Species with negative electron affinity and standard DFT methods

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Supplementary Material

Part 1. Calculation Details

Table S1. Detailed results with 6-31+G* and 6-311+G(2df,p) basis sets*

		B3LYP/6-31+G*								B3LYP/6-311+G(2df,p) // B3LYP/6-31+G*				
species	type	μ	LVUMO	E(neutral)	ZPE	E(vertical anion)	E(anion)	ZPE	VEA	AEA	E(n)	E(vertical anion)	E(anion)	VEA	AEA
1 1,1-dichloroethylene	V	1.51	-0.95	-997.7811	0.0336	-997.7453			-0.975		-997.8702	-997.8382		-0.873	
2 1,3-cyclohexadiene	V	0.49	-0.91	-233.4288	0.1225	-233.3924			-0.992		-233.4950	-233.4620		-0.898	
3 acetaldehyde	V	2.99	-1.08	-153.8397	0.0557	-153.7893			-1.372		-153.8891	-153.8414		-1.298	
4 adenine	V	2.46	-0.92	-467.3399	0.1120	-467.3100			-0.847		-467.4779	-467.4507		-0.740	
5 bromobenzene	V	1.85	-0.79	-2803.3846		-2803.3498			-0.946		-2805.8651	-2805.8331		-0.870	
6 butadiene	V	0.00	-1.10	-156.0011	0.0852	-155.9700			-0.846		-156.0487	-156.0207		-0.763	
7 chlorobenzene	V	1.89	-0.78	-691.8549		-691.8149			-1.091		-691.9511	-691.9151		-0.980	
8 chloroethylene	V	1.59	-0.59	-538.1910	0.0428	-538.1390			-1.417		-538.2480	-538.1995		-1.320	
9 chloroform	V	1.25	-1.62	-1419.2843	0.0199	-1419.2720			-0.335		-1419.3940	-1419.3818		-0.331	
10 cis-dichloroethylene	V	2.02	-0.76	-997.7843	0.0342	-997.7348			-1.345		-997.8727	-997.8282		-1.209	
11 cyclopentyl radical	V	0.20	5.44	-195.9017	0.1261	-195.8723	-195.8892	0.1233	-0.799	-0.263	-195.9572	-195.9315	-195.9473	-0.698	-0.192
12 cytosine	V	6.85	-1.32	-394.9498	0.0984	-394.9266	-394.9439	0.0944	-0.631	-0.051	-395.0752	-395.0550	-395.0687	-0.547	-0.068
13 dimethylaminomethyl radical	V	1.33	-0.86	-173.8273	0.1073	-173.7962	-173.8096	0.1042	-0.845	-0.399	-173.8807	-173.8524	-173.8643	-0.768	-0.364
14 ethylene	V	0.00	-0.22	-78.5933	0.0511	-78.5281			-1.774		-78.6192	-78.5565		-1.706	
15 ethyl radical	V	0.34	-1.52	-79.1629	0.0595	-79.1415	-79.1492	0.0578	-0.580	-0.323	-79.1879	-79.1698	-79.1769	-0.495	-0.253
16 fluorobenzene	V	1.75	-0.75	-331.5012	0.0924	-331.4576	-331.4640	0.0841	-1.187	-0.788	-331.5978	-331.5577	-331.5622	-1.092	-0.743
17 isopropyl radical	V	0.25	-1.20	-118.4837	0.0882	-118.4547	-118.4686	0.0860	-0.791	-0.352	-118.5199	-118.4943	-118.5068	-0.698	-0.296
18 naphtalene	V	0.00	-1.33	-385.9069	0.1476	-385.8930	-385.8973	0.1414	-0.378	-0.093	-386.0107	-386.0003	-386.0030	-0.283	-0.039
19 norbornadiene	V	0.04	-0.56	-271.4878	0.1286	-271.4460			-1.136		-271.5622	-271.5231		-1.065	
20 pyrazine	V	0.00	-1.83	-264.3286	0.0769	-264.3186	-264.3256	0.0726	-0.270	0.036	-264.4021	-264.3946	-264.4002	-0.203	0.068
21 pyridazine	V	4.43	-1.80	-264.2989	0.0763	-264.2876	-264.2954	0.0713	-0.308	0.039	-264.3725	-264.3635	-264.3700	-0.244	0.067
22 pyridine	V	2.38	-1.06	-248.2958	0.0889	-248.2616			-0.932		-248.3648	-248.3337		-0.846	
23 pyrimidine	V	2.48	-1.57	-264.3351	0.0772	-264.3156	-264.3230	0.0717	-0.531	-0.179	-264.4087	-264.3917	-264.3977	-0.461	-0.149
24 styrene	V	0.21	-1.29	-309.6613	0.1335	-309.6453			-0.434		-309.7477	-309.7351		-0.342	
25 t-buthyl	V	0.27	-4.75	-157.8045	0.1169	-157.7761	-157.7950	0.1143	-0.772	-0.186	-157.8515	-157.8264	-157.8432	-0.684	-0.152
26 thiophene	V	0.55	-0.64	-553.0114	0.0667	-552.9628			-1.322		-553.0895	-553.0438		-1.242	
27 thymine	V	4.63	-1.54	-454.1581	0.1149	-454.1444	-454.1587	0.1102	-0.372	0.145	-454.3001	-454.2890	-454.3004	-0.301	0.137
28 trans-dichloroethylene	V	0.00	-0.94	-997.7839	0.0339	-997.7433			-1.105		-997.8722	-997.8361		-0.984	
29 trichloroethylene	V	0.94	-1.12	-1457.3716	0.0248	-1457.3396			-0.872		-1457.4923	-1457.4652		-0.739	
30 uracil	V	4.67	-1.68	-414.8377	0.0871	-414.8246	-414.8401	0.0827	-0.355	0.184	-414.9689	-414.9588	-414.9708	-0.274	0.172
31 1,2,4-trimethylbenzene	NV	0.40	-0.21	-350.2132	0.1836	-350.1715	-350.1717	0.1817	-1.134	-1.079	-350.3106	-350.2735	-350.2734	-1.008	-0.961
32 acetone	NV	3.19	-0.75	-193.1663	0.0838	-193.1200			-1.258		-193.2267	-193.1882		-1.048	
33 aniline	NV	1.63	-0.28	-287.6161	0.1171	-287.5757			-1.099		-287.7028	-287.6654		-1.018	
34 anisole	NV	1.39	-0.37	-346.7855	0.1333	-346.7440			-1.129		-346.8870	-346.8512		-0.975	
35 cis-butene	NV	0.03	0.33	-157.2299	0.1079	-157.1767			-1.448		-157.2778	-157.2341		-1.190	
36 cyclohexene	NV	0.35	0.46	-234.6562	0.1466	-234.6094			-1.272		-234.7231	-234.6826		-1.101	
37 furan	NV	0.73	-0.07	-230.0314	0.0700	-229.9794			-1.417		-230.1010	-230.0560		-1.226	
38 m-xylene	NV	0.36	-0.29	-310.8956	0.1554	-310.8554			-1.092		-310.9822	-310.9457		-0.992	
39 o-xylene	NV	0.67	-0.20	-310.8950	0.1562	-310.8510			-1.198		-310.9815	-310.9431		-1.046	
40 phenol	NV	1.42	-0.48	-307.4803	0.1045	-307.4399			-1.099		-307.5753	-307.5388		-0.994	
41 propene	NV	0.43	0.10	-117.9139	0.0798	-117.8548			-1.610		-117.9509	-117.9020		-1.328	
42 pyrrole	NV	1.93	0.65	-210.1778	0.0825	-210.1375			-1.096		-210.2417	-210.2060		-0.973	
43 trans-butene	NV	0.00	0.42	-157.2336	0.1081	-157.1792			-1.480		-157.2815	-157.2301		-1.397	
44 trimethylethylene	NV	0.31	0.37	-196.5480		-196.4992			-1.329		-196.6068	-196.5657		-1.117	
45 CO2	NV	0.00	-0.56	-188.5904	0.0116	-188.5565	-188.5805	0.0083	-0.921	-0.182	-188.6569	-188.6233	-188.6415	-0.915	-0.332
46 guanine	NV	6.80	-0.58	-542.5764	0.1168	-542.5606	-542.5621	0.1139	-0.431	-0.311	-542.7433	-542.7286	-542.7297	-0.400	-0.291

