
10	6	0	3.806770	0.318769	-0.746458
11	6	0	5.209018	-0.272600	-0.597530
12	1	0	3.600411	0.499545	-1.811445
13	8	0	3.748625	1.549313	-0.024803
14	1	0	4.600120	1.988291	-0.215308
15	8	0	6.094146	0.771418	-1.013115
16	1	0	5.322384	-1.167946	-1.218603
17	1	0	5.386261	-0.544020	0.451205
18	1	0	6.960936	0.614575	-0.608789
19	8	0	-0.043790	-1.045464	0.916248
20	1	0	-0.843730	0.507296	1.733232
21	1	0	-0.782125	-1.724359	0.912378
22	8	0	-1.335510	1.331827	1.931819
23	1	0	-1.180853	2.078583	0.352623
24	1	0	-2.288117	1.037207	2.037258
25	8	0	-0.865302	2.270412	-0.570434
26	1	0	-0.675602	0.776476	-1.020289
27	1	0	0.039347	2.684238	-0.422361
28	8	0	-3.311945	-0.856881	-0.679641
29	1	0	-2.401641	-0.665347	-1.007575
30	1	0	-3.828266	-1.204737	-1.460591
31	8	0	-3.828643	0.349714	1.937510
32	1	0	-3.805270	-0.014705	1.030229
33	1	0	-3.788847	-0.455259	2.514258
34	8	0	1.486561	3.331488	0.159946
35	1	0	1.265226	3.300494	1.124290
36	1	0	2.190677	2.658566	0.045059
37	1	0	1.243634	-1.266498	2.394172
38	8	0	2.017588	-1.336993	2.985000
39	1	0	2.247014	-2.278596	2.942033
40	8	0	-4.852246	-1.273691	-2.864021
41	1	0	-5.696417	-1.672349	-2.596704
42	1	0	-5.016191	-0.304441	-2.822676
43	8	0	-2.173627	-2.682255	0.961350
44	1	0	-2.751081	-2.179276	0.326786
45	1	0	-2.058183	-3.569449	0.582549
46	1	0	-4.178081	0.856185	-1.285982
47	8	0	-4.690946	1.359430	-1.952848
48	1	0	-5.484519	1.654743	-1.475752
49	8	0	-3.480849	-2.012941	3.328384
50	1	0	-3.005998	-2.440904	2.580061
51	1	0	-2.780894	-1.823440	3.973649
52	1	0	-2.166329	3.278472	-1.503145
53	8	0	-2.911013	3.693421	-1.985375
54	1	0	-3.546696	2.958085	-2.074030
55	8	0	0.558304	3.157573	2.775753
56	1	0	0.110250	4.005542	2.923245
57	1	0	-0.179200	2.519470	2.625815

SCF Done: E(RB3LYP) = -1677.16425507 A.U. after 1 cycles

Zero-point correction= 0.456698 (a.u.)
Thermal correction to Energy= 0.499974
Thermal correction to Enthalpy= 0.500919
Thermal correction to Gibbs Free Energy= 0.377791
Sum of electronic and zero-point Energies= -1676.707557
Sum of electronic and thermal Energies= -1676.664281
Sum of electronic and thermal Enthalpies= -1676.663336
Sum of electronic and thermal Free Energies= -1676.786464

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.739	150.417	259.143

==== Ring cleavage TS, TS11, in Figure 4 ====
trionexpext.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.837377	0.261035	-1.213491
2	6	0	-2.396763	-1.201050	-0.962855
3	6	0	-0.880559	-1.336662	-1.092521
4	6	0	-1.668999	1.163386	-0.828515
5	8	0	-0.229969	-2.187514	-0.422909
6	8	0	-0.790277	0.277622	-0.158958
7	8	0	-3.932843	0.550241	-1.638413
8	8	0	-3.174413	-2.084631	-0.665134
9	1	0	-1.211528	1.560587	-1.749816
10	6	0	-2.058265	2.347972	0.066475
11	6	0	-2.917508	3.385563	-0.655316
12	1	0	-2.616580	1.961991	0.931446
13	8	0	-0.842018	2.962323	0.487414
14	1	0	-1.114648	3.847447	0.793034
15	8	0	-3.041216	4.480631	0.261106
16	1	0	-3.897083	2.970386	-0.917854
17	1	0	-2.411316	3.705927	-1.576475
18	1	0	-3.288318	5.270446	-0.243444
19	8	0	-0.533698	-0.974911	-2.350273
20	1	0	2.901078	-1.948766	-0.540159
21	1	0	0.452877	-0.886332	-2.460000
22	8	0	2.208253	-1.639312	0.241570
23	1	0	1.274415	-1.983119	-0.006683
24	1	0	0.817027	0.837436	-0.105925
25	8	0	1.810075	0.808644	-0.236094
26	1	0	2.096318	-0.597267	0.118506
27	1	0	2.270833	1.379672	0.461817
28	8	0	2.095155	-0.269355	-2.679883
29	1	0	2.152015	0.243969	-3.502532
30	1	0	2.111542	0.387035	-1.937694
31	8	0	3.798949	-2.138798	-1.596170
32	1	0	3.429888	-1.485763	-2.236423
33	1	0	4.656999	-1.752855	-1.250722
34	8	0	3.193368	1.961614	1.672490
35	1	0	3.675246	1.141102	1.914464
36	1	0	3.879384	2.546568	1.267633
37	1	0	-3.191193	-3.729202	0.306412
38	8	0	-3.203427	-4.385231	1.031727
39	1	0	-2.769079	-5.165544	0.651377
40	1	0	-0.689946	-2.836103	1.238518
41	8	0	-1.007633	-3.063413	2.139193
42	1	0	-1.836477	-3.559807	1.945564
43	1	0	-1.141549	-0.080888	1.639298
44	8	0	-1.457971	-0.368202	2.525327
45	1	0	-1.349318	-1.352941	2.499820
46	1	0	-3.155948	-0.075899	2.220465
47	8	0	-4.076787	0.152662	1.930294
48	1	0	-4.304115	0.912602	2.487587
49	8	0	5.932582	-1.089971	-0.345057
50	1	0	5.495022	-0.896683	0.517465
51	1	0	6.548755	-1.813491	-0.147348
52	8	0	4.361932	-0.629562	1.932192
53	1	0	4.727464	-0.917957	2.784930

54	1	0	3.603659	-1.221478	1.763303
55	8	0	5.095766	3.597595	0.485343
56	1	0	4.865448	3.632155	-0.457353
57	1	0	4.929324	4.501843	0.798007

SCF Done: E(RB3LYP) = -1677.13827051 A.U. after 12 cycles

	1	2	3
	A	A	A
Frequencies --	-170.3750	13.9538	17.0979

Zero-point correction= 0.451670 (a.u.)
Thermal correction to Energy= 0.494709
Thermal correction to Enthalpy= 0.495653
Thermal correction to Gibbs Free Energy= 0.372047
Sum of electronic and zero-point Energies= -1676.686600
Sum of electronic and thermal Energies= -1676.643562
Sum of electronic and thermal Enthalpies= -1676.642618
Sum of electronic and thermal Free Energies= -1676.766223

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	310.434	148.482	260.150

=== DKG + (H2O)12 in Figure 4 ==== trionexpext.for.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.815139	-0.115355	-1.168041
2	6	0	-1.988117	-1.428596	-1.122936
3	6	0	-0.540363	-1.365620	-1.638456
4	6	0	-2.118527	1.059668	-0.484137
5	8	0	0.328249	-2.102056	-1.199622
6	8	0	-1.112775	0.461777	0.327639
7	8	0	-3.892261	-0.105152	-1.719395
8	8	0	-2.463300	-2.466777	-0.715816
9	1	0	-1.658145	1.671501	-1.272375
10	6	0	-3.039933	1.951721	0.359400
11	6	0	-4.104174	2.687325	-0.457152
12	1	0	-3.531039	1.313978	1.108857
13	8	0	-2.195961	2.910263	0.989876
14	1	0	-2.804958	3.626552	1.250783
15	8	0	-4.707374	3.610972	0.458010
16	1	0	-4.842660	1.989795	-0.864523
17	1	0	-3.626435	3.222934	-1.289304
18	1	0	-5.137923	4.309344	-0.058055
19	8	0	-0.380143	-0.436428	-2.556295
20	1	0	3.072141	-1.493897	0.331718
21	1	0	0.616351	-0.260282	-2.694198
22	8	0	2.603232	-1.179804	1.159494
23	1	0	2.006229	-1.900067	1.462724
24	1	0	-0.219597	0.890191	0.208205
25	8	0	1.462946	1.028113	0.008903
26	1	0	1.779021	0.208507	0.478367
27	1	0	1.991549	1.769007	0.441204
28	8	0	2.137820	0.220354	-2.431214
29	1	0	2.439776	0.901039	-3.055321
30	1	0	1.973167	0.683979	-1.554153
31	8	0	3.956110	-1.565447	-1.124602
32	1	0	3.390447	-1.037845	-1.728858
33	1	0	4.691520	-0.952715	-0.889917
34	8	0	3.099909	2.756571	1.211199
35	1	0	3.552710	2.087637	1.770673
36	1	0	3.759482	2.925982	0.490450
37	1	0	-1.616640	-4.174028	0.027707
38	8	0	-1.190687	-4.834824	0.608068
39	1	0	-0.661098	-5.374421	-0.000745
40	1	0	0.268557	-2.459925	0.591669
41	8	0	0.357149	-2.764065	1.520194
42	1	0	-0.037670	-3.667175	1.454375
43	1	0	-1.301858	-0.267191	2.056503
44	8	0	-1.431919	-0.964783	2.730585

45	1	0	-0.845314	-1.684137	2.397207
46	1	0	-3.114499	-1.183418	2.149194
47	8	0	-4.020173	-1.113663	1.758674
48	1	0	-4.504577	-0.589429	2.414825
49	8	0	5.752096	0.343461	-0.135622
50	1	0	5.414377	0.357111	0.800235
51	1	0	6.699444	0.140619	-0.075872
52	8	0	4.415994	0.472025	2.214424
53	1	0	4.825448	0.255208	3.066929
54	1	0	3.742134	-0.237390	2.032077
55	8	0	4.969785	2.903496	-0.816441
56	1	0	5.355439	2.007406	-0.657000
57	1	0	4.452600	2.793992	-1.629927

SCF Done: E(RB3LYP) = -1677.18771952 A.U. after 1 cycles

Zero-point correction= 0.457776 (a.u.)
Thermal correction to Energy= 0.500506
Thermal correction to Enthalpy= 0.501450
Thermal correction to Gibbs Free Energy= 0.381785
Sum of electronic and zero-point Energies= -1676.729944
Sum of electronic and thermal Energies= -1676.687214
Sum of electronic and thermal Enthalpies= -1676.686270
Sum of electronic and thermal Free Energies= -1676.805934

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	314.072	149.664	251.855

==== ionization of DKG, TS12, in Figure 4 ====
dkg01.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.120585	0.174982	0.890465
2	6	0	-2.290079	1.477675	1.010589
3	6	0	-0.870658	1.292487	1.583379
4	6	0	-2.453642	-0.891324	0.019487
5	8	0	0.013809	2.115350	1.276324
6	8	0	-1.564705	-0.165825	-0.827558
7	8	0	-4.198654	0.085549	1.439192
8	8	0	-2.777113	2.553973	0.718414
9	1	0	-1.886438	-1.548717	0.690589
10	6	0	-3.413025	-1.748039	-0.815691
11	6	0	-4.360846	-2.609469	0.022564
12	1	0	-4.010172	-1.082791	-1.460631
13	8	0	-2.597162	-2.600446	-1.612069
14	1	0	-3.196940	-3.323654	-1.875878
15	8	0	-5.003642	-3.484830	-0.913052
16	1	0	-5.088581	-1.990512	0.555414
17	1	0	-3.780495	-3.185810	0.756385
18	1	0	-5.343964	-4.250278	-0.425612
19	8	0	-0.759689	0.254579	2.305990
20	1	0	2.832158	1.757770	-0.343624
21	1	0	0.710981	-0.210243	2.196506
22	8	0	2.402176	1.605569	-1.237095
23	1	0	1.780908	2.360110	-1.392201
24	1	0	-0.657624	-0.545763	-0.804431
25	8	0	1.162244	-0.640520	-0.572568
26	1	0	1.526662	0.248568	-0.895833
27	1	0	1.747523	-1.352144	-1.052976
28	8	0	1.625350	-0.505926	1.810357
29	1	0	1.918232	-1.377740	2.205059
30	1	0	1.424359	-0.639629	0.656636
31	8	0	3.580552	1.575365	1.168864
32	1	0	2.936919	0.992876	1.618373
33	1	0	4.316855	0.966012	0.922287
34	8	0	2.788552	-2.236532	-1.760087
35	1	0	3.347652	-1.554249	-2.197138
36	1	0	3.369422	-2.576415	-1.020701
37	1	0	-1.752363	4.233642	0.485155
38	8	0	-1.257720	5.032001	0.205012

39	1	0	-0.665419	5.202913	0.954874
40	1	0	0.060108	2.709575	-0.371844
41	8	0	0.209395	3.189130	-1.224176
42	1	0	-0.131150	4.080968	-0.980281
43	1	0	-1.853471	1.123258	-2.284707
44	8	0	-1.766881	1.920083	-2.837671
45	1	0	-1.079554	2.427051	-2.355347
46	8	0	2.647069	-2.855445	2.578765
47	1	0	3.075457	-2.862867	3.451635
48	1	0	2.021929	-3.600023	2.595453
49	8	0	5.384243	-0.268180	0.114481
50	1	0	5.147808	-0.122603	-0.839065
51	1	0	6.338259	-0.101195	0.179636
52	8	0	4.290098	0.048233	-2.358759
53	1	0	4.791603	0.333139	-3.139028
54	1	0	3.630899	0.763880	-2.165638
55	8	0	4.421734	-2.886282	0.302133
56	1	0	4.860057	-2.005468	0.354614
57	1	0	3.864145	-2.934289	1.105580

SCF Done: E(RB3LYP) = -1677.18652750 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-442.9809	21.6115	25.3908

Zero-point correction= 0.453033 (a.u.)
Thermal correction to Energy= 0.494764
Thermal correction to Enthalpy= 0.495708
Thermal correction to Gibbs Free Energy= 0.377471
Sum of electronic and zero-point Energies= -1676.733494
Sum of electronic and thermal Energies= -1676.691763
Sum of electronic and thermal Enthalpies= -1676.690819
Sum of electronic and thermal Free Energies= -1676.809056

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	310.469	146.518	248.851

==== congugate base of DKG in Figure 4 ====
dkg01.rev.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.198126	0.158788	0.822579
2	6	0	-2.466686	1.522754	0.916515
3	6	0	-1.068376	1.453926	1.571358
4	6	0	-2.441229	-0.890073	0.007428
5	8	0	-0.234853	2.359097	1.311790
6	8	0	-1.601596	-0.140855	-0.864808
7	8	0	-4.284895	0.012695	1.343954
8	8	0	-3.017196	2.546424	0.560748
9	1	0	-1.831211	-1.464182	0.717079
10	6	0	-3.321218	-1.864026	-0.785893
11	6	0	-4.186423	-2.770441	0.093209
12	1	0	-3.977000	-1.285175	-1.456913
13	8	0	-2.433623	-2.675366	-1.549269
14	1	0	-2.967618	-3.459411	-1.778124
15	8	0	-4.749237	-3.741636	-0.799183
16	1	0	-4.966216	-2.196448	0.602281
17	1	0	-3.554920	-3.259205	0.848204
18	1	0	-5.015969	-4.513209	-0.276794
19	8	0	-0.915687	0.440239	2.301378
20	1	0	2.811561	1.694903	-0.397003
21	1	0	0.753977	-0.039005	2.257737
22	8	0	2.423629	1.540253	-1.312296
23	1	0	1.808918	2.291548	-1.495767
24	1	0	-0.679000	-0.499177	-0.858497
25	8	0	1.060519	-0.711786	-0.685870
26	1	0	1.442454	0.161759	-0.993401
27	1	0	2.117784	-1.691330	-1.262114
28	8	0	1.632697	-0.330788	1.892780

29	1	0	1.914474	-1.155151	2.347779
30	1	0	1.234117	-0.680934	0.304169
31	8	0	3.499939	1.576475	1.131356
32	1	0	2.865691	0.947331	1.550741
33	1	0	4.288254	1.023386	0.933514
34	8	0	2.960331	-2.177771	-1.618638
35	1	0	3.494315	-1.446803	-2.069373
36	1	0	3.545889	-2.464515	-0.756853
37	1	0	-1.981813	4.557155	0.128427
38	8	0	-1.084048	4.871922	0.332457
39	1	0	-0.768702	4.138880	0.905974
40	1	0	0.021024	2.595513	-0.512561
41	8	0	0.197185	3.087617	-1.347224
42	1	0	-0.095834	3.985788	-1.067455
43	1	0	-1.976365	1.117277	-2.311100
44	8	0	-1.916978	1.910375	-2.874195
45	1	0	-1.183743	2.400873	-2.447977
46	8	0	2.814237	-2.719010	2.658401
47	1	0	3.336868	-2.726015	3.478053
48	1	0	2.244054	-3.504164	2.718030
49	8	0	5.481736	-0.187783	0.157407
50	1	0	5.283715	-0.051757	-0.801846
51	1	0	6.434872	-0.034176	0.260478
52	8	0	4.315667	-0.016923	-2.321061
53	1	0	4.720016	0.144752	-3.188818
54	1	0	3.647027	0.708031	-2.161385
55	8	0	4.396905	-2.690151	0.359765
56	1	0	4.908661	-1.842230	0.425249
57	1	0	3.859207	-2.744115	1.187156

SCF Done: E(RB3LYP) = -1677.19352113 A.U. after 1 cycles

Zero-point correction= 0.457408 (a.u.)
Thermal correction to Energy= 0.499181
Thermal correction to Enthalpy= 0.500125
Thermal correction to Gibbs Free Energy= 0.381802
Sum of electronic and zero-point Energies= -1676.736113
Sum of electronic and thermal Energies= -1676.694341
Sum of electronic and thermal Enthalpies= -1676.693396
Sum of electronic and thermal Free Energies= -1676.811719

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.241	146.821	249.030

==== The conjugate base of DKG, OH. and H3O(+)(H2O)10 , the reactant in Figure 5 ===
dkg02a.for.txt

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.299949	0.263978	0.983679
2	6	0	3.611866	0.646517	0.531432
3	6	0	1.969519	-2.319205	-1.198274
4	6	0	1.037428	0.915567	0.431229
5	8	0	2.809158	-1.822780	-1.838458
6	8	0	0.677460	0.258255	-0.809628
7	8	0	2.125156	-0.727332	1.792582
8	8	0	3.891124	1.441595	-0.400696
9	1	0	0.252832	0.692304	1.167057
10	6	0	1.041848	2.434096	0.230733
11	6	0	1.459296	3.202934	1.481187
12	1	0	1.718396	2.687978	-0.592256
13	8	0	-0.299658	2.811497	-0.113383
14	1	0	-0.323837	3.773205	0.043451
15	8	0	1.207619	4.588046	1.198859
16	1	0	2.519801	3.035757	1.703923
17	1	0	0.861318	2.870801	2.341600
18	1	0	1.141926	5.060542	2.042384
19	8	0	1.142708	-2.875312	-0.583491
20	1	0	-4.336056	0.396179	-3.382968
21	1	0	-0.943265	-2.851882	-0.790882

22	8	0	-3.949612	1.005663	-2.731365
23	1	0	-3.647659	1.770773	-3.249995
24	1	0	-0.297290	0.344989	-0.918703
25	8	0	-2.074676	-0.051406	-0.943910
26	1	0	-2.607897	0.257935	-1.712690
27	1	0	-2.857016	0.416568	0.290379
28	8	0	-1.879364	-2.699691	-1.007276
29	1	0	-2.381944	-3.028881	-0.227726
30	1	0	-2.044221	-1.056164	-0.993849
31	8	0	4.632407	0.037639	1.229005
32	1	0	5.273839	-0.313562	0.564778
33	8	0	5.670311	-1.809182	-0.462927
34	8	0	-3.492066	0.772608	1.029335
35	1	0	-4.221121	1.251955	0.522672
36	1	0	-3.990144	-0.078817	1.491511
37	1	0	5.024923	-2.287527	0.118488
38	1	0	5.158118	-1.644411	-1.270761
39	1	0	3.288903	-1.966559	1.572482
40	8	0	3.811101	-2.784421	1.322705
41	1	0	3.142934	-3.472788	1.186777
42	1	0	1.655245	0.975526	-2.293606
43	8	0	2.379070	1.426113	-2.774677
44	1	0	3.035298	1.482560	-2.048031
45	8	0	-3.466035	-3.448913	1.183647
46	1	0	-4.083503	-4.155344	0.928005
47	1	0	-2.958429	-3.821108	1.925006
48	8	0	-6.931046	-0.590452	0.488615
49	1	0	-6.567230	0.203230	0.033542
50	1	0	-7.630514	-0.239571	1.063040
51	8	0	-5.472879	1.581373	-0.530261
52	1	0	-5.818509	2.488902	-0.512264
53	1	0	-5.062930	1.453244	-1.423433
54	8	0	-4.761825	-1.123981	2.005695
55	1	0	-5.619388	-1.043655	1.497495
56	1	0	-4.353656	-1.980055	1.729704

SCF Done: E(UB3LYP) = -1676.55702183 A.U. after 1 cycles

Zero-point correction= 0.442266 (a.u.)
Thermal correction to Energy= 0.486205
Thermal correction to Enthalpy= 0.487149
Thermal correction to Gibbs Free Energy= 0.359966
Sum of electronic and zero-point Energies= -1676.114755
Sum of electronic and thermal Energies= -1676.070817
Sum of electronic and thermal Enthalpies= -1676.069873
Sum of electronic and thermal Free Energies= -1676.197056

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.098	150.154	267.679

==== CO2 elimination TS13 in Figure 5 ====
dkg02a.txt

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.543648	0.473941	-0.766531
2	6	0	-2.282519	-0.563596	0.111646
3	6	0	-1.490249	-1.943866	0.288744
4	6	0	-0.816123	1.572881	0.017749
5	8	0	-1.999200	-2.823051	1.005035
6	8	0	-0.351882	1.065599	1.251382
7	8	0	-1.612140	0.444767	-1.977401
8	8	0	-3.226579	-0.216225	0.787776
9	1	0	0.003308	1.933589	-0.618631
10	6	0	-1.749783	2.763591	0.304889
11	6	0	-2.549175	3.240316	-0.911373
12	1	0	-2.456351	2.448037	1.087933
13	8	0	-0.935158	3.829686	0.777597
14	1	0	-1.491353	4.622530	0.656241
15	8	0	-3.182236	4.454906	-0.492100
16	1	0	-3.294250	2.494617	-1.215578

17	1	0	-1.871590	3.425090	-1.755758
18	1	0	-3.411127	4.965846	-1.283081
19	8	0	-0.352849	-1.850165	-0.223847
20	1	0	4.460743	0.488110	3.396892
21	1	0	1.108244	-2.522833	0.519871
22	8	0	4.077224	1.112149	2.757436
23	1	0	3.759287	1.858601	3.293356
24	1	0	0.539322	0.664232	1.109872
25	8	0	2.212902	0.087018	0.934112
26	1	0	2.752028	0.379363	1.706061
27	1	0	3.030523	0.565128	-0.290558
28	8	0	2.010492	-2.541371	0.922292
29	1	0	2.600929	-2.855192	0.203231
30	1	0	2.190156	-0.926351	0.963293
31	8	0	-3.320704	-1.895880	-1.616375
32	1	0	-3.908229	-2.355790	-0.959959
33	8	0	-4.620406	-3.203131	0.515378
34	8	0	3.677419	0.934044	-1.008465
35	1	0	4.387637	1.419599	-0.481768
36	1	0	4.203333	0.090932	-1.470724
37	1	0	-4.778902	-4.151411	0.380632
38	1	0	-3.688606	-3.140148	0.854864
39	1	0	-4.190934	-0.349108	-2.149566
40	8	0	-4.543362	0.489937	-2.524468
41	1	0	-3.760551	0.842378	-2.973990
42	1	0	-4.605907	-0.878817	2.216392
43	8	0	-5.317419	-1.424563	2.590635
44	1	0	-5.337886	-2.162475	1.949588
45	8	0	3.778652	-3.275929	-1.178853
46	1	0	4.409088	-3.961313	-0.899319
47	1	0	3.297852	-3.672867	-1.924980
48	8	0	7.142217	-0.354346	-0.442278
49	1	0	6.755561	0.424474	0.019745
50	1	0	7.840072	0.019818	-1.003804
51	8	0	5.618280	1.761175	0.591378
52	1	0	5.940329	2.677496	0.594043
53	1	0	5.201174	1.606093	1.476969
54	8	0	4.999653	-0.919379	-1.980632
55	1	0	5.852527	-0.821448	-1.466601
56	1	0	4.613324	-1.789710	-1.714214

SCF Done: E(UB3LYP) = -1676.46405379 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-222.8482	13.8201	17.4366

Zero-point correction= 0.437854 (a.u.)
Thermal correction to Energy= 0.481700
Thermal correction to Enthalpy= 0.482644
Thermal correction to Gibbs Free Energy= 0.356427
Sum of electronic and zero-point Energies= -1676.026200
Sum of electronic and thermal Energies= -1675.982354
Sum of electronic and thermal Enthalpies= -1675.981410
Sum of electronic and thermal Free Energies= -1676.107627

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	302.271	150.305	265.645

==== HO-CH2-CH(OH)-CH(OH)-C.(-O(-))-C(=O)-OH + CO2 + H3O(+)(H2O)10
in Figure 5 === dkg02a.rev.txt
Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.325410	-0.342386	-0.774418
2	6	0	-3.420968	-0.624573	0.108038
3	6	0	-0.898517	-3.268405	0.285255
4	6	0	-1.021173	0.224800	-0.220092
5	8	0	-1.634233	-3.424333	1.176941
6	8	0	-0.540455	-0.554880	0.878903
7	8	0	-2.440768	-0.478898	-2.046361

8	8	0	-3.532000	-0.227238	1.313464
9	1	0	-0.305954	0.167591	-1.054533
10	6	0	-1.134408	1.703601	0.183050
11	6	0	-1.584747	2.600741	-0.967382
12	1	0	-1.858621	1.782923	1.006872
13	8	0	0.153763	2.142834	0.628973
14	1	0	0.106253	3.115066	0.573057
15	8	0	-1.485985	3.948833	-0.476770
16	1	0	-2.608313	2.368530	-1.284152
17	1	0	-0.913677	2.457605	-1.826496
18	1	0	-1.457764	4.544558	-1.240680
19	8	0	-0.163180	-3.194404	-0.624969
20	1	0	4.397728	-0.713193	3.519411
21	1	0	1.903758	-3.068573	-0.481231
22	8	0	3.904887	0.047265	3.167063
23	1	0	3.460552	0.438946	3.938120
24	1	0	0.414412	-0.348141	0.978840
25	8	0	2.281595	-0.416224	0.924310
26	1	0	2.736932	-0.382354	1.797008
27	1	0	2.929973	0.706557	0.105443
28	8	0	2.783534	-2.793329	-0.171113
29	1	0	3.301848	-2.619988	-0.989608
30	1	0	2.496927	-1.314887	0.528774
31	8	0	-4.443704	-1.325739	-0.472631
32	1	0	-5.187107	-1.338969	0.174523
33	8	0	-6.131355	-0.790849	1.670874
34	8	0	3.490940	1.462228	-0.335292
35	1	0	4.116879	1.769592	0.393125
36	1	0	4.138334	1.025960	-1.088030
37	1	0	-6.459021	-1.466138	2.285763
38	1	0	-5.180784	-0.636219	1.906543
39	1	0	-5.001590	1.407206	-1.414719
40	8	0	-4.701459	1.315941	-2.343077
41	1	0	-4.033073	0.598547	-2.300776
42	1	0	-4.650526	1.336363	0.857152
43	8	0	-5.450063	1.741542	0.462026
44	1	0	-6.134639	1.102848	0.733296
45	8	0	4.329228	-2.131543	-2.417403
46	1	0	5.077198	-2.741816	-2.533961
47	1	0	3.826412	-2.194537	-3.247324
48	8	0	7.135145	0.628043	-0.180838
49	1	0	6.626074	1.044641	0.551696
50	1	0	7.759183	1.316073	-0.462588
51	8	0	5.289305	1.793646	1.580487
52	1	0	5.453833	2.655584	1.996976
53	1	0	4.915188	1.207162	2.286586
54	8	0	5.107513	0.503182	-1.964428
55	1	0	5.934215	0.487754	-1.402856
56	1	0	4.885037	-0.439965	-2.154206

SCF Done: E(UB3LYP) = -1676.55598216 A.U. after 1 cycles

Zero-point correction= 0.442230 (a.u.)
Thermal correction to Energy= 0.486511
Thermal correction to Enthalpy= 0.487455
Thermal correction to Gibbs Free Energy= 0.358196
Sum of electronic and zero-point Energies= -1676.113752
Sum of electronic and thermal Energies= -1676.069472
Sum of electronic and thermal Enthalpies= -1676.068527
Sum of electronic and thermal Free Energies= -1676.197786

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.290	150.608	272.048

==== precursor HO-CH2-CH(OH)-CH(OH)-C(.)(-O(-))-COOH
and H3O(+)(H2O)10 in Figure 5. It is similar to the
product in Figure 5
(the position of H3O(+) is different) ====

dkg03y.txt

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.002351	0.228938	-0.100780
2	6	0	3.525423	1.567953	0.032399
3	6	0	3.494661	-0.893928	0.786846
4	8	0	2.952487	-0.738310	2.130475
5	8	0	2.047208	-0.018709	-0.956775
6	8	0	4.437483	1.903572	0.825235
7	1	0	3.102617	-1.829217	0.363997
8	6	0	5.010972	-1.062210	0.922505
9	6	0	5.714735	-1.398151	-0.385318
10	1	0	5.438078	-0.143317	1.337295
11	8	0	5.184069	-2.145512	1.847747
12	1	0	6.133727	-2.358524	1.819592
13	8	0	7.075932	-1.666494	-0.031156
14	1	0	5.645159	-0.557365	-1.088483
15	1	0	5.248880	-2.280506	-0.845291
16	1	0	7.482437	-2.170163	-0.752587
17	1	0	1.201736	-1.136696	-0.741866
18	8	0	0.511773	-1.931512	-0.523111
19	1	0	0.359861	-1.879025	0.478400
20	1	0	-0.422618	-1.740528	-1.023267
21	1	0	3.482485	-1.344047	2.685424
22	8	0	-1.635294	-1.485527	-1.706855
23	1	0	-2.408959	-1.773976	-1.136302
24	1	0	-1.722973	-0.495774	-1.782947
25	8	0	2.943054	2.475492	-0.790091
26	1	0	3.389224	3.346086	-0.618566
27	8	0	4.523063	4.533695	0.116966
28	8	0	-1.873309	1.214389	-1.837765
29	1	0	-1.989609	1.497295	-0.905297
30	1	0	-2.769859	1.348193	-2.247055
31	1	0	4.751850	3.696639	0.589925
32	1	0	5.243878	4.646119	-0.524098
33	1	0	1.278890	1.149724	-2.293305
34	8	0	0.724908	1.479530	-3.029234
35	1	0	-0.175603	1.479854	-2.649730
36	8	0	-4.474429	1.336974	-2.651716
37	1	0	-4.583361	0.584509	-3.255191
38	1	0	-4.790302	0.993430	-1.779892
39	8	0	-3.737059	-2.197036	-0.193958
40	1	0	-4.228979	-1.348185	-0.111459
41	1	0	-4.289945	-2.746664	-0.797496
42	8	0	0.377609	-1.661864	2.090198
43	1	0	1.292644	-1.296995	2.218273
44	1	0	-0.213605	-0.921862	2.303187
45	8	0	-4.899659	0.350224	-0.113966
46	1	0	-5.734981	0.499605	0.361290
47	1	0	-4.216101	0.883868	0.358096
48	8	0	-2.724931	1.771733	0.801204
49	1	0	-2.235859	1.383906	1.545803
50	1	0	-2.860449	2.702506	1.045031
51	8	0	-5.236063	-3.754055	-1.970930
52	1	0	-4.610409	-3.975352	-2.679880
53	1	0	-5.398144	-4.605082	-1.532235
54	8	0	-7.520612	0.916287	1.293366
55	6	0	-7.973875	0.999456	2.369761
56	8	0	-8.431893	1.084524	3.438634

SCF Done: E(UB3LYP) = -1676.57111247 A.U. after 1 cycles

Zero-point correction= 0.438920 (a.u.)
Thermal correction to Energy= 0.484509
Thermal correction to Enthalpy= 0.485453
Thermal correction to Gibbs Free Energy= 0.346864
Sum of electronic and zero-point Energies= -1676.132192
Sum of electronic and thermal Energies= -1676.086604
Sum of electronic and thermal Enthalpies= -1676.085659
Sum of electronic and thermal Free Energies= -1676.224248

