In search for an optimal methodology to calculate the valence electron affinities of temporary anions.

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Electronic Supporting Information (ESI). Supplementary Material

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Part 1.Chemical structures of all compounds under study

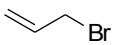
Chart 1A. compounds on Table 1

1,1-dichloroethylene

1

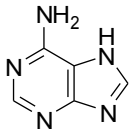
1,1-dibromoethylene

2



3-bromo-1-propene

3



adenine

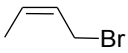
4

bromoethylene

5

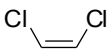
chloroethylene

6



cis-1-bromo-2-butene

7



cis-1,2-dichloroethylene

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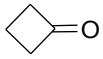


cyclobutanone

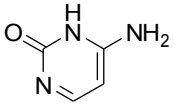
9

cyclopentadiene

10

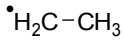
cyclopropene

11



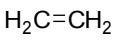
cytosine

12



ethyl radical

13



ethylene

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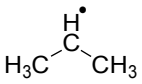


isopropyl radical

15

isothiazole

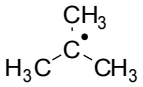
16

isooxazole

17

oxazole

18



tert-butyl radical

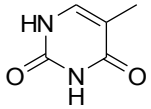
19

thiazole

20

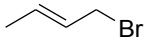
thiophene

21



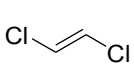
thymine

22



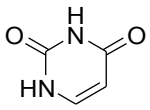
trans-bromo-2-butene

23



trans-1,2-dichloroethylene

24



uracil

25

Chart 1B compounds on Table 2


cyclohexa-1,4-diene

26


2-methylbut-2-ene

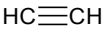
27


acetic acid

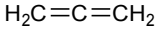
28


acetone

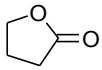
29


acetylene

30


allene

31


butyrolactone

32


cis-1-bromo-1-propene

33


cis-1,2-difluoro ethylene

34


cis-2-butene

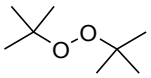
35


cyclobutene

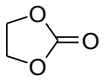
36


cyclopentene

37


di*tert*-butylperoxyde

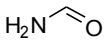
38


ethylene carbonate

39


fluoroethylene

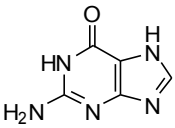
40


formamide

41


furan

42


guanine

43


imidazole

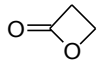
44


methyl vinyl ether

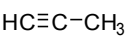
45


propene

46


propiolactone

47


propyne

48


pyrrole

49


tetramethyl ethylene

50


trans-1-bromo-1-propene

51


trans-1-chloro-1-propene

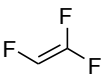
52


trans-1,2-difluoro ethylene

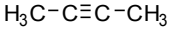
53


trans-2-butene

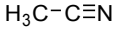
54


trifluorethylene

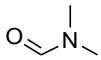
55


2-butyne

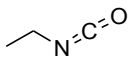
56


acetonitrile

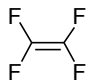
57


dimethyl formamide

58

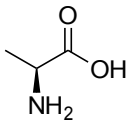

ethyl isocyanate

59


tetrafluoroethylene

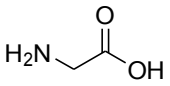
60

Chart 2. compounds on Table 4



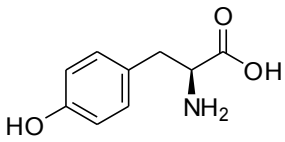
α -L-alanine

61



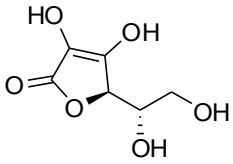
α -L-glycine

62



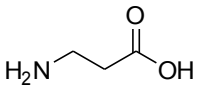
α -L-tyrosine

63



ascorbic acid (vitamin C)

64

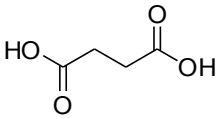


β -alanine

65

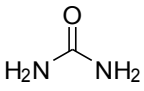
carbonic difluoride

66



succinic acid

67



urea

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Part 2. Details about DFT calculations by using B3LYP/6-311+G(2df,p)//B3LYP/6-31+G*