* Diple moment in Debyes, LVUMO energy in eV, Energies in Hartrees, VEA and AEA in eV

* Dipole moment in Debyes, LVUMO energy in eV, Energies in Hartrees, VEA and AEA in eV

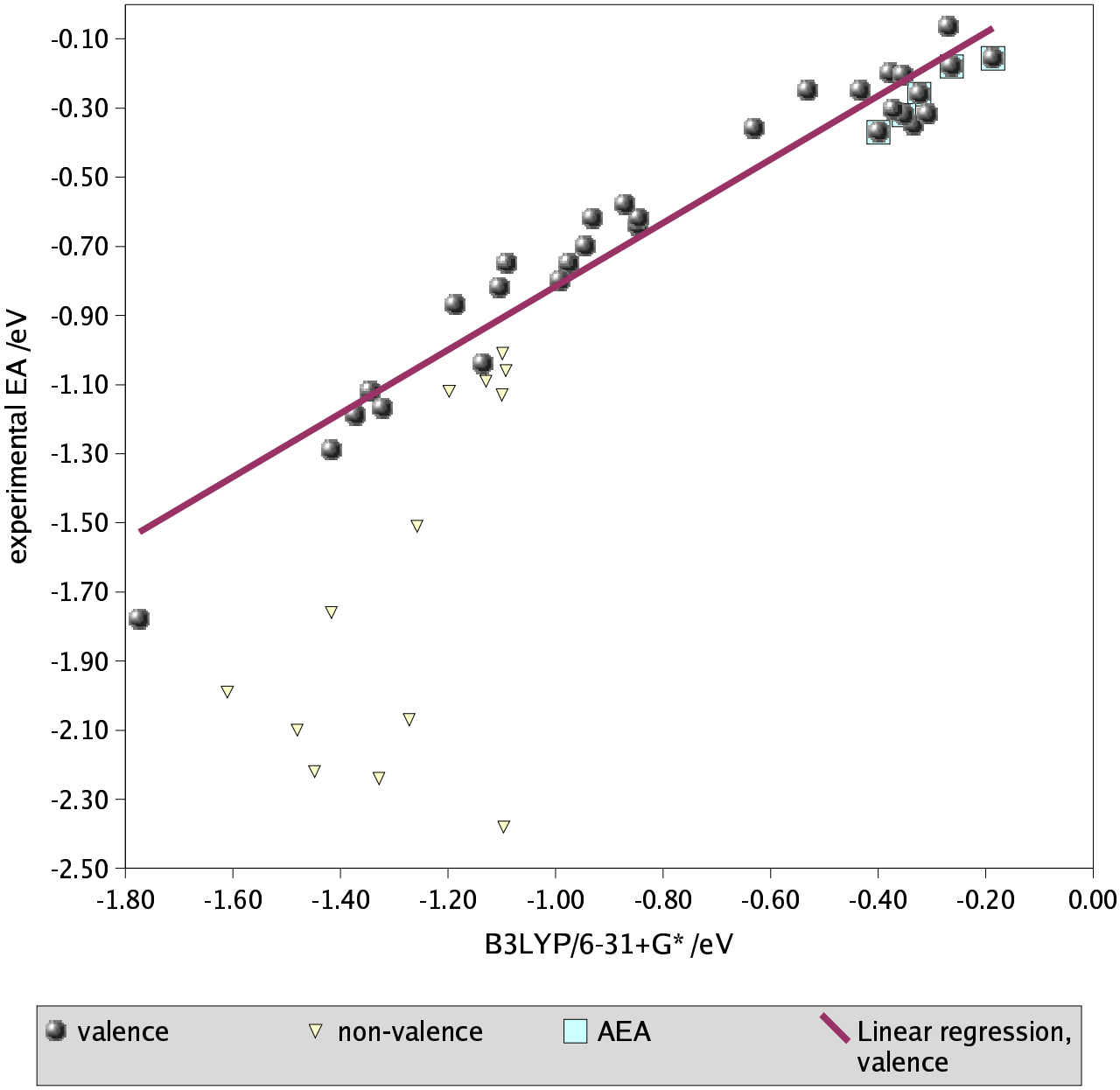

Figure S1. Correlation between the experimental and B3LYP/6-31+G* data. See text and Figure 1.

Table S2. Detailed results with AUG-CC-PVDZ and AUG-CC-PVTZ basis sets*

				B3LYP/AUG-cc-pVDZ							B3LYP/AUG-CC-PVTZ // B3LYP/AUG-CC-PVDZ				
species	type	μ	LVUMO	E(neutral)	ZPE	E(vertical anion)	E(anion)	ZPE	VEA	AEA	E(n)	E(vertical anion)	E(anion)	VEA	AEA
1 1,3-cyclohexadiene	V	0.50	-1.01	-233.4449	0.1216	-233.4261			-0.511		-233.5067	-233.4916		-0.411	
9 chloroform	V	1.11	-1.55	-1419.3600	0.0196	-1419.3492			-0.293		-1419.4135	-1419.4046		-0.243	
11 cyclopentyl radical	V	0.19		-195.9147	0.1249	-195.8921	-195.9085	0.1224	-0.614	-0.098	-195.9678	-195.9469	-195.9609	-0.567	-0.117
13 dimethylaminomethyl radical	V	1.30		-173.8398	0.1059	-173.8189	-173.8276	0.1030	-0.568	-0.252	-173.8902	-173.8711	-173.8776	-0.519	-0.265
15 ethyl radical	V	0.32		-79.1668	0.0588	-79.1495	-79.1576	0.0568	-0.470	-0.194	-79.1929	-79.1772	-79.1837	-0.428	-0.194
17 isopropyl radical	V	0.17		-118.4897	0.0870	-118.4684	-118.4803	0.0850	-0.578	-0.200	-118.5271	-118.5074	-118.5172	-0.535	-0.213
23 pyrimidine	V	2.38	-1.62	-264.3566	0.0767	-264.3393			-0.469		-264.4194	-264.4071		-0.335	
24 styrene	V	0.20	-1.38	-309.6830	0.1330	-309.6705			-0.339		-309.7624	-309.7509		-0.311	
25 t-buthyl	V	0.19		-157.8125	0.1154	-157.7953	-157.8085	0.1127	-0.467	-0.037	-157.8608	-157.8449	-157.8560	-0.431	-0.055
3 acetaldehyde	NV	2.91	-1.15	-153.8532	0.0550	-153.8342			-0.517		-153.8962	-153.8812		-0.408	
32 acetone	NV	3.11	-0.81	-193.1816	0.0827	-193.1664	-193.1665	0.0814	-0.414	-0.375	-193.2359	-193.2238	-193.2236	-0.328	-0.297
33 aniliine	NV	1.57	-0.40	-287.6438	0.1164	-287.6289			-0.405		-287.7167	-287.7052		-0.313	