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	304.034	151.057	291.685

==== the neutralization TS, TS14, in Figure 6 ====

dkg03yy.txt

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.979905	0.238868	-0.069481
2	6	0	3.525115	1.571526	0.043380
3	6	0	3.475868	-0.892256	0.803730
4	8	0	2.953920	-0.737619	2.154992
5	8	0	1.991848	0.012028	-0.898658
6	8	0	4.466151	1.893463	0.805343
7	1	0	3.071653	-1.823196	0.383237
8	6	0	4.992767	-1.073272	0.915960
9	6	0	5.675472	-1.401046	-0.405023
10	1	0	5.433283	-0.162504	1.334353
11	8	0	5.168148	-2.167354	1.827479
12	1	0	6.115508	-2.388080	1.785082
13	8	0	7.038787	-1.685037	-0.072602
14	1	0	5.603601	-0.551899	-1.097824
15	1	0	5.195507	-2.274143	-0.868121
16	1	0	7.431003	-2.183943	-0.805191
17	1	0	1.220237	-1.066750	-0.695166
18	8	0	0.533213	-1.915789	-0.483460
19	1	0	0.363263	-1.876050	0.512539
20	1	0	-0.385815	-1.760102	-0.984808
21	1	0	3.486184	-1.350811	2.699500
22	8	0	-1.637183	-1.529771	-1.704412
23	1	0	-2.408813	-1.803538	-1.128276
24	1	0	-1.727240	-0.544095	-1.802647
25	8	0	2.929792	2.483418	-0.762358
26	1	0	3.392917	3.349313	-0.608736
27	8	0	4.557012	4.523969	0.082096
28	8	0	-1.876803	1.178360	-1.890605
29	1	0	-1.983450	1.475380	-0.961461
30	1	0	-2.777617	1.305237	-2.291853
31	1	0	4.799336	3.691591	0.555218
32	1	0	5.258700	4.631053	-0.580789
33	1	0	1.265533	1.187367	-2.280386
34	8	0	0.728781	1.511643	-3.030173
35	1	0	-0.183865	1.480980	-2.681023
36	8	0	-4.489710	1.286691	-2.673838
37	1	0	-4.605552	0.518269	-3.255541
38	1	0	-4.793924	0.965638	-1.789398
39	8	0	-3.758411	-2.210332	-0.180995
40	1	0	-4.232898	-1.351831	-0.098871
41	1	0	-4.311604	-2.739029	-0.802258
42	8	0	0.372802	-1.666779	2.141702
43	1	0	1.285717	-1.297688	2.265392
44	1	0	-0.220863	-0.929603	2.357448
45	8	0	-4.883524	0.356577	-0.109493
46	1	0	-5.710864	0.519986	0.374942
47	1	0	-4.188868	0.890856	0.345066
48	8	0	-2.686180	1.778122	0.752506
49	1	0	-2.180908	1.397539	1.489955
50	1	0	-2.812422	2.712367	0.987791
51	8	0	-5.246767	-3.703356	-2.024507
52	1	0	-4.607420	-3.901497	-2.728118
53	1	0	-5.418099	-4.568559	-1.618220
54	8	0	-7.485144	0.949382	1.322976
55	6	0	-7.932868	1.022869	2.402389
56	8	0	-8.385454	1.098336	3.474307

SCF Done: E(UB3LYP) = -1676.57108782 A.U. after 1 cycles

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman

	1	2	3
	A	A	A
Frequencies --	-147.5267	7.3908	8.0740
Red. masses --	3.3745	7.6190	8.5117
Frc consts --	0.0433	0.0002	0.0003
IR Inten --	1455.8403	0.3600	0.9507

Zero-point correction= 0.437908 (a.u.)
Thermal correction to Energy= 0.482986
Thermal correction to Enthalpy= 0.483930
Thermal correction to Gibbs Free Energy= 0.346212
Sum of electronic and zero-point Energies= -1676.133180
Sum of electronic and thermal Energies= -1676.088102
Sum of electronic and thermal Enthalpies= -1676.087158
Sum of electronic and thermal Free Energies= -1676.224876

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	303.078	149.628	289.853

==== the neutral radical HO-CH2-CH(OH)-CH(OH)-C(.)(OH)-COOH + CO2 + (H2O)11 in Figure 6 ====

dkg03.for.txt

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.303053	0.752073	-0.585855
2	6	0	-1.716175	0.619754	-0.281743
3	6	0	-0.032412	-1.581818	2.203802
4	6	0	0.528513	1.978167	-0.311658
5	8	0	-1.155320	-1.390775	2.454360
6	8	0	1.044825	1.883411	1.045359
7	8	0	0.307078	-0.356464	-1.017352
8	8	0	-2.403084	1.508015	0.248926
9	1	0	1.384826	1.949504	-0.998216
10	6	0	-0.147988	3.340034	-0.503760
11	6	0	-0.752120	3.528833	-1.894574
12	1	0	-0.928085	3.466017	0.254319
13	8	0	0.882635	4.310485	-0.309942
14	1	0	0.522552	5.126448	-0.704267
15	8	0	-1.115070	4.913142	-1.970689
16	1	0	-1.629756	2.886384	-2.029788
17	1	0	-0.006728	3.280306	-2.662234
18	1	0	-1.155002	5.165280	-2.905647
19	8	0	1.097838	-1.771460	1.963618
20	1	0	1.319637	-0.238952	-1.173974
21	8	0	2.847888	-0.175175	-1.397908
22	1	0	3.211617	-0.099205	-0.486127
23	1	0	3.113775	-1.086620	-1.718992
24	1	0	1.731271	2.592365	1.173091
25	8	0	3.410217	3.098926	1.711734
26	1	0	3.343812	3.316033	2.655546
27	8	0	3.426348	-2.685844	-2.151152
28	1	0	4.313104	-2.901181	-1.776707
29	1	0	2.790608	-3.148157	-1.563132
30	1	0	3.726459	2.169932	1.700088
31	8	0	-2.228534	-0.564567	-0.642433
32	1	0	-3.171785	-0.703944	-0.256669
33	8	0	-4.482482	-1.282875	0.380039
34	8	0	1.559450	-3.701100	-0.281914
35	1	0	1.749978	-3.154190	0.500493
36	1	0	1.712695	-4.615220	0.010719
37	1	0	-5.078106	-1.551871	-0.360069
38	1	0	-4.114690	-2.133391	0.740219
39	1	0	-1.276676	-2.239220	-0.766919
40	8	0	-1.223069	-3.200778	-0.598501
41	1	0	-0.268057	-3.406193	-0.513555
42	1	0	-0.387726	2.242770	2.346786
43	8	0	-1.269267	2.410966	2.731393
44	1	0	-1.847606	2.123456	1.999893
45	8	0	5.939620	-3.264166	-1.070939
46	1	0	5.836300	-4.057225	-0.520154
47	1	0	6.495023	-3.566516	-1.807962
48	8	0	3.318064	0.340588	1.290948
49	1	0	2.377978	0.636626	1.327292
50	1	0	3.387957	-0.382259	1.935030
51	8	0	-3.170728	-3.519012	1.273753

52	1	0	-2.413529	-3.489435	0.629787
53	1	0	-2.782919	-3.195387	2.102136
54	8	0	-6.131373	-2.012036	-1.745831
55	1	0	-6.946669	-1.492487	-1.654868
56	1	0	-5.711144	-1.646170	-2.541159

SCF Done HF=-1676.573965 a.u.

Zero-point correction= 0.440744 (a.u.)
Thermal correction to Energy= 0.487281
Thermal correction to Enthalpy= 0.488225
Thermal correction to Gibbs Free Energy= 0.352935
Sum of electronic and zero-point Energies= -1676.133221
Sum of electronic and thermal Energies= -1676.086684
Sum of electronic and thermal Enthalpies= -1676.085740
Sum of electronic and thermal Free Energies= -1676.221030

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	305.773	154.259	284.741

==== the neutral radical HO-CH2-CH(OH)-CH(OH)-C(.)(OH)-COOH, threonic acid HO-CH2-CH(OH)-CH(OH)-COOH and (H2O)8 in the latter part of Figure 6 (before H abstraction) ====

habst2qr.for.txt

Stoichiometry C9H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.244813	1.033875	-0.506662
2	6	0	0.064969	1.739178	-0.039246
3	6	0	2.448793	0.791630	0.367187
4	8	0	2.119021	0.246784	1.655588
5	8	0	1.201603	0.528887	-1.753700
6	8	0	0.058341	2.410573	0.995545
7	1	0	3.095130	0.079647	-0.166053
8	6	0	3.303988	2.042048	0.624363
9	6	0	3.695624	2.770053	-0.662505
10	1	0	2.731034	2.719161	1.270707
11	8	0	4.500288	1.627877	1.293606
12	1	0	5.142720	2.340371	1.109856
13	8	0	4.658613	3.753438	-0.270797
14	1	0	2.818542	3.238374	-1.126771
15	1	0	4.135617	2.060998	-1.376742
16	1	0	5.191291	3.985167	-1.046703
17	1	0	1.293726	-0.284324	1.611797
18	8	0	-1.017735	1.574152	-0.826920
19	1	0	-1.816363	2.055986	-0.408021
20	1	0	-0.482707	-0.865792	-0.312832
21	6	0	-0.443998	-1.786655	0.281147
22	6	0	-1.818420	-2.514496	0.118579
23	6	0	0.738973	-2.555141	-0.290860
24	8	0	-0.215209	-1.458218	1.638122
25	1	0	-1.117641	-1.415290	2.024940
26	8	0	-2.683598	-2.073854	1.151766
27	1	0	-3.138905	-1.220646	0.916385
28	6	0	-2.399998	-2.310411	-1.284470
29	1	0	-1.676886	-3.589987	0.277246
30	8	0	0.813149	-2.785945	-1.498871
31	8	0	1.665336	-2.857614	0.591817
32	1	0	2.564884	-3.086920	0.151279
33	8	0	-2.797146	-0.959177	-1.532358
34	1	0	1.980494	-0.054436	-1.963902
35	8	0	2.994668	-1.414806	-2.406406
36	1	0	2.268248	-2.079868	-2.367472
37	1	0	3.292858	-1.389152	-3.331006
38	8	0	-3.180810	2.630541	0.196414
39	1	0	-3.790811	2.800418	-0.554328
40	1	0	-3.548839	1.809775	0.616669
41	8	0	-4.167307	0.218962	1.021595
42	1	0	-4.741281	0.195921	1.827144
43	1	0	-4.771854	0.108022	0.238186

44	1	0	-2.031161	-0.356526	-1.549006
45	1	0	-1.676255	-2.654207	-2.032168
46	1	0	-3.313356	-2.902821	-1.381600
47	8	0	4.089201	-2.950370	-0.289057
48	1	0	4.012493	-2.417795	-1.108695
49	1	0	4.383023	-2.300474	0.407286
50	8	0	4.540586	-1.169080	1.731740
51	1	0	4.906990	-0.296151	1.483482
52	1	0	3.612719	-0.911612	1.928493
53	8	0	-5.417213	-0.014096	-1.372372
54	1	0	-5.391173	0.922193	-1.666053
55	1	0	-4.550662	-0.374803	-1.658794
56	8	0	-5.038143	2.739198	-1.933008
57	1	0	-4.690572	2.967543	-2.810982
58	1	0	-5.803078	3.324668	-1.807014
59	8	0	-5.741489	0.168733	3.297656
60	1	0	-5.306271	-0.435942	3.920636
61	1	0	-5.647675	1.040149	3.715967

SCF Done: E(UB3LYP) = -1792.07529329 A.U. after 1 cycles

Zero-point correction= 0.491801 (a.u.)
Thermal correction to Energy= 0.534958
Thermal correction to Enthalpy= 0.535902
Thermal correction to Gibbs Free Energy= 0.411626
Sum of electronic and zero-point Energies= -1791.583492
Sum of electronic and thermal Energies= -1791.540336
Sum of electronic and thermal Enthalpies= -1791.539391
Sum of electronic and thermal Free Energies= -1791.663668

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	335.691	151.123	261.561

==== the hydrogen abstraction TS, TS15, in Figure 6 ====

habst2qr.txt

Stoichiometry C9H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.768643	0.662817	-0.216751
2	6	0	-0.370297	1.465970	0.333045
3	6	0	2.100838	0.716939	0.546365
4	8	0	2.032327	0.164941	1.861616
5	8	0	0.886886	0.778061	-1.590059
6	8	0	-0.452137	1.793472	1.508289
7	1	0	2.823038	0.140597	-0.048655
8	6	0	2.670721	2.139087	0.691834
9	6	0	2.805305	2.900862	-0.629802
10	1	0	2.016071	2.699881	1.371025
11	8	0	3.975926	2.035635	1.276639
12	1	0	4.421668	2.867280	1.021871
13	8	0	3.544003	4.085373	-0.306396
14	1	0	1.824340	3.150146	-1.048723
15	1	0	3.352566	2.292308	-1.361189
16	1	0	3.963375	4.412626	-1.116638
17	1	0	1.383465	-0.567093	1.887786
18	8	0	-1.318830	1.706561	-0.578999
19	1	0	-2.157861	2.097232	-0.117768
20	1	0	0.310330	-0.634881	-0.017486
21	6	0	0.074850	-1.985135	0.277912
22	6	0	-1.279929	-2.473424	-0.292132
23	6	0	1.306097	-2.547680	-0.337431
24	8	0	0.083333	-1.997421	1.664411
25	1	0	-0.875520	-1.968088	1.900168
26	8	0	-2.276844	-2.274125	0.696085
27	1	0	-2.759220	-1.414680	0.575790
28	6	0	-1.683829	-1.930766	-1.678127
29	1	0	-1.177885	-3.562186	-0.405380
30	8	0	1.373770	-2.773653	-1.552433
31	8	0	2.326617	-2.651403	0.498540

32	1	0	3.217183	-2.678600	-0.007683
33	8	0	-2.359549	-0.681112	-1.626481
34	1	0	1.670995	0.264171	-1.911692
35	8	0	3.001104	-0.807700	-2.484394
36	1	0	2.482786	-1.645086	-2.458593
37	1	0	3.225342	-0.655118	-3.417496
38	8	0	-3.523323	2.467084	0.526152
39	1	0	-4.146525	2.638778	-0.214954
40	1	0	-3.769217	1.553656	0.834610
41	8	0	-4.033282	-0.165685	0.951538
42	1	0	-4.600686	-0.462096	1.705481
43	1	0	-4.580465	-0.271660	0.126731
44	1	0	-1.755203	0.069055	-1.457078
45	1	0	-0.802782	-1.892267	-2.325594
46	1	0	-2.402589	-2.629342	-2.114751
47	8	0	4.630398	-2.179263	-0.571001
48	1	0	4.352568	-1.605067	-1.315626
49	1	0	4.825082	-1.555058	0.181341
50	8	0	4.787796	-0.598119	1.643344
51	1	0	4.827786	0.358145	1.427473
52	1	0	3.857293	-0.660180	1.945154
53	8	0	-5.114288	-0.283778	-1.531638
54	1	0	-5.262411	0.672269	-1.695720
55	1	0	-4.178968	-0.428522	-1.794425
56	8	0	-5.283559	2.548072	-1.671359
57	1	0	-4.935411	2.971971	-2.473140
58	1	0	-6.158538	2.948394	-1.537070
59	8	0	-5.598394	-0.980177	3.088339
60	1	0	-5.021137	-1.509577	3.662521
61	1	0	-5.779501	-0.183130	3.612669

SCF Done: E(UB3LYP) = -1792.04030318 A.U. after 1 cycles
NFock= 1 Conv=0.46D-08 -V/T= 2.0087

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman

	1	2	3
	A	A	A
Frequencies --	-1752.1604	15.1322	23.7380
Red. masses --	1.1645	5.7459	5.0070
Frc consts --	2.1063	0.0008	0.0017
IR Inten --	1020.5828	1.8864	5.1460

Zero-point correction= 0.487472 (a.u.)
Thermal correction to Energy= 0.529374
Thermal correction to Enthalpy= 0.530318
Thermal correction to Gibbs Free Energy= 0.411915
Sum of electronic and zero-point Energies= -1791.552832
Sum of electronic and thermal Energies= -1791.510929
Sum of electronic and thermal Enthalpies= -1791.509985
Sum of electronic and thermal Free Energies= -1791.628388

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	332.187	149.397	249.199

==== after the H migration, L-lyxonic acid,
HO-CH2-CH(OH)-C(.)(OH)-COOH and (H2O)8 in Figure 6 ====

habst2qr.rev.txt

Stoichiometry C9H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.519981	0.597018	-0.705896
2	6	0	0.480570	1.633647	-0.280934
3	6	0	2.634554	0.407491	0.355430
4	8	0	2.080880	-0.104916	1.575211
5	8	0	2.049310	0.935071	-1.973646
6	8	0	0.635856	2.838906	-0.343738
7	1	0	3.332958	-0.320755	-0.077358
8	6	0	3.448241	1.647341	0.735663

9	6	0	4.030274	2.434081	-0.441283
10	1	0	2.809254	2.319020	1.326642
11	8	0	4.540377	1.200935	1.554510
12	1	0	5.196921	1.921698	1.485655
13	8	0	4.936918	3.376823	0.156004
14	1	0	3.238118	2.942098	-0.995646
15	1	0	4.566118	1.761549	-1.121078
16	1	0	5.592360	3.628354	-0.511794
17	1	0	1.542707	-0.896450	1.361893
18	8	0	-0.617012	1.036343	0.195429
19	1	0	-1.302099	1.705330	0.593636
20	1	0	0.996232	-0.360865	-0.772942
21	6	0	-1.254479	-2.437290	0.297671
22	6	0	-2.517041	-2.475646	-0.558459
23	6	0	0.074155	-2.691334	-0.176101
24	8	0	-1.451759	-2.275830	1.609609
25	1	0	-2.437796	-2.184454	1.684533
26	8	0	-3.616547	-2.159129	0.287770
27	1	0	-3.773388	-1.174324	0.321755
28	6	0	-2.475562	-1.617508	-1.832691
29	1	0	-2.667281	-3.513331	-0.891724
30	8	0	0.332339	-2.891143	-1.381803
31	8	0	1.026302	-2.662497	0.780369
32	1	0	1.940803	-2.924750	0.396420
33	8	0	-2.496983	-0.219233	-1.573103
34	1	0	2.381863	0.082885	-2.335759
35	8	0	2.688998	-1.796338	-2.387686
36	1	0	1.830155	-2.242722	-2.186496
37	1	0	2.961790	-2.132380	-3.256877
38	8	0	-2.495106	2.435848	1.243417
39	1	0	-2.808693	3.085305	0.574306
40	1	0	-3.188626	1.723403	1.227647
41	8	0	-4.315114	0.432196	0.816213
42	1	0	-5.108103	0.376612	1.406359
43	1	0	-4.629756	0.819947	-0.046102
44	1	0	-1.724443	0.053328	-1.038672
45	1	0	-1.602201	-1.904938	-2.426234
46	1	0	-3.379775	-1.825903	-2.410725
47	8	0	3.460709	-3.116367	-0.037515
48	1	0	3.491711	-2.651188	-0.902656
49	1	0	3.976920	-2.562705	0.605966
50	8	0	4.492253	-1.559566	1.983786
51	1	0	4.936513	-0.730800	1.712196
52	1	0	3.609924	-1.195246	2.206286
53	8	0	-4.700190	1.475329	-1.651444
54	1	0	-4.345696	2.380730	-1.519040
55	1	0	-3.904915	0.937507	-1.858684
56	8	0	-3.470799	3.930743	-0.914775
57	1	0	-2.765598	4.254918	-1.499177
58	1	0	-4.036368	4.703485	-0.751258
59	8	0	-6.516598	0.245880	2.476994
60	1	0	-6.616079	-0.696586	2.689207
61	1	0	-6.268357	0.649966	3.324524

SCF Done: E(UB3LYP) = -1792.08184043 A.U. after 1 cycles
NFock= 1 Conv=0.38D-08 -V/T= 2.0087

Zero-point correction= 0.493675 (a.u.)
Thermal correction to Energy= 0.536042
Thermal correction to Enthalpy= 0.536986
Thermal correction to Gibbs Free Energy= 0.416073
Sum of electronic and zero-point Energies= -1791.588166
Sum of electronic and thermal Energies= -1791.545799
Sum of electronic and thermal Enthalpies= -1791.544854
Sum of electronic and thermal Free Energies= -1791.665767

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	336.371	149.690	254.482

==== precursor DKG + H2O2 + (H2O)10 in Figure 7 ====
dkgr6b.for.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.090758	-0.796571	-0.011719
2	6	0	1.695483	-2.158887	-0.615498
3	6	0	0.208907	-2.476269	-0.858006
4	6	0	2.682914	0.229040	-0.947215
5	8	0	-0.216120	-2.560688	-1.993318
6	8	0	2.367588	-0.141726	-2.273051
7	8	0	2.025512	-0.631402	1.202072
8	8	0	2.579187	-2.947101	-0.882064
9	1	0	2.225810	1.193679	-0.688304
10	6	0	4.230157	0.369243	-0.787189
11	6	0	4.661803	1.077920	0.500107
12	1	0	4.692751	-0.620135	-0.860404
13	8	0	4.681639	1.115685	-1.915533
14	1	0	4.514805	2.049985	-1.679079
15	8	0	4.232774	2.436526	0.476613
16	1	0	5.756297	1.080210	0.533612
17	1	0	4.296487	0.546576	1.385576
18	1	0	3.357678	2.483135	0.921073
19	8	0	-0.463771	-2.645395	0.260930
20	1	0	-1.521127	-2.702217	0.114057
21	8	0	-0.207653	0.445121	-0.239156
22	8	0	-1.080307	0.852623	-1.325207
23	1	0	-0.824287	0.106889	0.472395
24	1	0	-1.495308	1.673088	-0.939292
25	1	0	3.056616	0.289283	-2.816321
26	8	0	-1.509833	-0.190538	2.058683
27	1	0	-0.827621	-0.754393	2.508915
28	1	0	-1.383291	0.744302	2.384994
29	8	0	-1.096604	2.442534	2.398620
30	1	0	-0.165782	2.466615	2.091425
31	1	0	-1.641021	2.606168	1.594053
32	8	0	0.298312	-2.031842	2.986817
33	1	0	0.003344	-2.615287	2.262838
34	1	0	1.101029	-1.634202	2.597797
35	8	0	-2.676430	2.453669	0.082536
36	1	0	-3.164126	3.228898	-0.300050
37	1	0	-3.286028	1.686282	0.022330
38	8	0	-3.604866	-0.153531	-0.780366
39	1	0	-2.735437	0.027334	-1.202641
40	1	0	-4.270404	-0.114271	-1.513340
41	8	0	-4.008566	4.590281	-0.983931
42	1	0	-3.843726	5.357959	-0.412204
43	1	0	-3.562897	4.818282	-1.816222
44	8	0	-5.468407	-0.079677	-2.813015
45	1	0	-5.579613	-0.996264	-3.114237
46	1	0	-6.324238	0.138035	-2.408687
47	8	0	-2.980521	-2.681455	0.095806
48	1	0	-3.255261	-2.535795	1.043158
49	1	0	-3.255994	-1.824614	-0.326874
50	8	0	-3.616920	-1.827074	2.595110
51	1	0	-4.463954	-1.371670	2.464252
52	1	0	-2.934831	-1.113785	2.489635
53	8	0	1.778505	2.156613	1.906837
54	1	0	2.064772	2.318332	2.822242
55	1	0	1.777090	1.179744	1.819358

SCF Done: E(RB3LYP) = -1675.86904548 A.U. after 1 cycles

Zero-point correction= 0.434536 (a.u.)
Thermal correction to Energy= 0.477206
Thermal correction to Enthalpy= 0.478150
Thermal correction to Gibbs Free Energy= 0.356302
Sum of electronic and zero-point Energies= -1675.434509
Sum of electronic and thermal Energies= -1675.391840
Sum of electronic and thermal Enthalpies= -1675.390895
Sum of electronic and thermal Free Energies= -1675.512743

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.451	145.561	256.450

==== HOOH nucleophilic addtition, TS16, in Figure 7 ====
dkgr6b.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.583897	-0.692709	-0.126665
2	6	0	1.201359	-2.002441	-0.857933
3	6	0	-0.279776	-2.343615	-1.068568
4	6	0	2.391056	0.299481	-0.964300
5	8	0	-0.777661	-2.268712	-2.175011
6	8	0	1.981921	0.193532	-2.317534
7	8	0	1.850284	-0.825693	1.112036
8	8	0	2.080008	-2.751227	-1.235181
9	1	0	2.176090	1.302812	-0.570105
10	6	0	3.926568	0.068422	-0.885261
11	6	0	4.582088	0.452168	0.443487
12	1	0	4.146530	-0.975020	-1.130460
13	8	0	4.507898	0.860622	-1.931982
14	1	0	4.554361	1.763805	-1.562235
15	8	0	4.435809	1.850970	0.688441
16	1	0	5.655678	0.251327	0.358819
17	1	0	4.182096	-0.150711	1.263790
18	1	0	3.599995	1.973024	1.189558
19	8	0	-0.895010	-2.711391	0.045258
20	1	0	-1.936061	-2.701859	-0.078013
21	8	0	-0.005102	0.161541	-0.004896
22	8	0	-0.719023	0.717400	-1.142343
23	1	0	-0.775515	-0.172433	0.952389
24	1	0	-0.957473	1.607781	-0.764030
25	1	0	2.742768	0.546384	-2.819588
26	8	0	-1.311276	-0.322046	1.983114
27	1	0	-0.759656	-1.058699	2.433752
28	1	0	-1.115677	0.591310	2.436736
29	8	0	-0.745167	2.071105	2.677426
30	1	0	0.224140	2.088239	2.491034
31	1	0	-1.177970	2.447386	1.870807
32	8	0	0.215228	-2.291675	2.729805
33	1	0	-0.167594	-2.924614	2.094610
34	1	0	0.971580	-1.907438	2.217908
35	8	0	-2.006554	2.584919	0.271942
36	1	0	-2.311054	3.469142	-0.062731
37	1	0	-2.760399	1.966940	0.148572
38	8	0	-3.423947	0.246549	-0.687346
39	1	0	-2.516585	0.238795	-1.066382
40	1	0	-4.019956	0.493037	-1.439815
41	8	0	-2.833937	5.014739	-0.658201
42	1	0	-2.544640	5.691170	-0.024024
43	1	0	-2.316655	5.206143	-1.457652
44	8	0	-5.097011	0.898542	-2.783830
45	1	0	-5.195825	0.092317	-3.316216
46	1	0	-5.981594	1.039131	-2.408239
47	8	0	-3.439895	-2.458996	-0.087112
48	1	0	-3.671723	-2.344928	0.870972
49	1	0	-3.528423	-1.529735	-0.423377
50	8	0	-3.804772	-1.637009	2.494227
51	1	0	-4.577528	-1.050196	2.462224
52	1	0	-3.039690	-1.036623	2.369160
53	8	0	2.030465	1.673876	2.229715
54	1	0	2.386898	1.605738	3.131786
55	1	0	1.944662	0.733578	1.917974

SCF Done: E(RB3LYP) = -1675.84955069 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-655.5605	19.0045	23.8461

Zero-point correction= 0.431363 (a.u.)
Thermal correction to Energy= 0.471965
Thermal correction to Enthalpy= 0.472909
Thermal correction to Gibbs Free Energy= 0.356680
Sum of electronic and zero-point Energies= -1675.418188
Sum of electronic and thermal Energies= -1675.377586
Sum of electronic and thermal Enthalpies= -1675.376642

Sum of electronic and thermal Free Energies= -1675.492870

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.162	141.118	244.624

==== HOO(-) adduct to DKG in Figure 7 ===
dkgr12b.rev.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.377297	0.659064	-0.646791
2	6	0	0.475992	0.494594	-1.933283
3	6	0	1.969418	0.227551	-1.673302
4	6	0	-1.800925	0.053292	-0.746736
5	8	0	2.428937	-0.899360	-1.823729
6	8	0	-1.796261	-1.232824	-1.390307
7	8	0	-0.382313	1.953878	-0.296541
8	8	0	0.043827	0.608452	-3.061392
9	1	0	-2.152125	-0.074081	0.285676
10	6	0	-2.822783	0.944732	-1.508995
11	6	0	-3.331731	2.173741	-0.752789
12	1	0	-2.397018	1.243095	-2.470310
13	8	0	-3.950437	0.103323	-1.822690
14	1	0	-4.471332	0.055090	-0.997991
15	8	0	-3.963174	1.795266	0.471407
16	1	0	-4.098667	2.649590	-1.373795
17	1	0	-2.518723	2.883946	-0.591338
18	1	0	-3.266880	1.788142	1.160209
19	8	0	2.624649	1.296104	-1.278327
20	1	0	3.523656	1.073245	-0.806969
21	8	0	0.380711	0.007249	0.452411
22	8	0	0.429197	-1.449628	0.332292
23	1	0	1.847668	0.713756	1.323004
24	1	0	0.274769	-1.672910	1.286190
25	1	0	-2.678308	-1.272256	-1.823171
26	8	0	2.286304	1.267941	2.008094
27	1	0	2.156770	2.187158	1.618859
28	1	0	1.081433	1.066069	3.020635
29	8	0	0.183663	0.853623	3.486850
30	1	0	-0.553725	1.347058	2.939607
31	1	0	0.035485	-0.153491	3.384667
32	8	0	1.677739	3.456320	0.597908
33	1	0	2.371481	3.491729	-0.080035
34	1	0	0.953580	2.933987	0.154035
35	8	0	0.017168	-1.706926	3.025507
36	1	0	-0.790818	-2.325250	3.035337
37	1	0	0.726792	-2.187500	3.483639
38	1	0	1.011165	-2.712832	-1.509621
39	8	0	0.293706	-3.232560	-1.914390
40	1	0	-0.392146	-2.546328	-2.026783
41	8	0	-1.895815	-3.441351	2.741851
42	1	0	-2.783186	-3.064417	2.853448
43	1	0	-1.803711	-3.586088	1.756069
44	8	0	4.771605	-1.769172	-0.480110
45	1	0	3.983543	-1.606361	-1.043104
46	1	0	5.505994	-1.841939	-1.111149
47	8	0	4.608914	0.825082	0.263822
48	1	0	4.071833	0.892126	1.081855
49	1	0	4.802317	-0.143979	0.142970
50	1	0	-0.846518	-3.807247	-0.396273
51	8	0	-1.701317	-3.649665	0.060956
52	1	0	-1.894914	-2.740179	-0.252845
53	8	0	-1.526626	2.087444	2.017355
54	1	0	-1.570748	3.017870	2.298381
55	1	0	-1.047512	2.088595	1.102442

SCF Done: E(RB3LYP) = -1675.87144945 A.U. after 1 cycles

Zero-point correction= 0.437087 (a.u.)
Thermal correction to Energy= 0.475669
Thermal correction to Enthalpy= 0.476613

Thermal correction to Gibbs Free Energy= 0.368131
Sum of electronic and zero-point Energies= -1675.434362
Sum of electronic and thermal Energies= -1675.395780
Sum of electronic and thermal Enthalpies= -1675.394836
Sum of electronic and thermal Free Energies= -1675.503318

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.487	138.841	228.319

==== TS17 to the conjugate base of threonic acid and neutral oxalic acid in Figure 7 ====
dkgr7b.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.895292	-0.538982	0.285204
2	6	0	-1.104608	-0.055134	-1.383731
3	6	0	-1.411554	1.474825	-1.330512
4	6	0	-1.535870	-1.956467	0.507748
5	8	0	-2.709425	1.665048	-1.381018
6	8	0	-0.738225	-2.967274	-0.116672
7	8	0	-1.435241	0.389827	1.046012
8	8	0	-1.485183	-0.776775	-2.266419
9	1	0	-1.486680	-2.085985	1.596953
10	6	0	-3.004622	-2.151275	0.086290
11	6	0	-3.967480	-1.098735	0.643166
12	1	0	-3.072461	-2.167589	-1.003995
13	8	0	-3.356336	-3.486042	0.497055
14	1	0	-3.464725	-3.459676	1.464679
15	8	0	-3.707776	-0.789049	2.006602
16	1	0	-4.984059	-1.502284	0.577870
17	1	0	-3.915936	-0.198692	0.018315
18	1	0	-2.880720	-0.250784	1.951201
19	8	0	-0.548181	2.331080	-1.306092
20	1	0	-2.931204	2.652219	-1.202075
21	8	0	0.438841	-0.681889	0.224594
22	8	0	0.884699	0.086271	-1.469526
23	1	0	1.413526	0.486065	1.106771
24	1	0	1.097064	-0.813379	-1.846956
25	1	0	-1.283248	-3.777560	-0.066370
26	8	0	2.035012	1.064990	1.610883
27	1	0	1.395637	1.639098	2.119745
28	1	0	3.078584	-0.419999	1.882203
29	8	0	3.643411	-1.180434	1.602382
30	1	0	3.019205	-1.874791	1.271739
31	1	0	4.318883	-0.644667	0.379858
32	8	0	-0.152940	2.290325	2.569001
33	1	0	-0.326491	3.085741	2.023268
34	1	0	-0.641662	1.577076	2.080892
35	8	0	4.695920	-0.184066	-0.485385
36	1	0	5.610100	0.197968	-0.277343
37	1	0	4.022654	0.619183	-0.697097
38	8	0	3.012519	1.645984	-0.832335
39	1	0	2.242869	1.176177	-1.253899
40	1	0	2.702752	1.713443	0.111137
41	8	0	7.083981	0.816754	0.025554
42	1	0	7.116691	1.147852	0.938556
43	1	0	7.741560	0.101544	0.004426
44	8	0	-3.258401	4.132296	-0.723913
45	1	0	-4.000511	4.074107	-0.099528
46	1	0	-2.475753	4.370758	-0.166048
47	8	0	1.229465	-2.531258	-2.247008
48	1	0	0.328190	-2.717701	-1.920593
49	1	0	1.774812	-2.815795	-1.482081
50	8	0	2.053192	-3.117932	0.399853
51	1	0	2.233286	-4.034068	0.667049
52	1	0	1.076481	-3.013220	0.464955
53	8	0	-0.852067	4.298423	0.606978
54	1	0	-0.337298	5.119562	0.538433
55	1	0	-0.521102	3.719787	-0.115440