2.1. Table S1. Gas phase calculation details for the compounds on Table 1 in main text

	Species	Anion Type	B3LYP/6-31+G* - E(neutral)	ZPE	E(anion)	ZPE	B3LYP/6-311+G(2df,p)//B3LYP/6-31+G* E(neutral)	E(anion)
1	**1,1-dichloroethylene**	V	-997.7811	0.0336	-997.7453		-997.8702	-997.8382
2	**2-bromo-1-propene**	V	-2689.0391	0.0708	-2688.9958		-2691.4954	-2691.4541
3	**3-bromo-1-propene**	V	-2689.0335	0.0713	-2689.0153		-2691.4925	-2691.4762
4	**Adenine**	V	-467.3399	0.1120	467.3100		-467.4799	-467.4507
5	**Bromoethylene**	V	-2649.7127	0.0422	-2649.6670		-2652.1622	-2652.1190
6	**Chloroethylene**	V	-538.2480	0.0428	-538.1995		-538.2480	-538.1995
7	***cis*-1-bromo-2-butene**	V	-2728.3537	0.0999	-2728.3347		-2730.8221	-2730.8051
8	***cis*-1,2-dichloroethylene**	V	-997.7843	0.0342	-997.7348		-997.8727	-997.8282
9	**Cyclobutanone**	V	-231.2396	0.0909	-231.1958		-231.3081	-231.2691
10	**Cyclopentadiene**	V	-194.1103	0.0926	-194.0641		-194.1659	-194.1226
11	**Cyclopropene**	V	-116.6248	0.0560	-116.5621		-116.6603	-116.6000
12	**Cytosine**	V	-395.0575	0.0984	-395.0550		-395.0752	-395.0550
13	**Cytosine***	V			-395.0687	0.0944		-395.0687
13a	**Ethyl Radical***	V	-79.1879	0.0595	-79.1769	0.0578	-79.1879	-79.1769
14	**Ethylene**	V	-78.6192	0.0511	-78.5565		-78.6192	-78.5565
15	**Isopropil radical***	V	-118.4837	0.0882	-118.4686	0.0860	-118.5199	-118.5068
16	**isothiazole**	V	-569.0498	0.0551	-569.0213		-569.1355	-569.1072
17	**Isoxazole**	V	-246.0455	0.0580	-246.0002		-246.1189	-246.0760
18	**Oxazole**	V	-246.0812	0.0586	-246.0296		-246.1552	-246.1043
19	***t*-Butyl radical***	V	-157.8045	0.1169	-157.7761	0.1142	-157.8515	-157.8432
20	**Thiazole**	V	-569.0563	0.0552	-569.0210		-569.1386	-569.1053
21	**Thiophene**	V	-553.0895	0.0667	-553.0438		-553.0895	-553.0438
22	**Thymine**	V	-454.3001	0.1149	-454.2890		-454.3001	-454.2890
23	***trans*-1-bromo-2-butene**	V	-2728.3558	0.0996	-2728.3331		-2730.8247	-2730.8040
24	***trans*-1,2-dichloroethylene**	V	-997.7839	0.0339	-997.7433		-997.8722	-997.8361
25	**Uracil**	V	-414.9689	0.0871	-414.9588		-414.9689	-414.9588
25a	**Uracil***	V			-414.8401	0.0827		-414.9708

* AEA were calculated for these compounds. All energies in Hartree

2.2. **Table S2.** Gas phase calculation details for the compounds on Table 2 in main text

	Species	Anion Type	B3LYP/6-31+G*			B3LYP/6-311+G(2df,p)//B3LYP/6-31+G*	
			E(neutral)	ZPE	E(anion)	E(neutral)	E(anion)
26	**1,4-Cyclohexadiene**	N	-233.4280	0.1222	-233.3770	-233.4951	-233.4548
27	**2-methyl-2-butene**	N	-196.6068	0.1356	-196.5657	-196.6068	-196.5657
28	**acetic acid**	N	-229.0961	0.0618	-229.0548	-229.1754	-229.1379
29	**Acetone**	N	-193.2267	0.0838	-193.1882	-193.2267	-193.1882
30	**Acetylene**	N	-77.3331	0.0268	-77.2804	-77.3602	-77.3115
31	**Allene**	N	-116.6651	0.0553	-116.6092	-116.7017	-116.6515
32	**Butyrolactone**	N	-306.5062	0.0988	-306.4651	-306.6008	-306.5656
33	***cis*-1-bromo-1-propene**	N	-2689.0354	0.0708	-2688.9946	-2691.4952	-2691.4580
34	**cis-1,2-difluorethylene**	N	-277.0666	0.0370	-277.0218	-277.1563	-277.1144
35	***cis*-2-butene**	N	-157.2778	0.1079	-157.2341	-157.2778	-157.2341
36	**Cyclobutene**	N	-155.9797	0.0866	-155.9151	-156.0244	-155.9721
37	**Cyclopentene**	N	-195.3345	0.1169	-195.2780	-195.3905	-195.3443
38	**di-tert-butil-peroxide**	N	-466.0834	0.2514	-466.0407	-466.2245	-466.1880
39	**Ethylene Carbonate**	N	-305.2452	0.0719	-305.2772	-342.5234	-342.4911
40	**Fluorethylene**	N	-177.8355	0.0440	-177.7757	-177.8931	-177.8355
41	**Formamide**	N	-169.9025	0.0454	-169.8592	-169.9624	-169.9215
42	**Furan**	N	-230.1010	0.0700	-230.0560	-230.1010	-230.0560
43	**Guanine**	N	-542.7286	0.1168	-542.7297	-542.7433	-542.7286
44	**Imidazole**	N	-226.2269	0.0712	-226.1892	-226.2950	-226.2620
45	**vinyl ether**	N	-193.1212	0.0844	-193.0672	-193.1841	-193.1381
46	**Propene**	N	-117.9509	0.0798	-117.9020	-117.9509	-117.9020
47	**propyne**	N	-116.6611	0.0568	-117.9020	-116.6987	-116.6550
48	**Propiolactone**	N	-267.1665	0.0689	-267.1249	-267.2501	-267.2128
49	**Pyrrole**	N	-210.2417	0.0825	-210.2060	-210.2417	-210.2060
50	**tetramethylethylene**	N	-235.8592	0.1627	-235.8106	-235.9288	-235.8889
51	***trans*-1-bromo-1-propene**	N	-2689.0358	0.0707	-2688.9989	-2691.4935	-2691.4592
52	***trans*-1-chloro-1-propene**	N	-577.5113	0.0711	-577.4629	-577.5792	-577.5373
53	***trans*-1,2-difluorethylene**	N	-277.0657	0.0366	-277.0144	-277.1563	-277.1144
54	***trans*-2-butene**	N	-157.2815	0.1081	-157.2301	-157.2815	-157.2301
55	**trifluorethylene**	N	-376.3042	0.0292	-376.2596	-376.4265	-376.3837
56	**2-butyne**	N	-155.9867	0.0847	-155.9392	-156.0349	-155.9925
57	**acetonitrile**	N	-132.7617	0.0455	-132.7243	-132.8024	-132.7701
58	**dimethylformamide**	N	-248.5242	0.1027	-248.4822	-248.6018	-248.5665
59	**ethyl isocyanate**	N	-247.3160	0.0791	-247.2796	-247.3955	-247.3642
60	**tetrafluoroethylene**	N	-475.5364	0.0213	-475.4951	-475.6918	-475.6504

All energies in Hartrees

Part 3. Details concerning the extrapolation of ΔE *vs.* (1/ε).