34 anisole	NV	1.31	-0.49	-346.8126	0.1323	-346.7962			-0.445		-346.9028	-346.8900		-0.347	
5 bromobenzene	NV	1.86	-0.91	-2805.8307	0.0900	-2805.8160	-2805.8438	0.0865	-0.398	0.453	-2805.9609	-2805.9494	-2805.9715	-0.311	0.385
6 butadiene	NV	0.00	-1.19	-156.0121	0.0849	-155.9875			-0.669		-156.0569	-156.0380		-0.517	
7 chlorobenzene	NV	1.89	-0.87	-691.8948	0.0906	-691.8786	-691.8788	0.0892	-0.442	-0.398	-691.9672	-691.9544	-691.9542	-0.349	-0.315
35 cis-butene	NV	0.31	0.19	-157.2389	0.1068	-157.2188			-0.546		-157.2868	-157.2704		-0.444	
36 cyclohexene	NV	0.37	0.38	-234.6720	0.1454	-234.6535			-0.504		-234.7354	-234.7205		-0.405	
14 ethylene	NV	0.00	-0.34	-78.5984	0.0508	-78.5719	-78.5719	0.0503	-0.720		-78.6237	-78.6029	-78.6028	-0.568	-0.555
16 fluorobenzene	NV	1.62	-0.85	-331.5256	0.0918	-331.5078	-331.5080	0.0908	-0.484	-0.454	-331.6124	-331.5982	-331.5981	-0.386	-0.364
37 furan	NV	0.67	-0.20	-230.0517	0.0695	-230.0304			-0.581		-230.1114	-230.0942		-0.467	
19 norbornadiene	NV	0.09	-0.66	-271.5072	0.1276	-271.4881			-0.520		-271.5751	-271.5597		-0.420	
40 phenol	NV	1.27	-0.60	-307.5119	0.1043	-307.4969			-0.408		-307.5897	-307.5780		-0.317	
41 propene	NV	0.43	-0.03	-117.9209	0.0791	-117.8981	-117.8982	0.0785	-0.620	-0.600	-117.9576	-117.9390	-117.9389	-0.507	-0.491
22 pyridine	NV	2.28	-1.14	-248.3142	0.0883	-248.2980			-0.440		-248.3756	-248.3630		-0.343	
42 pyrrole	NV	1.84	0.52	-210.1982	0.0822	-210.1820			-0.441		-210.2518	-210.2392		-0.345	
43 trans-butene	NV	0.00	0.28	-157.2425	0.1070	-157.2201			-0.610		-157.2903	-157.2720		-0.497	
44 trimethylethylene	NV	0.29	0.28	-196.5592	0.1341	-196.5401			-0.519		-196.6178	-196.6023		-0.420	
30 uracil	NV	4.54	-1.74	-414.8843	0.0868	-414.8805	-414.8813	0.0856	-0.102	-0.046	-414.9845	-414.9831	-414.9834	-0.038	0.004
45 CO2	NV	0.00	-0.53	-188.6142	0.0116	-188.5812			-0.898		-188.6632	-188.6355		-0.754	