SCF Done: E(RB3LYP) = -1675.81800487   A.U. after   1 cycles

	1	2	3
	A	A	A
Frequencies --	-707.1115	19.9025	24.7971

Zero-point correction= 0.433103 (a.u.)
Thermal correction to Energy= 0.472364
Thermal correction to Enthalpy= 0.473308
Thermal correction to Gibbs Free Energy= 0.361766
Sum of electronic and zero-point Energies= -1675.384902
Sum of electronic and thermal Energies= -1675.345641
Sum of electronic and thermal Enthalpies= -1675.344697
Sum of electronic and thermal Free Energies= -1675.456239

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	296.413	139.913	234.761

==== Conjugate base of DKG and the neutral oxalic acid in Figure 7 ===
dkgr7b.rev.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.289616	-0.913348	1.150649
2	6	0	-0.344607	0.423738	-2.221057
3	6	0	-0.326236	1.875609	-1.693008
4	6	0	-2.359895	-1.881992	0.621599
5	8	0	-1.496175	2.448866	-1.782983
6	8	0	-1.756137	-2.972908	-0.080819
7	8	0	-1.703224	-0.003546	1.920041
8	8	0	-1.352094	-0.071517	-2.690383
9	1	0	-2.874423	-2.270297	1.512646
10	6	0	-3.442406	-1.254815	-0.290479
11	6	0	-4.112506	0.002445	0.267877
12	1	0	-2.985810	-1.014594	-1.255012
13	8	0	-4.391756	-2.297546	-0.572965
14	1	0	-4.923450	-2.413516	0.234667
15	8	0	-4.459134	-0.121668	1.642664
16	1	0	-5.038055	0.171782	-0.292974
17	1	0	-3.453871	0.865102	0.101026
18	1	0	-3.589933	-0.054348	2.096329
19	8	0	0.688066	2.378999	-1.214172
20	1	0	-1.497066	3.382638	-1.351609
21	8	0	-0.087128	-1.097271	0.800812
22	8	0	0.814000	-0.173601	-2.044522
23	1	0	1.177635	-0.195024	1.477545
24	1	0	0.676109	-1.191942	-2.143138
25	1	0	-2.512643	-3.466265	-0.451292
26	8	0	1.934260	0.275548	1.927385
27	1	0	1.443857	0.895360	2.536313
28	1	0	3.060484	-1.137046	1.976341
29	8	0	3.572886	-1.888178	1.584524
30	1	0	2.870262	-2.508121	1.258100
31	1	0	4.115346	-1.289672	0.339014
32	8	0	0.090335	1.839677	3.092471
33	1	0	0.128974	2.593352	2.464411
34	1	0	-0.585641	1.232970	2.703833
35	8	0	4.403526	-0.775143	-0.535592
36	1	0	5.395328	-0.577657	-0.486316
37	1	0	3.870528	0.143212	-0.503206
38	8	0	3.101755	1.347145	-0.212579
39	1	0	2.350574	1.472453	-0.829771
40	1	0	2.655773	1.082709	0.646410
41	8	0	6.987607	-0.246156	-0.455558
42	1	0	7.239345	0.072988	0.427013
43	1	0	7.490757	-1.070014	-0.566681
44	8	0	-1.588779	4.759818	-0.589335
45	1	0	-2.456891	4.794835	-0.154577
46	1	0	-0.938196	4.639515	0.147581
47	8	0	0.343324	-2.723264	-2.019213
48	1	0	-0.508215	-2.707231	-1.524267

49	1	0	0.955678	-3.056247	-1.322860
50	8	0	1.470379	-3.238406	0.456518
51	1	0	1.144945	-4.068942	0.840023
52	1	0	0.763292	-2.562600	0.649500
53	8	0	0.365296	3.908049	1.117903
54	1	0	1.070807	4.532571	1.355348
55	1	0	0.710024	3.403013	0.348545

SCF Done: E(RB3LYP) = -1676.04514711 A.U. after 1 cycles

Zero-point correction= 0.437981 (a.u.)
Thermal correction to Energy= 0.477526
Thermal correction to Enthalpy= 0.478470
Thermal correction to Gibbs Free Energy= 0.363044
Sum of electronic and zero-point Energies= -1675.607166
Sum of electronic and thermal Energies= -1675.567621
Sum of electronic and thermal Enthalpies= -1675.566677
Sum of electronic and thermal Free Energies= -1675.682103

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.652	137.952	242.936

===== Neutralization TS18 in Figure 7 ====
dkgr12b.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.376751	0.643653	-0.631471
2	6	0	0.469456	0.475941	-1.923395
3	6	0	1.958671	0.182024	-1.662922
4	6	0	-1.802359	0.043497	-0.727628
5	8	0	2.395805	-0.957560	-1.785127
6	8	0	-1.791418	-1.247754	-1.356952
7	8	0	-0.381219	1.956572	-0.291349
8	8	0	0.032762	0.593928	-3.047553
9	1	0	-2.157590	-0.071872	0.304888
10	6	0	-2.823449	0.924107	-1.505575
11	6	0	-3.332374	2.169177	-0.775609
12	1	0	-2.398380	1.202468	-2.473077
13	8	0	-3.949759	0.075601	-1.801366
14	1	0	-4.470642	0.038719	-0.976212
15	8	0	-3.940192	1.822372	0.468822
16	1	0	-4.113954	2.617288	-1.398632
17	1	0	-2.527839	2.896681	-0.650528
18	1	0	-3.230235	1.827820	1.142772
19	8	0	2.632043	1.248026	-1.301154
20	1	0	3.529005	1.025770	-0.812373
21	8	0	0.382474	0.020839	0.463411
22	8	0	0.397007	-1.436277	0.385869
23	1	0	1.865932	0.735503	1.356102
24	1	0	0.212907	-1.625976	1.345050
25	1	0	-2.675256	-1.298426	-1.785071
26	8	0	2.336053	1.307026	2.001116
27	1	0	2.214162	2.209696	1.585043
28	1	0	0.988669	1.167494	3.056049
29	8	0	0.070002	1.006831	3.440213
30	1	0	-0.680274	1.545751	2.736727
31	1	0	-0.082157	0.014296	3.375630
32	8	0	1.751367	3.487023	0.510388
33	1	0	2.440814	3.486719	-0.172803
34	1	0	1.015359	2.974995	0.087632
35	8	0	-0.079070	-1.637095	3.052064
36	1	0	-0.837376	-2.308716	3.064937
37	1	0	0.659997	-2.071977	3.508898
38	1	0	1.052925	-2.690631	-1.595086
39	8	0	0.308085	-3.221091	-1.932004
40	1	0	-0.387263	-2.540918	-2.017253
41	8	0	-1.855962	-3.533248	2.766949
42	1	0	-2.772638	-3.232427	2.871914
43	1	0	-1.745319	-3.663471	1.782369

44	8	0	4.727862	-1.823014	-0.402126
45	1	0	3.945670	-1.672794	-0.975753
46	1	0	5.465772	-1.925246	-1.024973
47	8	0	4.590365	0.795929	0.256111
48	1	0	4.046210	0.898241	1.068583
49	1	0	4.773080	-0.178797	0.168179
50	1	0	-0.778141	-3.814733	-0.390583
51	8	0	-1.631189	-3.684668	0.078697
52	1	0	-1.847878	-2.773791	-0.212522
53	8	0	-1.449285	2.152710	1.909666
54	1	0	-1.483767	3.091626	2.165173
55	1	0	-0.946805	2.097124	0.899111

SCF Done: E(RB3LYP) = -1675.86992126 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-767.0546	21.9239	28.3646

Zero-point correction= 0.432735 (a.u.)
Thermal correction to Energy= 0.470853
Thermal correction to Enthalpy= 0.471797
Thermal correction to Gibbs Free Energy= 0.364385
Sum of electronic and zero-point Energies= -1675.437186
Sum of electronic and thermal Energies= -1675.399069
Sum of electronic and thermal Enthalpies= -1675.398124
Sum of electronic and thermal Free Energies= -1675.505537

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	295.464	137.643	226.068

==== HO-CH2-CH(OH)-CH(OH)-C(OH)(OOH)-C(=O)-COOH + (H2O)10
in Figure 7 ==== dkgr14b.rev.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000175	-0.949378	-0.097347
2	6	0	-1.103299	-1.881062	0.486737
3	6	0	-2.534772	-1.364310	0.229538
4	6	0	1.478532	-1.267774	0.242189
5	8	0	-3.146957	-1.703976	-0.769971
6	8	0	1.917438	-2.338860	-0.604632
7	8	0	-0.373736	0.334985	0.256860
8	8	0	-0.903112	-2.890094	1.122821
9	1	0	2.028467	-0.366064	-0.051258
10	6	0	1.849259	-1.625233	1.709319
11	6	0	1.883338	-0.442398	2.670400
12	1	0	1.158837	-2.380480	2.087056
13	8	0	3.128792	-2.275948	1.670551
14	1	0	3.807425	-1.583691	1.570674
15	8	0	2.796830	0.564739	2.225051
16	1	0	2.212962	-0.816966	3.646771
17	1	0	0.876701	-0.029594	2.796042
18	1	0	2.255201	1.375521	2.078978
19	8	0	-2.966546	-0.561792	1.181962
20	1	0	-3.786874	0.023696	0.857002
21	8	0	-0.160844	-0.976341	-1.540983
22	8	0	-0.348527	-2.352680	-1.969739
23	1	0	-1.735523	1.740567	-0.435757
24	1	0	0.554154	-2.709214	-1.798584
25	1	0	2.567857	-2.837625	-0.063086
26	8	0	-2.245236	2.529116	-0.164081
27	1	0	-2.155196	2.496723	0.817667
28	1	0	-0.668672	3.720273	-0.417600
29	8	0	0.222657	4.087759	-0.235080
30	1	0	0.691113	3.049808	0.974748
31	1	0	0.816222	3.702033	-0.925236
32	8	0	-1.746807	1.790885	2.485177
33	1	0	-2.267396	2.048319	3.263312
34	1	0	-1.989288	0.863262	2.293348
35	8	0	2.084863	2.820347	-1.830981

36	1	0	2.732054	2.345436	-1.228607
37	1	0	2.626161	3.455830	-2.327329
38	1	0	0.856799	0.130738	-2.875386
39	8	0	1.539995	0.591373	-3.397518
40	1	0	1.658156	1.450046	-2.924567
41	8	0	3.884747	1.375141	-0.453709
42	1	0	3.643396	1.036769	0.429970
43	1	0	3.909053	0.575881	-1.048477
44	8	0	-5.486363	-0.434499	-1.746367
45	1	0	-4.740251	-1.029345	-1.517321
46	1	0	-6.277282	-0.918246	-1.457765
47	8	0	-4.658855	1.096909	0.315900
48	1	0	-3.985423	1.730593	-0.027063
49	1	0	-5.079400	0.680078	-0.485523
50	1	0	2.958973	-0.244724	-2.773994
51	8	0	3.674821	-0.675267	-2.235382
52	1	0	3.205331	-1.409213	-1.791964
53	8	0	0.826999	2.255982	1.579109
54	1	0	0.032962	2.233061	2.158909
55	1	0	0.334896	0.945208	0.618131

SCF Done: E(RB3LYP) = -1675.88748186 A.U. after 1 cycles

Zero-point correction= 0.440678 (a.u.)
Thermal correction to Energy= 0.479339
Thermal correction to Enthalpy= 0.480283
Thermal correction to Gibbs Free Energy= 0.370798
Sum of electronic and zero-point Energies= -1675.446803
Sum of electronic and thermal Energies= -1675.408143
Sum of electronic and thermal Enthalpies= -1675.407199
Sum of electronic and thermal Free Energies= -1675.516684

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	300.790	139.648	230.431

==== C-C cleavage TS, TS19, to threonic acid and oxalic acid in Figure 7====

dkgr14b.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.204282	-0.717225	-0.488850
2	6	0	-1.059105	-1.863717	-0.741019
3	6	0	-2.436530	-1.134033	-0.547882
4	6	0	1.528048	-1.359963	0.017382
5	8	0	-3.101552	-0.809486	-1.512007
6	8	0	2.053577	-2.099955	-1.079388
7	8	0	-0.314906	0.258898	0.352814
8	8	0	-0.947852	-3.034113	-0.427751
9	1	0	2.197921	-0.514767	0.239097
10	6	0	1.488846	-2.284989	1.261956
11	6	0	1.344187	-1.585928	2.613787
12	1	0	0.706874	-3.036035	1.140454
13	8	0	2.734782	-3.002503	1.258204
14	1	0	3.383179	-2.384642	1.649636
15	8	0	2.476840	-0.758923	2.869398
16	1	0	1.322088	-2.364846	3.384082
17	1	0	0.406109	-1.027715	2.679375
18	1	0	2.223171	0.161314	2.645596
19	8	0	-2.764857	-1.019628	0.715988
20	1	0	-3.570666	-0.338846	0.815406
21	8	0	0.298376	-0.361765	-1.764823
22	8	0	-0.855208	-1.620158	-2.463480
23	1	0	-1.628671	1.822465	0.271175
24	1	0	-0.104012	-2.224487	-2.644719
25	1	0	2.645975	-2.757426	-0.654763
26	8	0	-2.108183	2.467329	0.829488
27	1	0	-1.969569	2.090397	1.729127
28	1	0	-0.471194	3.633946	0.912720

29	8	0	0.456362	3.879893	1.114224
30	1	0	0.978787	2.486257	1.880437
31	1	0	0.943149	3.789157	0.257857
32	8	0	-1.515636	0.752136	2.941300
33	1	0	-2.025609	0.598107	3.753341
34	1	0	-1.691315	-0.014803	2.363572
35	8	0	2.017269	3.418277	-1.122689
36	1	0	2.782697	2.863289	-0.782118
37	1	0	2.424688	4.245661	-1.427560
38	1	0	0.759440	1.204660	-2.972960
39	8	0	1.525914	1.721699	-3.275013
40	1	0	1.635584	2.406524	-2.571621
41	8	0	4.049072	1.828032	-0.437166
42	1	0	3.975078	1.430790	0.444041
43	1	0	3.922705	1.077690	-1.086600
44	8	0	-5.624501	0.521125	-1.458207
45	1	0	-4.835874	-0.010495	-1.691654
46	1	0	-6.337779	-0.132383	-1.373019
47	8	0	-4.449275	0.847851	0.951781
48	1	0	-3.814463	1.593500	0.834815
49	1	0	-5.010124	0.841921	0.128222
50	1	0	2.815332	0.570030	-2.792265
51	8	0	3.517517	0.020135	-2.360268
52	1	0	3.047377	-0.777144	-2.036625
53	8	0	1.074918	1.532484	2.187860
54	1	0	0.297700	1.376763	2.766913
55	1	0	0.391787	0.735619	0.883702

SCF Done: E(RB3LYP) = -1675.82480637 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-772.6574	18.8640	30.7936

Zero-point correction= 0.436107 (a.u.)
Thermal correction to Energy= 0.475135
Thermal correction to Enthalpy= 0.476079
Thermal correction to Gibbs Free Energy= 0.365819
Sum of electronic and zero-point Energies= -1675.388699
Sum of electronic and thermal Energies= -1675.349671
Sum of electronic and thermal Enthalpies= -1675.348727
Sum of electronic and thermal Free Energies= -1675.458987

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	298.152	140.491	232.063

==== product threonic acid and oxalic acid with (H2O)9 in Figure 7 ====
dkgr14b.for.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.912382	0.047378	-1.185863
2	6	0	-3.117137	-2.341605	-1.357450
3	6	0	-3.658407	-0.964292	-0.936034
4	6	0	3.168721	-0.206895	-0.350787
5	8	0	-3.550420	-0.001375	-1.680677
6	8	0	4.084960	0.849633	-0.604644
7	8	0	0.766490	-0.404255	-0.694619
8	8	0	-2.579639	-3.110642	-0.580889
9	1	0	2.905081	-0.227078	0.714006
10	6	0	3.866284	-1.545334	-0.718628
11	6	0	3.118120	-2.810785	-0.282195
12	1	0	4.035873	-1.552230	-1.800749
13	8	0	5.149954	-1.527571	-0.094462
14	1	0	4.983090	-1.882452	0.802801
15	8	0	3.184815	-2.953591	1.132325
16	1	0	3.625969	-3.675699	-0.721005
17	1	0	2.083551	-2.806171	-0.646765
18	1	0	2.415441	-2.467761	1.510493
19	8	0	-4.154792	-1.011108	0.268731
20	1	0	-4.380354	-0.057816	0.672770

21	8	0	1.959507	0.612863	-2.267336
22	8	0	-3.268104	-2.561870	-2.657423
23	1	0	-1.564379	0.867611	1.572644
24	1	0	-2.881379	-3.435344	-2.870327
25	1	0	4.941365	0.511777	-0.274541
26	8	0	-1.970212	0.524272	2.387046
27	1	0	-1.993475	-0.456510	2.243277
28	1	0	-0.287915	0.661217	3.296465
29	8	0	0.694124	0.668259	3.289117
30	1	0	0.929969	-0.696697	2.356236
31	1	0	0.888880	1.434662	2.697529
32	8	0	-1.691013	-2.193359	1.938412
33	1	0	-2.007943	-2.780267	2.644110
34	1	0	-2.102295	-2.524889	1.106543
35	8	0	0.801930	2.871726	1.576450
36	1	0	1.630902	2.997082	1.005855
37	1	0	0.812653	3.622299	2.193882
38	1	0	-0.423804	3.271890	0.387471
39	8	0	-0.979700	3.538484	-0.394143
40	1	0	-1.095743	4.498142	-0.294410
41	8	0	2.822649	3.308520	-0.057566
42	1	0	3.371836	2.505535	-0.192691
43	1	0	2.305487	3.399667	-0.901685
44	8	0	-3.644734	2.676137	-0.642574
45	1	0	-2.701329	2.930259	-0.511034
46	1	0	-3.605373	1.860122	-1.181181
47	8	0	-4.487956	1.203903	1.424253
48	1	0	-3.684048	1.098248	1.986893
49	1	0	-4.221710	1.888129	0.741603
50	1	0	0.315457	3.385813	-1.702722
51	8	0	1.145912	3.334055	-2.230177
52	1	0	1.248444	2.382422	-2.430223
53	8	0	0.940658	-1.463620	1.703223
54	1	0	0.068236	-1.915222	1.820388
55	1	0	0.852296	-0.791234	0.239744

SCF Done: E(RB3LYP) = -1676.04916219 A.U. after 1 cycles

Zero-point correction= 0.441475 (a.u.)
Thermal correction to Energy= 0.480388
Thermal correction to Enthalpy= 0.481332
Thermal correction to Gibbs Free Energy= 0.367832
Sum of electronic and zero-point Energies= -1675.607687
Sum of electronic and thermal Energies= -1675.568774
Sum of electronic and thermal Enthalpies= -1675.567830
Sum of electronic and thermal Free Energies= -1675.681331

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	301.448	137.801	238.883

==== HO-CH2-CH(OH)-CH(OH)-C(OH)(OOH)-C(=O)-COOH + H3O(+)(H2O)9 in Figure 8 ==== dkgr17b.rev.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.883242	-0.009183	-0.863496
2	6	0	-0.257750	-0.435428	0.097483
3	6	0	-1.269410	-1.456830	-0.457963
4	6	0	1.651172	1.276210	-0.489011
5	8	0	-2.064548	-1.916923	0.474750
6	8	0	2.555940	0.989937	0.593018
7	8	0	0.526235	0.102640	-2.185461
8	8	0	-0.244039	-0.139424	1.275377
9	1	0	2.255428	1.505687	-1.375193
10	6	0	0.784016	2.510918	-0.107322
11	6	0	0.346486	3.336660	-1.322024
12	1	0	-0.088147	2.195488	0.461762
13	8	0	1.567600	3.337068	0.760805
14	1	0	2.085002	3.910329	0.157600
15	8	0	1.453907	4.105562	-1.808645

16	1	0	-0.409259	4.058962	-1.002566
17	1	0	-0.084670	2.697867	-2.096426
18	1	0	1.945524	3.571856	-2.452517
19	8	0	-1.282631	-1.809681	-1.637959
20	1	0	-2.761340	-2.523196	0.070955
21	8	0	1.831188	-1.139525	-0.861209
22	8	0	2.116534	-1.607386	0.502884
23	1	0	2.340217	-0.748558	0.949995
24	1	0	2.523953	1.800052	1.156378
25	1	0	-0.118396	-0.619497	-2.368183
26	1	0	3.690886	-2.179926	0.113626
27	8	0	4.649886	-2.184186	-0.182571
28	1	0	4.928815	-1.170024	-0.231006
29	1	0	5.225066	-2.671125	0.525393
30	8	0	5.140158	0.299242	-0.209052
31	1	0	5.299855	0.627451	-1.109842
32	1	0	4.280042	0.698601	0.071299
33	8	0	6.139777	-3.378286	1.534391
34	1	0	5.782014	-3.301560	2.435291
35	1	0	6.158064	-4.333853	1.355059
36	8	0	-1.962999	1.063040	-0.818354
37	1	0	-2.734409	1.024547	-0.181087
38	1	0	-2.344675	0.806617	-1.688733
39	8	0	-4.043996	0.895670	0.900687
40	1	0	-4.636955	0.194138	0.541657
41	1	0	-3.611830	0.485065	1.692429
42	8	0	-5.784229	-1.056120	-0.120915
43	1	0	-5.272074	-1.870041	-0.308999
44	1	0	-6.345030	-1.298923	0.632622
45	8	0	-2.629993	-0.190303	3.002152
46	1	0	-1.849124	-0.407970	2.459086
47	1	0	-2.354519	0.606653	3.512753
48	8	0	-4.069463	-3.299967	-0.577455
49	1	0	-4.288714	-4.140075	-0.138857
50	1	0	-3.903032	-3.529239	-1.508062
51	8	0	-1.912282	2.139336	4.384675
52	1	0	-2.205969	2.853471	3.795914
53	1	0	-2.513713	2.205320	5.144237
54	8	0	-3.056721	-0.084519	-3.141442
55	1	0	-2.583792	0.155254	-3.954743
56	1	0	-2.678336	-0.946840	-2.891247

SCF Done: E(RB3LYP) = -1676.28805960 A.U. after 1 cycles

Zero-point correction= 0.445957 (a.u.)
Thermal correction to Energy= 0.489001
Thermal correction to Enthalpy= 0.489945
Thermal correction to Gibbs Free Energy= 0.365101
Sum of electronic and zero-point Energies= -1675.842102
Sum of electronic and thermal Energies= -1675.799059
Sum of electronic and thermal Enthalpies= -1675.798114
Sum of electronic and thermal Free Energies= -1675.922959

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.853	147.887	262.757

==== H2O addition toward the tetrahedral intermediate TS20 in Figure 8 ==== dkgr17b.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.715167	0.201034	-0.900274
2	6	0	-0.508705	-0.167820	0.007595
3	6	0	-1.265764	-1.398108	-0.576963
4	6	0	1.584287	1.381025	-0.408110
5	8	0	-1.797387	-2.169931	0.347932
6	8	0	2.478104	0.903732	0.616551
7	8	0	0.404027	0.446020	-2.227827
8	8	0	-0.318751	-0.108272	1.259425
9	1	0	2.194046	1.669301	-1.274686
10	6	0	0.839401	2.626182	0.140167

11	6	0	0.319614	3.559548	-0.957561
12	1	0	0.029049	2.304771	0.791402
13	8	0	1.761648	3.350841	0.965616
14	1	0	2.266627	3.912689	0.343038
15	8	0	1.411851	4.282473	-1.541268
16	1	0	-0.332122	4.310464	-0.502595
17	1	0	-0.250715	3.007891	-1.709277
18	1	0	1.779453	3.753525	-2.266630
19	8	0	-1.401773	-1.592795	-1.789916
20	1	0	-2.405032	-2.824524	-0.103353
21	8	0	1.586283	-0.980955	-1.004116
22	8	0	1.763936	-1.661572	0.286475
23	1	0	1.926825	-0.890852	0.886466
24	1	0	2.568272	1.671360	1.226943
25	1	0	-0.218346	-0.267773	-2.492156
26	1	0	3.288078	-2.260956	-0.046983
27	8	0	4.260812	-2.354438	-0.299244
28	1	0	4.630195	-1.366485	-0.318704
29	1	0	4.749132	-2.893743	0.429170
30	8	0	4.947941	0.073146	-0.264928
31	1	0	5.099104	0.411431	-1.163465
32	1	0	4.106122	0.499041	0.043334
33	8	0	5.531765	-3.705645	1.494790
34	1	0	5.129945	-3.589593	2.372481
35	1	0	5.450391	-4.656735	1.309836
36	8	0	-1.647077	0.994360	-0.427008
37	1	0	-2.678019	0.806756	0.234677
38	1	0	-1.912498	0.961464	-1.386117
39	8	0	-3.651837	0.599668	0.897781
40	1	0	-4.236192	-0.081929	0.446627
41	1	0	-3.290814	0.176733	1.762958
42	8	0	-5.258897	-1.186004	-0.311145
43	1	0	-4.774645	-1.962772	-0.669242
44	1	0	-5.840301	-1.557242	0.371725
45	8	0	-2.438674	-0.446065	2.921496
46	1	0	-1.600778	-0.472674	2.385178
47	1	0	-2.293238	0.275352	3.579639
48	8	0	-3.624237	-3.317441	-1.205902
49	1	0	-3.898747	-4.243844	-1.309784
50	1	0	-3.128590	-3.083348	-2.012503
51	8	0	-2.092391	1.638186	4.748140
52	1	0	-2.462267	2.421564	4.309413
53	1	0	-2.711322	1.467591	5.476751
54	8	0	-2.718371	0.775093	-2.941586
55	1	0	-2.227209	1.155239	-3.687857
56	1	0	-2.636182	-0.187083	-3.057511

SCF Done: E(RB3LYP) = -1676.27507834 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-659.8236	16.1580	18.1641

Zero-point correction= 0.443248 (a.u.)
Thermal correction to Energy= 0.484102
Thermal correction to Enthalpy= 0.485046
Thermal correction to Gibbs Free Energy= 0.366409
Sum of electronic and zero-point Energies= -1675.831831
Sum of electronic and thermal Energies= -1675.790977
Sum of electronic and thermal Enthalpies= -1675.790033
Sum of electronic and thermal Free Energies= -1675.908669

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	303.778	142.352	249.691

==== A tetrahedral intermediate in Figure 8 ====
dkgr17b.for.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.735202	0.409835	-0.952180

2	6	0	-0.553093	0.070581	-0.120158
3	6	0	-1.386333	-1.003613	-0.876114
4	6	0	1.762572	1.359755	-0.284805
5	8	0	-1.874402	-1.950062	-0.109545
6	8	0	2.571834	0.611859	0.628122
7	8	0	0.416414	0.979145	-2.174922
8	8	0	-0.144588	-0.307858	1.140131
9	1	0	2.396142	1.698801	-1.117097
10	6	0	1.212111	2.602459	0.466087
11	6	0	0.755173	3.740579	-0.452153
12	1	0	0.403045	2.303648	1.131176
13	8	0	2.266685	3.088283	1.307806
14	1	0	2.810624	3.657377	0.726398
15	8	0	1.893155	4.386392	-1.036131
16	1	0	0.255429	4.499542	0.156116
17	1	0	0.056755	3.384942	-1.213716
18	1	0	2.131049	3.915031	-1.850040
19	8	0	-1.624879	-0.890863	-2.081123
20	1	0	-2.533037	-2.486279	-0.649062
21	8	0	1.444930	-0.817662	-1.319598
22	8	0	1.303756	-1.905984	-0.339652
23	1	0	1.119663	-1.432418	0.515653
24	1	0	2.837000	1.280031	1.298956
25	1	0	-0.270852	0.403749	-2.578005
26	1	0	2.824869	-2.563258	-0.465356
27	8	0	3.798742	-2.774584	-0.615083
28	1	0	4.304853	-1.844046	-0.536521
29	1	0	4.124145	-3.408906	0.123943
30	8	0	4.827517	-0.502529	-0.367347
31	1	0	5.021938	-0.115987	-1.237684
32	1	0	4.041353	0.001671	-0.017524
33	8	0	4.679552	-4.368027	1.223234
34	1	0	4.091172	-4.376480	1.997160
35	1	0	4.667234	-5.283013	0.894795
36	8	0	-1.397929	1.206653	-0.020429
37	1	0	-3.191299	0.859063	0.809552
38	1	0	-1.759351	1.470307	-0.913454
39	8	0	-3.913126	0.478363	1.345647
40	1	0	-4.432793	-0.087400	0.722588
41	1	0	-2.851316	-0.467207	2.343308
42	8	0	-5.501738	-1.091148	-0.317011
43	1	0	-4.989528	-1.731924	-0.853981
44	1	0	-5.998180	-1.647383	0.304003
45	8	0	-2.060221	-0.866343	2.795483
46	1	0	-0.930954	-0.564985	1.752892
47	1	0	-1.888891	-0.277418	3.569087
48	8	0	-3.758437	-2.844633	-1.734910
49	1	0	-3.942908	-3.768624	-1.973722
50	1	0	-3.370941	-2.428897	-2.526963
51	8	0	-1.573518	0.804273	4.978776
52	1	0	-2.025325	1.642730	4.789105
53	1	0	-2.078695	0.432549	5.720144
54	8	0	-2.719938	1.825683	-2.294959
55	1	0	-2.290041	2.411127	-2.939461
56	1	0	-2.755417	0.958421	-2.734268

SCF Done: E(RB3LYP) = -1676.29977468 A.U. after 1 cycles

Zero-point correction= 0.447421 (a.u.)
Thermal correction to Energy= 0.488870
Thermal correction to Enthalpy= 0.489815
Thermal correction to Gibbs Free Energy= 0.369918
Sum of electronic and zero-point Energies= -1675.852353
Sum of electronic and thermal Energies= -1675.810904
Sum of electronic and thermal Enthalpies= -1675.809960
Sum of electronic and thermal Free Energies= -1675.929857

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.771	144.430	252.344

==== C.....C cleavage toward threonic acid and oxalic acid
TS21 in Figure 8 === dkgr16b.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.057366	-0.580755	0.964868
2	6	0	-0.380110	-0.138248	0.122630
3	6	0	-1.374611	0.401652	1.243006
4	6	0	2.115027	-1.266950	0.018436
5	8	0	-2.165455	1.324632	0.740939
6	8	0	2.709875	-0.261968	-0.786741
7	8	0	0.709519	-1.532149	1.937603
8	8	0	-0.086110	0.728977	-0.805855
9	1	0	2.862327	-1.668368	0.719114
10	6	0	1.660425	-2.422215	-0.909082
11	6	0	1.320893	-3.734653	-0.198261
12	1	0	0.823730	-2.097823	-1.526277
13	8	0	2.756287	-2.662362	-1.807068
14	1	0	3.367864	-3.240429	-1.308950
15	8	0	2.507765	-4.320180	0.351382
16	1	0	0.949798	-4.443628	-0.943984
17	1	0	0.555261	-3.590243	0.566370
18	1	0	2.645765	-3.947333	1.236559
19	8	0	-1.490974	-0.072678	2.368424
20	1	0	-2.920962	1.509323	1.378276
21	8	0	1.638904	0.510283	1.457785
22	8	0	0.706518	2.057984	1.210177
23	1	0	0.482329	1.847199	0.245558
24	1	0	3.098580	-0.762450	-1.534971
25	1	0	-0.026462	-1.151607	2.467493
26	1	0	1.656215	2.653972	1.230796
27	8	0	2.804124	3.324041	1.277550
28	1	0	3.502361	2.688008	0.937776
29	1	0	2.771378	4.076330	0.627203
30	8	0	4.526504	1.502638	0.342497
31	1	0	4.899376	1.050760	1.116262
32	1	0	3.896264	0.846727	-0.043805
33	8	0	2.678923	5.373428	-0.517970
34	1	0	1.836410	5.295706	-0.994907
35	1	0	2.592347	6.203638	-0.021387
36	8	0	-0.996044	-1.303030	-0.363013
37	1	0	-2.761119	-1.058912	-1.246632
38	1	0	-1.312170	-1.893650	0.380487
39	8	0	-3.443718	-0.581645	-1.761324
40	1	0	-4.154123	-0.318566	-1.109247
41	1	0	-2.670073	0.568441	-2.211080
42	8	0	-5.461119	0.098940	-0.088916
43	1	0	-5.177785	0.591492	0.711102
44	1	0	-6.010706	0.731014	-0.579144
45	8	0	-1.952760	1.313295	-2.449906
46	1	0	-1.166479	1.122142	-1.800858
47	1	0	-1.626744	1.155533	-3.400330
48	8	0	-4.409331	1.532824	2.138300
49	1	0	-4.766459	2.415089	2.337756
50	1	0	-4.375999	1.065717	2.990654
51	8	0	-1.102661	0.925850	-4.901578
52	1	0	-1.010521	-0.026309	-5.073175
53	1	0	-1.782876	1.220867	-5.530021
54	8	0	-2.236296	-2.796489	1.505884
55	1	0	-1.755940	-3.534931	1.914441
56	1	0	-2.367152	-2.159814	2.229979