3.3. Table S3. ΔE vs (1/ε) extrapolation details for the V anions on Table 1 (main text)

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-997.8708	-997.8614	-0.2543
1,1-dichloroethylene	Krypton	1.52	*V*	-997.8708	-997.8646	-0.1687
	Heptane	1.92	*V*	-997.8711	-997.8755	0.1203
	Ciclohexane	2.02	*V*	-997.8712	-997.8777	0.1764
	Benzene	2.25	*V*	-997.8713	-997.8816	0.2812
	Ethyl Ether	4.34	*V*	-997.8719	-997.8992	0.7424
	Chloroform	4.90	*V*	-997.8720	-997.9014	0.8006
	Chlorobenzene	5.62	*V*	-997.8721	-997.9036	0.8576
	Tetrahydrofuran	7.58	*V*	-997.8723	-997.9075	0.9588
	Dichloroethane	10.36	*V*	-997.8724	-997.9105	1.0370
	Acetone	20.70	*V*	-997.8726	-997.9147	1.1442
	Ethanol	24.55	*V*	-997.8727	-997.9153	1.1612
	Acetonitrile	36.64	*V*	-997.8727	-997.9165	1.1912
	Dimethylsulfoxide	46.70	*V*	-997.8727	-997.9170	1.2042
	Water	78.39	*V*	-997.8728	-997.9178	1.2241
	EA experimental /eV		-0.7500			
	EA Linear extrap./eV		-0.9100			
	R^2		0.9999			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2691.4959	-2691.4750	-0.5689
2-bromo-1-propene	Krypton	1.52	*V*	-2691.4960	-2691.4780	-0.4908
	Heptane	1.92	*V*	-2691.4964	-2691.4881	-0.2237
	Ciclohexane	2.02	*V*	-2691.4964	-2691.4901	-0.1712
	Benzene	2.25	*V*	-2691.4966	-2691.4939	-0.0729
	Ethyl Ether	4.34	*V*	-2691.4973	-2691.5108	0.3673
	Chloroform	4.90	*V*	-2691.4974	-2691.5129	0.4239
	Chlorobenzene	5.62	*V*	-2691.4975	-2691.5151	0.4793
	Tetrahydrofuran	7.58	*V*	-2691.4977	-2691.5189	0.5786
	Dichloroethane	10.36	*V*	-2691.4978	-2691.5219	0.6558
	Acetone	20.70	*V*	-2691.4980	-2691.5261	0.7625
	Ethanol	24.55	*V*	-2691.4981	-2691.5267	0.7800
	Acetonitrile	36.64	*V*	-2691.4981	-2691.5279	0.8119
	Dimethylsulfoxide	46.70	*V*	-2691.4982	-2691.5284	0.8224
	EA experimental /eV		-1.3100			
	EA Linear extrap./eV		-1.2000			
	R^2		0.9996			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2691.4937	-2691.4990	0.1449
3-bromo-1-propene	Krypton	1.52	*V*	-2691.4938	-2691.5022	0.2270
	Heptane	1.92	*V*	-2691.4945	-2691.5130	0.5051
	Ciclohexane	2.02	*V*	-2691.4946	-2691.5152	0.5597
	Benzene	2.25	*V*	-2691.4949	-2691.5192	0.6612
	Ethyl Ether	4.34	*V*	-2691.4962	-2691.5370	1.1108
	Chloroform	4.90	*V*	-2691.4964	-2691.5393	1.1682
	Chlorobenzene	5.62	*V*	-2691.4966	-2691.5416	1.2240
	Tetrahydrofuran	7.58	*V*	-2691.4970	-2691.5456	1.3242
	Dichloroethane	10.36	*V*	-2691.4973	-2691.5488	1.4018
	Acetone	20.70	*V*	-2691.4977	-2691.5532	1.5088
	Ethanol	24.55	*V*	-2691.4978	-2691.5539	1.5264
	Acetonitrile	36.64	*V*	-2691.4982	-2691.5551	1.5505
	Dimethylsulfoxide	46.70	*V*	-2691.4980	-2691.5556	1.5688
	Water	78.39	*V*	-2691.4981	-2691.5566	1.5917
	EA experimental /eV		-0.6000			
	EA Linear extrap./eV		-0.5011			
	R^2		0.9998			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-467.4833	-467.4773	-0.165
Adenine	Krypton	1.52	*V*	-467.4842	-467.4811	-0.085
	Heptane	1.92	*V*	-467.4873	-467.4941	0.187
	Ciclohexane	2.02	*V*	-467.4880	-467.4968	0.240
	Benzene	2.25	*V*	-467.4894	-467.5018	0.339
	Ethyl Ether	4.34	*V*	-467.4960	-467.5247	0.781
	Chloroform	4.90	*V*	-467.4971	-467.5279	0.837
	Chlorobenzene	5.62	*V*	-467.4980	-467.5308	0.893
	Tetrahydrofuran	7.58	*V*	-467.4999	-467.5364	0.993
	Dichloroethane	10.36	*V*	-467.5014	-467.5408	1.070
	Acetone	20.70	*V*	-467.5036	-467.5469	1.177
	Ethanol	24.55	*V*	-467.5040	-467.5479	1.194
	Acetonitrile	36.64	*V*	-467.5049	-467.5497	1.219
	Dimethylsulfoxide	46.70	*V*	-467.5055	-467.5504	1.220
	Water	78.39	*V*	-467.5055	-467.5518	1.259
	EA experimental /eV		-0.64			
	EA Linear extrap./eV		-0.80			
	R^2		0.9997			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2652.1630	-2652.1427	-0.553