* Diple moment in Debyes, LVUMO energy in eV, Energies in Hartrees, VEA and AEA in eV

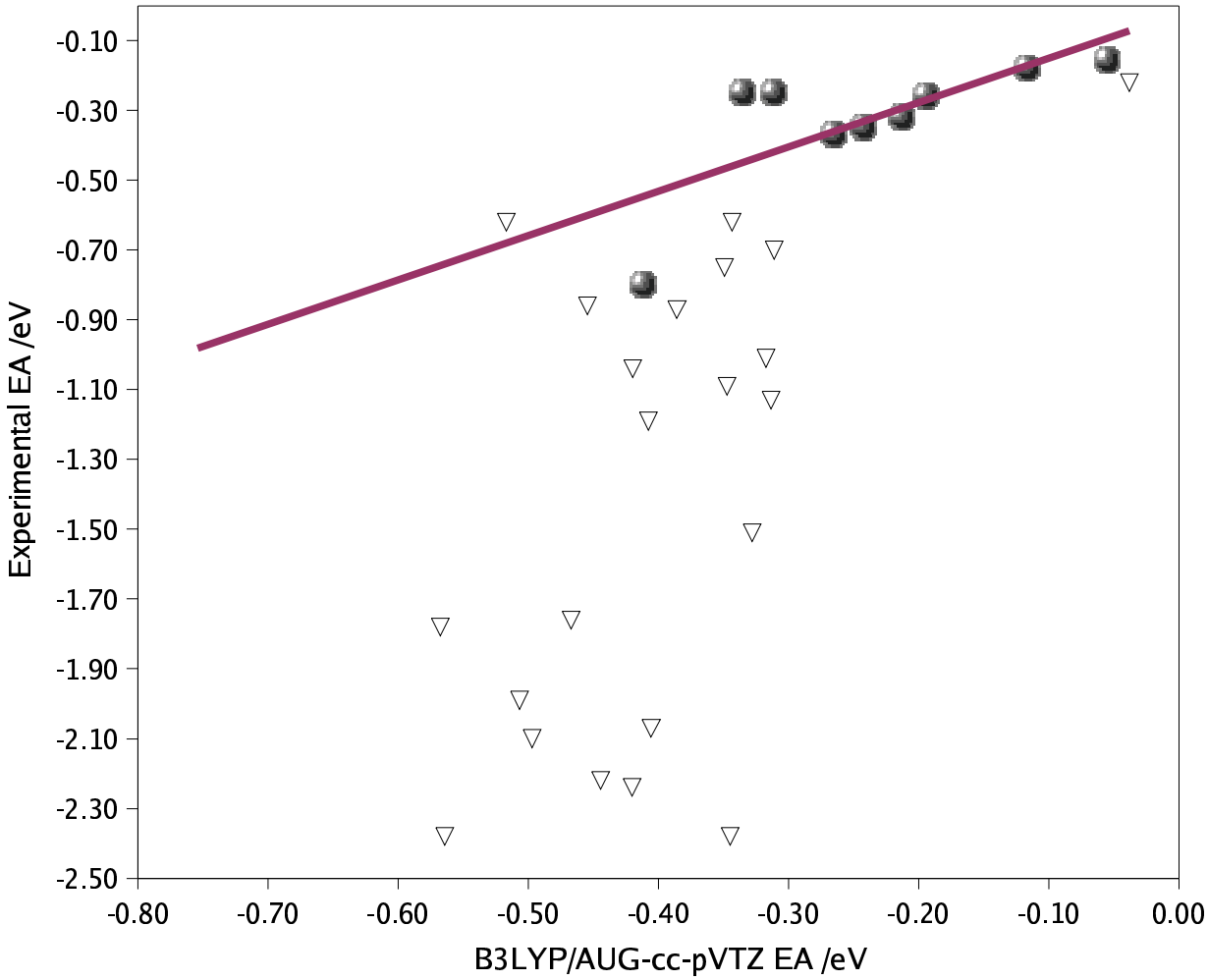

Figure S2. Correlation between experimental and calculated electron affinities (B3LYP/AUG-cc-pVTZ basis). Same as figure S1.