SCF Done: E(RB3LYP) = -1676.25701237 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-756.2613	14.1874	17.9199

Zero-point correction= 0.439701 (a.u.)
Thermal correction to Energy= 0.481165
Thermal correction to Enthalpy= 0.482109
Thermal correction to Gibbs Free Energy= 0.361920
Sum of electronic and zero-point Energies= -1675.817311
Sum of electronic and thermal Energies= -1675.775847
Sum of electronic and thermal Enthalpies= -1675.774903
Sum of electronic and thermal Free Energies= -1675.895092

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	301.936	143.918	252.960

==== product of threonic acid and oxalic acid with H3O(+)(H2O)9 in Figure 8 ==== dkgr16b.rev.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.196695	-0.157392	0.844074
2	6	0	-1.381787	-1.869599	-1.577998
3	6	0	-1.600312	-2.292736	-0.111392
4	6	0	3.696972	0.068719	0.936827
5	8	0	-2.845828	-2.640802	0.096691
6	8	0	3.905527	1.352191	1.498224
7	8	0	1.853444	-1.443145	0.966055
8	8	0	-2.260022	-1.267083	-2.172959
9	1	0	4.131808	-0.705115	1.583503
10	6	0	4.373162	0.027147	-0.473626
11	6	0	4.652861	-1.377664	-1.020851
12	1	0	3.745719	0.590040	-1.172390
13	8	0	5.607165	0.732632	-0.368742
14	1	0	6.257074	0.056320	-0.086984
15	8	0	5.772697	-1.951282	-0.340224
16	1	0	4.951790	-1.285308	-2.068445
17	1	0	3.771320	-2.024245	-0.975310
18	1	0	5.460173	-2.391569	0.465979
19	8	0	-0.719997	-2.254016	0.736737
20	1	0	-3.035083	-2.808981	1.072792
21	8	0	1.399767	0.744297	0.660124
22	8	0	-1.064100	1.901414	0.092862
23	1	0	-0.398714	1.206407	0.268602
24	1	0	4.777211	1.624142	1.139066
25	1	0	0.868090	-1.545551	0.868713
26	1	0	-0.739458	2.706084	0.605377
27	8	0	-0.179479	4.225615	0.994587
28	1	0	0.800191	4.088280	0.929566
29	1	0	-0.446575	4.536709	0.098319
30	8	0	2.535112	3.764696	0.783880
31	1	0	2.967649	4.254223	1.501134
32	1	0	2.758801	2.827184	0.970940
33	8	0	-1.184356	4.219319	-1.613393
34	1	0	-1.047826	3.268422	-1.433281
35	1	0	-2.147711	4.323920	-1.473172
36	8	0	-0.217819	-2.141390	-2.115437
37	1	0	-3.824709	-0.727070	-1.298404
38	1	0	0.409299	-2.700234	-1.548054
39	8	0	-4.552107	-0.206736	-0.888627
40	1	0	-5.004083	-0.795611	-0.219570
41	1	0	-3.998815	0.856049	-0.204112
42	8	0	-5.879462	-1.596350	1.014813
43	1	0	-5.265695	-2.017282	1.653435
44	1	0	-6.327485	-0.904354	1.527192
45	8	0	-3.591464	1.705611	0.347419
46	1	0	-2.556106	1.686829	0.307783
47	1	0	-3.860123	2.552083	-0.117480
48	8	0	-3.823415	-2.850985	2.527509
49	1	0	-3.378394	-2.348053	3.230832
50	1	0	-3.966353	-3.740969	2.892651
51	8	0	-3.995148	4.035413	-0.930888
52	1	0	-4.618878	4.005522	-1.676445
53	1	0	-4.333448	4.734961	-0.346245
54	8	0	1.627073	-3.583995	-0.944681
55	1	0	1.951497	-3.184632	-0.118118
56	1	0	1.372585	-4.492284	-0.711661

SCF Done: E(RB3LYP) = -1676.46232535 A.U. after 1 cycles

Zero-point correction= 0.446486 (a.u.)
Thermal correction to Energy= 0.489235
Thermal correction to Enthalpy= 0.490179
Thermal correction to Gibbs Free Energy= 0.365330

Sum of electronic and zero-point Energies= -1676.015839
Sum of electronic and thermal Energies= -1675.973090
Sum of electronic and thermal Enthalpies= -1675.972146
Sum of electronic and thermal Free Energies= -1676.096995

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	307.000	145.595	262.768

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Hereafter, data of Figure Ss in Supporting Information

==== Figure S2 AA.(-) + H3O(+)(H2O)12 reactant, same as the ion pair between the anion radical and hydronium ion included in Figure 1. ====
vitacoh2p.rev.txt

==== TS-S1 of the neutralization of teh anion radical in FIgure S2 ====

vitachat1.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.201932	-1.194634	-0.276109
2	6	0	3.184629	-2.197890	0.019872
3	6	0	4.483493	-1.734695	-0.528605
4	6	0	2.927171	-0.091387	-1.049138
5	8	0	5.562837	-2.284367	-0.483077
6	8	0	4.304354	-0.534402	-1.150207
7	8	0	0.981025	-1.178887	-0.001153
8	1	0	-0.597253	-0.171999	-0.259327
9	8	0	3.099352	-3.324355	0.628585
10	1	0	2.035221	-3.837472	0.955662
11	1	0	2.532949	-0.023907	-2.070086
12	6	0	2.907880	1.305763	-0.419908
13	6	0	1.487649	1.878926	-0.332679
14	1	0	3.344577	1.242875	0.589938
15	8	0	3.696520	2.146623	-1.248903
16	1	0	3.390686	3.049023	-1.035232
17	8	0	1.554671	3.292088	-0.110617
18	1	0	0.913417	1.392869	0.457056
19	1	0	0.972230	1.734849	-1.287568
20	1	0	1.531388	3.444706	0.870579
21	8	0	-1.467476	0.270127	-0.172956
22	1	0	-2.943721	-0.697031	-0.328874
23	1	0	-1.413259	0.841622	0.646814
24	8	0	-1.441932	2.132144	1.750202
25	1	0	-0.624192	2.361565	2.239613
26	1	0	-1.486114	2.856913	1.080693
27	8	0	-3.776169	-1.151665	-0.610439
28	1	0	-3.973267	-0.723901	-1.483853
29	1	0	-3.156447	-2.825335	-0.596980
30	8	0	-1.145195	4.036197	-0.272525
31	1	0	-0.183654	3.860265	-0.399994
32	1	0	-1.603586	3.546758	-0.997977
33	8	0	0.844374	3.613687	2.463067
34	1	0	0.318484	4.458278	2.383268
35	1	0	1.421099	3.719750	3.236046
36	8	0	-4.567053	0.635406	-2.541629
37	1	0	-5.163280	0.867148	-1.793448
38	1	0	-3.813939	1.259642	-2.442219
39	8	0	1.117407	-4.507472	1.321233
40	1	0	0.966079	-5.195869	0.649720
41	1	0	-0.218532	6.467207	1.569685
42	8	0	-0.755444	5.716437	1.870039

43	1	0	-1.096101	5.311255	1.040448
44	8	0	-2.196895	2.140659	-2.011951
45	1	0	-1.858037	1.413553	-1.420864
46	1	0	-1.659365	2.082038	-2.819284
47	8	0	-2.679888	-3.675156	-0.428987
48	1	0	-1.526386	-3.217590	0.662067
49	1	0	-3.318498	-4.218675	0.089744
50	8	0	-5.822644	0.651357	-0.024458
51	1	0	-6.663859	0.175991	-0.115672
52	1	0	-5.150503	-0.067612	0.037738
53	8	0	-0.830858	-2.929979	1.334819
54	1	0	0.245500	-3.909765	1.351902
55	1	0	-0.338317	-2.199659	0.907551
56	8	0	-4.484873	-5.173916	1.097843
57	1	0	-4.639136	-4.644189	1.896887
58	1	0	-5.337616	-5.146008	0.634276

SCF Done: E(UB3LYP) = -1677.78653265 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-543.9209	10.8599	16.6985

Zero-point correction= 0.464555 a.u.)
Thermal correction to Energy= 0.507141
Thermal correction to Enthalpy= 0.508085
Thermal correction to Gibbs Free Energy= 0.384144
Sum of electronic and zero-point Energies= -1677.321978
Sum of electronic and thermal Energies= -1677.279392
Sum of electronic and thermal Enthalpies= -1677.278448
Sum of electronic and thermal Free Energies= -1677.402389

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	318.236	148.660	260.856

==== the neutral radical AAH. and H3O(+)(H2O)13 in Figure S2 ====
vitachat1.for.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.218976	-1.231338	-0.287693
2	6	0	3.201882	-2.233712	0.005823
3	6	0	4.505489	-1.782238	-0.526122
4	6	0	2.957616	-0.128292	-1.051327
5	8	0	5.577688	-2.342433	-0.470550
6	8	0	4.333909	-0.579756	-1.141137
7	8	0	1.003076	-1.224355	-0.016326
8	1	0	-0.596083	-0.189432	-0.285638
9	8	0	3.117331	-3.376257	0.612503
10	1	0	2.152801	-3.733117	0.897601
11	1	0	2.572799	-0.058625	-2.075262
12	6	0	2.940136	1.266452	-0.416793
13	6	0	1.522636	1.848676	-0.340411
14	1	0	3.366977	1.197575	0.596686
15	8	0	3.741614	2.102630	-1.236681
16	1	0	3.441418	3.006992	-1.023042
17	8	0	1.600167	3.258710	-0.106902
18	1	0	0.936562	1.361663	0.440235
19	1	0	1.016039	1.715998	-1.301674
20	1	0	1.576670	3.403555	0.875796
21	8	0	-1.457774	0.264866	-0.193942
22	1	0	-2.966485	-0.664368	-0.352148
23	1	0	-1.392479	0.831185	0.629230
24	8	0	-1.404776	2.111373	1.739464
25	1	0	-0.585875	2.328150	2.232729
26	1	0	-1.442408	2.844495	1.078638
27	8	0	-3.815476	-1.087265	-0.631429
28	1	0	-4.003341	-0.648355	-1.501312
29	1	0	-3.247502	-2.788875	-0.622111
30	8	0	-1.091920	4.036575	-0.260649
31	1	0	-0.132592	3.852288	-0.391531

32	1	0	-1.555372	3.558597	-0.990521
33	8	0	0.893267	3.564295	2.468192
34	1	0	0.375794	4.415052	2.398020
35	1	0	1.472346	3.656314	3.241232
36	8	0	-4.566608	0.729682	-2.550156
37	1	0	-5.152270	0.974339	-1.797719
38	1	0	-3.795762	1.331872	-2.450947
39	8	0	1.035630	-4.514116	1.352291
40	1	0	0.845833	-5.174181	0.665047
41	1	0	-0.141991	6.438215	1.609518
42	8	0	-0.685815	5.688778	1.900606
43	1	0	-1.030288	5.296978	1.066186
44	8	0	-2.157165	2.167394	-2.018241
45	1	0	-1.829091	1.429142	-1.435884
46	1	0	-1.621095	2.110170	-2.826612
47	8	0	-2.792680	-3.648283	-0.448844
48	1	0	-1.646105	-3.168753	0.699341
49	1	0	-3.447681	-4.172305	0.068165
50	8	0	-5.802163	0.772932	-0.023755
51	1	0	-6.657141	0.321304	-0.107472
52	1	0	-5.149693	0.035283	0.030501
53	8	0	-0.982079	-2.866622	1.387298
54	1	0	0.200243	-3.938722	1.409850
55	1	0	-0.461362	-2.171955	0.944414
56	8	0	-4.655981	-5.089798	1.077150
57	1	0	-4.804405	-4.542987	1.865705
58	1	0	-5.500820	-5.041560	0.600995

SCF Done: E(UB3LYP) = -1677.78747616 A.U. after 1 cycles

Zero-point correction= 0.467959 (a.u.)
Thermal correction to Energy= 0.511301
Thermal correction to Enthalpy= 0.512245
Thermal correction to Gibbs Free Energy= 0.386954
Sum of electronic and zero-point Energies= -1677.319517
Sum of electronic and thermal Energies= -1677.276175
Sum of electronic and thermal Enthalpies= -1677.275231
Sum of electronic and thermal Free Energies= -1677.400523

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.846	150.755	263.699

==== DHA +(H2O)0 before ring closure n=0 in Figure S3 ====
trione0r.rev.txt

Stoichiometry C6H6O6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.078416	1.130177	-0.418566
2	6	0	-1.436847	0.707220	0.141809
3	6	0	-1.632775	-0.742176	-0.314052
4	6	0	0.510097	-0.115207	-1.077161
5	8	0	-2.582562	-1.456171	-0.119816
6	8	0	-0.552687	-1.117841	-1.041029
7	8	0	0.370754	2.252799	-0.413727
8	8	0	-2.233266	1.372377	0.755237
9	1	0	0.741041	0.085931	-2.125737
10	6	0	1.750224	-0.696359	-0.364013
11	6	0	1.377979	-1.186177	1.035816
12	1	0	2.128847	-1.537006	-0.960295
13	8	0	2.685614	0.372642	-0.310669
14	1	0	3.569097	-0.006668	-0.178333
15	8	0	0.609595	-0.195453	1.725847
16	1	0	0.753424	-2.080257	0.983207
17	1	0	2.289478	-1.435141	1.593211
18	1	0	1.196949	0.561459	1.898214

SCF Done: E(RB3LYP) = -683.547023949 A.U. after 1 cycles

Zero-point correction= 0.126417
(Hartree/Particle)
Thermal correction to Energy= 0.137496

```
Thermal correction to Enthalpy=               0.138441
Thermal correction to Gibbs Free Energy=       0.089441
Sum of electronic and zero-point Energies=          -683.420607
Sum of electronic and thermal Energies=             -683.409527
Sum of electronic and thermal Enthalpies=           -683.408583
Sum of electronic and thermal Free Energies=        -683.457583

                E (Thermal)           CV              S
                 KCal/Mol       Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total               86.280           40.274           103.128

  ====  n=0 TS in Figure S3  ====
   trione0r.txt

Stoichiometry   C6H6O6

                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type           X         Y         Z
---------------------------------------------------------------------
    1         6          0       0.012374    0.827740   -0.321580
    2         6          0      -1.490778    0.680626   -0.076516
    3         6          0      -1.763234   -0.833325   -0.063274
    4         6          0       0.458553   -0.572639   -0.777445
    5         8          0      -2.791687   -1.394877    0.209764
    6         8          0      -0.615082   -1.479030   -0.383298
    7         8          0       0.570897    1.935506   -0.732734
    8         8          0      -2.320530    1.543341    0.054695
    9         1          0       0.597441   -0.634827   -1.857584
   10         6          0       1.733722   -0.931186   -0.006037
   11         6          0       1.507244   -0.318334    1.383790
   12         1          0       1.861255   -2.018601    0.054067
   13         8          0       2.793245   -0.305130   -0.709722
   14         1          0       3.630640   -0.603433   -0.319749
   15         8          0       0.695227    0.874253    1.172938
   16         1          0       0.939696   -0.978945    2.042420
   17         1          0       2.434036   -0.015657    1.873557
   18         1          0       1.133081    1.741658    0.480518
---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -683.488549039    A.U. after    1 cycles

                 1                  2                  3
                 A                  A                  A
Frequencies --  -1753.7409            75.6003            111.4806

Zero-point correction=                          0.121907 (a.u.)
Thermal correction to Energy=                    0.131901
Thermal correction to Enthalpy=                  0.132846
Thermal correction to Gibbs Free Energy=         0.086451
Sum of electronic and zero-point Energies=          -683.366642
Sum of electronic and thermal Energies=             -683.356648
Sum of electronic and thermal Enthalpies=           -683.355704
Sum of electronic and thermal Free Energies=        -683.402098

                E (Thermal)           CV              S
                 KCal/Mol       Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total               82.769           37.826            97.646

 ==== n=0 the ring-closure product in Figure S3 ====
              trione0r.for.txt

Stoichiometry   C6H6O6

                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type           X         Y         Z
---------------------------------------------------------------------
    1         6          0       0.107173    0.793413   -0.068453
    2         6          0      -1.410448    0.723431    0.005479
    3         6          0      -1.742748   -0.777300   -0.148589
    4         6          0       0.475163   -0.510213   -0.808796
    5         8          0      -2.800046   -1.317947    0.041765
    6         8          0      -0.622516   -1.428643   -0.549506
    7         8          0       0.583047    1.968975   -0.604489
    8         8          0      -2.222052    1.596763    0.175318
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     9        1          0       0.596261   -0.393184   -1.885919
    10        6          0       1.740937   -0.951061   -0.086432
    11        6          0       1.400980   -0.592029    1.360121
    12        1          0       1.983938   -2.010185   -0.222546
    13        8          0       2.739179   -0.090769   -0.638502
    14        1          0       3.560030   -0.201623   -0.131396
    15        8          0       0.539868    0.568808    1.279337
    16        1          0       0.865539   -1.407435    1.857612
    17        1          0       2.282095   -0.328705    1.951833
    18        1          0       1.545946    1.846191   -0.720941
---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -683.557727410    A.U. after   1 cycles
         NFock=  1  Conv=0.31D-08    -V/T= 2.0086

Zero-point correction=                          0.127971 (a.u.)
Thermal correction to Energy=                    0.137986
Thermal correction to Enthalpy=                  0.138930
Thermal correction to Gibbs Free Energy=         0.092612
Sum of electronic and zero-point Energies=          -683.429756
Sum of electronic and thermal Energies=             -683.419742
Sum of electronic and thermal Enthalpies=           -683.418798
Sum of electronic and thermal Free Energies=        -683.465116

                 E (Thermal)             CV              S
                  KCal/Mol       Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                86.587           38.186           97.484

==== n=1 before ring closure in Figure S3 ====
   trione1r.for.txt

Stoichiometry   C6H8O7

                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X         Y         Z
---------------------------------------------------------------------
     1         6          0      -0.133281    0.719518   -0.872473
     2         6          0      -1.430245    0.979052   -0.109622
     3         6          0      -2.089356   -0.394024    0.050884
     4         6          0      -0.046510   -0.792866   -1.056476
     5         8          0      -3.139966   -0.653123    0.578320
     6         8          0      -1.310152   -1.324416   -0.554053
     7         8          0       0.616016    1.562531   -1.315280
     8         8          0      -1.893881    2.035406    0.241230
     9         1          0       0.025463   -1.044682   -2.117152
    10         6          0       1.095429   -1.466973   -0.268038
    11         6          0       0.885097   -1.248291    1.236047
    12         1          0       1.082699   -2.540218   -0.490509
    13         8          0       2.308656   -0.879024   -0.751101
    14         1          0       3.023488   -1.527918   -0.648258
    15         8          0       0.456574    0.083114    1.512505
    16         1          0       0.103679   -1.919968    1.599622
    17         1          0       1.813295   -1.484731    1.771396
    18         1          0       1.244272    0.683813    1.402739
    19         8          0       2.693812    1.442351    0.809886
    20         1          0       2.811965    0.731356    0.142786
    21         1          0       2.359865    2.189139    0.285386
---------------------------------------------------------------------
SCF Done:  E(RB3LYP) =  -759.984367412    A.U. after   1 cycles

Zero-point correction=                          0.152548 (a.u.)
Thermal correction to Energy=                    0.165733
Thermal correction to Enthalpy=                  0.166677
Thermal correction to Gibbs Free Energy=         0.113475
Sum of electronic and zero-point Energies=          -759.831819
Sum of electronic and thermal Energies=             -759.818634
Sum of electronic and thermal Enthalpies=           -759.817690
Sum of electronic and thermal Free Energies=        -759.870892

                 E (Thermal)             CV              S
                  KCal/Mol       Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total              103.999           48.403          111.973

==== n=1 TS in Figure S3 ====
    trione1r.txt
```

Stoichiometry C6H8O7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.081234	0.477373	-0.582558
2	6	0	-1.334984	0.913914	-0.206493
3	6	0	-2.114971	-0.380644	0.077486
4	6	0	-0.030880	-1.045390	-0.781952
5	8	0	-3.234710	-0.490226	0.509983
6	8	0	-1.332381	-1.436839	-0.241455
7	8	0	0.835435	1.201177	-1.321085
8	8	0	-1.804589	2.024879	-0.164286
9	1	0	0.007701	-1.327281	-1.834754
10	6	0	1.053238	-1.722539	0.054372
11	6	0	1.041664	-0.926143	1.367578
12	1	0	0.809707	-2.778669	0.225576
13	8	0	2.261249	-1.574573	-0.676798
14	1	0	2.947452	-2.089157	-0.222693
15	8	0	0.631680	0.416277	1.045290
16	1	0	0.323598	-1.347857	2.078056
17	1	0	2.032434	-0.903869	1.831796
18	1	0	1.561727	1.344343	0.972636
19	8	0	2.203527	2.135801	0.476445
20	1	0	1.717380	1.976040	-0.458284
21	1	0	1.946504	3.015053	0.812302

SCF Done: E(RB3LYP) = -759.951895829 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-832.2090	33.0170	79.0066

Zero-point correction= 0.147254 (a.u)
Thermal correction to Energy= 0.159157
Thermal correction to Enthalpy= 0.160101
Thermal correction to Gibbs Free Energy= 0.108899
Sum of electronic and zero-point Energies= -759.804642
Sum of electronic and thermal Energies= -759.792739
Sum of electronic and thermal Enthalpies= -759.791795
Sum of electronic and thermal Free Energies= -759.842997

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	99.872	44.833	107.764

==== n=1 ring closure product in Figure S3 ====
trione1r.rev.txt

Stoichiometry C6H8O7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.147377	0.433492	-0.216043
2	6	0	-1.196990	-0.665828	-0.050243
3	6	0	-0.423871	-1.995429	-0.084194
4	6	0	1.078260	-0.327799	-0.755819
5	8	0	-0.844938	-3.096044	0.160284
6	8	0	0.852232	-1.734042	-0.441275
7	8	0	-0.491345	1.504927	-0.995309
8	8	0	-2.395095	-0.584318	0.105901
9	1	0	1.221135	-0.226968	-1.831170
10	6	0	2.251368	0.189503	0.072763
11	6	0	1.580478	0.486126	1.420957
12	1	0	3.039812	-0.567113	0.164685
13	8	0	2.711119	1.355229	-0.594038
14	1	0	3.463560	1.706868	-0.091932
15	8	0	0.191491	0.773415	1.136095
16	1	0	1.634113	-0.375526	2.095243
17	1	0	2.018786	1.355618	1.918978
18	1	0	-2.782384	2.598257	0.896974
19	8	0	-2.898710	2.231918	0.004823

20	1	0	-1.341696	1.892281	-0.644812
21	1	0	-3.102563	1.287527	0.155654

SCF Done: E(RB3LYP) = -759.990871654 A.U. after 1 cycles

Zero-point correction= 0.152669 (a.u.)
Thermal correction to Energy= 0.165642
Thermal correction to Enthalpy= 0.166586
Thermal correction to Gibbs Free Energy= 0.113031
Sum of electronic and zero-point Energies= -759.838202
Sum of electronic and thermal Energies= -759.825230
Sum of electronic and thermal Enthalpies= -759.824286
Sum of electronic and thermal Free Energies= -759.877840

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	103.942	47.367	112.715

==== n=2 before ring closure in Figure S3 ====
trione2.for.log

Stoichiometry C6H10O8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.299882	0.439513	-1.006854
2	6	0	-1.497793	1.118317	-0.348445
3	6	0	-2.429940	-0.020285	0.074426
4	6	0	-0.549515	-1.062411	-0.894282
5	8	0	-3.498908	0.063446	0.621920
6	8	0	-1.881493	-1.198409	-0.310916
7	8	0	0.594002	1.001474	-1.603515
8	8	0	-1.720309	2.298057	-0.235609
9	1	0	-0.570286	-1.518991	-1.886872
10	6	0	0.433419	-1.816183	0.019689
11	6	0	0.358383	-1.235766	1.441978
12	1	0	0.137969	-2.871720	0.039966
13	8	0	1.722707	-1.694658	-0.587179
14	1	0	2.263232	-2.449169	-0.303517
15	8	0	0.114000	0.165840	1.421485
16	1	0	-0.469498	-1.710047	1.977287
17	1	0	1.287568	-1.467139	1.976259
18	1	0	0.983275	0.666869	1.480209
19	1	0	2.863600	-0.244808	-0.770826
20	8	0	3.343248	0.609587	-0.838222
21	1	0	2.765964	1.110713	-1.439302
22	8	0	2.426732	1.462583	1.563474
23	1	0	2.870833	1.222611	0.704663
24	1	0	2.979495	1.059216	2.251553

SCF Done: E(RB3LYP) = -836.418004267 A.U. after 1 cycles

Zero-point correction= 0.177408 (a.u.)
Thermal correction to Energy= 0.193270
Thermal correction to Enthalpy= 0.194215
Thermal correction to Gibbs Free Energy= 0.134746
Sum of electronic and zero-point Energies= -836.240597
Sum of electronic and thermal Energies= -836.224734
Sum of electronic and thermal Enthalpies= -836.223790
Sum of electronic and thermal Free Energies= -836.283258

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.279	57.281	125.162

==== n=2 TS in Figure S3 ====
trione2.log

Stoichiometry C6H10O8

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.142098	0.456911	-0.512000
2	6	0	-1.454059	1.160276	-0.163136
3	6	0	-2.513568	0.056158	-0.013005
4	6	0	-0.575456	-1.000846	-0.817042
5	8	0	-3.655807	0.170788	0.358461
6	8	0	-1.968856	-1.123183	-0.384306
7	8	0	0.738930	1.073316	-1.191484
8	8	0	-1.683713	2.341353	-0.053404
9	1	0	-0.526966	-1.228855	-1.882472
10	6	0	0.264364	-1.938156	0.040356
11	6	0	0.310669	-1.208731	1.388608
12	1	0	-0.199433	-2.929131	0.129216
13	8	0	1.531460	-2.006245	-0.601160
14	1	0	2.103735	-2.586152	-0.073862
15	8	0	0.311887	0.194600	1.100972
16	1	0	-0.566672	-1.463305	1.995252
17	1	0	1.209597	-1.472822	1.958078
18	1	0	1.611226	0.798471	1.314789
19	1	0	2.258499	0.661277	-1.213545
20	8	0	3.246217	0.668503	-0.936624
21	1	0	3.629318	1.452606	-1.367315
22	8	0	2.606227	1.177972	1.360441
23	1	0	3.029324	0.957583	0.338734
24	1	0	3.101511	0.679840	2.035257

SCF Done: E(RB3LYP) = -836.391482455 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-371.3607	29.4286	66.2293

Zero-point correction= 0.172911 (a.u.)
Thermal correction to Energy= 0.186984
Thermal correction to Enthalpy= 0.187928
Thermal correction to Gibbs Free Energy= 0.131726
Sum of electronic and zero-point Energies= -836.218571
Sum of electronic and thermal Energies= -836.204498
Sum of electronic and thermal Enthalpies= -836.203554
Sum of electronic and thermal Free Energies= -836.259757

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	117.334	52.295	118.288

==== After the ring closure n=2 in Figure S3 ====
trione2.rev.log

Stoichiometry C6H10O8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.161118	0.373660	-0.363214
2	6	0	-1.457794	1.168663	-0.187987
3	6	0	-2.574470	0.130481	0.013530
4	6	0	-0.673774	-1.056798	-0.675985
5	8	0	-3.719040	0.331156	0.329015
6	8	0	-2.063907	-1.096977	-0.230921
7	8	0	0.675861	0.987113	-1.244784
8	8	0	-1.620040	2.362209	-0.186271
9	1	0	-0.639575	-1.309922	-1.735449
10	6	0	0.159034	-1.979529	0.204957
11	6	0	0.376886	-1.106218	1.444207
12	1	0	-0.368945	-2.910013	0.446103
13	8	0	1.348676	-2.211333	-0.532490
14	1	0	1.971670	-2.694797	0.033420
15	8	0	0.402449	0.261843	0.968317
16	1	0	-0.439312	-1.223024	2.164651
17	1	0	1.326656	-1.308071	1.945856
18	1	0	2.024844	1.204096	1.338300
19	1	0	1.586540	0.565004	-1.251657
20	8	0	3.276802	0.366277	-1.143231
21	1	0	3.648797	1.058559	-1.713674

22	8	0	2.969114	1.466954	1.332065
23	1	0	3.348679	0.742883	-0.228016
24	1	0	3.368751	0.955796	2.053831

SCF Done: E(RB3LYP) = -836.420475687 A.U. after 1 cycles

Zero-point correction= 0.177907 (a.u.)
Thermal correction to Energy= 0.193317
Thermal correction to Enthalpy= 0.194261
Thermal correction to Gibbs Free Energy= 0.135362
Sum of electronic and zero-point Energies= -836.242569
Sum of electronic and thermal Energies= -836.227159
Sum of electronic and thermal Enthalpies= -836.226215
Sum of electronic and thermal Free Energies= -836.285114

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	121.308	56.198	123.963

==== n=3 before ring closure in Figure S3 ====
trione3a.for.log

Stoichiometry C6H12O9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.428235	-0.872306	-0.514046
2	6	0	1.678542	-1.202472	0.295118
3	6	0	2.722284	-0.166100	-0.132529
4	6	0	0.760543	0.360930	-1.332708
5	8	0	3.859952	-0.064413	0.251014
6	8	0	2.177583	0.634014	-1.076583
7	8	0	-0.573494	-1.561341	-0.562264
8	8	0	1.856048	-2.120245	1.056820
9	1	0	0.650760	0.156152	-2.400295
10	6	0	-0.050849	1.630619	-0.959777
11	8	0	-1.779227	0.142455	2.638648
12	1	0	0.352723	2.448965	-1.567883
13	8	0	-1.395168	1.477946	-1.343443
14	1	0	-1.938740	1.065115	-0.632289
15	8	0	0.425191	0.770907	1.293081
16	1	0	1.090969	2.578793	0.616176
17	1	0	-0.654671	2.518256	0.924372
18	1	0	-2.458088	0.167550	1.918772
19	8	0	-3.249315	0.358838	0.376874
20	1	0	-3.429095	-0.456108	-0.172379
21	1	0	-4.049786	0.905362	0.326154
22	6	0	0.197559	1.953678	0.529046
23	1	0	-0.397671	0.517772	1.809192
24	1	0	-2.002833	0.888497	3.217806
25	8	0	-3.292389	-1.730491	-1.284969
26	1	0	-2.313536	-1.710514	-1.304792
27	1	0	-3.501375	-2.567302	-0.838875

SCF Done: E(RB3LYP) = -912.852101088 A.U. after 1 cycles

Zero-point correction= 0.202569 (a.u.)
Thermal correction to Energy= 0.220910
Thermal correction to Enthalpy= 0.221854
Thermal correction to Gibbs Free Energy= 0.156124
Sum of electronic and zero-point Energies= -912.649532
Sum of electronic and thermal Energies= -912.631191
Sum of electronic and thermal Enthalpies= -912.630247
Sum of electronic and thermal Free Energies= -912.695977

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.623	65.749	138.340

==== n=3 ring-closing TS in Figure S3 ====
trione3a.log

Stoichiometry C6H12O9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.399077	-0.498967	-0.299091
2	6	0	1.787087	-1.118254	-0.103990
3	6	0	2.803304	0.033213	-0.185515
4	6	0	0.716425	0.948217	-0.773595
5	8	0	3.991429	-0.009372	0.025728
6	8	0	2.152931	1.158100	-0.547995
7	8	0	-0.505125	-1.221527	-0.863722
8	8	0	2.093881	-2.277679	0.048019
9	1	0	0.516248	1.100656	-1.834525
10	6	0	-0.044047	1.919313	0.136034
11	8	0	-2.203371	-1.361234	1.729370
12	1	0	0.454915	2.892823	0.154171
13	8	0	-1.361746	2.147691	-0.333060
14	1	0	-1.961644	1.440034	-0.032396
15	8	0	0.068650	-0.193553	1.237427
16	1	0	0.954095	1.512658	2.031171
17	1	0	-0.819266	1.457565	2.132858
18	1	0	-2.886419	-0.682742	0.983249
19	8	0	-3.386253	0.072686	0.187575
20	1	0	-3.221406	-0.264904	-0.820870
21	1	0	-4.336096	0.213755	0.345992
22	6	0	0.041617	1.218879	1.499291
23	1	0	-1.256606	-1.000488	1.587172
24	1	0	-2.445541	-1.181498	2.655575
25	8	0	-2.661939	-0.596666	-2.077049
26	1	0	-1.719155	-0.794477	-1.718568
27	1	0	-3.007566	-1.455357	-2.372984

SCF Done: E(RB3LYP) = -912.825920064 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-501.6169	38.9452	59.5938

Zero-point correction= 0.197323 (a.u.)
Thermal correction to Energy= 0.213413
Thermal correction to Enthalpy= 0.214357
Thermal correction to Gibbs Free Energy= 0.153901
Sum of electronic and zero-point Energies= -912.628597
Sum of electronic and thermal Energies= -912.612507
Sum of electronic and thermal Enthalpies= -912.611563
Sum of electronic and thermal Free Energies= -912.672019