Bromoethylene	Krypton	1.52	*V*	-2652.1631	-2652.1460	-0.466
	Heptane	1.92	*V*	-2652.1636	-2652.1572	-0.172
	Ciclohexane	2.02	*V*	-2652.1636	-2652.1594	-0.115
	Benzene	2.25	*V*	-2652.1638	-2652.1635	-0.008
	Ethyl Ether	4.34	*V*	-2652.1648	-2652.1818	0.463
	Chloroform	4.90	*V*	-2652.1649	-2652.1841	0.522
	Chlorobenzene	5.62	*V*	-2652.1651	-2652.1864	0.580
	Tetrahydrofuran	7.58	*V*	-2652.1653	-2652.1905	0.684
	Dichloroethane	10.36	*V*	-2652.1655	-2652.1936	0.764
	Acetone	20.70	*V*	-2652.1659	-2652.1980	0.874
	Ethanol	24.55	*V*	-2652.1659	-2652.1987	0.891
	Acetonitrile	36.64	*V*	-2652.1660	-2652.1999	0.922
	Dimethylsulfoxide	46.70	*V*	-2652.1660	-2652.2004	0.935
	EA experimental /eV		-1.17			
	EA Linear extrap./eV		-1.22			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-538.2488	-538.2244	-0.663
Chloroethylene	Krypton	1.52	*V*	-538.2489	-538.2279	-0.572
	Heptane	1.92	*V*	-538.2494	-538.2396	-0.265
	Ciclohexane	2.02	*V*	-538.2494	-538.2419	-0.206
	Benzene	2.25	*V*	-538.2496	-538.2462	-0.095
	Ethyl Ether	4.34	*V*	-538.2506	-538.2650	0.394
	Chloroform	4.90	*V*	-538.2507	-538.2674	0.455
	Chlorobenzene	5.62	*V*	-538.2508	-538.2698	0.515
	Tetrahydrofuran	7.58	*V*	-538.2511	-538.2740	0.622
	Dichloroethane	10.36	*V*	-538.2513	-538.2772	0.704
	Acetone	20.70	*V*	-538.2516	-538.2817	0.817
	Ethanol	24.55	*V*	-538.2517	-538.2824	0.835
	Acetonitrile	36.64	*V*	-538.2518	-538.2836	0.867
	Dimethylsulfoxide	46.70	*V*	-538.2518	-538.2842	0.881
	Water	78.39	*V*	-538.2519	-538.2850	0.902
	EA experimental /eV		-1.29			
	EA Linear extrap./eV		-1.36			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-997.8737	-997.8530	-0.564
***cis*-1,2-dichloro-**	Krypton	1.52	*V*	-997.8739	-997.8564	-0.475
Ethylene	Heptane	1.92	*V*	-997.8746	-997.8681	-0.177
	Ciclohexane	2.02	*V*	-997.8747	-997.8703	-0.119
	Benzene	2.25	*V*	-997.8750	-997.8746	-0.011
	Ethyl Ether	4.34	*V*	-997.8764	-997.8933	0.460
	Chloroform	4.90	*V*	-997.8766	-997.8957	0.520
	Chlorobenzene	5.62	*V*	-997.8768	-997.8980	0.577
	Tetrahydrofuran	7.58	*V*	-997.8772	-997.9022	0.680
	Dichloroethane	10.36	*V*	-997.8775	-997.9054	0.759
	Acetone	20.70	*V*	-997.8780	-997.9099	0.868
	Ethanol	24.55	*V*	-997.8781	-997.9106	0.885
	Acetonitrile	36.64	*V*	-997.8782	-997.9118	0.915
	Dimethylsulfoxide	46.70	*V*	-997.8783	-997.9124	0.928
	Water	78.39	*V*	-997.8784	-997.9133	0.951
	EA experimental /eV		-1.12			
	EA Linear extrap./eV		-1.23			
	R^2		1.0000			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2730.8233	-2730.8272	0.107
***cis*-1-bromo-**	Krypton	1.52	*V*	-2730.8235	-2730.8303	0.187
-2-butene	Heptane	1.92	*V*	-2730.8241	-2730.8411	0.461
	Ciclohexane	2.02	*V*	-2730.8243	-2730.8432	0.515
	Benzene	2.25	*V*	-2730.8245	-2730.8472	0.616
	Ethyl Ether	4.34	*V*	-2730.8259	-2730.8651	1.067
	Chloroform	4.90	*V*	-2730.8262	-2730.8675	1.125
	Chlorobenzene	5.62	*V*	-2730.8263	-2730.8698	1.182
	Tetrahydrofuran	7.58	*V*	-2730.8267	-2730.8739	1.284
	Dichloroethane	10.36	*V*	-2730.8271	-2730.8772	1.364
	Acetone	20.70	*V*	-2730.8275	-2730.8817	1.474
	Ethanol	24.55	*V*	-2730.8276	-2730.8825	1.492
	Acetonitrile	36.64	*V*	-2730.8280	-2730.8838	1.518
	Dimethylsulfoxide	46.70	*V*	-2730.8278	-2730.8843	1.537
	Water	78.39	*V*	-2730.8280	-2730.8853	1.561
	EA experimental /eV		-0.68			
	EA Linear extrap./eV		-0.55			
	R^2		0.9995			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-231.3099	-231.2947	-0.414
Cyclobutanone	Krypton	1.52	*V*	-231.3102	-231.2983	-0.324
	Heptane	1.92	*V*	-231.3112	-231.3107	-0.014
	Ciclohexane	2.02	*V*	-231.3114	-231.3132	0.047