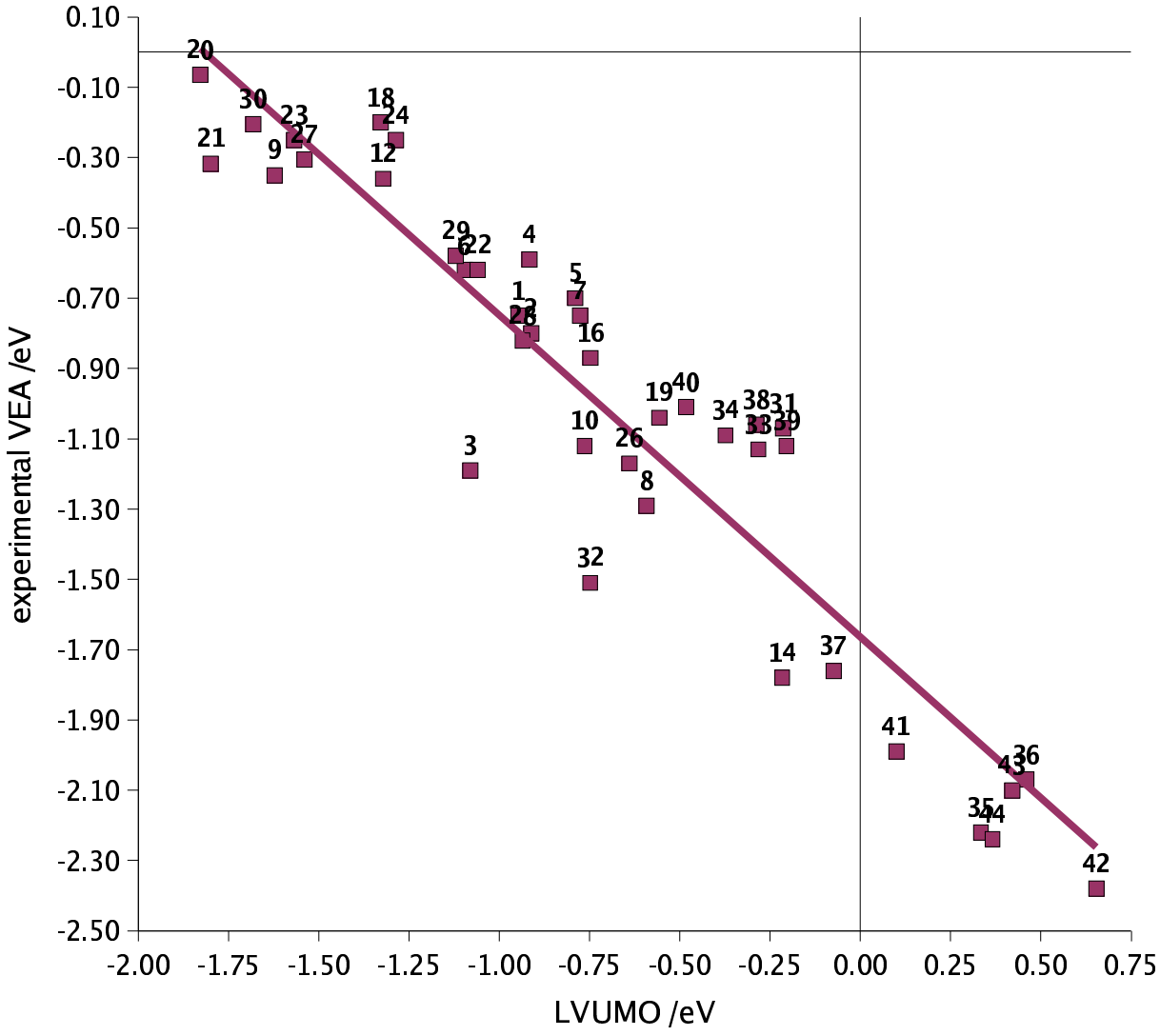

Figure S3. Koopman's Theorem correlation at the B3LYP/6-31+G* level.