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	133.919	60.118	127.240

==== After the ring closure n=3 in Figure S3 ====
trione3a.rev.log

Stoichiometry C6H12O9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.515137	-0.427910	-0.378512
2	6	0	1.915179	-1.023086	-0.208833
3	6	0	2.865888	0.161665	0.029504
4	6	0	0.794731	1.082085	-0.595574
5	8	0	4.031024	0.119644	0.333209
6	8	0	2.176616	1.305056	-0.164830
7	8	0	-0.189046	-1.127166	-1.309085
8	8	0	2.253577	-2.179075	-0.237339
9	1	0	0.706530	1.400925	-1.633747
10	6	0	-0.155746	1.817029	0.353388
11	8	0	-2.469620	-1.869432	1.491867
12	1	0	0.266654	2.779581	0.665085
13	8	0	-1.378957	2.021588	-0.323516
14	1	0	-2.105930	1.513898	0.101191
15	8	0	-0.089178	-0.485907	0.944444

16	1	0	0.581858	1.006149	2.238427
17	1	0	-1.183914	0.868785	2.055311
18	1	0	-3.226792	-0.474008	0.885541
19	8	0	-3.457851	0.365776	0.397387
20	1	0	-3.084788	-0.031813	-1.294327
21	1	0	-4.338099	0.639710	0.698220
22	6	0	-0.229875	0.834612	1.524257
23	1	0	-1.543014	-1.618128	1.286618
24	1	0	-2.507890	-1.889036	2.461672
25	8	0	-2.594880	-0.281637	-2.115119
26	1	0	-1.058198	-0.689185	-1.555314
27	1	0	-2.991783	-1.124018	-2.390192

SCF Done: E(RB3LYP) = -912.859713984 A.U. after 1 cycles

Zero-point correction= 0.203747 (a.u.)
Thermal correction to Energy= 0.221319
Thermal correction to Enthalpy= 0.222263
Thermal correction to Gibbs Free Energy= 0.158566
Sum of electronic and zero-point Energies= -912.655967
Sum of electronic and thermal Energies= -912.638395
Sum of electronic and thermal Enthalpies= -912.637451
Sum of electronic and thermal Free Energies= -912.701148

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	138.880	64.186	134.062

==== DHA + H3O(+)(H2O)12 in Figure S4 ====
trioneh1.rev.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.606828	-1.881109	0.057774
2	6	0	-1.180009	-1.842477	0.611286
3	6	0	-0.804488	-0.367202	0.605059
4	6	0	-2.982541	-0.436042	-0.263998
5	8	0	0.240263	0.137320	0.977534
6	8	0	-1.831218	0.365472	0.169062
7	8	0	-3.304727	-2.859411	-0.057184
8	8	0	-0.523015	-2.744347	1.071158
9	1	0	-3.068458	-0.303127	-1.345229
10	6	0	-4.219221	0.121755	0.433117
11	6	0	-5.510718	-0.591066	0.024418
12	1	0	-4.092221	0.045225	1.522391
13	8	0	-4.312220	1.492938	0.048019
14	1	0	-5.231743	1.749352	0.258352
15	8	0	-6.554725	0.197651	0.599285
16	1	0	-5.525736	-1.618660	0.403281
17	1	0	-5.591010	-0.615516	-1.069676
18	1	0	-7.367510	0.044390	0.093698
19	8	0	-0.756150	-1.506151	-1.741177
20	1	0	-0.494623	-0.599537	-2.072970
21	1	0	0.089111	-2.016596	-1.758879
22	8	0	0.115840	0.921897	-2.629685
23	1	0	0.061391	1.591865	-1.913715
24	1	0	1.078884	0.727801	-2.700681
25	1	0	0.254561	1.907179	0.278949
26	8	0	0.112267	2.655625	-0.341955
27	1	0	-0.817757	2.990976	-0.143876
28	8	0	3.736088	0.842156	0.129161
29	1	0	3.389358	0.195443	0.806467
30	1	0	4.550571	0.416196	-0.223015
31	1	0	1.149002	3.698713	-0.119896
32	8	0	1.904955	4.411370	0.027404
33	1	0	2.822390	3.913263	0.448889
34	8	0	-2.350754	3.527748	0.205368
35	1	0	-2.645830	4.092210	-0.527003
36	1	0	-2.986685	2.776352	0.203889
37	8	0	1.799479	-2.516836	-1.950730
38	1	0	2.461456	-2.791635	-1.241149
39	1	0	1.967676	-3.096865	-2.710582

40	8	0	3.858895	3.308787	1.003092
41	1	0	3.880812	2.346156	0.685828
42	1	0	4.684541	3.718223	0.692676
43	8	0	3.694481	-2.941026	-0.150156
44	1	0	4.375307	-2.366723	-0.566309
45	1	0	3.359130	-2.396204	0.601742
46	8	0	5.207202	-0.888593	-1.404660
47	1	0	6.065157	-0.912205	-1.857307
48	1	0	4.543648	-0.609042	-2.078085
49	8	0	2.708300	-1.099177	1.671096
50	1	0	1.752804	-0.927309	1.548359
51	1	0	2.869266	-1.114890	2.651515
52	8	0	2.777848	0.019618	-2.387707
53	1	0	2.404549	-0.891509	-2.260751
54	1	0	2.869354	0.384401	-1.475745
55	8	0	3.164933	-1.137523	4.359356
56	1	0	3.428912	-2.040476	4.600854
57	1	0	3.960633	-0.607065	4.529011
58	1	0	2.123943	4.786314	-0.845202

SCF Done: E(RB3LYP) = -1677.62593008 A.U. after 1 cycles

Zero-point correction= 0.466853 (a.u.)
Thermal correction to Energy= 0.509709
Thermal correction to Enthalpy= 0.510654
Thermal correction to Gibbs Free Energy= 0.389037
Sum of electronic and zero-point Energies= -1677.159077
Sum of electronic and thermal Energies= -1677.116221
Sum of electronic and thermal Enthalpies= -1677.115276
Sum of electronic and thermal Free Energies= -1677.236893

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	319.847	149.713	255.963

==== H2O addition TS, TS-S2, in Figure S4 ====
trioneh1.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.819494	-1.874522	0.420262
2	6	0	-1.297763	-1.861715	0.691271
3	6	0	-0.780539	-0.577637	0.022342
4	6	0	-3.119284	-0.591245	-0.345633
5	8	0	0.194452	0.072101	0.587312
6	8	0	-1.919107	0.204113	-0.194109
7	8	0	-3.578908	-2.751961	0.753346
8	8	0	-0.668613	-2.676515	1.316042
9	1	0	-3.273370	-0.821628	-1.408532
10	6	0	-4.287531	0.235612	0.185876
11	6	0	-5.645557	-0.434062	-0.025910
12	1	0	-4.136679	0.423908	1.258019
13	8	0	-4.271199	1.473597	-0.529011
14	1	0	-5.162100	1.850676	-0.385585
15	8	0	-6.603684	0.558749	0.347836
16	1	0	-5.734494	-1.335205	0.590899
17	1	0	-5.759017	-0.713754	-1.081139
18	1	0	-7.442242	0.355482	-0.093974
19	8	0	-0.414679	-1.074325	-1.420964
20	1	0	-0.081978	-0.201566	-2.003779
21	1	0	0.395935	-1.708093	-1.404323
22	8	0	0.484817	0.885061	-2.670509
23	1	0	0.458919	1.620832	-2.016850
24	1	0	1.450853	0.637947	-2.753604
25	1	0	0.208300	1.291113	0.206719
26	8	0	0.190082	2.346560	-0.276018
27	1	0	-0.760397	2.724308	-0.203151
28	8	0	3.985694	0.758619	-0.074025
29	1	0	3.503316	0.253097	0.638621
30	1	0	4.775024	0.210117	-0.271955
31	1	0	0.834537	3.000507	0.207366
32	8	0	1.714268	3.986437	0.976465

33	1	0	2.687355	3.770480	0.857163
34	8	0	-2.219352	3.333497	-0.100235
35	1	0	-2.352912	3.938664	-0.847678
36	1	0	-2.904952	2.632402	-0.222251
37	8	0	1.731449	-2.472679	-1.685640
38	1	0	2.368305	-2.761058	-0.940770
39	1	0	1.635937	-3.224861	-2.292526
40	8	0	4.296964	3.362817	0.649872
41	1	0	4.265187	2.404498	0.392311
42	1	0	4.597054	3.817199	-0.153476
43	8	0	3.511425	-2.948212	0.140146
44	1	0	4.276068	-2.525777	-0.312180
45	1	0	3.228951	-2.277453	0.812027
46	8	0	5.338432	-1.312941	-1.297474
47	1	0	6.216772	-1.536703	-1.644689
48	1	0	4.808288	-1.023591	-2.068780
49	8	0	2.611885	-0.824825	1.608642
50	1	0	1.679859	-0.642930	1.348553
51	1	0	2.666043	-0.704765	2.592131
52	8	0	2.998677	-0.130386	-2.496538
53	1	0	2.602822	-1.011677	-2.290152
54	1	0	3.205153	0.267644	-1.610749
55	8	0	2.777099	-0.496517	4.319124
56	1	0	3.011355	-1.357238	4.703364
57	1	0	3.553905	0.058579	4.497181
58	1	0	1.601578	4.864757	0.578434

SCF Done: E(RB3LYP) = -1677.60632113 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-586.3059	15.1412	21.0529

Zero-point correction= 0.462877 (a.u.)
Thermal correction to Energy= 0.504144
Thermal correction to Enthalpy= 0.505088
Thermal correction to Gibbs Free Energy= 0.386673
Sum of electronic and zero-point Energies= -1677.143444
Sum of electronic and thermal Energies= -1677.102177
Sum of electronic and thermal Enthalpies= -1677.101233
Sum of electronic and thermal Free Energies= -1677.219649

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	316.355	145.371	249.227

==== H2O adduct to DHA in Figure S4 ====
trioneh1.for.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.929097	-1.941353	0.236260
2	6	0	-1.398908	-1.966710	0.466020
3	6	0	-0.887585	-0.657745	-0.146021
4	6	0	-3.236368	-0.582004	-0.381907
5	8	0	0.088492	-0.071566	0.610109
6	8	0	-2.023703	0.176222	-0.189635
7	8	0	-3.688454	-2.840101	0.510441
8	8	0	-0.771790	-2.850136	0.996615
9	1	0	-3.436145	-0.701192	-1.456352
10	6	0	-4.375364	0.193249	0.275910
11	6	0	-5.747517	-0.443044	0.054318
12	1	0	-4.179198	0.269228	1.355080
13	8	0	-4.376818	1.497650	-0.308540
14	1	0	-5.254071	1.864976	-0.082847
15	8	0	-6.681444	0.508416	0.571727
16	1	0	-5.819066	-1.404268	0.575190
17	1	0	-5.908676	-0.608482	-1.018747
18	1	0	-7.539299	0.355746	0.147037
19	8	0	-0.525926	-0.918006	-1.486900
20	1	0	0.034153	0.647622	-2.429779
21	1	0	0.297545	-1.477757	-1.521714

22	8	0	0.630751	1.409808	-2.607820
23	1	0	0.515910	1.963877	-1.784288
24	1	0	1.934699	0.791350	-2.526902
25	1	0	0.169057	0.911090	0.354837
26	8	0	0.201799	2.422929	-0.175117
27	1	0	-0.715097	2.801294	-0.052905
28	8	0	4.062948	0.554210	-0.217159
29	1	0	3.493256	0.104504	0.475519
30	1	0	4.839497	-0.050924	-0.310271
31	1	0	0.848714	3.031938	0.291527
32	8	0	1.934832	4.035322	1.072984
33	1	0	2.862856	3.724334	0.886530
34	8	0	-2.311320	3.390599	0.122080
35	1	0	-2.479173	3.979725	-0.630417
36	1	0	-2.960614	2.659554	0.003067
37	8	0	1.855853	-2.149973	-1.968312
38	1	0	2.440239	-2.569134	-1.242976
39	1	0	1.803622	-2.793949	-2.694070
40	8	0	4.467897	3.183493	0.549815
41	1	0	4.389629	2.235459	0.283474
42	1	0	4.741072	3.636812	-0.263489
43	8	0	3.385152	-3.036292	-0.049177
44	1	0	4.281592	-2.703699	-0.272976
45	1	0	3.085028	-2.409898	0.656059
46	8	0	5.782672	-1.575430	-0.541028
47	1	0	6.502497	-1.719816	0.095730
48	1	0	6.202252	-1.648014	-1.414648
49	8	0	2.583213	-0.913321	1.462990
50	1	0	1.638830	-0.741430	1.249680
51	1	0	2.684766	-0.784246	2.442809
52	8	0	2.833633	0.214978	-2.463303
53	1	0	2.529891	-0.754742	-2.381420
54	1	0	3.317753	0.423358	-1.575283
55	8	0	2.864423	-0.555171	4.152411
56	1	0	3.101754	-1.411390	4.544726
57	1	0	3.650152	-0.003606	4.299677
58	1	0	1.877924	4.898278	0.633214

SCF Done: E(RB3LYP) = -1677.62830482 A.U. after 1 cycles

Zero-point correction= 0.468176 (a.u.)
Thermal correction to Energy= 0.510131
Thermal correction to Enthalpy= 0.511075
Thermal correction to Gibbs Free Energy= 0.391010
Sum of electronic and zero-point Energies= -1677.160129
Sum of electronic and thermal Energies= -1677.118174
Sum of electronic and thermal Enthalpies= -1677.117229
Sum of electronic and thermal Free Energies= -1677.237295

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.112	147.329	252.699

==== Ring opening TS, TS-S3, in Figure S4 ====
trioneh3.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.003018	1.501027	-1.655987
2	6	0	-1.865984	0.228520	-1.554043
3	6	0	-0.899764	-0.955792	-1.405878
4	6	0	0.392635	1.114235	-1.157609
5	8	0	-1.280136	-1.999810	-0.701889
6	8	0	0.177183	-0.184927	-0.563189
7	8	0	-1.400916	2.568303	-2.058401
8	8	0	-3.076361	0.207932	-1.527452
9	1	0	1.075775	1.027753	-2.013066
10	6	0	0.952366	2.105192	-0.136167
11	6	0	1.221533	3.491973	-0.733294
12	1	0	0.252967	2.206293	0.700773
13	8	0	2.209773	1.610792	0.373798
14	1	0	2.626745	2.431227	0.725757

15	8	0	1.949813	4.189474	0.284023
16	1	0	0.283377	4.000085	-0.972214
17	1	0	1.819726	3.398102	-1.648177
18	1	0	2.516445	4.851756	-0.140288
19	8	0	-0.388371	-1.171119	-2.661224
20	1	0	0.044539	-4.188244	1.179408
21	1	0	0.141686	-2.024229	-2.686467
22	8	0	0.256704	-3.241655	1.139025
23	1	0	-0.391948	-2.828734	0.502526
24	1	0	1.661193	-1.415407	-0.512996
25	8	0	2.190143	-2.243689	-0.421929
26	1	0	1.635839	-2.781918	0.206888
27	1	0	3.529367	-1.814819	0.312906
28	8	0	1.236669	-3.308425	-2.783496
29	1	0	1.812286	-3.118618	-3.542312
30	1	0	1.773803	-3.061167	-1.994670
31	8	0	4.266126	-1.321329	0.823927
32	1	0	4.537945	-0.559200	0.187791
33	1	0	3.734674	-0.851091	1.622157
34	8	0	4.601582	0.681235	-0.779237
35	1	0	4.589031	0.381092	-1.703305
36	1	0	3.718156	1.086828	-0.625383
37	8	0	2.861054	-0.118431	2.522560
38	1	0	2.422878	0.513773	1.909492
39	1	0	2.132546	-0.703781	2.857544
40	1	0	-0.708379	-0.134050	1.189995
41	8	0	-1.136867	0.021914	2.058702
42	1	0	-2.818341	-0.520068	2.019598
43	1	0	-0.556628	-0.459388	2.699532
44	8	0	-3.772696	-0.705444	1.815905
45	1	0	-4.101775	0.156643	1.418684
46	1	0	-3.729856	-1.640174	0.820308
47	8	0	0.684679	-1.603568	3.257481
48	1	0	0.610282	-1.995298	4.142549
49	1	0	0.522966	-2.334592	2.605834
50	8	0	-4.352791	1.662080	0.684485
51	1	0	-3.561018	2.140142	1.041793
52	1	0	-4.118341	1.480762	-0.243724
53	8	0	-3.595363	-2.362602	0.000125
54	1	0	-2.570033	-2.179953	-0.387940
55	1	0	-3.615164	-3.257396	0.384574
56	8	0	-1.978756	2.613018	1.698060
57	1	0	-2.039605	3.181404	2.482327
58	1	0	-1.629494	1.751358	2.027789

SCF Done: E(RB3LYP) = -1677.61620797 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-295.4755	34.9435	39.4312

Zero-point correction= 0.467162 (a.u.)
Thermal correction to Energy= 0.506439
Thermal correction to Enthalpy= 0.507383
Thermal correction to Gibbs Free Energy= 0.397976
Sum of electronic and zero-point Energies= -1677.149046
Sum of electronic and thermal Energies= -1677.109769
Sum of electronic and thermal Enthalpies= -1677.108825
Sum of electronic and thermal Free Energies= -1677.218232

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	317.795	142.683	230.268

==== An ion-pair intermediate with the alkoxide form in Figure S4 ====
trioneh3.for.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.402808	1.234836	-1.820095
2	6	0	-1.573756	0.236071	-1.616426
3	6	0	-1.309037	-1.254859	-1.806593

4	6	0	0.809393	0.761672	-1.017429
5	8	0	-1.925753	-2.108181	-1.166504
6	8	0	0.257832	-0.173109	-0.135463
7	8	0	-0.582224	2.266941	-2.426756
8	8	0	-2.698265	0.629799	-1.355253
9	1	0	1.528623	0.294039	-1.713681
10	6	0	1.530070	1.917671	-0.301459
11	6	0	2.188321	2.939250	-1.226923
12	1	0	0.824954	2.433409	0.362130
13	8	0	2.579096	1.343437	0.517664
14	1	0	3.125662	2.122050	0.759331
15	8	0	2.962502	3.783895	-0.364134
16	1	0	1.429864	3.510521	-1.770381
17	1	0	2.833060	2.426730	-1.952928
18	1	0	3.690518	4.163726	-0.879103
19	8	0	-0.414366	-1.484095	-2.734571
20	1	0	-1.240367	-4.005007	1.553684
21	1	0	-0.081055	-2.460412	-2.716483
22	8	0	-0.888242	-3.114470	1.390983
23	1	0	-1.432924	-2.739775	0.668803
24	1	0	0.989334	-1.590841	-0.124040
25	8	0	1.354842	-2.547029	-0.054091
26	1	0	0.693819	-2.977632	0.541624
27	1	0	2.698110	-2.417135	0.671722
28	8	0	0.711249	-3.768152	-2.409912
29	1	0	1.459705	-3.830291	-3.026415
30	1	0	1.101981	-3.446781	-1.555269
31	8	0	3.548993	-2.131805	1.192237
32	1	0	4.068164	-1.526564	0.542911
33	1	0	3.166391	-1.471346	1.924505
34	8	0	4.594386	-0.373667	-0.391940
35	1	0	4.504248	-0.630740	-1.324439
36	1	0	3.899352	0.311213	-0.241716
37	8	0	2.492393	-0.432505	2.731980
38	1	0	2.304011	0.263943	2.062258
39	1	0	1.612565	-0.792044	3.007972
40	1	0	-0.590342	0.359259	1.123518
41	8	0	-1.111641	0.649499	1.948798
42	1	0	-2.617277	0.485656	1.809073
43	1	0	-0.776994	0.055465	2.665887
44	8	0	-3.644975	0.560753	1.666868
45	1	0	-3.755411	1.448200	1.124274
46	1	0	-3.948070	-0.232587	1.082521
47	8	0	-0.026936	-1.379986	3.370012
48	1	0	-0.240427	-1.647385	4.278203
49	1	0	-0.381600	-2.085210	2.775182
50	8	0	-3.595111	2.721751	0.310764
51	1	0	-2.775002	3.112587	0.722486
52	1	0	-3.279879	2.329623	-0.528811
53	8	0	-4.336314	-1.423836	0.170132
54	1	0	-3.547588	-1.611140	-0.388700
55	1	0	-4.473438	-2.227649	0.697774
56	8	0	-1.254195	3.356090	1.536172
57	1	0	-1.333966	3.920039	2.322065
58	1	0	-1.095293	2.445609	1.883714

SCF Done: E(RB3LYP) = -1677.63413465 A.U. after 2 cycles

Zero-point correction= 0.468659 (a.u.)
Thermal correction to Energy= 0.509058
Thermal correction to Enthalpy= 0.510002
Thermal correction to Gibbs Free Energy= 0.398035
Sum of electronic and zero-point Energies= -1677.165476
Sum of electronic and thermal Energies= -1677.125077
Sum of electronic and thermal Enthalpies= -1677.124133
Sum of electronic and thermal Free Energies= -1677.236100

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	319.439	144.363	235.655

==== neutralization TS, TS-S4, to form DKG in Figure S4 ====
trioneh2a.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.349003	1.240103	-1.825164
2	6	0	-1.573334	0.294814	-1.668892
3	6	0	-1.354446	-1.207928	-1.856380
4	6	0	0.842604	0.744701	-1.003767
5	8	0	-1.997815	-2.040807	-1.220063
6	8	0	0.287342	-0.188330	-0.115198
7	8	0	-0.462043	2.262045	-2.463318
8	8	0	-2.682756	0.734926	-1.433857
9	1	0	1.554130	0.263939	-1.696833
10	6	0	1.577524	1.883494	-0.274638
11	6	0	2.263658	2.899661	-1.186904
12	1	0	0.873707	2.407163	0.384594
13	8	0	2.604028	1.280467	0.547525
14	1	0	3.166971	2.043831	0.798836
15	8	0	3.045586	3.720407	-0.308865
16	1	0	1.522923	3.490980	-1.732994
17	1	0	2.905373	2.380239	-1.910736
18	1	0	3.783749	4.093500	-0.814226
19	8	0	-0.441788	-1.451999	-2.760197
20	1	0	-1.218518	-4.054827	1.476557
21	1	0	-0.107401	-2.431987	-2.729252
22	8	0	-0.935039	-3.133973	1.353346
23	1	0	-1.516274	-2.768206	0.657588
24	1	0	0.874934	-1.353089	-0.110384
25	8	0	1.289550	-2.418217	-0.072910
26	1	0	0.632675	-2.878122	0.506642
27	1	0	2.414785	-2.391180	0.535295
28	8	0	0.689801	-3.710380	-2.392766
29	1	0	1.435363	-3.786034	-3.011397
30	1	0	1.081062	-3.358279	-1.549385
31	8	0	3.407107	-2.257338	1.114884
32	1	0	3.982083	-1.676145	0.518427
33	1	0	3.130595	-1.637261	1.881163
34	8	0	4.609384	-0.461455	-0.398457
35	1	0	4.512186	-0.676681	-1.340388
36	1	0	3.926460	0.226376	-0.221908
37	8	0	2.481524	-0.508936	2.800864
38	1	0	2.306482	0.185964	2.130017
39	1	0	1.596044	-0.851721	3.065513
40	1	0	-0.603031	0.332926	1.186596
41	8	0	-1.117300	0.614906	2.005400
42	1	0	-2.640721	0.494160	1.837531
43	1	0	-0.800711	-0.005196	2.710898
44	8	0	-3.656262	0.604655	1.667215
45	1	0	-3.724414	1.503252	1.132710
46	1	0	-3.970906	-0.171401	1.064220
47	8	0	-0.091324	-1.452381	3.396045
48	1	0	-0.342164	-1.721059	4.294232
49	1	0	-0.444543	-2.143440	2.785552
50	8	0	-3.519360	2.782460	0.351791
51	1	0	-2.687288	3.139369	0.771530
52	1	0	-3.223611	2.422278	-0.507944
53	8	0	-4.391640	-1.315981	0.116194
54	1	0	-3.606577	-1.523137	-0.440518
55	1	0	-4.568106	-2.127037	0.620853
56	8	0	-1.170271	3.329934	1.596461
57	1	0	-1.234896	3.903344	2.376914
58	1	0	-1.042164	2.418409	1.952004

SCF Done: E(RB3LYP) = -1677.63216167 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-808.6113	28.9410	46.9137

Zero-point correction= 0.464115 (a.u.)
Thermal correction to Energy= 0.504147
Thermal correction to Enthalpy= 0.505091
Thermal correction to Gibbs Free Energy= 0.394091
Sum of electronic and zero-point Energies= -1677.168047
Sum of electronic and thermal Energies= -1677.128015

Sum of electronic and thermal Enthalpies= -1677.127071
Sum of electronic and thermal Free Energies= -1677.238070

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	316.357	143.510	233.618

==== DKG + H3O(+)(H2O)11 in the end of Figure S4 ====
trioneh2a.rev.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.421622	1.329972	-1.763700
2	6	0	-1.618186	0.333556	-1.710184
3	6	0	-1.324506	-1.159576	-1.922438
4	6	0	0.803145	0.877895	-0.966879
5	8	0	-1.950942	-2.027440	-1.320797
6	8	0	0.311096	-0.099027	-0.057597
7	8	0	-0.548916	2.370222	-2.365999
8	8	0	-2.746652	0.727788	-1.507481
9	1	0	1.505713	0.416151	-1.673698
10	6	0	1.512215	2.009827	-0.210840
11	6	0	2.170730	3.062508	-1.103060
12	1	0	0.797786	2.499103	0.463987
13	8	0	2.547815	1.394128	0.581030
14	1	0	3.107738	2.151955	0.852891
15	8	0	2.942252	3.870419	-0.206876
16	1	0	1.415156	3.654439	-1.627775
17	1	0	2.816150	2.572651	-1.843660
18	1	0	3.671818	4.269485	-0.704875
19	8	0	-0.349745	-1.332641	-2.770288
20	1	0	-0.969389	-4.230886	1.287015
21	1	0	0.031286	-2.308878	-2.773099
22	8	0	-0.747309	-3.290938	1.183241
23	1	0	-1.363303	-2.948248	0.507279
24	1	0	0.859104	-0.945175	-0.090321
25	8	0	1.489426	-2.460441	-0.184367
26	1	0	0.843063	-2.932439	0.392469
27	1	0	2.381424	-2.472481	0.303844
28	8	0	0.830732	-3.562536	-2.542852
29	1	0	1.551050	-3.601621	-3.193990
30	1	0	1.258817	-3.288734	-1.684384
31	8	0	3.738850	-2.278630	1.149573
32	1	0	4.213934	-1.632353	0.570593
33	1	0	3.362394	-1.699761	1.864303
34	8	0	4.668051	-0.236250	-0.465617
35	1	0	4.471432	-0.499253	-1.378912
36	1	0	3.926173	0.356712	-0.217668
37	8	0	2.477924	-0.514436	2.821773
38	1	0	2.293282	0.160015	2.137979
39	1	0	1.610458	-0.931260	3.016880
40	1	0	-0.729322	0.257161	1.357094
41	8	0	-1.254507	0.444519	2.172121
42	1	0	-2.789584	0.301483	1.905875
43	1	0	-0.914650	-0.229041	2.819159
44	8	0	-3.785541	0.398901	1.670339
45	1	0	-3.844570	1.315849	1.161752
46	1	0	-4.043870	-0.366353	1.025259
47	8	0	-0.082561	-1.665203	3.331069
48	1	0	-0.281633	-2.037436	4.205003
49	1	0	-0.376773	-2.335030	2.667718
50	8	0	-3.656007	2.625132	0.449337
51	1	0	-2.828451	2.976046	0.883303
52	1	0	-3.369342	2.343709	-0.440910
53	8	0	-4.381209	-1.490398	0.032459
54	1	0	-3.580766	-1.640722	-0.519963
55	1	0	-4.518808	-2.324238	0.511672
56	8	0	-1.331901	3.171932	1.737556
57	1	0	-1.403423	3.782098	2.488973
58	1	0	-1.200401	2.281169	2.135809

SCF Done: E(RB3LYP) = -1677.64546436 A.U. after 1 cycles

Zero-point correction= 0.469962 (a.u.)
Thermal correction to Energy= 0.511660
Thermal correction to Enthalpy= 0.512604
Thermal correction to Gibbs Free Energy= 0.397121
Sum of electronic and zero-point Energies= -1677.175502
Sum of electronic and thermal Energies= -1677.133804
Sum of electronic and thermal Enthalpies= -1677.132860
Sum of electronic and thermal Free Energies= -1677.248343

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	321.072	147.896	243.055

Cartesian coordinates of the optimized transition-state geometries and energies by M06-2X/ 6-311+G** SCRF=(PCM, solvent=water).

[TS6 in Figure 3 and TS16 in Figure 6 could not be obtained by M06-2X/ 6-311+G**. Alternatively, their geometries were obtained by B3LYP / 6-311+G** SCRF=(PCM, solvent=water)]

==== TS1 in Figure 1 ====
vitacoh2k.high.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.832063	-1.761407	0.111133
2	6	0	-2.974350	-2.492905	0.127468
3	6	0	-2.964726	-3.433865	-0.958721
4	6	0	-1.007806	-2.272940	-1.061045
5	8	0	-3.819488	-4.237808	-1.264210
6	8	0	-1.806677	-3.303735	-1.660547
7	8	0	-1.464017	-0.800128	0.891955
8	1	0	-0.609887	0.230596	0.581126
9	8	0	-4.030225	-2.380342	0.988289
10	1	0	-4.690936	-3.038069	0.733703
11	1	0	-0.867271	-1.484546	-1.809114
12	6	0	0.350149	-2.857637	-0.698809
13	6	0	1.238238	-1.824292	-0.015394
14	1	0	0.200472	-3.722992	-0.039812
15	8	0	0.952930	-3.267055	-1.913402
16	1	0	1.880445	-3.443948	-1.711256
17	8	0	2.589195	-2.272942	-0.061228
18	1	0	0.918156	-1.654860	1.014155
19	1	0	1.174718	-0.880577	-0.565491
20	1	0	2.932578	-2.284569	0.849818
21	8	0	0.024519	1.073582	0.401886
22	1	0	-0.506828	2.101445	0.457081
23	1	0	0.851797	1.004972	0.956356
24	8	0	2.362621	0.815160	1.577181
25	1	0	2.550060	0.012013	2.092305
26	1	0	2.937710	0.738061	0.794666
27	8	0	-1.041615	3.220112	0.393382
28	1	0	-0.712158	3.634698	-0.441670
29	1	0	-2.041221	3.151540	0.385153
30	8	0	3.617624	0.211546	-0.885276
31	1	0	3.397367	-0.735454	-0.818780
32	1	0	2.967090	0.616330	-1.485772
33	8	0	3.326955	-1.668102	2.516496
34	1	0	4.279797	-1.462383	2.573478
35	1	0	3.098633	-2.160981	3.311189
36	8	0	0.158091	3.997606	-1.853202
37	1	0	0.704937	4.802088	-1.896466
38	1	0	0.725704	3.252307	-2.101770
39	8	0	5.998063	-0.850325	2.333715
40	1	0	6.077538	-0.267028	1.526384
41	1	0	6.831866	0.677059	-0.444161
42	8	0	6.088872	0.714538	0.164796
43	1	0	5.279463	0.605911	-0.369328
44	8	0	1.323767	1.367351	-2.093248
45	1	0	0.729685	1.165091	-1.348846
46	1	0	0.953518	0.917857	-2.860895
47	8	0	-3.621370	2.872563	0.449107
48	1	0	-3.808475	2.013607	0.878021
49	1	0	-4.175840	3.540065	0.888882
50	8	0	1.686727	6.319028	-1.975989
51	1	0	1.412831	7.027391	-2.566626
52	1	0	1.946447	6.753862	-1.157964
53	8	0	-3.796248	0.424198	1.682737
54	1	0	-4.396449	-0.306270	1.490280
55	1	0	-2.915465	0.029624	1.521496
56	8	0	-5.224690	4.800105	1.680599
57	1	0	-4.876207	5.313247	2.415971
58	1	0	-5.707014	5.429369	1.135775

```
---------------------------------------------------------------------
SCF Done:  E(UM062X) =  -1677.79363950    A.U. after   1 cycles

                 1                  2                  3
                 A                  A                  A
Frequencies --   -400.5722            13.2373             16.7030

Zero-point correction=                          0.462113 (a.u.)
Thermal correction to Energy=                    0.507294
Thermal correction to Enthalpy=                  0.508238
Thermal correction to Gibbs Free Energy=         0.378493
Sum of electronic and zero-point Energies=          -1677.331526
Sum of electronic and thermal Energies=             -1677.286346
Sum of electronic and thermal Enthalpies=           -1677.285401
Sum of electronic and thermal Free Energies=        -1677.415147

                E (Thermal)          CV              S
                 KCal/Mol       Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total               318.332          154.658          273.072

 ==== TS2 in Figure 1 ====
  vitacoh2f.high.txt

Stoichiometry   C6H33O19(2)

                    Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X          Y          Z
---------------------------------------------------------------------
     1          6          0       -1.644643   -1.396280    0.425828
     2          6          0       -3.000031   -1.765039    0.372341
     3          6          0       -3.190192   -2.612049   -0.813435
     4          6          0       -1.033371   -1.811788   -0.901454
     5          8          0       -4.149358   -3.258250   -1.143717
     6          8          0       -2.062207   -2.562897   -1.567493
     7          8          0       -1.051574   -0.756516    1.327374
     8          1          0        0.235047    0.384707    1.171065
     9          8          0       -3.848347   -1.772225    1.430375
    10          1          0       -4.480005   -1.064857    1.220975
    11          1          0       -0.821437   -0.921972   -1.505710
    12          6          0        0.223048   -2.666511   -0.825697
    13          6          0        1.346877   -1.966308   -0.066739
    14          1          0       -0.020397   -3.618632   -0.336476
    15          8          0        0.627071   -2.895366   -2.163623
    16          1          0        1.513615   -3.275394   -2.120687
    17          8          0        2.568735   -2.620161   -0.394620
    18          1          0        1.162103   -1.987639    1.008706
    19          1          0        1.409413   -0.922379   -0.392003
    20          1          0        3.084605   -2.765384    0.420753
    21          8          0        0.901440    1.094445    1.038934
    22          1          0        0.270863    2.550936    1.052603
    23          1          0        1.742726    0.788386    1.449933
    24          8          0        3.329579    0.177450    1.738254
    25          1          0        3.463391   -0.711946    2.100814
    26          1          0        3.695309    0.115599    0.838279
    27          8          0       -0.232298    3.390724    0.819412
    28          1          0        0.234345    3.781339   -0.023513
    29          1          0       -1.219331    3.086697    0.623324
    30          8          0        3.999351   -0.269874   -0.986272
    31          1          0        3.539344   -1.124550   -1.066451
    32          1          0        3.420112    0.398025   -1.390038
    33          8          0        4.181041   -2.511161    1.806452
    34          1          0        5.032800   -2.213624    1.424882
    35          1          0        4.378164   -3.191969    2.456686
    36          8          0        0.981748    4.163642   -1.221552
    37          1          0        1.633189    4.889002   -1.136901
    38          1          0        1.450077    3.373700   -1.543470
    39          8          0       -3.904617   -0.205451   -0.514720
    40          1          0       -3.266275    0.518014   -0.435043
    41          1          0        6.934383   -1.585996    0.012879
    42          8          0        6.161993   -1.221146    0.453611
    43          1          0        5.651415   -0.754307   -0.227690
    44          8          0        1.823707    1.500914   -1.582305
    45          1          0        1.378197    1.289360   -0.738307
    46          1          0        1.276424    1.122400   -2.279413
    47          8          0       -2.505327    2.482263    0.444332
```