	Benzene	2.25	*V*	-231.3118	-231.3178	0.162
	Ethyl Ether	4.34	*V*	-231.3139	-231.3387	0.674
	Chloroform	4.90	*V*	-231.3142	-231.3415	0.741
	Chlorobenzene	5.62	*V*	-231.3145	-231.3441	0.805
	Tetrahydrofuran	7.58	*V*	-231.3151	-231.3490	0.922
	Dichloroethane	10.36	*V*	-231.3156	-231.3528	1.013
	Acetone	20.70	*V*	-231.3162	-231.3581	1.139
	Ethanol	24.55	*V*	-231.3163	-231.3589	1.159
	Acetonitrile	36.64	*V*	-231.3165	-231.3604	1.195
	Dimethylsulfoxide	46.70	*V*	-231.3166	-231.3610	1.209
	Water	78.39	*V*	-231.3168	-231.3628	1.250
	EA experimental /eV		-1.00			
	EA Linear extrap./eV		-1.16			
	R^2		0.9993			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-194.1669	-194.1474	-0.530
Cyclopentadiene	Krypton	1.52	*V*	-194.1670	-194.1508	-0.440
	Heptane	1.92	*V*	-194.1676	-194.1625	-0.137
	Ciclohexane	2.02	*V*	-194.1677	-194.1648	-0.078
	Benzene	2.25	*V*	-194.1679	-194.1691	0.032
	Ethyl Ether	4.34	*V*	-194.1691	-194.1881	0.517
	Chloroform	4.90	*V*	-194.1693	-194.1906	0.578
	Chlorobenzene	5.62	*V*	-194.1695	-194.1930	0.638
	Tetrahydrofuran	7.58	*V*	-194.1699	-194.1973	0.746
	Dichloroethane	10.36	*V*	-194.1701	-194.2006	0.829
	Acetone	20.70	*V*	-194.1706	-194.2052	0.943
	Ethanol	24.55	*V*	-194.1706	-194.2060	0.961
	Acetonitrile	36.64	*V*	-194.1708	-194.2073	0.993
	Dimethylsulfoxide	46.70	*V*	-194.1708	-194.2078	1.007
	EA experimental /eV		-1.19			
	EA Linear extrap./eV		-1.22			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-116.6610	-116.6251	-0.977
Cyclopropene	Krypton	1.52	*V*	-116.6611	-116.6286	-0.884
	Heptane	1.92	*V*	-116.6615	-116.6405	-0.570
	Ciclohexane	2.02	*V*	-116.6616	-116.6429	-0.508
	Benzene	2.25	*V*	-116.6617	-116.6473	-0.394
	Ethyl Ether	4.34	*V*	-116.6626	-116.6668	0.115
	Chloroform	4.90	*V*	-116.6627	-116.6693	0.179
	Chlorobenzene	5.62	*V*	-116.6628	-116.6717	0.242
	Tetrahydrofuran	7.58	*V*	-116.6631	-116.6761	0.355
	Dichloroethane	10.36	*V*	-116.6633	-116.6795	0.442
	Acetone	20.70	*V*	-116.6635	-116.6842	0.562
	Ethanol	24.55	*V*	-116.6636	-116.6849	0.581
	Acetonitrile	36.64	*V*	-116.6637	-116.6863	0.615
	Dimethylsulfoxide	46.70	*V*	-116.6637	-116.6868	0.629
	Water	78.39	*V*	-116.6638	-116.6878	0.653
	EA experimental /eV		-1.73			
	EA Linear extrap./eV		-1.71			
	R^2		0.9998			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-395.0822	-395.0833	0.031
Cytosine	Krypton	1.52	*V*	-395.0833	-395.0873	0.110
	Heptane	1.92	*V*	-395.0874	-395.1012	0.377
	Ciclohexane	2.02	*V*	-395.0883	-395.1040	0.428
	Benzene	2.25	*V*	-395.0900	-395.1093	0.525
	Ethyl Ether	4.34	*V*	-395.0988	-395.1335	0.946
	Chloroform	4.90	*V*	-395.1001	-395.1368	1.000
	Chlorobenzene	5.62	*V*	-395.1013	-395.1400	1.052
	Tetrahydrofuran	7.58	*V*	-395.1038	-395.1458	1.144
	Dichloroethane	10.36	*V*	-395.1058	-395.1505	1.216
	Acetone	20.70	*V*	-395.1087	-395.1570	1.314
	Ethanol	24.55	*V*	-395.1092	-395.1581	1.330
	Dimethylsulfoxide	46.70	*V*	-395.1104	-395.1607	1.369
	EA experimental /eV		-0.36			
	EA Linear extrap./eV		-0.57			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	AEA/ eV
	Argon	1.43	*V*	-395.0822	-395.0970	0.511
Cytosine	Krypton	1.52	*V*	-395.0833	-395.1010	0.590
(adiabatic)	Heptane	1.92	*V*	-395.0874	-395.1148	0.854
	Ciclohexane	2.02	*V*	-395.0883	-395.1176	0.906
	Benzene	2.25	*V*	-395.0900	-395.1228	1.001
	Ethyl Ether	4.34	*V*	-395.0988	-395.1468	1.416
	Chloroform	4.90	*V*	-395.1001	-395.1500	1.468
	Chlorobenzene	5.62	*V*	-395.1013	-395.1532	1.519
	Tetrahydrofuran	7.58	*V*	-395.1038	-395.1589	1.608
	Dichloroethane	10.36	*V*	-395.1058	-395.1635	1.678
	Acetone	20.70	*V*	-395.1087	-395.1699	1.774
	Ethanol	24.55	*V*	-395.1092	-395.1710	1.789