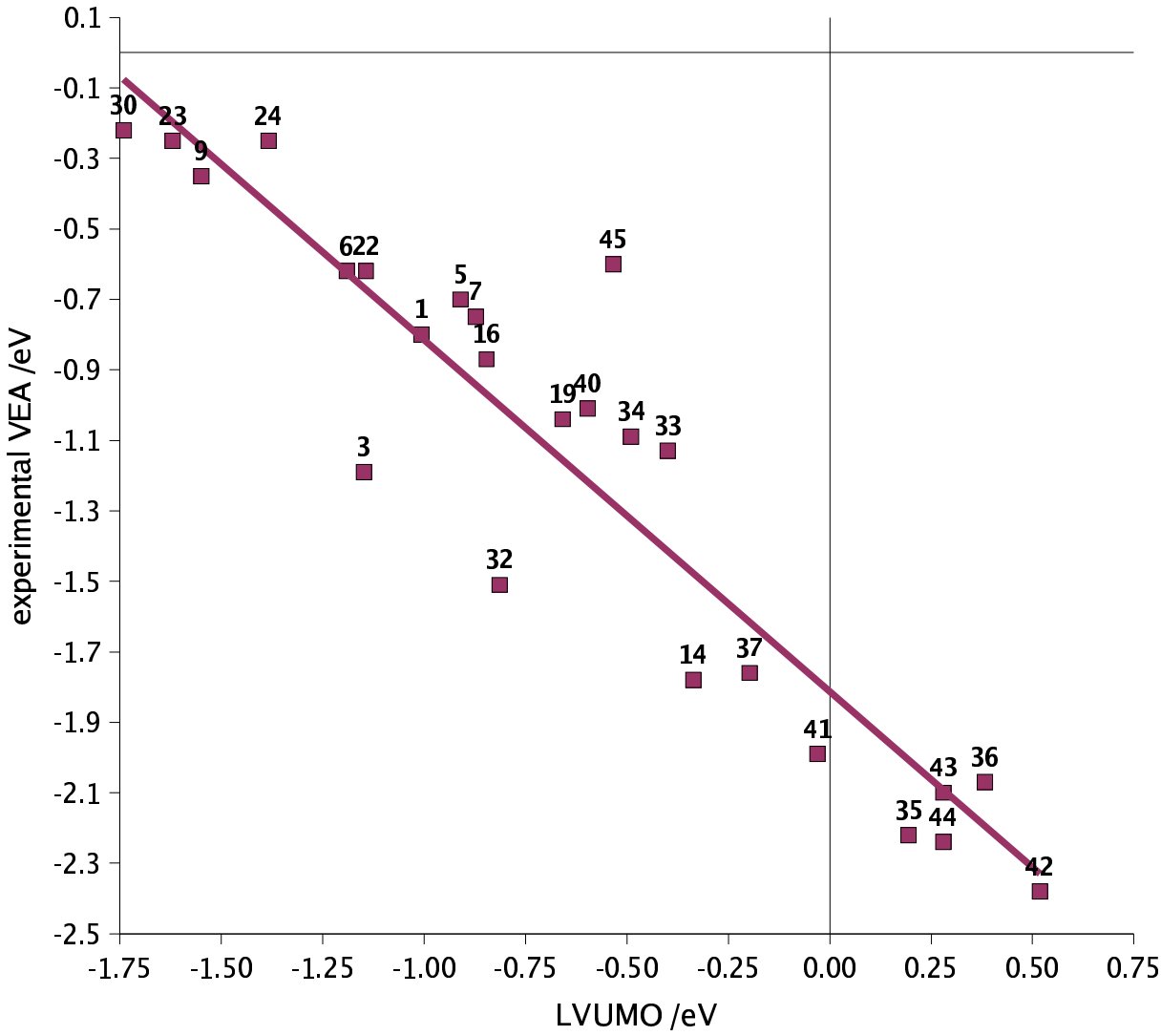

Figure S4. Koopman's Theorem correlation at the B3LYP/AUG-cc-pVDZ level.

Part 2. Structure, Dipole, SOMO diagrmas and spin density of some species under study

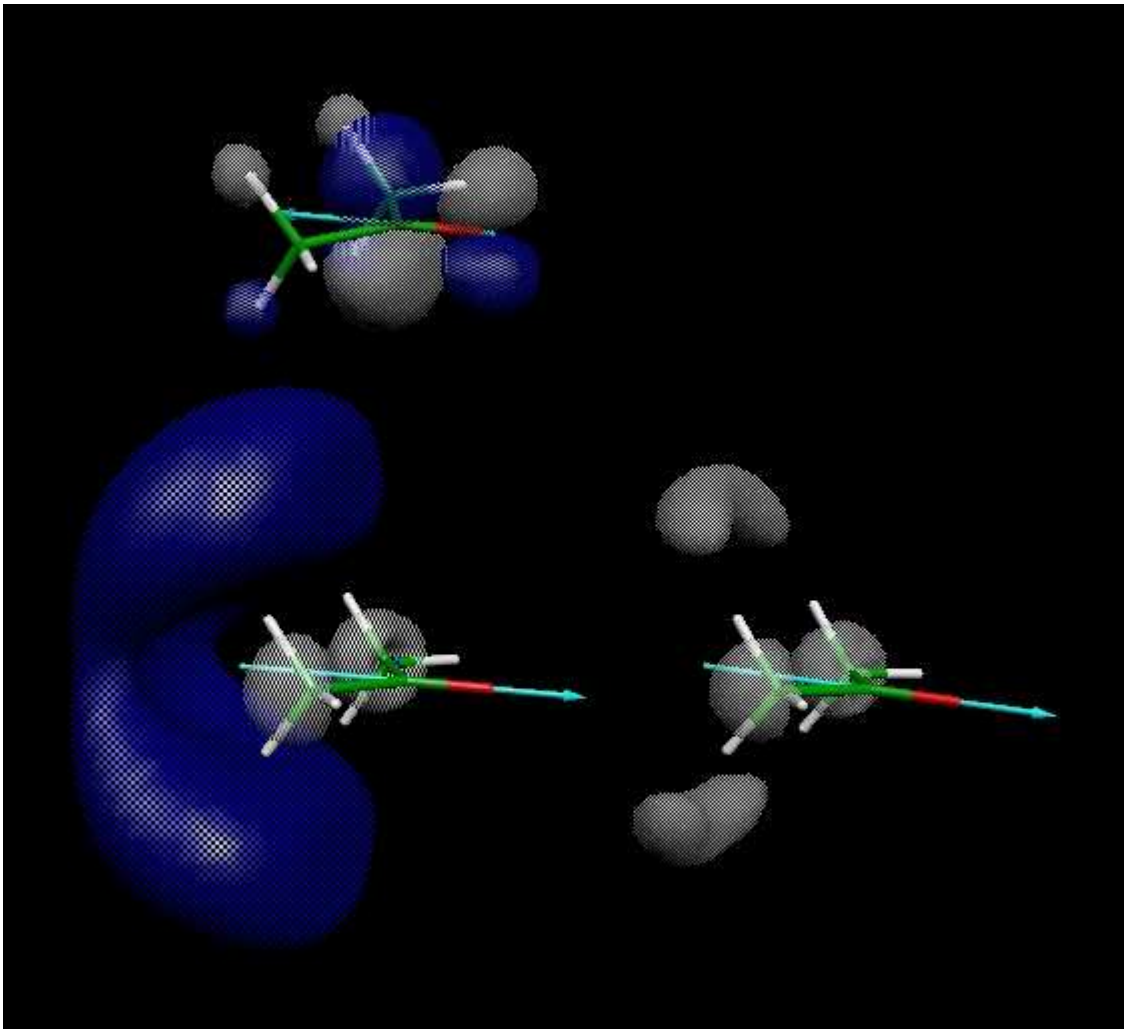

Figure S5. Acetone B3LYP/6-31+G*, Non -Valence RA. Top: LUMO of the neutral. Lower left corner: SOMO of the vertical RA. Lower right corner: spin density. The cyan arrow show the dipole orientation.