48	1	0	-2.748138	1.966128	1.245934
49	1	0	-3.267120	3.039782	0.185372
50	8	0	2.781751	6.210051	-0.998530
51	1	0	2.710514	6.947138	-1.613441
52	1	0	2.942379	6.607545	-0.136885
53	8	0	-2.693820	0.984401	2.664862
54	1	0	-3.491580	0.653444	3.087196
55	1	0	-2.198370	0.200126	2.357584
56	8	0	-4.658960	3.989208	-0.310674
57	1	0	-4.517769	4.833045	-0.751340
58	1	0	-5.337370	3.540722	-0.825476

SCF Done: E(UM062X) = -1677.80654463 A.U. after 20 cycles

	1	2	3
	A	A	A
Frequencies --	-59.9158	15.8200	19.9567

Zero-point correction= 0.466686 (a.u.)
Thermal correction to Energy= 0.511674
Thermal correction to Enthalpy= 0.512618
Thermal correction to Gibbs Free Energy= 0.385286
Sum of electronic and zero-point Energies= -1677.339859
Sum of electronic and thermal Energies= -1677.294871
Sum of electronic and thermal Enthalpies= -1677.293926
Sum of electronic and thermal Free Energies= -1677.421258

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	321.080	154.408	267.993

=== TS3 in Figure 1 ====
vitacoh2p.high.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.468307	-0.658287	0.509183
2	6	0	-2.775325	-0.110552	0.370763
3	6	0	-3.445973	-0.889448	-0.695224
4	6	0	-1.277136	-1.646698	-0.630560
5	8	0	-4.604808	-0.869644	-1.022742
6	8	0	-2.535724	-1.658143	-1.329061
7	8	0	-0.585414	-0.349993	1.347219
8	1	0	1.194706	-0.608999	1.410549
9	8	0	-3.539872	0.375515	1.367661
10	1	0	-3.241637	1.266565	1.636479
11	1	0	-0.505851	-1.303283	-1.328055
12	6	0	-0.976776	-3.079476	-0.202552
13	6	0	0.274467	-3.162631	0.656275
14	1	0	-1.842353	-3.456470	0.360866
15	8	0	-0.800720	-3.831506	-1.388074
16	1	0	-0.389446	-4.667046	-1.134871
17	8	0	0.657910	-4.520774	0.867017
18	1	0	0.127877	-2.651434	1.608691
19	1	0	1.106895	-2.705465	0.117610
20	1	0	0.044582	-4.930771	1.488273
21	8	0	2.162885	-0.698735	1.296208
22	1	0	3.046769	0.632301	1.086740
23	1	0	2.444313	-1.543194	1.703423
24	8	0	2.898128	-3.226522	2.101196
25	1	0	3.230670	-3.493023	2.963104
26	1	0	2.308620	-3.937175	1.804270
27	8	0	3.461608	1.484170	0.760477
28	1	0	3.921746	1.282477	-0.176835
29	1	0	2.677145	2.144579	0.622916
30	8	0	-2.526623	1.508116	-0.637542
31	1	0	-1.646602	1.432951	-1.041017
32	8	0	0.241552	1.403501	-1.596973
33	1	0	0.243760	1.855748	-2.447746
34	1	0	0.648008	2.028206	-0.963461
35	1	0	-4.069103	1.877427	-1.453257
36	8	0	4.369349	0.948419	-1.463896

37	1	0	5.262235	0.554615	-1.545200
38	1	0	3.707482	0.287037	-1.754334
39	8	0	-4.993806	1.951477	-1.761577
40	1	0	-5.335241	1.067795	-1.585688
41	1	0	-2.622368	2.645509	0.513806
42	8	0	-2.706086	3.002676	1.445312
43	1	0	-3.332295	3.731626	1.443710
44	8	0	2.162215	-0.643306	-1.563976
45	1	0	2.198555	-0.827434	-0.611203
46	1	0	1.454346	0.021474	-1.652866
47	8	0	1.435465	2.923646	0.416897
48	1	0	0.807266	2.756751	1.173131
49	1	0	1.547571	3.891824	0.310407
50	8	0	6.862265	-0.136019	-1.707263
51	1	0	7.577401	0.397252	-2.067900
52	1	0	7.242152	-0.605841	-0.958274
53	8	0	-0.235915	2.232231	2.328273
54	1	0	-1.086809	2.683546	2.182195
55	1	0	-0.418876	1.299604	2.106831
56	8	0	1.739740	5.616228	0.107753
57	1	0	2.585059	6.030675	0.307179
58	1	0	1.430527	6.034017	-0.702040

SCF Done: E(UM062X) = -1677.81804099 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-238.6184	19.2149	21.1382

Zero-point correction= 0.467155 (a.u.)
Thermal correction to Energy= 0.511353
Thermal correction to Enthalpy= 0.512297
Thermal correction to Gibbs Free Energy= 0.386915
Sum of electronic and zero-point Energies= -1677.350886
Sum of electronic and thermal Energies= -1677.306688
Sum of electronic and thermal Enthalpies= -1677.305744
Sum of electronic and thermal Free Energies= -1677.431126

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.879	152.581	263.890

=== TS4 in Figure 3 ===
trione9bx.high.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.413799	-0.360996	-1.022217
2	6	0	0.299783	0.398085	-0.281230
3	6	0	0.739459	0.273904	1.194000
4	6	0	2.203374	-1.120959	0.034393
5	8	0	0.278699	0.853951	2.137301
6	8	0	1.711689	-0.628242	1.307356
7	8	0	1.582583	-0.380697	-2.205191
8	8	0	-0.759673	-0.959363	-0.228182
9	1	0	-1.435890	-0.874264	-0.975975
10	1	0	1.934759	-2.179515	-0.035897
11	6	0	3.719067	-0.989345	0.044289
12	6	0	4.357245	-0.977739	-1.336005
13	1	0	3.960981	-0.050369	0.551296
14	8	0	4.201058	-2.086247	0.800136
15	1	0	5.164577	-2.052729	0.757458
16	8	0	5.759855	-0.897775	-1.080210
17	1	0	4.025439	-0.112569	-1.913889
18	1	0	4.113540	-1.893966	-1.880873
19	1	0	6.245685	-1.146238	-1.872488
20	8	0	-0.258027	1.413763	-0.739782
21	1	0	-1.273575	-1.001062	0.652797
22	8	0	-1.991105	-1.183221	1.991947
23	1	0	-1.811955	-0.509979	2.658123
24	1	0	-2.975650	-1.206113	1.811228
25	8	0	-4.448847	-1.466342	1.170601

26	1	0	-4.633817	-0.728500	0.559071
27	1	0	-4.235643	-2.222261	0.588331
28	8	0	-4.526474	0.558554	-0.717065
29	1	0	-5.326901	0.915834	-1.144904
30	1	0	-4.000230	1.313567	-0.371290
31	8	0	-3.327828	-3.360969	-0.513613
32	1	0	-3.016598	-2.753076	-1.199565
33	1	0	-2.543263	-3.622356	0.000824
34	8	0	-2.735458	2.390709	0.073275
35	1	0	-2.484337	2.754346	0.939701
36	1	0	-1.901658	2.018177	-0.264318
37	8	0	-6.797668	1.552412	-1.948392
38	1	0	-7.020317	1.245445	-2.832627
39	1	0	-7.630493	1.570541	-1.466958
40	8	0	-1.246589	-3.802074	1.316479
41	1	0	-1.387985	-3.019646	1.870955
42	1	0	-1.266607	-4.557668	1.910946
43	8	0	-2.682467	-0.941656	-1.943669
44	1	0	-2.538278	-0.745962	-2.875495
45	1	0	-3.416507	-0.359498	-1.625408
46	1	0	2.650277	2.093017	-1.310020
47	8	0	2.788102	1.896307	-0.374897
48	1	0	2.321660	2.621142	0.079968
49	1	0	0.277608	3.051573	-0.147540
50	8	0	0.763192	3.720133	0.372220
51	1	0	0.778211	4.522730	-0.159916
52	1	0	4.734715	1.937613	-0.216638
53	8	0	5.700450	1.871310	-0.190114
54	1	0	5.900214	0.974913	-0.494047
55	1	0	-0.586622	3.711621	1.795362
56	8	0	-1.278338	3.269883	2.312847
57	1	0	-0.882923	2.404081	2.484029

SCF Done: E(RM062X) = -1677.25112619 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-163.6308	16.7814	26.5786

Zero-point correction= 0.457633 (a.u.)
Thermal correction to Energy= 0.502028
Thermal correction to Enthalpy= 0.502973
Thermal correction to Gibbs Free Energy= 0.379231
Sum of electronic and zero-point Energies= -1676.793493
Sum of electronic and thermal Energies= -1676.749098
Sum of electronic and thermal Enthalpies= -1676.748154
Sum of electronic and thermal Free Energies= -1676.871895

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	315.028	154.020	260.435

==== TS5 in Figure 3 ====
rot1.high.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.936078	-1.565529	-1.089231
2	6	0	3.134148	-2.894421	-0.348709
3	6	0	3.836216	-2.520735	0.961543
4	6	0	3.405487	-0.475282	-0.137471
5	8	0	4.208169	-3.259902	1.817903
6	8	0	3.988389	-1.192172	0.990476
7	8	0	2.557406	-1.456679	-2.214144
8	8	0	2.831576	-3.987159	-0.706002
9	1	0	4.214837	0.084697	-0.608828
10	6	0	2.344524	0.509083	0.404522
11	6	0	0.912385	0.315893	-0.088260
12	1	0	2.318800	0.341981	1.488068
13	8	0	2.808803	1.814901	0.124716
14	1	0	2.108356	2.472588	0.349168
15	8	0	0.693641	0.674049	-1.438723

16	1	0	0.270694	0.902896	0.576771
17	1	0	0.616277	-0.731282	0.019351
18	1	0	1.014342	1.575287	-1.624546
19	8	0	1.364878	3.235934	-2.420269
20	1	0	2.335336	3.240615	-2.541182
21	1	0	0.968831	3.442138	-3.271916
22	8	0	-2.033954	0.777298	-0.780761
23	1	0	-1.213420	0.798366	-1.303931
24	1	0	-1.902248	1.437271	-0.067190
25	8	0	-5.921118	-1.512443	-2.627208
26	1	0	-5.515299	-0.742974	-2.173217
27	1	0	-6.677589	-1.170200	-3.111066
28	8	0	-1.492962	2.533647	1.272996
29	1	0	-2.246519	3.041604	1.628722
30	1	0	-1.036269	2.103843	2.024710
31	8	0	0.845145	3.641014	0.271499
32	1	0	0.796067	3.758174	-0.690487
33	1	0	-0.043265	3.374228	0.572391
34	1	0	3.799911	2.426542	-1.282212
35	8	0	4.024366	2.778564	-2.161605
36	1	0	4.748499	3.397003	-2.030414
37	1	0	-5.950605	-4.079381	-0.654231
38	8	0	-6.247433	-3.184286	-0.469928
39	1	0	-6.189741	-2.698467	-1.316666
40	1	0	-2.032233	-0.802590	0.004539
41	8	0	-2.052519	-1.634419	0.527525
42	1	0	-1.903886	-2.349209	-0.100822
43	1	0	-0.838475	-1.581977	1.868855
44	8	0	-0.193794	-1.418291	2.583519
45	1	0	0.513831	-2.058729	2.466815
46	8	0	-3.661685	3.969976	2.215289
47	1	0	-3.699514	4.916639	2.047114
48	1	0	-4.541037	3.638293	2.008591
49	8	0	0.199523	1.250362	2.982965
50	1	0	0.320645	1.467453	3.911618
51	1	0	0.102997	0.277450	2.935256
52	1	0	-5.308497	-2.104625	0.677503
53	8	0	-4.833109	-1.372348	1.110972
54	1	0	-3.893380	-1.609478	1.061122
55	8	0	-4.812317	0.405195	-1.044708
56	1	0	-4.865806	-0.098568	-0.209268
57	1	0	-3.868720	0.610438	-1.145093

SCF Done: E(RM062X) = -1677.24981295 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-37.6005	11.9435	15.3517

Zero-point correction= 0.457456
(Hartree/Particle)
Thermal correction to Energy= 0.503158
Thermal correction to Enthalpy= 0.504102
Thermal correction to Gibbs Free Energy= 0.372974
Sum of electronic and zero-point Energies= -1676.792356
Sum of electronic and thermal Energies= -1676.746655
Sum of electronic and thermal Enthalpies= -1676.745711
Sum of electronic and thermal Free Energies= -1676.876839

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	315.736	155.980	275.983

==== TS6 in Figure 3 (B3LYP/6-311+G** SCRF=PCM) ====
trione24ext.bhigh.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.066255	0.239677	0.445726
2	6	0	2.902475	1.169442	-0.430479
3	6	0	3.976191	0.290964	-1.097149
4	6	0	2.768423	-1.131849	0.342525

5	8	0	4.802592	0.626846	-1.900016
6	8	0	3.872045	-0.956457	-0.611067
7	8	0	1.516187	0.666912	1.488973
8	8	0	2.826798	2.360956	-0.550596
9	1	0	3.199272	-1.432210	1.295416
10	6	0	1.825888	-2.176519	-0.248684
11	6	0	1.095193	-1.417182	-1.358353
12	1	0	2.393558	-3.023218	-0.649152
13	8	0	0.961512	-2.588904	0.803127
14	1	0	0.224427	-3.125247	0.428619
15	8	0	0.846314	-0.100297	-0.860296
16	1	0	1.715245	-1.377157	-2.259575
17	1	0	0.153483	-1.906599	-1.620135
18	1	0	-0.548659	-0.063240	-0.178545
19	1	0	0.104247	0.142338	2.523613
20	8	0	-0.852682	0.035284	2.712760
21	1	0	-1.153929	0.893436	3.085523
22	8	0	-1.467694	-0.015315	0.277331
23	1	0	-1.306480	-0.029090	1.308543
24	1	0	-2.087255	-0.769133	-0.026431
25	8	0	-1.671160	2.587471	3.372567
26	1	0	-2.329315	2.884369	2.696767
27	1	0	-1.979227	2.901787	4.229895
28	8	0	-3.016858	-1.900813	-0.531247
29	1	0	-3.827987	-2.003066	0.016553
30	1	0	-3.307808	-1.695979	-1.457649
31	8	0	-1.131849	-3.938151	-0.308974
32	1	0	-1.469381	-4.749107	0.087069
33	1	0	-1.894898	-3.327298	-0.385984
34	1	0	1.629218	-3.377262	2.334866
35	8	0	1.965223	-3.756318	3.170200
36	1	0	2.305056	-4.624775	2.930414
37	1	0	1.057274	2.469147	1.678364
38	8	0	0.646618	3.343627	1.839210
39	1	0	-0.036116	3.175481	2.512756
40	1	0	0.261535	1.200633	-1.945217
41	8	0	-0.204933	1.929157	-2.416456
42	1	0	0.458426	2.347416	-2.978885
43	1	0	-1.612981	1.329901	-3.398180
44	8	0	-2.391707	1.011710	-3.902625
45	1	0	-2.127473	1.028016	-4.829147
46	8	0	-5.277136	-2.209553	1.002882
47	1	0	-5.368631	-3.039435	1.486202
48	1	0	-5.486919	-1.517047	1.640911
49	8	0	-3.654670	-1.274817	-3.070872
50	1	0	-4.587034	-1.176530	-3.293289
51	1	0	-3.211785	-0.451206	-3.380800
52	1	0	-0.345079	3.676474	0.348989
53	8	0	-1.022204	3.805793	-0.351742
54	1	0	-0.787102	3.180307	-1.061261
55	8	0	-3.185362	3.408713	1.269462
56	1	0	-2.491804	3.523058	0.575116
57	1	0	-3.836702	2.801291	0.902148

SCF Done: E(RB3LYP) = -1677.97049607 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-116.5951	12.3935	16.0594

Zero-point correction= 0.448515 (a.u.)
Thermal correction to Energy= 0.493558
Thermal correction to Enthalpy= 0.494502
Thermal correction to Gibbs Free Energy= 0.364435
Sum of electronic and zero-point Energies= -1677.521981
Sum of electronic and thermal Energies= -1677.476938
Sum of electronic and thermal Enthalpies= -1677.475994
Sum of electronic and thermal Free Energies= -1677.606061

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	309.712	152.249	273.750

==== TS7 in Figure 3 ====
trione3bext.high.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.634971	-1.472066	0.087709
2	6	0	0.582121	-0.423614	-0.419985
3	6	0	1.305307	0.224693	-1.617575
4	6	0	2.560940	-1.644778	-1.136809
5	8	0	1.028537	1.259743	-2.162560
6	8	0	2.240833	-0.607365	-2.083085
7	8	0	2.366290	-1.053520	1.179288
8	8	0	-0.562266	-0.916115	-0.837853
9	1	0	3.608840	-1.533276	-0.864722
10	6	0	2.277077	-3.051522	-1.659256
11	6	0	0.993326	-3.437065	-0.918672
12	1	0	2.151000	-3.058888	-2.744584
13	8	0	3.386828	-3.840809	-1.261225
14	1	0	3.224692	-4.753752	-1.518893
15	8	0	1.048491	-2.726395	0.321933
16	1	0	0.112639	-3.128456	-1.484817
17	1	0	0.941797	-4.502503	-0.694581
18	1	0	1.831602	-1.136303	1.998784
19	8	0	0.367561	0.601120	0.624397
20	1	0	-0.481786	1.291437	0.313149
21	1	0	1.219284	1.219079	0.773356
22	1	0	-1.769442	-0.016386	-1.584304
23	8	0	-2.498599	0.626606	-1.777892
24	1	0	-3.291695	0.230261	-1.370799
25	8	0	-1.410709	2.118573	-0.016874
26	1	0	-1.911239	1.673637	-0.782363
27	1	0	-0.920728	2.900211	-0.352289
28	8	0	-4.422966	-0.515030	-0.133564
29	1	0	-4.287522	0.104500	0.609216
30	1	0	-5.380364	-0.653426	-0.242278
31	8	0	2.238613	2.186831	0.734974
32	1	0	1.847230	2.982052	0.328856
33	1	0	2.666623	2.428794	1.583035
34	8	0	0.596031	3.722172	-0.872501
35	1	0	0.800156	3.162008	-1.635508
36	1	0	0.635626	4.652909	-1.168820
37	8	0	1.022635	-1.434260	3.540733
38	1	0	1.308524	-0.977235	4.336933
39	1	0	0.069490	-1.257609	3.447275
40	8	0	3.450686	2.790891	3.090814
41	1	0	3.031053	2.510437	3.910366
42	1	0	4.381293	2.564817	3.186820
43	1	0	-1.632309	-1.967793	0.019339
44	8	0	-2.361291	-2.340251	0.566365
45	1	0	-3.155875	-1.864558	0.269314
46	1	0	-1.813771	-1.400240	1.947276
47	8	0	-1.428300	-0.695747	2.518204
48	1	0	-0.814686	-0.233386	1.926632
49	8	0	0.699605	6.341137	-1.692341
50	1	0	-0.122673	6.810592	-1.863481
51	1	0	1.262114	6.967227	-1.226204
52	8	0	-3.458548	1.166588	1.842829
53	1	0	-2.833498	0.559859	2.276691
54	1	0	-2.889060	1.778663	1.356456
55	8	0	-7.156353	-0.937597	-0.480590
56	1	0	-7.561480	-0.703400	-1.321215
57	1	0	-7.524900	-1.795741	-0.249530

SCF Done: E(RM062X) = -1677.26675197 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-279.1260	18.6710	19.3633

Zero-point correction= 0.456535 (a.u.)
Thermal correction to Energy= 0.499120
Thermal correction to Enthalpy= 0.500064
Thermal correction to Gibbs Free Energy= 0.377940
Sum of electronic and zero-point Energies= -1676.810217
Sum of electronic and thermal Energies= -1676.767632
Sum of electronic and thermal Enthalpies= -1676.766688

Sum of electronic and thermal Free Energies= -1676.888812

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.202	147.665	257.031

==== TS8 in Figure 3 ===
trione10a.high.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.734765	-0.534031	-0.768643
2	6	0	1.357091	-0.848549	-1.434105
3	6	0	0.326298	-0.026900	-0.585285
4	6	0	2.374615	0.402648	0.412785
5	8	0	-0.685879	0.439277	-1.222141
6	8	0	1.112118	0.959501	0.071047
7	8	0	3.355881	-1.732789	-0.405614
8	8	0	1.317378	-0.343756	-2.719615
9	1	0	2.341770	-0.118247	1.371806
10	6	0	3.459175	1.461954	0.347114
11	6	0	3.684410	1.547193	-1.156298
12	1	0	3.164746	2.413055	0.797650
13	8	0	4.564699	0.871073	1.009816
14	1	0	5.340427	1.428675	0.891289
15	8	0	3.598872	0.189010	-1.598743
16	1	0	2.905615	2.150415	-1.631908
17	1	0	4.667494	1.930326	-1.427699
18	1	0	4.253955	-1.514037	-0.119110
19	8	0	-0.098307	-0.919455	0.578298
20	1	0	-0.789872	-0.287019	1.212373
21	1	0	-0.624347	-1.699657	0.204309
22	8	0	-1.624747	0.446060	1.884038
23	1	0	-1.876634	1.214690	1.309324
24	1	0	-2.452476	-0.122254	1.969135
25	8	0	-1.998044	2.398101	0.070993
26	1	0	-1.496236	1.815691	-0.547010
27	1	0	-1.345563	3.058890	0.375347
28	8	0	-3.149774	-0.785842	-1.043374
29	1	0	-2.326918	-0.272771	-1.179713
30	1	0	-3.839649	-0.371585	-1.601691
31	8	0	-3.691529	-1.096311	1.685345
32	1	0	-3.697133	-1.027694	0.711725
33	1	0	-3.473937	-2.028717	1.877844
34	8	0	0.308554	3.542071	1.065285
35	1	0	0.264354	3.201236	1.977061
36	1	0	0.736877	2.820807	0.582654
37	1	0	1.113581	-2.253650	1.682810
38	8	0	1.862371	-2.838119	1.843327
39	1	0	2.440398	-2.664885	1.088033
40	8	0	-4.976252	0.672476	-2.456393
41	1	0	-5.908093	0.447534	-2.523360
42	1	0	-4.928917	1.516215	-1.963202
43	8	0	-1.541678	-2.837196	-0.440125
44	1	0	-2.263954	-2.341666	-0.879526
45	1	0	-0.951207	-3.160334	-1.133705
46	1	0	-3.619150	2.826787	-0.567493
47	8	0	-4.490279	2.945344	-0.993357
48	1	0	-5.090680	3.222370	-0.295808
49	8	0	-2.851821	-3.738059	1.864632
50	1	0	-2.252285	-3.705509	1.102352
51	1	0	-2.337044	-4.089205	2.596723
52	8	0	1.033209	-2.207064	-1.383464
53	1	0	1.834544	-2.725027	-1.536295
54	1	0	0.407907	-0.024082	-2.846163
55	8	0	0.073568	2.098941	3.450445
56	1	0	-0.179499	2.408398	4.324765
57	1	0	-0.582903	1.431248	3.200876

SCF Done: E(RM062X) = -1677.27408966 A.U. after 1 cycles

1 2 3

```
                 A                  A                  A
Frequencies --   -155.2756            22.7629            30.7443

 Zero-point correction=                          0.462001
(Hartree/Particle)
 Thermal correction to Energy=                   0.502353
 Thermal correction to Enthalpy=                 0.503297
 Thermal correction to Gibbs Free Energy=        0.389498
 Sum of electronic and zero-point Energies=          -1676.812088
 Sum of electronic and thermal Energies=             -1676.771737
 Sum of electronic and thermal Enthalpies=           -1676.770793
 Sum of electronic and thermal Free Energies=        -1676.884592

                 E (Thermal)             CV                S
                  KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total               315.231            145.295           239.511

  ==== TS9 in Figure 3 ====
  trione10k.high.txt

Stoichiometry   C6H32O19

                     Standard orientation:
---------------------------------------------------------------------
Center     Atomic     Atomic           Coordinates (Angstroms)
Number     Number      Type             X           Y           Z
---------------------------------------------------------------------
    1          6          0        2.764180   -0.543859   -0.700780
    2          6          0        1.427160   -0.678815   -1.505827
    3          6          0        0.286037   -0.038295   -0.667202
    4          6          0        2.531255    0.552004    0.379057
    5          8          0       -0.656934    0.510212   -1.275720
    6          8          0        1.311523    1.168625   -0.000237
    7          8          0        3.099605   -1.800897   -0.184388
    8          8          0        1.543212    0.037877   -2.681916
    9          1          0        2.476284    0.133805    1.385089
   10          6          0        3.715557    1.491984    0.194202
   11          6          0        4.018279    1.298511   -1.286246
   12          1          0        3.472911    2.526080    0.450488
   13          8          0        4.736402    0.960480    1.018725
   14          1          0        5.555439    1.438684    0.853491
   15          8          0        3.823873   -0.102940   -1.497339
   16          1          0        3.319599    1.869333   -1.903712
   17          1          0        5.045235    1.539710   -1.557458
   18          1          0        4.054459   -1.807190   -0.030236
   19          8          0        0.010485   -0.763900    0.491484
   20          1          0       -1.285581    0.021040    1.647009
   21          1          0       -0.528899   -1.543283    0.197500
   22          8          0       -2.038591    0.426217    2.109490
   23          1          0       -2.361058    1.765251    0.874361
   24          1          0       -2.758432   -0.239518    2.025824
   25          8          0       -2.152081    2.400055    0.160452
   26          1          0       -1.656354    1.854191   -0.478951
   27          1          0       -0.611542    2.930360    1.130461
   28          8          0       -3.172195   -0.755932   -1.222622
   29          1          0       -2.377440   -0.197260   -1.281458
   30          1          0       -3.876551   -0.299389   -1.727913
   31          8          0       -3.871816   -1.426940    1.417185
   32          1          0       -3.737584   -1.232729    0.471947
   33          1          0       -3.550675   -2.337232    1.544631
   34          8          0        0.250406    2.736276    1.545885
   35          1          0        0.055068    2.437039    2.466552
   36          1          0        0.865737    1.817397    0.734694
   37          1          0        1.008935   -1.653950    2.085485
   38          8          0        1.731268   -2.218841    2.382495
   39          1          0        2.258472   -2.316314    1.578906
   40          8          0       -5.071396    0.757047   -2.486158
   41          1          0       -5.999143    0.521636   -2.398633
   42          1          0       -4.968417    1.627890   -2.052077
   43          8          0       -1.423916   -2.751087   -0.654402
   44          1          0       -2.163059   -2.276994   -1.080804
   45          1          0       -0.750620   -2.889924   -1.336119
   46          1          0       -3.659908    2.939495   -0.673567
   47          8          0       -4.448648    3.114893   -1.222596
   48          1          0       -5.063665    3.596714   -0.662992
   49          8          0       -2.702322   -3.984577    1.483299
   50          1          0       -2.085852   -3.793637    0.757559
```

51	1	0	-2.161978	-4.279910	2.221527
52	8	0	1.088077	-2.016997	-1.747872
53	1	0	1.821787	-2.578327	-1.457314
54	1	0	0.661565	0.396630	-2.869574
55	8	0	-0.481425	1.720530	3.916306
56	1	0	-0.830793	2.252482	4.636806
57	1	0	-1.226973	1.207925	3.552665

SCF Done: E(RM062X) = -1677.27084615 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-155.1931	26.3775	30.7552

Zero-point correction= 0.463417 (a.u.)
Thermal correction to Energy= 0.504075
Thermal correction to Enthalpy= 0.505019
Thermal correction to Gibbs Free Energy= 0.391140
Sum of electronic and zero-point Energies= -1676.807429
Sum of electronic and thermal Energies= -1676.766772
Sum of electronic and thermal Enthalpies= -1676.765827
Sum of electronic and thermal Free Energies= -1676.879706

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	316.312	146.801	239.678

==== TS10 in Figure 4 ====
trione5zzext.high.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.370622	-1.626646	-0.966166
2	6	0	0.843142	-1.729315	-1.147123
3	6	0	0.261391	-0.421789	-0.561491
4	6	0	2.583900	-0.323382	-0.209323
5	8	0	-0.739938	0.104902	-1.163741
6	8	0	1.393905	0.425053	-0.486787
7	8	0	3.175514	-2.403714	-1.387157
8	8	0	0.248236	-2.596927	-1.710029
9	1	0	2.650171	-0.539965	0.864825
10	6	0	3.776613	0.497620	-0.659448
11	6	0	5.100516	-0.177131	-0.337740
12	1	0	3.706805	0.673712	-1.740050
13	8	0	3.697744	1.736264	0.031292
14	1	0	4.558722	2.164655	-0.068859
15	8	0	6.095598	0.783869	-0.669798
16	1	0	5.216508	-1.090980	-0.923489
17	1	0	5.136901	-0.418015	0.730114
18	1	0	6.939353	0.507769	-0.301677
19	8	0	-0.029689	-0.729001	0.906711
20	1	0	-0.600372	0.175536	1.354550
21	1	0	-0.618257	-1.536752	0.941773
22	8	0	-1.260474	1.149262	1.799729
23	1	0	-1.285836	1.819070	1.053066
24	1	0	-2.183101	0.782206	1.936794
25	8	0	-0.957431	2.650156	-0.322411
26	1	0	-0.817368	1.814217	-0.824669
27	1	0	-0.060191	3.004549	-0.128430
28	8	0	-3.139099	-0.908751	-0.716253
29	1	0	-2.262576	-0.522009	-0.982427
30	1	0	-3.637045	-1.105298	-1.532436
31	8	0	-3.543534	-0.116317	1.950916
32	1	0	-3.605268	-0.476549	1.049809
33	1	0	-3.448458	-0.897796	2.529581
34	8	0	1.488234	3.433370	0.587330
35	1	0	1.344963	3.221476	1.526425
36	1	0	2.172564	2.808604	0.293934
37	1	0	1.315275	-2.727983	2.016601
38	8	0	1.365795	-3.076408	1.120146
39	1	0	1.856055	-3.901470	1.195206
40	8	0	-4.742388	-0.759126	-2.955820

41	1	0	-5.480432	-1.282122	-3.280761
42	1	0	-5.117290	0.073523	-2.631093
43	8	0	-1.699400	-2.756184	0.734910
44	1	0	-2.340183	-2.374175	0.100922
45	1	0	-1.247632	-3.483539	0.289576
46	1	0	-4.241577	0.789982	-0.746350
47	8	0	-4.820403	1.433469	-1.184424
48	1	0	-5.544379	1.594272	-0.570113
49	8	0	-3.049697	-2.540714	3.188302
50	1	0	-2.481268	-2.863719	2.471003
51	1	0	-2.548502	-2.653643	4.000845
52	1	0	-2.394219	3.534920	-1.154347
53	8	0	-3.218138	3.816727	-1.581791
54	1	0	-3.802796	3.050554	-1.491156
55	8	0	0.805982	2.532067	3.155773
56	1	0	0.658228	3.059800	3.945490
57	1	0	-0.022447	2.059038	2.987894

SCF Done: E(RM062X) = -1677.23634497 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-421.8563	15.6749	23.9192

Zero-point correction= 0.454927
(Hartree/Particle)
Thermal correction to Energy= 0.498926
Thermal correction to Enthalpy= 0.499871
Thermal correction to Gibbs Free Energy= 0.376522
Sum of electronic and zero-point Energies= -1676.781418
Sum of electronic and thermal Energies= -1676.737419
Sum of electronic and thermal Enthalpies= -1676.736474
Sum of electronic and thermal Free Energies= -1676.859823