	Dimethylsulfoxide	46.70	*V*	-395.1104	-395.1736	1.826
	EA experimental /eV		-0.06			
	EA Linear extrap./eV		-0.07			
	R^2		1.0000			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	AEA/ eV
	Argon	1.43	*V*	-79.1882	-79.2054	0.508
Ethyl Radical	Krypton	1.52	*V*	-79.1882	-79.2093	0.615
(adiabatic)	Heptane	1.92	*V*	-79.1883	-79.2227	0.977
	Benzene	2.25	*V*	-79.1884	-79.2303	1.180
	Ethyl Ether	*4.34*	*V*	-79.1886	-79.2521	1.768
	Chloroform	4.90	*V*	-79.1886	-79.2549	1.843
	Chlorobenzene	5.62	*V*	-79.1887	-79.2576	1.917
	Tetrahydrofuran	7.58	*V*	-79.1887	-79.2625	2.049
	Dichloroethane	10.36	*V*	-79.1888	-79.2663	2.151
	Acetone	20.70	*V*	-79.1888	-79.2716	2.293
	Ethanol	24.55	*V*	-79.1888	-79.2725	2.316
	Acetonitrile	36.64	*V*	-79.1889	-79.2740	2.356
	Dimethylsulfoxide	46.70	*V*	-79.1889	-79.2746	2.373
	Water	78.39	*V*	-79.1889	-79.2756	2.400
	EA experimental /eV		-0.26			
	EA Linear extrap./eV		-0.34			
	R^2		0.9997			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-78.6195	-78.5823	-1.012
Ethylene	Krypton	1.52	*V*	-78.6196	-78.5859	-0.916
	Heptane	1.92	*V*	-78.6198	-78.5980	-0.591
	Ciclohexane	2.02	*V*	-78.6198	-78.6004	-0.528
	Benzene	2.25	*V*	-78.6199	-78.6048	-0.410
	Ethyl Ether	*4.34*	*V*	-78.6204	-78.6244	0.109
	Chloroform	4.90	*V*	-78.6204	-78.6268	0.174
	Chlorobenzene	5.62	*V*	-78.6205	-78.6293	0.238
	Tetrahydrofuran	7.58	*V*	-78.6206	-78.6335	0.352
	Dichloroethane	10.36	*V*	-78.6207	-78.6369	0.440
	Acetone	20.70	*V*	-78.6209	-78.6414	0.560
	Ethanol	24.55	*V*	-78.6209	-78.6422	0.579
	Acetonitrile	36.64	*V*	-78.6209	-78.6434	0.613
	Dimethylsulfoxide	46.70	*V*	-78.6209	-78.6440	0.627
	Water	78.39	*V*	-78.6210	-78.6448	0.649
	EA experimental /eV		-1.78			
	EA Linear extrap./eV		-1.75			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-118.520	-118.533	0.437
Isopropil radical	Krypton	1.52	*V*	-118.517	-118.537	0.627
(adiabatic)	Heptane	1.92	*V*	-118.520	-118.549	0.872
	Ciclohexane	2.02	*V*	-118.520	-118.551	0.926
	Benzene	2.25	*V*	-118.520	-118.556	1.062
	Ethyl Ether	*4.34*	*V*	-118.521	-118.577	1.607
	Chloroform	4.90	*V*	-118.521	-118.580	1.688
	Chlorobenzene	5.62	*V*	-118.521	-118.582	1.743
	Tetrahydrofuran	7.58	*V*	-118.518	-118.587	1.960
	Dichloroethane	10.36	*V*	-118.521	-118.591	1.988
	Acetone	20.70	*V*	-118.521	-118.596	2.124
	Ethanol	24.55	*V*	-118.521	-118.597	2.151
	Acetonitrile	36.64	*V*	-118.521	-118.599	2.205
	Dimethylsulfoxide	46.70	*V*	-118.521	-118.599	2.205
	Water	78.39	*V*	-118.521	-118.600	2.233
	EA experimental /eV		-0.32			
	EA Linear extrap./eV		-0.35			
	R^2		-0.9965			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-569.137	-569.133	-0.115
isothiazole	Krypton	1.52	*V*	-569.137	-569.137	-0.024
	Heptane	1.92	*V*	-569.138	-569.149	0.283
	Ciclohexane	2.02	*V*	-569.139	-569.151	0.343
	Benzene	2.25	*V*	-569.139	-569.156	0.454
	Ethyl Ether	*4.34*	*V*	-569.141	-569.176	0.947
	Chloroform	4.90	*V*	-569.141	-569.179	1.010
	Chlorobenzene	5.62	*V*	-569.142	-569.181	1.071
	Tetrahydrofuran	7.58	*V*	-569.142	-569.186	1.180
	Dichloroethane	10.36	*V*	-569.143	-569.189	1.264
	Acetone	20.70	*V*	-569.144	-569.194	1.381
	Ethanol	24.55	*V*	-569.144	-569.195	1.399
	Acetonitrile	36.64	*V*	-569.144	-569.197	1.432
	Dimethylsulfoxide	46.70	*V*	-569.144	-569.197	1.446
	EA experimental /eV		-0.63			
	EA Lineal extrap./eV		-0.82			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-246.121	-246.103	-0.491
Isoxazole	Krypton	1.52	*V*	-246.121	-246.107	-0.397
	Heptane	1.92	*V*	-246.123	-246.120	-0.079
	Ciclohexane	2.02	*V*	-246.123	-246.122	-0.017
	Benzene	2.25	*V*	-246.123	-246.127	0.099