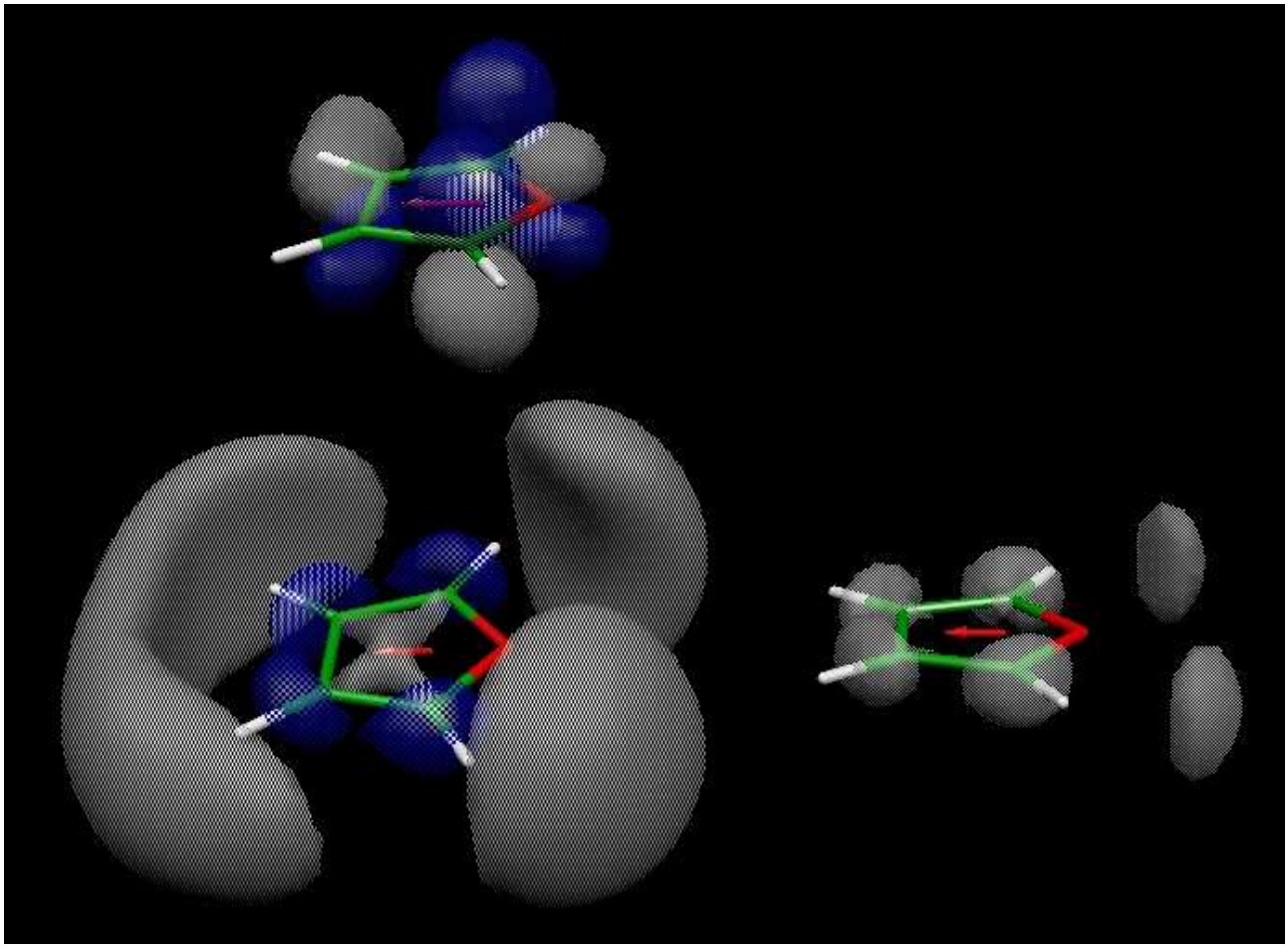

Figure S6. Neutral and non valence RA obtained at the B3LYP/6-31+G* level for furan presented as in figure S5.