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.081	152.444	259.610

==== TS11 in Figure 4 ====
trionexpext.high.txt
Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.788052	0.642801	-1.088323
2	6	0	-2.593641	-0.886082	-0.947920
3	6	0	-1.101882	-1.243163	-1.059853
4	6	0	-1.437052	1.302237	-0.853563
5	8	0	-0.593975	-2.169629	-0.386221
6	8	0	-0.637741	0.270021	-0.308530
7	8	0	-3.811208	1.147503	-1.448845
8	8	0	-3.478482	-1.677225	-0.798175
9	1	0	-1.053323	1.605712	-1.839540
10	6	0	-1.402242	2.513516	0.064501
11	6	0	-2.273540	3.658192	-0.420449
12	1	0	-1.721656	2.210882	1.067430
13	8	0	-0.037522	2.906992	0.095036
14	1	0	-0.007241	3.766097	0.533605
15	8	0	-1.981684	4.747476	0.447887
16	1	0	-3.328811	3.380249	-0.367346
17	1	0	-2.016206	3.908579	-1.455601
18	1	0	-2.376614	5.548452	0.093006
19	8	0	-0.756496	-1.040105	-2.361994
20	1	0	2.602076	-2.498802	-0.337140
21	1	0	0.200262	-1.204907	-2.494703
22	8	0	2.011692	-2.043599	0.308687
23	1	0	1.083093	-2.281749	0.092236
24	1	0	0.726149	0.482492	-0.343632
25	8	0	1.798459	0.409757	-0.377917
26	1	0	1.979001	-0.555343	-0.099476
27	1	0	2.285333	1.023700	0.309458
28	8	0	1.999194	-0.920766	-2.859691
29	1	0	2.108862	-0.692014	-3.789808
30	1	0	2.180592	-0.109143	-2.363657

31	8	0	3.807062	-2.736865	-1.557854
32	1	0	3.373839	-2.190522	-2.230800
33	1	0	4.503772	-2.175912	-1.169587
34	8	0	3.081397	1.629864	1.374363
35	1	0	3.414870	0.861517	1.871157
36	1	0	3.860513	2.137757	1.070084
37	1	0	-4.325695	-2.829166	0.588147
38	8	0	-4.364897	-3.288492	1.437123
39	1	0	-4.731829	-4.155768	1.241835
40	1	0	-1.320141	-2.844117	1.119594
41	8	0	-1.614112	-2.995781	2.037174
42	1	0	-2.569229	-3.158968	1.967527
43	1	0	-0.658364	-0.144083	1.576581
44	8	0	-0.923277	-0.337023	2.490520
45	1	0	-1.111713	-1.295188	2.490830
46	1	0	-2.633543	0.185292	2.071522
47	8	0	-3.405195	0.330597	1.493869
48	1	0	-3.878673	1.083430	1.859613
49	8	0	5.403061	-1.038079	-0.048511
50	1	0	4.984768	-1.004918	0.828446
51	1	0	6.350559	-1.080063	0.108064
52	8	0	3.694393	-0.961404	2.196068
53	1	0	3.883627	-1.300650	3.076518
54	1	0	2.993048	-1.521359	1.818079
55	8	0	5.284891	3.020744	0.535816
56	1	0	5.580617	2.943686	-0.376603
57	1	0	5.396040	3.947934	0.767383

SCF Done: E(RM062X) = -1677.23405001 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-269.5189	15.3130	21.6475

Zero-point correction= 0.454412 (a.u.)
Thermal correction to Energy= 0.499145
Thermal correction to Enthalpy= 0.500089
Thermal correction to Gibbs Free Energy= 0.374060
Sum of electronic and zero-point Energies= -1676.779638
Sum of electronic and thermal Energies= -1676.734905
Sum of electronic and thermal Enthalpies= -1676.733961
Sum of electronic and thermal Free Energies= -1676.859990

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	313.218	153.596	265.252

==== TS12 in Figure 4 ====
dkg01.high.txt

Stoichiometry C6H32O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.006804	0.100171	0.863598
2	6	0	-2.121740	1.352735	1.105191
3	6	0	-0.685644	1.062618	1.585921
4	6	0	-2.329606	-0.972899	0.021321
5	8	0	0.216144	1.848518	1.249428
6	8	0	-1.398565	-0.256895	-0.772527
7	8	0	-4.123001	0.059546	1.298819
8	8	0	-2.574735	2.455199	0.960315
9	1	0	-1.806268	-1.646070	0.710589
10	6	0	-3.278004	-1.783235	-0.856001
11	6	0	-4.228010	-2.660885	-0.054464
12	1	0	-3.858611	-1.098882	-1.489617
13	8	0	-2.445495	-2.599164	-1.661649
14	1	0	-3.015277	-3.283565	-2.034716
15	8	0	-4.883939	-3.480396	-1.017207
16	1	0	-4.943176	-2.053201	0.500519
17	1	0	-3.649292	-3.277664	0.642626
18	1	0	-5.377289	-4.168405	-0.562433
19	8	0	-0.592873	0.018062	2.266789
20	1	0	2.558470	2.063480	-0.559279

21	1	0	0.890404	-0.522747	2.090403
22	8	0	2.200386	1.808957	-1.442961
23	1	0	1.504139	2.461100	-1.635746
24	1	0	-0.542185	-0.708201	-0.822673
25	8	0	1.395778	-0.611980	-0.686854
26	1	0	1.600473	0.315507	-0.995804
27	1	0	2.011759	-1.245672	-1.220315
28	8	0	1.771533	-0.789847	1.680718
29	1	0	2.021843	-1.682711	2.000442
30	1	0	1.615560	-0.721892	0.469016
31	8	0	2.992215	1.983463	1.112255
32	1	0	2.107548	1.774701	1.456520
33	1	0	3.520062	1.170670	1.163576
34	8	0	3.046697	-2.068012	-1.927740
35	1	0	3.635587	-1.386361	-2.295793
36	1	0	3.553937	-2.486034	-1.196610
37	1	0	-1.977038	4.337707	0.821774
38	8	0	-1.638113	5.128075	0.377906
39	1	0	-1.356791	5.722624	1.079024
40	1	0	-0.012993	2.849876	-0.196291
41	8	0	-0.048934	3.340096	-1.043442
42	1	0	-0.445043	4.191085	-0.795190
43	1	0	-1.798495	1.016615	-2.164930
44	8	0	-1.839606	1.842970	-2.664219
45	1	0	-1.244674	2.428240	-2.167315
46	8	0	2.583335	-3.282691	2.478334
47	1	0	2.955833	-3.357175	3.364469
48	1	0	1.948721	-4.004031	2.398441
49	8	0	4.879771	-0.038328	0.406176
50	1	0	4.843538	0.158331	-0.549901
51	1	0	5.749774	0.251189	0.700911
52	8	0	4.352644	0.377273	-2.309426
53	1	0	4.998914	0.678481	-2.955835
54	1	0	3.636556	1.039564	-2.288318
55	8	0	4.393035	-2.789539	0.314758
56	1	0	4.635560	-1.871394	0.530609
57	1	0	3.847064	-3.098675	1.052644

SCF Done: E(RM062X) = -1677.27466673 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-461.2241	21.0655	24.6894

Zero-point correction= 0.456327 (a.u.)
Thermal correction to Energy= 0.499701
Thermal correction to Enthalpy= 0.500646
Thermal correction to Gibbs Free Energy= 0.378399
Sum of electronic and zero-point Energies= -1676.818340
Sum of electronic and thermal Energies= -1676.774965
Sum of electronic and thermal Enthalpies= -1676.774021
Sum of electronic and thermal Free Energies= -1676.896268

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	313.567	150.819	257.289

==== TS13 in Figure 5 ====

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.144871	0.446620	-0.421247
2	6	0	-1.907772	-0.716241	0.246674
3	6	0	-0.944893	-1.958553	0.692787
4	6	0	-0.724596	1.542213	0.555430
5	8	0	-1.489029	-2.866027	1.315634
6	8	0	-0.472708	0.999506	1.829087
7	8	0	-0.964470	0.511511	-1.605938
8	8	0	-2.995675	-0.536030	0.723253
9	1	0	0.160097	2.030562	0.129108
10	6	0	-1.824888	2.594508	0.699299
11	6	0	-2.444739	3.013830	-0.625356

12	1	0	-2.609604	2.173712	1.341187
13	8	0	-1.229748	3.712710	1.332697
14	1	0	-1.866984	4.434684	1.263709
15	8	0	-3.306676	4.100462	-0.311998
16	1	0	-3.010004	2.185312	-1.064486
17	1	0	-1.661130	3.326827	-1.324661
18	1	0	-3.588576	4.525530	-1.126345
19	8	0	0.233789	-1.695077	0.435419
20	1	0	5.000412	2.080281	2.302319
21	1	0	1.620754	-2.385138	1.371998
22	8	0	4.153942	2.285170	1.887849
23	1	0	3.830793	3.073540	2.339866
24	1	0	0.442363	0.669369	1.848202
25	8	0	2.207119	0.276576	1.602163
26	1	0	2.904465	0.879417	1.917174
27	1	0	2.224579	0.271196	0.097832
28	8	0	2.440680	-2.338923	1.899887
29	1	0	3.123538	-2.767479	1.360902
30	1	0	2.430755	-0.653779	1.862434
31	8	0	-2.183241	-2.036257	-1.424497
32	1	0	-2.854489	-2.617825	-1.003318
33	8	0	-3.944165	-3.435862	0.301756
34	8	0	2.347524	0.350800	-0.920424
35	1	0	2.910726	1.159128	-1.049703
36	1	0	2.911625	-0.491660	-1.273339
37	1	0	-4.147038	-4.376037	0.295846
38	1	0	-3.177121	-3.312414	0.896492
39	1	0	-3.094699	-0.630240	-2.341338
40	8	0	-3.571615	0.066701	-2.820831
41	1	0	-2.871073	0.667717	-3.090135
42	1	0	-5.125941	-0.530253	0.160362
43	8	0	-5.730658	-1.259532	-0.006544
44	1	0	-5.175317	-2.043002	0.133911
45	8	0	4.322216	-3.490171	0.069535
46	1	0	5.242182	-3.537784	0.353843
47	1	0	4.091996	-4.383354	-0.210929
48	8	0	5.775730	0.319678	-2.039497
49	1	0	5.376553	1.142285	-1.711450
50	1	0	6.216301	0.543453	-2.864268
51	8	0	4.123339	2.320701	-0.896493
52	1	0	3.997006	3.185613	-1.301814
53	1	0	4.233732	2.468614	0.063203
54	8	0	3.764249	-1.466074	-1.766699
55	1	0	4.601899	-0.986680	-1.947501
56	1	0	3.967919	-2.194756	-1.149493

SCF Done: E(UM062X) = -1676.54314430 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-1357.1148	11.6293	16.5135

Zero-point correction= 0.440162 (a.u.)
Thermal correction to Energy= 0.485530
Thermal correction to Enthalpy= 0.486475
Thermal correction to Gibbs Free Energy= 0.356668
Sum of electronic and zero-point Energies= -1676.102982
Sum of electronic and thermal Energies= -1676.057614
Sum of electronic and thermal Enthalpies= -1676.056670
Sum of electronic and thermal Free Energies= -1676.186477

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	304.675	154.485	273.202

==== the neutralizationTS, TS14, in Figure 6 ====
dkg03yy.higha.txt

Stoichiometry C6H31O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.369410	-0.443774	-0.111095
2	6	0	-2.287401	-0.586348	1.321827

3	6	0	-2.429464	0.929881	-0.732727
4	8	0	-1.195983	1.643986	-0.513571
5	8	0	-2.398098	-1.495733	-0.873613
6	8	0	-2.209709	0.362409	2.114360
7	1	0	-2.551664	0.796567	-1.815267
8	6	0	-3.596242	1.782452	-0.240386
9	6	0	-4.932990	1.217480	-0.677274
10	1	0	-3.564079	1.851103	0.850820
11	8	0	-3.389294	3.070548	-0.808964
12	1	0	-4.144807	3.619067	-0.566775
13	8	0	-5.910318	2.147451	-0.229526
14	1	0	-5.090507	0.230591	-0.229472
15	1	0	-4.954873	1.127209	-1.768833
16	1	0	-6.753701	1.941600	-0.641620
17	1	0	-1.715294	-1.408311	-1.970871
18	8	0	-1.003328	-1.386814	-2.836748
19	1	0	-0.796955	-0.444816	-3.067566
20	1	0	-0.105113	-1.791833	-2.500219
21	1	0	-1.417115	2.586651	-0.455585
22	8	0	1.142015	-2.312955	-1.943834
23	1	0	1.921355	-1.716866	-2.006887
24	1	0	1.030466	-2.443946	-0.979811
25	8	0	-2.263463	-1.862232	1.737940
26	1	0	-2.162767	-1.862582	2.713741
27	8	0	-1.945013	-1.210077	4.378899
28	8	0	1.055350	-2.312604	0.816331
29	1	0	0.793524	-1.396843	1.015354
30	1	0	2.004773	-2.369893	1.049309
31	1	0	-2.117616	-0.335639	3.996071
32	1	0	-2.554063	-1.314133	5.115775
33	1	0	-1.693791	-3.187878	-0.223884
34	8	0	-1.081876	-3.937680	-0.157987
35	1	0	-0.361417	-3.572832	0.374732
36	8	0	3.768928	-2.155127	1.314451
37	1	0	4.307100	-2.489758	0.580494
38	1	0	3.791352	-1.187426	1.224449
39	8	0	3.374380	-0.759175	-1.808835
40	1	0	3.329531	-0.225583	-0.996033
41	1	0	4.093768	-1.392559	-1.658648
42	8	0	-0.367362	1.175429	-3.136958
43	1	0	-0.384350	1.515722	-2.226374
44	1	0	0.491213	1.408382	-3.503478
45	8	0	3.245666	0.526417	0.703411
46	1	0	3.729673	1.334948	0.904061
47	1	0	2.323341	0.662458	0.995450
48	8	0	0.572996	0.468887	1.296399
49	1	0	-0.010469	0.905991	0.646354
50	1	0	0.106249	0.575862	2.134527
51	8	0	5.208497	-2.819117	-1.072421
52	1	0	5.035710	-3.667917	-1.494394
53	1	0	6.165591	-2.711084	-1.089352
54	8	0	4.978822	2.952613	1.219758
55	6	0	5.551348	3.838144	0.743358
56	8	0	6.122778	4.720864	0.272373

SCF Done: E(UM062X) = -1676.67702472 A.U. after 19 cycles

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman

	1	2	3
	A	A	A
Frequencies --	-89.8095	10.6229	13.3651

Zero-point correction= 0.444668 (a.u.)
Thermal correction to Energy= 0.489046
Thermal correction to Enthalpy= 0.489990
Thermal correction to Gibbs Free Energy= 0.360403
Sum of electronic and zero-point Energies= -1676.232357
Sum of electronic and thermal Energies= -1676.187979
Sum of electronic and thermal Enthalpies= -1676.187035
Sum of electronic and thermal Free Energies= -1676.316622

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	306.881	150.769	272.739

==== the hydrogen abstraction TS, TS15, in Figure 6 ====
habst2qr.high.txt

Stoichiometry C9H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.668342	0.566578	-0.067046
2	6	0	-0.522082	1.179078	0.605998
3	6	0	2.020652	0.680449	0.632438
4	8	0	2.060514	0.048140	1.896768
5	8	0	0.703625	0.797300	-1.425651
6	8	0	-0.828311	0.870914	1.740421
7	1	0	2.763231	0.220380	-0.039925
8	6	0	2.435547	2.135034	0.856455
9	6	0	2.352378	3.000023	-0.392756
10	1	0	1.783437	2.556963	1.632667
11	8	0	3.778490	2.121637	1.326086
12	1	0	4.112920	3.024260	1.239417
13	8	0	2.941776	4.241807	-0.024522
14	1	0	1.312477	3.132884	-0.700763
15	1	0	2.915294	2.534059	-1.209981
16	1	0	3.083088	4.771719	-0.813593
17	1	0	1.511717	-0.752537	1.900490
18	8	0	-1.197689	2.015529	-0.154423
19	1	0	-2.095222	2.210500	0.274262
20	1	0	0.335270	-0.777724	0.055144
21	6	0	0.211495	-2.102840	0.252044
22	6	0	-1.139543	-2.564317	-0.305653
23	6	0	1.448432	-2.502534	-0.464564
24	8	0	0.310260	-2.242239	1.623207
25	1	0	-0.597857	-2.150930	1.959949
26	8	0	-2.111428	-2.343394	0.694853
27	1	0	-2.601279	-1.507211	0.558102
28	6	0	-1.539711	-1.940491	-1.638315
29	1	0	-1.076791	-3.649688	-0.455711
30	8	0	1.481986	-2.638334	-1.678350
31	8	0	2.508510	-2.553266	0.315168
32	1	0	3.354450	-2.485498	-0.226482
33	8	0	-1.793664	-0.547230	-1.502150
34	1	0	1.513663	0.414761	-1.828391
35	8	0	2.868156	-0.456889	-2.588266
36	1	0	2.462416	-1.331781	-2.709938
37	1	0	3.100522	-0.129016	-3.464332
38	8	0	-3.563434	2.306566	0.816212
39	1	0	-4.155143	2.612230	0.108264
40	1	0	-3.795915	1.366972	0.964548
41	8	0	-4.087312	-0.398143	0.748242
42	1	0	-4.774447	-0.846880	1.273648
43	1	0	-4.421247	-0.308346	-0.166856
44	1	0	-1.009140	-0.035027	-1.751775
45	1	0	-0.771912	-2.134329	-2.387539
46	1	0	-2.474414	-2.408158	-1.956420
47	8	0	4.700636	-1.837555	-0.858930
48	1	0	4.384336	-1.224034	-1.539862
49	1	0	4.941332	-1.281523	-0.088436
50	8	0	4.864821	-0.444019	1.499285
51	1	0	4.782802	0.519039	1.400354
52	1	0	4.001334	-0.669681	1.877268
53	8	0	-4.432434	0.204977	-1.887408
54	1	0	-4.614151	1.156552	-1.914389
55	1	0	-3.466811	0.102561	-1.946688
56	8	0	-5.093169	2.964950	-1.485112
57	1	0	-4.740317	3.672023	-2.036192
58	1	0	-6.036710	3.144086	-1.407906
59	8	0	-6.009453	-1.682613	2.304566
60	1	0	-5.874770	-2.610566	2.520442
61	1	0	-6.280261	-1.267044	3.129060

SCF Done: E(UM062X) = -1792.11140148 A.U. after 2 cycles

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman

		1			2			3		
		A			A			A		
Frequencies --		-1574.1536			22.3428			27.1441		
Red. masses --		1.2107			5.4748			5.0437		
Frc consts --		1.7676			0.0016			0.0022		
IR Inten --		996.1822			2.5819			4.9216		
Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	-0.02	-0.09	0.01	0.01	-0.01	0.02	-0.01	0.01	-0.01
2	6	0.00	0.01	0.01	0.01	-0.02	0.04	-0.01	0.01	-0.01
3	6	0.00	0.01	0.00	0.02	0.01	-0.01	-0.01	0.01	-0.01
4	8	0.00	0.00	0.00	0.05	0.02	-0.01	-0.02	0.03	0.00
5	8	0.00	0.01	-0.01	-0.02	-0.01	0.01	-0.01	0.00	-0.01
6	8	0.00	0.00	0.00	0.04	-0.02	0.04	-0.01	0.02	-0.01
7	1	-0.01	0.00	0.00	0.01	0.02	-0.03	-0.02	-0.01	0.00
8	6	0.00	0.00	0.00	0.01	0.02	-0.03	0.00	0.01	-0.03
9	6	0.00	0.00	0.00	-0.03	0.01	-0.03	0.00	-0.01	-0.05
10	1	0.00	0.00	0.00	0.03	0.01	-0.01	0.00	0.03	-0.04
11	8	0.00	0.00	0.00	0.02	0.03	-0.07	0.00	0.01	-0.04
12	1	0.00	0.00	0.00	0.01	0.04	-0.07	0.01	0.00	-0.05
13	8	0.00	0.00	0.00	-0.04	0.02	-0.05	0.02	-0.01	-0.07
14	1	0.00	0.00	0.00	-0.04	-0.01	-0.01	0.00	0.00	-0.05
15	1	0.00	0.00	0.00	-0.05	0.02	-0.04	-0.01	-0.03	-0.04
16	1	0.00	0.00	0.00	-0.06	0.02	-0.06	0.02	-0.02	-0.08
17	1	0.01	0.00	0.00	0.06	0.02	0.01	-0.03	0.03	0.01
18	8	0.00	0.00	0.00	-0.01	-0.02	0.05	-0.01	0.01	-0.01
19	1	0.00	0.01	0.00	0.00	-0.03	0.07	-0.01	0.02	0.00
20	1	0.23	0.96	-0.02	0.02	-0.01	0.03	-0.02	0.01	0.00
21	6	0.01	-0.08	0.02	0.02	-0.01	0.05	-0.03	0.01	0.02
22	6	0.00	0.01	0.00	0.01	-0.02	0.09	-0.03	0.02	0.02
23	6	-0.01	0.02	0.01	0.01	-0.01	0.02	-0.03	-0.01	0.04
24	8	0.00	0.01	-0.02	0.06	0.01	0.05	-0.04	0.04	0.03
25	1	-0.01	-0.01	-0.01	0.06	0.03	0.07	-0.04	0.05	0.02
26	8	0.00	0.00	0.00	0.03	0.00	0.11	-0.03	0.04	0.01
27	1	0.00	0.00	0.00	0.00	-0.02	0.08	-0.02	0.05	-0.01
28	6	0.00	0.00	0.00	-0.02	-0.04	0.08	-0.01	0.00	0.01
29	1	0.01	0.01	0.00	0.01	-0.02	0.11	-0.04	0.01	0.03
30	8	0.00	0.00	0.00	-0.02	-0.02	0.02	-0.02	-0.03	0.04
31	8	0.00	0.00	0.00	0.03	0.01	0.00	-0.03	-0.01	0.05
32	1	0.00	0.01	0.00	0.01	0.01	-0.02	-0.03	-0.02	0.05
33	8	0.00	0.00	0.00	0.01	-0.04	0.05	-0.01	0.00	-0.01
34	1	-0.02	-0.01	0.00	-0.03	-0.01	0.00	-0.02	-0.02	-0.01
35	8	0.00	0.00	0.00	-0.05	-0.02	-0.02	-0.02	-0.04	0.02
36	1	0.00	0.00	0.00	-0.05	-0.02	-0.01	-0.02	-0.04	0.03
37	1	0.00	0.00	0.00	-0.07	-0.03	-0.03	-0.01	-0.06	0.01
38	8	0.00	0.00	0.00	0.00	-0.04	0.09	0.00	0.05	0.03
39	1	0.00	0.00	0.00	0.01	-0.01	0.09	0.01	0.07	0.04
40	1	0.00	0.00	0.00	-0.01	-0.04	0.06	-0.01	0.05	0.03
41	8	0.00	0.00	0.00	-0.01	-0.04	-0.02	0.00	0.05	-0.01
42	1	0.00	0.00	0.00	-0.07	-0.04	-0.09	0.04	-0.06	-0.04
43	1	0.00	0.00	0.00	0.05	0.02	-0.04	0.00	0.07	-0.01
44	1	0.01	0.00	0.01	0.02	-0.06	0.04	0.00	0.00	-0.01
45	1	0.00	0.00	0.00	-0.05	-0.08	0.06	-0.01	-0.01	0.02
46	1	0.00	0.00	0.00	-0.04	-0.04	0.12	-0.01	0.00	0.00
47	8	0.00	0.00	0.00	0.00	0.01	-0.05	-0.03	-0.04	0.04
48	1	0.00	0.00	0.00	-0.02	0.00	-0.05	-0.02	-0.04	0.03
49	1	0.00	0.00	0.00	0.01	0.02	-0.07	-0.03	-0.02	0.03
50	8	0.00	0.00	0.00	0.05	0.04	-0.08	-0.02	0.00	0.02
51	1	0.00	0.00	0.00	0.04	0.04	-0.08	-0.01	0.00	0.00
52	1	0.00	0.00	0.00	0.06	0.04	-0.05	-0.03	0.02	0.02
53	8	0.00	0.00	0.00	0.06	0.07	0.00	0.02	0.11	0.00
54	1	0.00	0.00	0.00	0.08	0.08	0.02	0.05	0.12	0.01
55	1	0.00	0.00	0.00	0.05	0.04	0.00	0.01	0.08	0.00
56	8	0.00	0.00	0.00	0.08	0.07	0.07	0.06	0.13	0.02
57	1	0.00	0.00	0.00	0.11	0.08	0.11	0.09	0.13	0.04
58	1	0.00	0.00	0.00	0.08	0.07	0.04	0.06	0.14	-0.01
59	8	0.00	0.00	0.00	-0.28	-0.03	-0.32	0.22	-0.37	-0.08
60	1	0.00	0.00	0.00	-0.34	-0.04	-0.35	0.37	-0.37	-0.17
61	1	0.00	0.00	0.00	-0.34	-0.05	-0.33	0.20	-0.48	-0.03

Zero-point correction= 0.492003 (a.u.)
Thermal correction to Energy= 0.534877
Thermal correction to Enthalpy= 0.535821
Thermal correction to Gibbs Free Energy= 0.416109
Sum of electronic and zero-point Energies= -1791.619399
Sum of electronic and thermal Energies= -1791.576524
Sum of electronic and thermal Enthalpies= -1791.575580
Sum of electronic and thermal Free Energies= -1791.695293

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	335.641	152.344	251.957

==== TS16 in Figure 7 ====
dkgr6b.high.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.677045	-0.486582	-0.097042
2	6	0	1.564701	-1.848876	-0.825308
3	6	0	0.273510	-2.698630	-0.729139
4	6	0	2.389012	0.617137	-0.876761
5	8	0	-0.003783	-3.479798	-1.599881
6	8	0	1.884986	0.605259	-2.201868
7	8	0	1.829033	-0.549847	1.150242
8	8	0	2.512169	-2.283131	-1.416945
9	1	0	2.115121	1.560678	-0.386937
10	6	0	3.924348	0.500011	-0.896300
11	6	0	4.574378	0.839924	0.441034
12	1	0	4.214976	-0.500219	-1.220006
13	8	0	4.392572	1.408970	-1.887307
14	1	0	4.448970	2.274389	-1.456786
15	8	0	4.409059	2.222290	0.723768
16	1	0	5.646378	0.652214	0.357224
17	1	0	4.169080	0.213923	1.238903
18	1	0	3.591502	2.332121	1.236599
19	8	0	-0.416264	-2.452028	0.356177
20	1	0	-1.385337	-2.777895	0.293074
21	8	0	0.025103	0.172830	-0.374483
22	8	0	-0.550786	-0.299140	-1.579354
23	1	0	-0.668749	-0.073013	0.556963
24	1	0	0.003936	0.169128	-2.232889
25	1	0	2.527458	1.074644	-2.751156
26	8	0	-1.253326	-0.123167	1.638667
27	1	0	-0.762688	-0.774919	2.215057
28	1	0	-1.112002	0.795324	2.033974
29	8	0	-0.811156	2.328646	2.304808
30	1	0	0.131787	2.471131	2.119047
31	1	0	-1.336479	2.655397	1.552812
32	8	0	0.296439	-1.722849	3.075648
33	1	0	0.068272	-2.653587	2.985313
34	1	0	0.996192	-1.562918	2.413288
35	8	0	-2.739174	2.245788	0.397657
36	1	0	-3.335693	2.781211	-0.146699
37	1	0	-2.885404	1.328275	0.112934
38	8	0	-3.213457	-0.313016	-0.829029
39	1	0	-2.425501	-0.251144	-1.390872
40	1	0	-3.966168	0.028245	-1.354381
41	8	0	-4.638341	3.591673	-1.285020
42	1	0	-5.307379	4.110545	-0.824899
43	1	0	-4.291967	4.170287	-1.973490
44	8	0	-5.233816	0.971594	-2.148925
45	1	0	-6.160417	0.731125	-2.061974
46	1	0	-5.168752	1.905676	-1.887983
47	8	0	-2.920117	-2.860681	0.206907
48	1	0	-3.290649	-2.653460	1.083185
49	1	0	-3.143366	-2.050161	-0.295609
50	8	0	-3.777498	-1.281881	2.320581
51	1	0	-4.608928	-0.837561	2.130323
52	1	0	-3.082512	-0.683479	2.004290
53	8	0	2.011799	1.949867	2.203754
54	1	0	2.227739	1.976822	3.142548
55	1	0	1.945097	0.998260	1.966050

SCF Done: E(RM062X) = -1675.93813608 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-662.6299	18.8622	28.5100

Zero-point correction= 0.436430 (a.u.)
Thermal correction to Energy= 0.477183
Thermal correction to Enthalpy= 0.478127
Thermal correction to Gibbs Free Energy= 0.364094
Sum of electronic and zero-point Energies= -1675.501706
Sum of electronic and thermal Energies= -1675.460953
Sum of electronic and thermal Enthalpies= -1675.460009
Sum of electronic and thermal Free Energies= -1675.574042

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.437	144.695	240.002

==== TS17 in Figure 7 ===
dkgr7b.high.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.939585	-0.613828	0.426867
2	6	0	-0.597940	-0.101259	-1.211027
3	6	0	-0.798422	1.436177	-1.180916
4	6	0	-1.786157	-1.911891	0.419909
5	8	0	-2.018167	1.764095	-1.479976
6	8	0	-1.016597	-2.993501	-0.094024
7	8	0	-1.463564	0.367125	1.128763
8	8	0	-0.899138	-0.749633	-2.191731
9	1	0	-2.008800	-2.100782	1.477774
10	6	0	-3.119248	-1.838983	-0.333099
11	6	0	-3.968427	-0.629049	0.024220
12	1	0	-2.923910	-1.840807	-1.406750
13	8	0	-3.800457	-3.066019	-0.061652
14	1	0	-4.143307	-3.014345	0.839505
15	8	0	-4.053607	-0.436679	1.426736
16	1	0	-4.978723	-0.798834	-0.354676
17	1	0	-3.553743	0.257098	-0.461321
18	1	0	-3.185269	-0.053049	1.658312
19	8	0	0.116174	2.206294	-0.970124
20	1	0	-2.162359	2.764643	-1.385325
21	8	0	0.355861	-0.923281	0.633373
22	8	0	1.058047	-0.240970	-0.858042
23	1	0	1.154163	0.405476	1.605647
24	1	0	1.289545	-1.122393	-1.273283
25	1	0	-1.628324	-3.732655	-0.219711
26	8	0	1.755072	0.998779	2.092005
27	1	0	1.136848	1.654113	2.472260
28	1	0	2.812898	-0.731179	2.050849
29	8	0	3.225301	-1.404496	1.489189
30	1	0	2.566800	-2.117339	1.351551
31	1	0	3.739248	-0.763001	0.254294
32	8	0	-0.503566	2.510036	2.465038
33	1	0	-0.468915	3.284157	1.884963
34	1	0	-0.889365	1.781604	1.925908
35	8	0	4.045301	-0.211128	-0.563390
36	1	0	5.039082	-0.116752	-0.579292
37	1	0	3.559082	0.729866	-0.492668
38	8	0	2.838992	1.919544	-0.226882
39	1	0	1.998353	1.860608	-0.716262
40	1	0	2.547250	1.776850	0.701569
41	8	0	6.642109	0.055335	-0.665231
42	1	0	7.126885	0.217336	0.150727
43	1	0	7.149429	-0.604053	-1.150010
44	8	0	-2.385402	4.290791	-1.144423
45	1	0	-3.248474	4.539691	-0.798536
46	1	0	-1.719013	4.616918	-0.509353
47	8	0	1.338972	-2.695640	-1.782761
48	1	0	0.382198	-2.832278	-1.700183
49	1	0	1.703573	-3.190365	-1.031800
50	8	0	1.565803	-3.518042	0.901082
51	1	0	1.637253	-4.365963	1.350271
52	1	0	0.614862	-3.335498	0.785105
53	8	0	-0.173283	4.570552	0.439718
54	1	0	0.428125	5.316448	0.530748

55	1	0	0.260462	3.922186	-0.137392

SCF Done: E(RM062X) = -1675.87643484 A.U. after 1 cycles

1	2	3
A	A	A
-1268.1741	25.8373	34.9900

Frequencies --

Zero-point correction= 0.436853 (a.u.)
Thermal correction to Energy= 0.476847
Thermal correction to Enthalpy= 0.477791
Thermal correction to Gibbs Free Energy= 0.366244
Sum of electronic and zero-point Energies= -1675.439582
Sum of electronic and thermal Energies= -1675.399588
Sum of electronic and thermal Enthalpies= -1675.398644
Sum of electronic and thermal Free Energies= -1675.510191