	Ethyl Ether	*4.34*	*V*	-246.126	-246.149	0.610
	Chloroform	4.90	*V*	-246.127	-246.151	0.675
	Chlorobenzene	5.62	*V*	-246.127	-246.154	0.739
	Tetrahydrofuran	7.58	*V*	-246.128	-246.159	0.852
	Dichloroethane	10.36	*V*	-246.128	-246.163	0.940
	Acetone	20.70	*V*	-246.129	-246.168	1.061
	Ethanol	24.55	*V*	-246.129	-246.169	1.081
	Acetonitrile	36.64	*V*	-246.130	-246.171	1.115
	Dimethylsulfoxide	46.70	*V*	-246.130	-246.171	1.129
	Water	78.39	*V*	-246.130	-246.172	1.154
	EA experimental /eV		-1.09			
	EA Linear extrap./eV		-1.22			
	R^2		0.9998			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-246.1573	-246.1290	-0.770
Oxazole	Krypton	1.52	*V*	-246.1576	-246.1325	-0.683
	Heptane	1.92	*V*	-246.1588	-246.1446	-0.386
	Ciclohexane	2.02	*V*	-246.1590	-246.1469	-0.328
	Benzene	2.25	*V*	-246.1595	-246.1514	-0.219
	Ethyl Ether	*4.34*	*V*	-246.1619	-246.1716	0.265
	Chloroform	4.90	*V*	-246.1622	-246.1742	0.326
	Chlorobenzene	5.62	*V*	-246.1626	-246.1768	0.387
	Tetrahydrofuran	7.58	*V*	-246.1632	-246.1814	0.495
	Dichloroethane	10.36	*V*	-246.1638	-246.1850	0.579
	Acetone	20.70	*V*	-246.1645	-246.1901	0.694
	Ethanol	24.55	*V*	-246.1647	-246.1909	0.712
	Acetonitrile	36.64	*V*	-246.1649	-246.1923	0.745
	Dimethylsulfoxide	46.70	*V*	-246.1650	-246.1929	0.759
	EA experimental /eV		-1.44			
	EA Linear extrap./eV		-1.47			
	R^2		0.9997			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	AEA/ eV
	Argon	1.43	*V*	-157.8516	-157.8669	0.417
***t*-Butyl radical**	Krypton	1.52	*V*	-157.8516	-157.8702	0.506
(adiabatic)	Heptane	1.92	*V*	-157.8516	-157.8813	0.808
	Ciclohexane	2.02	*V*	-157.8517	-157.8838	0.872
	Benzene	2.25	*V*	-157.8517	-157.8880	0.986
	Ethyl Ether	*4.34*	*V*	-157.8519	-157.9069	1.497
	Chloroform	4.90	*V*	-157.8519	-157.9092	1.558
	Chlorobenzene	5.62	*V*	-157.8519	-157.9119	1.630
	Tetrahydrofuran	7.58	*V*	-157.8520	-157.9163	1.751
	Dichloroethane	10.36	*V*	-157.8520	-157.9199	1.847
	Acetone	20.70	*V*	-157.8523	-157.9249	1.977
	Ethanol	24.55	*V*	-157.8521	-157.9257	2.003
	Acetonitrile	36.64	*V*	-157.8521	-157.9272	2.044
	Dimethylsulfoxide	46.70	*V*	-157.8521	-157.9278	2.058
	Water	78.39	*V*	-157.8522	-157.9290	2.091
	EA experimental /eV		-0.16			
	EA Linear extrap./eV		-0.27			
	R^2		0.9987			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-569.1403	-569.1313	-0.246
Thiazole	Kripton	1.52	*V*	-569.1406	-569.1349	-0.155
	Heptane	1.92	*V*	-569.1416	-569.1473	0.153
	Ciclohexane	2.02	*V*	-569.1419	-569.1497	0.213
	Benzene	2.25	*V*	-569.1423	-569.1542	0.324
	Ether	4.34	*V*	-569.1445	-569.1745	0.815
	Chloroform	4.90	*V*	-569.1449	-569.1771	0.877
	Dichloroethane	5.62	*V*	-569.1452	-569.1796	0.937
	THF	7.58	*V*	-569.1458	-569.1842	1.046
	Chlorobenzene	10.36	*V*	-569.1463	-569.1878	1.129
	Acetone	20.70	*V*	-569.1471	-569.1928	1.244
	Ethanol	24.55	*V*	-569.1472	-569.1936	1.263
	Acetonitrile	36.64	*V*	-569.1474	-569.1950	1.295
	DMSO	46.70	*V*	-569.1475	-569.1956	1.309
	EA experimental /eV		-0.800			
	EA Linear extrap./eV		-0.94			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-553.0906	-553.0686	-0.600
Thiophene	Krypton	1.52	*V*	-553.0908	-553.0720	-0.511
	Heptane	1.92	*V*	-553.0915	-553.0838	-0.210
	Ciclohexane	2.02	*V*	-553.0916	-553.0861	-0.151
	Benzene	2.25	*V*	-553.0919	-553.0904	-0.042
	Ethyl	*4.34*	*V*	-553.0934	-553.1097	0.442
	Chloroform	4.90	*V*	-553.0937	-553.1121	0.503
	Chlorobenzene	5.62	*V*	-553.0939	-553.1146	0.563
	Tetrahydrofuran	7.58	*V*	-553.0943	-553.1190	0.671
	Dichloroethane	10.36	*V*	-553.0947	-553.1224	0.754
	Acetone	20.70	*V*	-553.0952	-553.1271	0.868
	Ethanol	24.55	*V*	-553.0953	-553.1279	0.887
