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-Supporting Information-

**Relationship Between Superelectrophilicity and the
Electrophilicity Index of Isolated Species**

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Supporting Information

Optimized Geometries and total energies of the most stable structures of alkyloxonium and carboxonium ions and diprotonated carboxylic acids at the B3LYP/6-31G(d) level of theory using Gaussian98 package of programs. See the manuscript for details

I. Alkyloxonium mono- and dications

1. H₂O E = -76.4089514383 a.u.

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	0.968619
H	0.941227	0.000000	-0.228724

2. H₃O⁺ E = -76.6887862621 a.u.

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	0.990130
H	0.929958	0.000000	-0.339914
H	-0.464984	0.805377	-0.339871

3. H₄O²⁺ E = -76.6000088481 a.u.

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.056637
H	0.996200	0.000000	-0.352247
H	-0.498123	-0.862732	-0.352213
H	-0.498125	0.862731	-0.352213

4. CH₃OH E = -115.714405542 a.u.

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.093458
H	1.046954	0.000000	-0.341769
H	-0.476970	-0.932016	-0.341728
O	-0.708784	1.159233	-0.407866
H	-0.717321	1.173374	-1.376437

5. CH_3OH_2^+ $E = -116.015745074$ a.u.

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.087859
H	0.998862	0.000000	-0.434366
H	-0.649196	-0.773192	-0.405184
O	-0.687578	1.304443	-0.377330
H	-0.831161	1.419430	-1.342948
H	-0.256195	2.108576	-0.011675

6. $\text{CH}_4\text{OH}_2^{2+}$ $E = -115.969794852$ a.u.

C	-0.000104	-0.000066	0.000113
H	0.000000	0.000000	1.220184
H	1.112533	-0.000066	0.041301
H	-0.253172	-0.855152	-0.666738
O	-0.558520	1.250527	-0.434468
H	-1.269564	1.255824	-1.139064
H	0.020653	2.066540	-0.461910
H	-0.759507	-0.481732	0.824555

7. CH_3OCH_3 $E = -155.025043937$ a.u.

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.093399
H	1.043351	0.000000	-0.357399
H	-0.485003	-0.923933	-0.356924
O	-0.697095	1.152316	-0.418362
C	-0.763469	1.256741	-1.823193
H	0.239561	1.323186	-2.276817
H	-1.287788	0.397261	-2.273351
H	-1.317817	2.170377	-2.054535

8. $\text{CH}_3(\text{OH})\text{CH}_3^+$ $E = -155.334313899$ a.u.

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.088591
H	1.012298	0.000000	-0.403109
H	-0.613944	-0.804293	-0.404276
O	-0.631381	1.280022	-0.409520
C	-0.804633	1.675013	-1.830924
H	0.190846	1.730203	-2.270327
H	-1.430261	0.915994	-2.299626
H	-1.293481	2.647511	-1.815048
H	-0.948754	1.885060	0.284081

9. $(\text{CH}_3)_3\text{O}^+$ E = -194.657238627 a.u.

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.092187
H	1.008006	0.000000	-0.410819
H	-0.586864	-0.819769	-0.410359
O	-0.642171	1.247105	-0.483694
C	0.122507	2.483307	-0.185240
H	0.123413	2.648145	0.894470
H	1.124992	2.320359	-0.576677
H	-0.379712	3.285559	-0.722865
C	-2.092541	1.342691	-0.184577
H	-2.541623	0.430096	-0.572182
H	-2.226549	1.441785	0.894832
H	-2.454975	2.215140	-0.725262

10. $(\text{CH}_3)_3(\text{OH})^{2+}$ E = -194.704748319 a.u.

C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.089276
H	0.985135	0.000000	-0.467230
H	-0.732665	-0.659149	-0.466428
O	-0.582350	1.514082	-0.358902
C	0.431637	2.727600	0.154474
H	0.412817	2.606530	1.236882
H	1.376556	2.475219	-0.327477
H	-0.055292	3.627011	-0.223402
C	-2.148791	1.733648	0.152909
H	-2.678558	0.909465	-0.325471
H	-2.054279	1.661607	1.235737
H	-2.392584	2.725115	-0.229639
H	-0.604847	1.573916	-1.354596

II. Carboxonium mono- and dications

11. H_2CO E = -114.500476929 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.206480
H	0.937807	0.000000	-0.594633
H	-0.937807	-0.000027	-0.594633

12. H_2COH^+ $E = -114.782499665$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.252309
H	0.927913	0.000000	-0.579749
H	-0.984346	-0.000001	-0.471338
H	0.889055	-0.000000	1.686552

13. $\text{H}_2\text{C}(\text{OH}_2)^{2+}$ $E = -114.746458143$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.315662
H	0.987333	0.000000	-0.497116
H	-0.987031	-0.000001	-0.497752
H	0.865203	0.000002	1.870716
H	-0.865059	-0.000000	1.870659