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	299.226	142.644	234.770

==== TS18 in Figure 7 by B3LYP / 6-311+G** SCRF=PCM ====

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.102794	0.106671	-0.776808
2	6	0	-1.107461	0.934402	-1.289533
3	6	0	-2.481566	0.674049	-0.633524
4	6	0	1.418066	0.929699	-0.682826
5	8	0	-2.922657	1.465790	0.185055
6	8	0	1.194847	2.184748	-0.006749
7	8	0	0.202556	-0.978874	-1.588021
8	8	0	-1.046896	1.737696	-2.187761
9	1	0	2.113003	0.333587	-0.080991
10	6	0	2.085025	1.259915	-2.052514
11	6	0	2.792925	0.112981	-2.769798
12	1	0	1.337122	1.690110	-2.718556
13	8	0	3.036208	2.316255	-1.808680
14	1	0	3.841323	1.903444	-1.462872
15	8	0	3.846914	-0.439057	-1.976145
16	1	0	3.254195	0.527076	-3.669366
17	1	0	2.075998	-0.650296	-3.069370
18	1	0	3.465239	-1.166407	-1.456581
19	8	0	-3.101269	-0.378237	-1.103270
20	1	0	-4.037964	-0.500062	-0.713097
21	8	0	-0.274606	-0.487885	0.507148
22	8	0	-0.176174	0.431640	1.636263
23	1	0	-1.483088	-4.353505	1.484124
24	1	0	0.380857	-0.120213	2.228695
25	1	0	1.828491	2.798555	-0.422545
26	8	0	-0.798901	-4.384215	0.805959
27	1	0	-1.168542	-3.925041	0.009781
28	1	0	0.613626	-3.731872	1.192009
29	8	0	1.533098	-3.320958	1.276328
30	1	0	1.801813	-2.899645	0.261703
31	1	0	1.505594	-2.599797	1.965613
32	8	0	-1.579453	-3.072461	-1.442093
33	1	0	-2.474660	-2.714460	-1.450113
34	1	0	-1.002666	-2.274131	-1.507148
35	8	0	1.424124	-1.359041	3.094369
36	1	0	2.268363	-0.866635	3.284657
37	1	0	1.072906	-1.642768	3.947560
38	1	0	-1.859551	3.048420	0.798366
39	8	0	-1.149942	3.690230	0.954846
40	1	0	-0.355231	3.205256	0.680876
41	8	0	3.532915	0.206202	3.531357
42	1	0	4.377623	0.035889	3.100104
43	1	0	3.201934	1.062713	3.173474
44	8	0	-5.458033	1.364257	1.497155
45	1	0	-4.582984	1.600889	1.140354
46	1	0	-6.013180	2.144390	1.385301
47	8	0	-5.508890	-0.734947	-0.210877
48	1	0	-5.682511	-1.588532	0.203085

49	1	0	-5.695979	-0.044395	0.467068
50	1	0	1.768344	2.902967	3.167150
51	8	0	2.374245	2.477575	2.549893
52	1	0	1.850643	2.302712	1.741692
53	8	0	2.048851	-2.426261	-0.921978
54	1	0	2.137139	-3.153947	-1.551428
55	1	0	1.187941	-1.770270	-1.241912

SCF Done: E(RB3LYP) = -1676.63028802 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-689.0076	17.9928	23.7032

Zero-point correction= 0.426567 (a.u.)
Thermal correction to Energy= 0.467817
Thermal correction to Enthalpy= 0.468761
Thermal correction to Gibbs Free Energy= 0.351017
Sum of electronic and zero-point Energies= -1676.203721
Sum of electronic and thermal Energies= -1676.162471
Sum of electronic and thermal Enthalpies= -1676.161527
Sum of electronic and thermal Free Energies= -1676.279271

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	293.559	143.978	247.813

==== TS19 in Figure 7 ====
dkgr14b.high.txt

Stoichiometry C6H30O19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.627781	-0.913904	-0.461930
2	6	0	-0.471812	-2.184138	-0.014791
3	6	0	-1.860827	-1.474637	0.005618
4	6	0	2.071619	-1.271459	-0.072128
5	8	0	-2.453033	-1.167919	-0.999802
6	8	0	2.357139	-2.455138	-0.802022
7	8	0	0.113629	0.268517	0.039479
8	8	0	-0.191774	-3.036742	0.798981
9	1	0	2.722267	-0.466778	-0.428697
10	6	0	2.372332	-1.477617	1.415994
11	6	0	2.078738	-0.272550	2.283322
12	1	0	1.809077	-2.334074	1.787462
13	8	0	3.747383	-1.849460	1.495413
14	1	0	4.277406	-1.051458	1.372705
15	8	0	2.762765	0.866618	1.771732
16	1	0	2.420143	-0.493937	3.299942
17	1	0	1.002086	-0.091793	2.307800
18	1	0	2.223244	1.641812	2.031883
19	8	0	-2.268685	-1.285726	1.230488
20	1	0	-3.191349	-0.792241	1.221825
21	8	0	0.406185	-1.118692	-1.757757
22	8	0	-0.360565	-2.694107	-1.544566
23	1	0	-1.796264	1.305088	0.015483
24	1	0	0.509724	-3.144128	-1.556548
25	1	0	3.147967	-2.848810	-0.410556
26	8	0	-2.336047	1.847766	0.608403
27	1	0	-2.001195	1.616253	1.494678
28	1	0	-1.382950	3.494450	0.402746
29	8	0	-0.622997	4.096643	0.444145
30	1	0	0.411283	3.207980	1.650893
31	1	0	-0.263174	4.109292	-0.458242
32	8	0	-1.287754	0.792679	2.974482
33	1	0	-1.715711	0.825444	3.837056
34	1	0	-1.358120	-0.124023	2.670609
35	8	0	0.626557	3.759889	-2.050736
36	1	0	1.391358	3.335278	-1.619668
37	1	0	0.966978	4.489200	-2.578165
38	1	0	-0.589562	0.780168	-2.772467
39	8	0	0.032774	1.283654	-3.308588
40	1	0	0.060311	2.179321	-2.929555

41	8	0	2.158942	1.900734	-0.830371
42	1	0	2.711962	1.737537	-0.050659
43	1	0	2.520175	1.351346	-1.557706
44	8	0	-5.277362	-0.872449	-1.256351
45	1	0	-4.364650	-1.130064	-1.452863
46	1	0	-5.821662	-1.642463	-1.445211
47	8	0	-4.395478	0.044259	1.146004
48	1	0	-4.001109	0.891735	0.874446
49	1	0	-4.920338	-0.262524	0.377685
50	1	0	1.671340	0.474136	-3.251081
51	8	0	2.577809	0.247951	-2.963695
52	1	0	2.585867	-0.709523	-2.850382
53	8	0	0.815028	2.643777	2.339509
54	1	0	0.110021	2.042960	2.625355
55	1	0	0.721767	0.997605	-0.223255

SCF Done: E(RM062X) = -1675.88948898 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-1151.1374	22.5711	38.2723

Zero-point correction= 0.439466 (a.u.)
Thermal correction to Energy= 0.480089
Thermal correction to Enthalpy= 0.481033
Thermal correction to Gibbs Free Energy= 0.369098
Sum of electronic and zero-point Energies= -1675.450023
Sum of electronic and thermal Energies= -1675.409400
Sum of electronic and thermal Enthalpies= -1675.408456
Sum of electronic and thermal Free Energies= -1675.520391

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	301.260	145.644	235.587

==== TS20 in Figure 8 ====
dkgr17b.high.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.670693	0.387585	-0.829818
2	6	0	-0.536777	-0.046269	0.076452
3	6	0	-1.029262	-1.452276	-0.384573
4	6	0	1.384907	1.666119	-0.364719
5	8	0	-1.563043	-2.156120	0.591259
6	8	0	2.235828	1.315480	0.726581
7	8	0	0.350455	0.568216	-2.159645
8	8	0	-0.384924	0.127036	1.336424
9	1	0	2.020448	1.967053	-1.208646
10	6	0	0.487116	2.845559	0.036786
11	6	0	-0.179981	3.529051	-1.151706
12	1	0	-0.261091	2.501690	0.749423
13	8	0	1.303117	3.788279	0.725043
14	1	0	1.759542	4.310072	0.049683
15	8	0	0.797569	4.218761	-1.926637
16	1	0	-0.869918	4.283399	-0.770361
17	1	0	-0.733971	2.814696	-1.759066
18	1	0	1.104188	3.645973	-2.635526
19	8	0	-0.968532	-1.822826	-1.539212
20	1	0	-1.929603	-2.985268	0.209348
21	8	0	1.672544	-0.663021	-0.821763
22	8	0	1.634809	-1.426075	0.382851
23	1	0	1.593197	-0.752894	1.094046
24	1	0	2.285935	2.094822	1.300831
25	1	0	-0.160509	-0.204619	-2.457670
26	1	0	3.236502	-2.129382	0.145956
27	8	0	4.176918	-2.080254	-0.140303
28	1	0	4.430362	-1.041145	-0.134706
29	1	0	4.777160	-2.645030	0.456231
30	8	0	4.617345	0.327192	-0.068336
31	1	0	4.897126	0.736630	-0.894531

32	1	0	3.779539	0.766003	0.212323
33	8	0	5.744570	-3.474024	1.290104
34	1	0	5.552388	-3.583420	2.227861
35	1	0	5.982266	-4.346270	0.957120
36	8	0	-1.699531	0.863009	-0.443183
37	1	0	-2.645716	0.588370	0.165382
38	1	0	-1.925849	0.723013	-1.407022
39	8	0	-3.651627	0.168893	0.783850
40	1	0	-3.972533	-0.595412	0.267691
41	1	0	-3.322836	-0.143253	1.690733
42	8	0	-4.105104	-1.609938	-1.306389
43	1	0	-3.742706	-2.515129	-1.279818
44	1	0	-5.027400	-1.703732	-1.570200
45	8	0	-2.447783	-0.481421	2.945489
46	1	0	-1.593712	-0.348377	2.465972
47	1	0	-2.478845	0.177697	3.660112
48	8	0	-2.668620	-3.993637	-1.068785
49	1	0	-2.991698	-4.900317	-1.028729
50	1	0	-2.003515	-3.955067	-1.768450
51	8	0	-2.560414	1.416688	5.010120
52	1	0	-3.366985	1.925019	5.138681
53	1	0	-2.269985	1.171996	5.894052
54	8	0	-2.563228	0.196182	-2.841001
55	1	0	-3.102584	0.812061	-3.347367
56	1	0	-3.162175	-0.507156	-2.529613

SCF Done: E(RM062X) = -1676.36398187 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-450.5361	19.4762	25.3868

Zero-point correction= 0.448731 (a.u.)
Thermal correction to Energy= 0.489079
Thermal correction to Enthalpy= 0.490023
Thermal correction to Gibbs Free Energy= 0.375395
Sum of electronic and zero-point Energies= -1675.915250
Sum of electronic and thermal Energies= -1675.874903
Sum of electronic and thermal Enthalpies= -1675.873959
Sum of electronic and thermal Free Energies= -1675.988586

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	306.902	142.704	241.255

==== TS21 in Figure 8 ====
dkgr16b.high.txt

Stoichiometry C6H31O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.207176	-0.369963	-0.886284
2	6	0	0.308341	-0.205487	0.014877
3	6	0	1.175108	0.755249	-0.899702
4	6	0	-2.155253	-1.393285	-0.179719
5	8	0	1.971911	1.471042	-0.150731
6	8	0	-2.697052	-0.783719	0.969308
7	8	0	-0.907914	-0.905639	-2.140338
8	8	0	0.050060	0.257850	1.193131
9	1	0	-2.951274	-1.543435	-0.921551
10	6	0	-1.604545	-2.782887	0.178399
11	6	0	-1.073719	-3.587599	-1.001139
12	1	0	-0.841723	-2.698392	0.951628
13	8	0	-2.702086	-3.471023	0.781549
14	1	0	-3.295691	-3.752652	0.072593
15	8	0	-2.024601	-3.641068	-2.055801
16	1	0	-0.918916	-4.612296	-0.658041
17	1	0	-0.125748	-3.186398	-1.353954
18	1	0	-1.924845	-2.825975	-2.562856
19	8	0	1.190866	0.733937	-2.109814
20	1	0	2.578184	2.022552	-0.712751
21	8	0	-1.806680	0.786994	-0.897042
22	8	0	-0.826577	2.171184	-0.278482

23	1	0	-0.621921	1.787105	0.608579
24	1	0	-3.063183	-1.498614	1.509147
25	1	0	-0.208119	-0.372916	-2.556684
26	1	0	-1.742479	2.779307	-0.228743
27	8	0	-2.920033	3.380855	-0.232807
28	1	0	-3.574730	2.730555	0.118442
29	1	0	-2.987913	4.211720	0.282263
30	8	0	-4.410344	1.405640	0.753838
31	1	0	-5.218636	1.108055	0.326470
32	1	0	-3.820416	0.628741	0.791427
33	8	0	-3.134046	5.711702	1.155004
34	1	0	-2.500821	5.935455	1.844045
35	1	0	-3.288982	6.528047	0.669658
36	8	0	0.913597	-1.437897	0.016048
37	1	0	3.659358	-1.022294	0.004706
38	1	0	1.465863	-1.584231	-0.778409
39	8	0	3.911385	-0.697404	0.883950
40	1	0	4.451081	0.108239	0.729017
41	1	0	2.804630	-0.458946	1.832659
42	8	0	5.399307	1.524154	0.367822
43	1	0	4.983843	2.145635	-0.249760
44	1	0	5.749061	2.054748	1.089512
45	8	0	2.048993	-0.295233	2.524819
46	1	0	1.158741	-0.037495	2.005323
47	1	0	1.885439	-1.135610	3.035312
48	8	0	3.766177	2.925665	-1.487989
49	1	0	3.654135	3.883315	-1.457439
50	1	0	3.917356	2.704895	-2.414916
51	8	0	1.504351	-2.493134	3.850197
52	1	0	1.500629	-3.325151	3.365414
53	1	0	1.937939	-2.677272	4.689933
54	8	0	2.970661	-1.537026	-1.744391
55	1	0	3.357617	-2.343854	-2.103154
56	1	0	2.941173	-0.904030	-2.472648

SCF Done: E(RM062X) = -1676.32616233 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-1028.4998	21.1769	25.6540

Zero-point correction= 0.445677 (a.u.)
Thermal correction to Energy= 0.487279
Thermal correction to Enthalpy= 0.488223
Thermal correction to Gibbs Free Energy= 0.370639
Sum of electronic and zero-point Energies= -1675.880485
Sum of electronic and thermal Energies= -1675.838883
Sum of electronic and thermal Enthalpies= -1675.837939
Sum of electronic and thermal Free Energies= -1675.955523

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	305.772	145.881	247.476

Hereafter, data of TSs in Figures S2 and S4 in the Supporting Information

==== TS-S1 in Figure S2 ====

vitachat1.high.txt

Stoichiometry C6H33O19(2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.383181	-1.055465	-0.334737
2	6	0	3.429221	-1.971021	0.001295

3	6	0	4.706351	-1.377021	-0.462178
4	6	0	3.049469	0.133705	-1.011435
5	8	0	5.814175	-1.829411	-0.371496
6	8	0	4.452182	-0.186693	-1.050667
7	8	0	1.166053	-1.177845	-0.153012
8	1	0	-0.412986	-0.285123	-0.596136
9	8	0	3.385185	-3.107069	0.568940
10	1	0	2.334340	-3.654245	0.845646
11	1	0	2.698513	0.225140	-2.043629
12	6	0	2.876305	1.468391	-0.300161
13	6	0	1.407028	1.859103	-0.154641
14	1	0	3.340140	1.401823	0.693684
15	8	0	3.548368	2.431008	-1.087156
16	1	0	3.229690	3.292817	-0.787899
17	8	0	1.327035	3.237755	0.188019
18	1	0	0.916730	1.244547	0.602614
19	1	0	0.892988	1.730088	-1.112793
20	1	0	1.227140	3.314332	1.156910
21	8	0	-1.312941	0.076545	-0.546148
22	1	0	-2.805295	-0.862093	-0.812971
23	1	0	-1.360609	0.587420	0.293052
24	8	0	-1.594674	1.797495	1.528077
25	1	0	-0.903855	2.036442	2.165059
26	1	0	-1.669705	2.587542	0.963598
27	8	0	-3.675649	-1.274396	-0.979391
28	1	0	-4.010421	-0.817560	-1.770097
29	1	0	-3.299839	-3.011595	-0.592192
30	8	0	-1.330989	3.909483	-0.335219
31	1	0	-0.363222	3.796620	-0.363888
32	1	0	-1.682917	3.458992	-1.123112
33	8	0	0.425719	3.344783	2.757695
34	1	0	-0.171214	4.121139	2.722412
35	1	0	0.890531	3.375075	3.599193
36	8	0	-4.684475	0.845222	-2.564452
37	1	0	-5.134226	1.037350	-1.726988
38	1	0	-3.882849	1.393001	-2.554242
39	8	0	1.409422	-4.309867	1.165881
40	1	0	1.359110	-5.125133	0.653393
41	1	0	-1.386569	6.153921	2.151098
42	8	0	-1.455407	5.196375	2.100492
43	1	0	-1.599611	4.980218	1.163931
44	8	0	-2.102243	2.053266	-2.308489
45	1	0	-1.727442	1.298627	-1.809313
46	1	0	-1.621195	2.093291	-3.141690
47	8	0	-2.837503	-3.801373	-0.258947
48	1	0	-1.480169	-3.298694	0.584064
49	1	0	-3.487277	-4.319380	0.246303
50	8	0	-5.455635	0.597083	0.148232
51	1	0	-6.267936	0.332894	0.588229
52	1	0	-4.920369	-0.208480	0.057021
53	8	0	-0.682136	-2.975775	1.075338
54	1	0	0.495252	-3.812852	1.115106
55	1	0	-0.349913	-2.193156	0.614749
56	8	0	-4.606207	-5.374923	1.230203
57	1	0	-4.886526	-5.076914	2.100945
58	1	0	-5.391856	-5.755518	0.825908

SCF Done: E(UM062X) = -1677.86971787 A.U. after 1 cycles

Harmonic frequencies (cm**-1), IR intensities (KM/Mole),
activities (A**4/AMU), depolarization ratios for plane

	1	2	3
	A	A	A
Frequencies --	-528.7415	13.5030	16.9287

Zero-point correction= 0.465688 (a.u.)
Thermal correction to Energy= 0.510686
Thermal correction to Enthalpy= 0.511630
Thermal correction to Gibbs Free Energy= 0.382280
Sum of electronic and zero-point Energies= -1677.404030
Sum of electronic and thermal Energies= -1677.359032
Sum of electronic and thermal Enthalpies= -1677.358088
Sum of electronic and thermal Free Energies= -1677.487438

	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	320.460	155.125	272.239

==== TS-S2 in Figure S4 ====
trioneh1.high.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.688519	-1.907282	0.194082
2	6	0	-1.180467	-1.848406	0.513844
3	6	0	-0.736912	-0.477386	-0.000155
4	6	0	-3.043102	-0.547096	-0.388671
5	8	0	0.284859	0.121093	0.409848
6	8	0	-1.884662	0.273163	-0.140090
7	8	0	-3.397928	-2.849644	0.373043
8	8	0	-0.515669	-2.679660	1.044326
9	1	0	-3.193067	-0.637108	-1.470137
10	6	0	-4.240333	0.120826	0.265461
11	6	0	-5.544111	-0.595996	-0.048591
12	1	0	-4.089746	0.158029	1.351168
13	8	0	-4.290513	1.444280	-0.251041
14	1	0	-5.183146	1.774524	-0.072154
15	8	0	-6.558343	0.252943	0.469829
16	1	0	-5.563244	-1.579946	0.424559
17	1	0	-5.648926	-0.708437	-1.132885
18	1	0	-7.414146	-0.034369	0.139324
19	8	0	-0.529428	-0.989513	-1.628984
20	1	0	-0.319843	-0.111086	-2.126337
21	1	0	0.292770	-1.565525	-1.701155
22	8	0	0.200469	1.175322	-2.729472
23	1	0	0.051635	1.930758	-2.144888
24	1	0	1.170182	0.994765	-2.696977
25	1	0	0.193086	1.588395	0.141665
26	8	0	0.035116	2.566771	-0.142914
27	1	0	-0.918275	2.850030	0.137271
28	8	0	4.119463	0.506835	-0.121393
29	1	0	3.606491	0.141442	0.628473
30	1	0	4.859580	-0.108131	-0.259096
31	1	0	0.773797	3.208491	0.227721
32	8	0	1.822266	4.050076	0.738796
33	1	0	2.736026	3.794387	0.454393
34	8	0	-2.299518	3.178489	0.541947
35	1	0	-2.618781	4.065773	0.348636
36	1	0	-2.987175	2.552672	0.232374
37	8	0	1.654355	-2.383385	-1.920927
38	1	0	2.254584	-2.597990	-1.155209
39	1	0	1.574565	-3.180101	-2.455685
40	8	0	4.252908	3.236144	0.033813
41	1	0	4.298594	2.261476	-0.045517
42	1	0	4.648086	3.591616	-0.767431
43	8	0	3.303969	-2.781897	0.092991
44	1	0	4.207138	-2.527328	-0.155776
45	1	0	3.047669	-2.164434	0.804477
46	8	0	5.849969	-1.669216	-0.601068
47	1	0	6.616841	-1.864345	-0.051136
48	1	0	6.147408	-1.783583	-1.510481
49	8	0	2.530351	-0.723850	1.747611
50	1	0	1.638336	-0.488565	1.434826
51	1	0	2.541228	-0.648716	2.720150
52	8	0	2.696371	0.203800	-2.523802
53	1	0	2.490640	-0.744182	-2.511001
54	1	0	3.162898	0.368489	-1.683043
55	8	0	2.563939	-0.533093	4.502310
56	1	0	2.704564	-1.332522	5.018972
57	1	0	3.095726	0.145801	4.928973
58	1	0	1.721388	4.992496	0.571512

SCF Done: E(RM062X) = -1677.67981415 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-254.5633	19.5581	20.7633

Zero-point correction= 0.467160 (a.u.)
Thermal correction to Energy= 0.510815
Thermal correction to Enthalpy= 0.511759
Thermal correction to Gibbs Free Energy= 0.387795
Sum of electronic and zero-point Energies= -1677.212654
Sum of electronic and thermal Energies= -1677.169000
Sum of electronic and thermal Enthalpies= -1677.168055
Sum of electronic and thermal Free Energies= -1677.292020

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.541	151.103	260.905

==== TS-S3 in Figure S4 ====
trioneh3.high.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.824479	1.820010	-1.429751
2	6	0	-1.803558	0.631002	-1.379262
3	6	0	-0.924819	-0.629911	-1.319423
4	6	0	0.524413	1.261570	-0.974692
5	8	0	-1.386769	-1.679628	-0.694371
6	8	0	0.221228	-0.063408	-0.518702
7	8	0	-1.075643	2.909967	-1.849357
8	8	0	-2.996707	0.693341	-1.363184
9	1	0	1.187269	1.220566	-1.848516
10	6	0	1.195860	2.053762	0.134435
11	6	0	1.362750	3.527618	-0.212324
12	1	0	0.610105	1.958150	1.052306
13	8	0	2.490736	1.486533	0.367694
14	1	0	3.000454	2.197524	0.793348
15	8	0	2.214369	4.043669	0.802129
16	1	0	0.393656	4.028945	-0.212297
17	1	0	1.825276	3.632557	-1.199325
18	1	0	2.537268	4.910496	0.540612
19	8	0	-0.488832	-0.802591	-2.621823
20	1	0	-0.446013	-4.176143	0.966747
21	1	0	-0.117824	-1.707794	-2.731696
22	8	0	-0.090354	-3.281881	0.985800
23	1	0	-0.652785	-2.728263	0.387593
24	1	0	1.478983	-1.465590	-0.597912
25	8	0	1.930312	-2.332205	-0.563583
26	1	0	1.368185	-2.864515	0.038605
27	1	0	3.346805	-2.083183	0.017113
28	8	0	0.724758	-3.228603	-2.918519
29	1	0	1.177894	-3.435264	-3.741408
30	1	0	1.412107	-3.125644	-2.241757
31	8	0	4.154353	-1.697274	0.499382
32	1	0	4.488117	-0.950749	-0.099569
33	1	0	3.707776	-1.237916	1.339198
34	8	0	4.669305	0.340635	-0.962348
35	1	0	4.824545	0.269164	-1.909669
36	1	0	3.855644	0.857672	-0.839575
37	8	0	2.917568	-0.527031	2.294802
38	1	0	2.547035	0.214241	1.784677
39	1	0	2.164388	-1.033837	2.666801
40	1	0	-0.605670	-0.312152	1.218817
41	8	0	-1.079180	-0.164515	2.057195
42	1	0	-2.735308	-0.604844	1.925769
43	1	0	-0.552595	-0.637645	2.726589
44	8	0	-3.695333	-0.747486	1.727341
45	1	0	-4.082565	0.146026	1.468985
46	1	0	-3.783711	-1.468021	0.828300
47	8	0	0.731122	-1.913846	3.196649
48	1	0	0.751870	-2.354414	4.052132
49	1	0	0.445730	-2.575576	2.533312
50	8	0	-4.504273	1.593953	0.941109
51	1	0	-3.629607	2.030728	0.925773
52	1	0	-4.759462	1.523827	0.014039
53	8	0	-3.768945	-2.159518	-0.208142

54	1	0	-2.800934	-1.987144	-0.542580
55	1	0	-3.882778	-3.102469	-0.045086
56	8	0	-1.850803	2.291444	1.142052
57	1	0	-1.645593	3.155314	1.515838
58	1	0	-1.544571	1.629207	1.785943

SCF Done: E(RM062X) = -1677.68959847 A.U. after 2 cycles

	1	2	3
	A	A	A
Frequencies --	-304.1176	31.1810	35.0589

Zero-point correction= 0.469147 (a.u.)
Thermal correction to Energy= 0.509990
Thermal correction to Enthalpy= 0.510935
Thermal correction to Gibbs Free Energy= 0.397595
Sum of electronic and zero-point Energies= -1677.220452
Sum of electronic and thermal Energies= -1677.179608
Sum of electronic and thermal Enthalpies= -1677.178664
Sum of electronic and thermal Free Energies= -1677.292003

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.024	146.516	238.542

==== An ion pair intermediate with the alkoxide form in Figure S4 ====
trioneh2a.for.high.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.648170	1.196912	-1.450065
2	6	0	-1.644212	0.006341	-1.583993
3	6	0	-1.125940	-1.424014	-1.749119
4	6	0	0.714350	0.818091	-0.883424
5	8	0	-1.654257	-2.339542	-1.146665
6	8	0	0.423321	-0.171845	0.056391
7	8	0	-1.090262	2.301179	-1.615405
8	8	0	-2.823072	0.215805	-1.527677
9	1	0	1.345568	0.423643	-1.694340
10	6	0	1.394356	2.041400	-0.266944
11	6	0	1.869311	3.057630	-1.291338
12	1	0	0.706625	2.525946	0.436516
13	8	0	2.534151	1.567262	0.460895
14	1	0	3.020749	2.359531	0.735670
15	8	0	2.589909	4.032414	-0.545096
16	1	0	1.018141	3.503155	-1.808555
17	1	0	2.525971	2.566297	-2.018404
18	1	0	3.070156	4.605354	-1.149096
19	8	0	-0.145950	-1.500928	-2.589879
20	1	0	-1.062204	-4.112920	1.704179
21	1	0	0.286189	-2.435991	-2.609785
22	8	0	-0.759047	-3.233524	1.453697
23	1	0	-1.282658	-2.976379	0.679087
24	1	0	1.070483	-1.499105	-0.011174
25	8	0	1.485233	-2.450839	0.026282
26	1	0	0.892807	-2.946420	0.620884
27	1	0	2.780874	-2.238799	0.610475
28	8	0	1.073264	-3.689380	-2.375918
29	1	0	1.787229	-3.900416	-2.986512
30	1	0	1.477423	-3.438997	-1.522406
31	8	0	3.648221	-1.882939	1.086506
32	1	0	4.107975	-1.289946	0.415194
33	1	0	3.238159	-1.242959	1.798784
34	8	0	4.525143	-0.110201	-0.577694
35	1	0	4.547889	-0.278300	-1.525169
36	1	0	3.845478	0.571230	-0.425043
37	8	0	2.448547	-0.272565	2.572332
38	1	0	2.214524	0.403225	1.908892
39	1	0	1.611391	-0.663955	2.891890
40	1	0	-0.460085	0.239016	1.098092
41	8	0	-1.121420	0.574499	1.848472
42	1	0	-2.499063	0.427361	1.600709

43	1	0	-0.848316	0.106535	2.657082
44	8	0	-3.536937	0.459746	1.366941
45	1	0	-3.676930	1.277831	0.777133
46	1	0	-3.816329	-0.394408	0.900074
47	8	0	0.042545	-1.382229	3.387724
48	1	0	-0.042151	-1.688177	4.296495
49	1	0	-0.288360	-2.099964	2.815064
50	8	0	-3.593785	2.621860	-0.010013
51	1	0	-2.925896	3.156726	0.461287
52	1	0	-3.204602	2.431329	-0.875386
53	8	0	-4.135423	-1.740722	0.192660
54	1	0	-3.398248	-2.009611	-0.381308
55	1	0	-4.346541	-2.498689	0.748020
56	8	0	-1.436190	3.357746	1.570027
57	1	0	-1.519015	3.698079	2.466001
58	1	0	-1.327315	2.395225	1.666305

SCF Done: E(RM062X) = -1677.70048177 A.U. after 1 cycles
NFock= 1 Conv=0.20D-08 -V/T= 2.0035

Zero-point correction= 0.468152 (a.u.)
Thermal correction to Energy= 0.510108
Thermal correction to Enthalpy= 0.511052
Thermal correction to Gibbs Free Energy= 0.395385
Sum of electronic and zero-point Energies= -1677.232330
Sum of electronic and thermal Energies= -1677.190374
Sum of electronic and thermal Enthalpies= -1677.189430
Sum of electronic and thermal Free Energies= -1677.305097

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	320.097	147.932	243.441

==== TS-S4 in Figure S4 =====
trioneh2a.high.txt

Stoichiometry C6H33O19(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.569555	1.244626	-1.503483
2	6	0	-1.669527	0.145118	-1.598042
3	6	0	-1.268528	-1.323236	-1.763020
4	6	0	0.739193	0.767971	-0.884697
5	8	0	-1.866859	-2.197652	-1.166692
6	8	0	0.350882	-0.181873	0.063227
7	8	0	-0.892921	2.374496	-1.748978
8	8	0	-2.824387	0.453378	-1.518222
9	1	0	1.355285	0.303398	-1.669577
10	6	0	1.502489	1.944196	-0.274061
11	6	0	2.119203	2.871816	-1.306930
12	1	0	0.834101	2.516969	0.378731
13	8	0	2.559183	1.391636	0.522234
14	1	0	3.089948	2.147154	0.817777
15	8	0	2.888704	3.807089	-0.559205
16	1	0	1.340529	3.371321	-1.885627
17	1	0	2.762931	2.293471	-1.979855
18	1	0	3.459956	4.298928	-1.155565
19	8	0	-0.290232	-1.469383	-2.598018
20	1	0	-1.336153	-4.194921	1.583485
21	1	0	0.069368	-2.433378	-2.630466
22	8	0	-1.008549	-3.318805	1.353192
23	1	0	-1.521082	-3.028540	0.582791
24	1	0	0.918216	-1.600966	-0.020760
25	8	0	1.275514	-2.560557	-0.009495
26	1	0	0.650071	-3.047123	0.558303
27	1	0	2.611019	-2.431124	0.591425
28	8	0	0.764764	-3.747047	-2.424250
29	1	0	1.446260	-4.005663	-3.053391
30	1	0	1.206730	-3.534839	-1.580369
31	8	0	3.476442	-2.121760	1.077655
32	1	0	3.974037	-1.535576	0.422682
33	1	0	3.084140	-1.475467	1.798395
34	8	0	4.480305	-0.364338	-0.509292

35	1	0	4.512752	-0.504413	-1.461160
36	1	0	3.838144	0.350803	-0.346172
37	8	0	2.335733	-0.494234	2.583140
38	1	0	2.142157	0.216976	1.943836
39	1	0	1.480008	-0.860710	2.880951
40	1	0	-0.406473	0.281627	1.083508
41	8	0	-1.021426	0.638082	1.911270
42	1	0	-2.281840	0.668695	1.664287
43	1	0	-0.832949	0.029741	2.649764
44	8	0	-3.379822	0.796240	1.427007
45	1	0	-3.459971	1.605816	0.833472
46	1	0	-3.748628	-0.016463	0.975087
47	8	0	-0.133135	-1.540885	3.319961
48	1	0	-0.260618	-1.848086	4.223374
49	1	0	-0.500293	-2.227871	2.731421
50	8	0	-3.216968	2.973787	0.036373
51	1	0	-2.457221	3.350680	0.522745
52	1	0	-2.881526	2.762198	-0.845053
53	8	0	-4.239430	-1.381476	0.266281
54	1	0	-3.547085	-1.710606	-0.330355
55	1	0	-4.482783	-2.118265	0.836194
56	8	0	-1.043748	3.429093	1.654710
57	1	0	-0.983286	4.046341	2.389698
58	1	0	-0.907790	2.540641	2.024658

SCF Done: E(RM062X) = -1677.70232036 A.U. after 1 cycles

	1	2	3
	A	A	A
Frequencies --	-278.2571	34.1578	38.3588

Zero-point correction= 0.466417 (a.u.)
Thermal correction to Energy= 0.507857
Thermal correction to Enthalpy= 0.508801
Thermal correction to Gibbs Free Energy= 0.394416
Sum of electronic and zero-point Energies= -1677.235904
Sum of electronic and thermal Energies= -1677.194464
Sum of electronic and thermal Enthalpies= -1677.193520
Sum of electronic and thermal Free Energies= -1677.307905

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	318.685	146.519	240.744