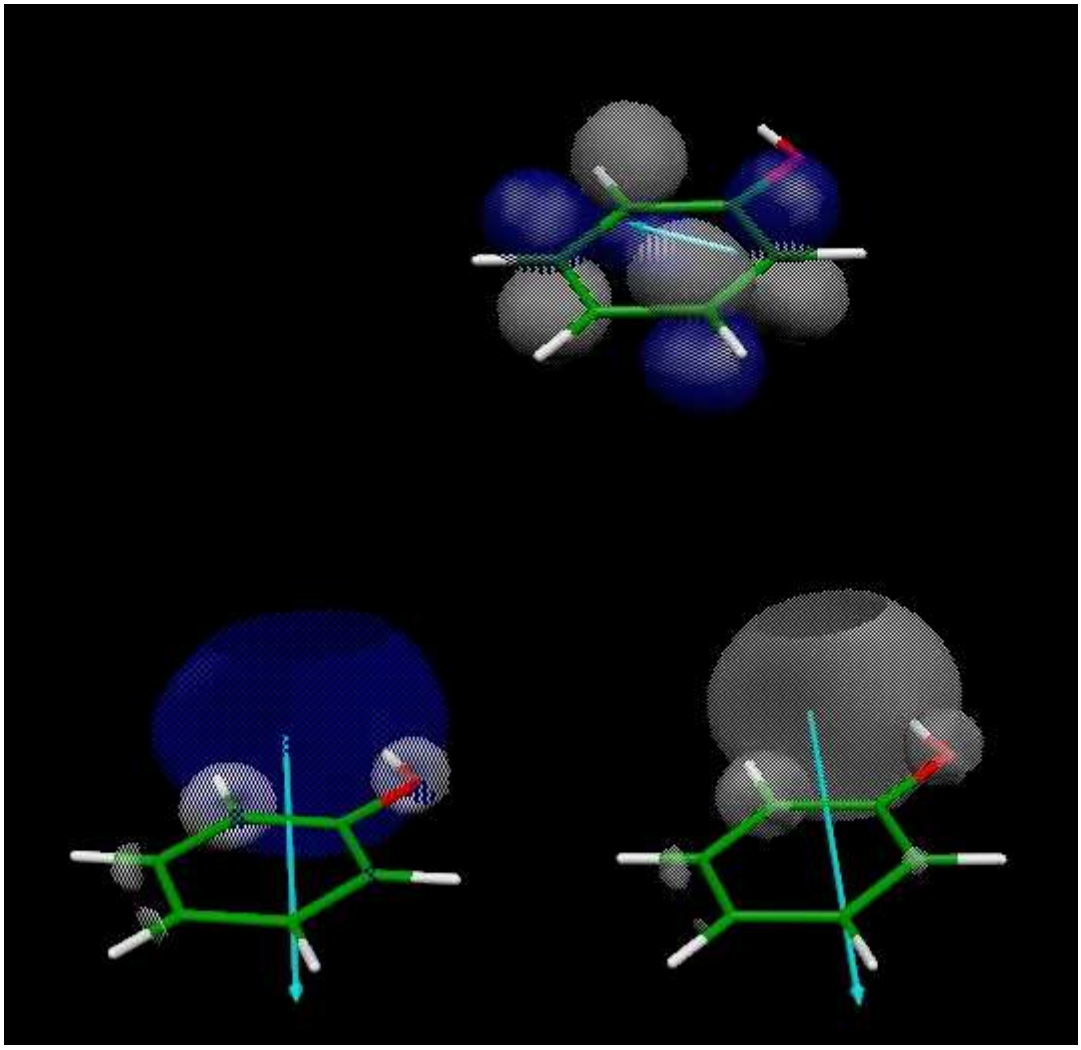

Figure S7. Non valence RA found for phenol (organized as Fig. S5).

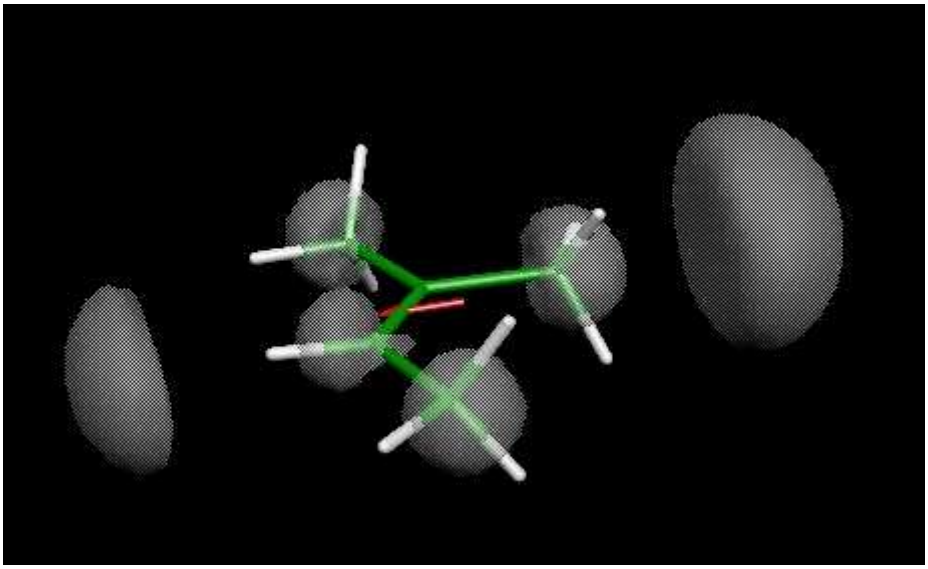

Figure S8. Spin density in the trimethylethylene RA.

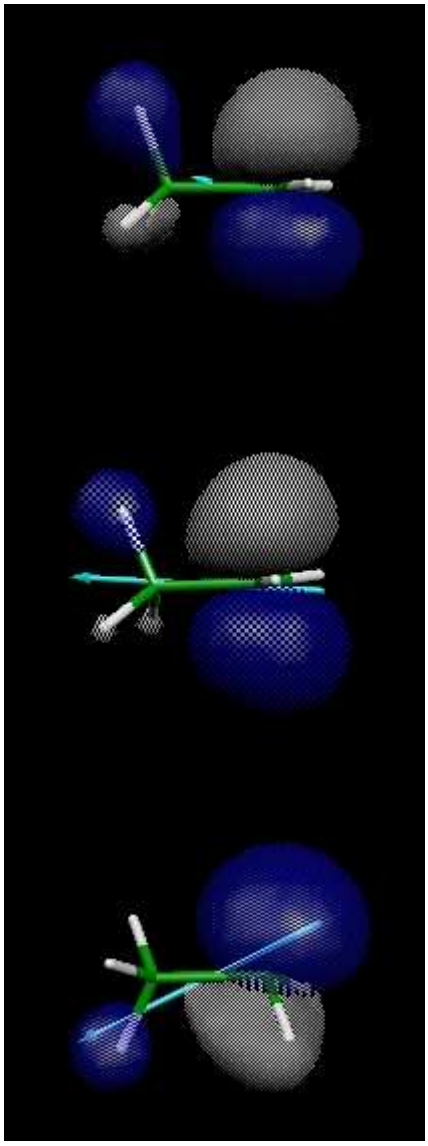

Figure S9. Ethyl radical and its anions. From top to bottom, SOMO of the neutral, HOMO of the vertical anion and HOMO of the optimized anion.

Part 3. Geometries of all species under study.

All the XYZ coordinates in Angstorms for all the optimized species under study have been gathered in a single ASCII file named Structures-xyz.txt