14. CH_3COH $E = -153.830121001$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.210288
H	0.959980	0.000000	-0.565781
C	-1.239770	-0.000003	-0.859741
H	-1.237439	0.881044	-1.515125
H	-1.237417	-0.881023	-1.515160
H	-2.137190	-0.000023	-0.236851

15. $\text{CH}_3\text{CH}(\text{OH})^+$ $E = -154.136701479$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.269657
H	0.960488	0.000000	-0.525848
C	-1.258760	0.000006	-0.725686
H	-1.266908	0.871351	-1.403062
H	-1.266880	-0.871265	-1.403154
H	-2.129463	-0.000034	-0.068242
H	0.890655	0.000004	1.688947

16. $\text{CH}_3\text{CH}(\text{OH}_2)^{2+}$ $E = -154.148380941$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.364713
H	1.021093	0.000000	-0.403108
C	-1.189536	0.000003	-0.746796
H	-1.102148	0.839858	-1.495867
H	-1.102152	-0.839822	-1.495898
H	-2.154338	0.000003	-0.228984
H	0.854432	0.000010	1.904016
H	-0.849414	-0.000001	1.910360

17. CH_3COCH_3 $E = -193.154660052$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.215244
C	1.286063	0.000000	-0.805890
H	1.323187	-0.880589	-1.460522
H	1.323184	0.880573	-1.460543
H	2.149710	0.000007	-0.137944
C	-1.310113	0.000008	-0.782419
H	-1.896816	-0.880737	-0.498524
H	-1.896814	0.880750	-0.498512
H	-1.165639	0.000015	-1.866547

18. $\text{CH}_3\text{C}(\text{OH})\text{CH}_3^+$ $E = -193.478719904$ a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.282560
C	1.322666	0.000000	-0.640382
H	1.392884	-0.874763	-1.305028
H	1.392854	0.874686	-1.305129
H	2.136497	0.000047	0.085356
C	-1.273721	-0.000009	-0.759002
H	-1.868631	-0.884768	-0.487141
H	-1.868648	0.884736	-0.487133
H	-1.105209	-0.000003	-1.836423
H	-0.894516	-0.000013	1.691322

19. $\text{CH}_3\text{C}(\text{OH}_2)\text{CH}_3^{2+}$ E = -193.518343442 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.402002
C	1.296561	0.000000	-0.617011
H	1.338297	-0.862241	-1.322806
H	1.338282	0.862191	-1.322864
H	2.169462	0.000024	0.042614
C	-1.310479	0.000001	-0.612579
H	-1.900787	-0.883700	-0.288022
H	-1.900748	0.883747	-0.288071
H	-1.231931	-0.000026	-1.704541
H	-0.843071	-0.000013	1.944223
H	0.847570	0.000006	1.937279

III. Mono and diprotonated Carboxylic Acids

20. HCOOH E = -189.755455746 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.204780
O	1.100962	0.000000	-0.776474
H	-0.895684	0.000004	-0.637656
H	1.868839	-0.000001	-0.171851

21. $\text{HC}(\text{OH})_2^+$ E = -190.050724023 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.276958
O	1.090956	0.000000	-0.645878
H	-0.912365	0.000009	-0.598802
H	1.902567	-0.000015	-0.083719
H	-0.891293	-0.000005	1.689627

22. $\text{HC}(\text{OH})(\text{OH}_2)^{2+}$ E = -190.055523403 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.228075
O	1.252967	0.000000	-0.559204
H	-0.843449	0.000009	-0.709745
H	2.093738	0.000360	0.009944
H	-0.868162	-0.000031	1.737720
H	1.390288	0.001284	-1.560807

23. CH₃COOH E = -229.081202924 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.210626
O	1.144836	0.000000	-0.729265
H	1.873843	0.000069	-0.079994
C	-1.230574	0.000195	-0.873793
H	-1.832776	0.882952	-0.637307
H	-0.980695	-0.001840	-1.935894
H	-1.835228	-0.880042	-0.634304

24. CH₃C(OH)₂⁺ E = -229.395083062 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.291035
O	1.144542	0.000000	-0.574786
H	1.901473	0.005821	0.054833
C	-1.215877	0.032138	-0.844990
H	-1.578146	1.070169	-0.890165
H	-0.977431	-0.295641	-1.858344
H	-2.008480	-0.589585	-0.416695
H	-0.892164	-0.001621	1.695186

25. CH₃C(OH)(OH₂)²⁺ E = -229.428800249 a.u.

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.403274
O	1.184437	0.000000	-0.392668
H	1.373832	-0.000150	-1.371633
C	-1.271307	-0.003319	-0.713627
H	-1.294562	0.862007	-1.405115
H	-1.315867	-0.908803	-1.352244
H	-2.149794	0.024967	-0.061493
H	-0.843197	0.004511	1.942859
H	0.864192	0.002663	1.921020