	Acetonitrile	36.64	*V*	-553.0954	-553.1292	0.919
	Dimethylsulfoxide	46.70	*V*	-553.0955	-553.1298	0.933
	Water	78.39	*V*	-553.0956	-553.1308	0.956
	EA experimental /eV		-1.17			
	EA Linear extrap./eV		-1.29			
	R^2		0.9998			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-454.3060	-454.3148	0.239
Thymine	Krypton	1.52	*V*	-454.3069	-454.3184	0.313
	Heptane	1.92	*V*	-454.3102	-454.3308	0.562
	Ciclohexane	2.02	*V*	-454.3109	-454.3334	0.611
	Benzene	2.25	*V*	-454.3124	-454.3381	0.700
	Ethyl Ether	*4.34*	*V*	-454.3194	-454.3596	1.093
	Chloroform	4.90	*V*	-454.3206	-454.3626	1.143
	Chlorobenzene	5.62	*V*	-454.3215	-454.3653	1.191
	Tetrahydrofuran	7.58	*V*	-454.3235	-454.3704	1.276
	Dichloroethane	10.36	*V*	-454.3251	-454.3745	1.343
	Acetone	20.70	*V*	-454.3275	-454.3802	1.434
	Ethanol	24.55	*V*	-454.3279	-454.3812	1.449
	Dimethylsulfoxide	46.70	*V*	-454.3288	-454.3833	1.485
	Water	78.39	*V*	-454.3295	-454.3849	1.466
	EA experimental /eV		-0.31			
	EA Linear extrap./eV		-0.34			
	R^2		0.9997			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2730.8259	-2730.8262	0.008
trans-1-bromo-	Kripton	1.52	*V*	-2730.8261	-2730.8293	0.089
2-butene	Heptane	1.92	*V*	-2730.8268	-2730.8401	0.363
	Ciclohexane	2.02	*V*	-2730.8269	-2730.8422	0.417
	Benzene	2.25	*V*	-2730.8272	-2730.8462	0.518
	Ether	4.34	*V*	-2730.8286	-2730.8643	0.971
	Chloroform	4.90	*V*	-2730.8289	-2730.8667	1.029
	Dichloroethane	5.62	*V*	-2730.8291	-2730.8690	1.086
	THF	7.58	*V*	-2730.8295	-2730.8732	1.189
	Chlorobenzene	10.36	*V*	-2730.8298	-2730.8765	1.270
	Dichloromethane	20.70	*V*	-2730.8303	-2730.8810	1.381
	Acetone	24.55	*V*	-2730.8304	-2730.8818	1.400
	DMSO	46.70	*V*	-2730.8306	-2730.8836	1.444
	Water	78.39	*V*	-2730.8307	-2730.8847	1.469
	EA experimental /eV		-0.68			
	EA Linear extrap./eV		-0.65			
	R^2		0.9994			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-997.8732	-997.8600	-0.358
***trans*-**	Krypton	1.52	*V*	-997.8733	-997.8634	-0.272
1,2-dichloroethylene	Heptane	1.92	*V*	-997.8739	-997.8746	0.019
	Ciclohexane	2.02	*V*	-997.8740	-997.8768	0.075
	Benzene	2.25	*V*	-997.8743	-997.8809	0.180
	Ethyl Ether	4.34	*V*	-997.8754	-997.8990	0.642
	Chloroform	4.90	*V*	-997.8756	-997.9013	0.700
	Chlorobenzene	5.62	*V*	-997.8758	-997.9036	0.757
	Tetrahydrofuran	7.58	*V*	-997.8761	-997.9076	0.857
	Dichloroethane	10.36	*V*	-997.8764	-997.9107	0.935
	Acetone	20.70	*V*	-997.8767	-997.9150	1.042
	Ethanol	24.55	*V*	-997.8768	-997.9157	1.058
	Acetonitrile	36.64	*V*	-997.8769	-997.9169	1.088
	Dimethylsulfoxide	46.70	*V*	-997.8770	-997.9174	1.101
	Water	78.39	*V*	-997.8770	-997.9183	1.122
	EA experimental /eV		-0.82			
	EA Linear extrap./eV		-1.01			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-414.9754	-414.9863	0.299
Uracil	Krypton	1.52	*V*	-414.9764	-414.9902	0.377
	Heptane	1.92	*V*	-414.9800	-415.0034	0.639
	Ciclohexane	2.02	*V*	-414.9808	-415.0061	0.689
	Benzene	2.25	*V*	-414.9823	-415.0111	0.782
	Ethyl Ether	*4.34*	*V*	-414.9900	-415.0337	1.188
	Chloroform	4.90	*V*	-414.9911	-415.0366	1.238
	Chlorobenzene	5.62	*V*	-414.9922	-415.0395	1.288
	Tetrahydrofuran	7.58	*V*	-414.9943	-415.0448	1.375
	Dichloroethane	10.36	*V*	-414.9960	-415.0490	1.442
	Acetone	20.70	*V*	-414.9984	-415.0548	1.534
	Ethanol	24.55	*V*	-414.9988	-415.0557	1.548
	Dimethylsulfoxide	46.70	*V*	-414.9998	-415.0581	1.585
	Water	78.39	*V*	-415.0004	-415.0594	1.569
	EA experimental /eV		-0.27			
	EA Linear extrap./eV		-0.27			
	R^2		1.0000			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	AEA/ eV
	Argon	1.43	*V*	-414.9754	-414.9985	0.747
Uracil	Krypton	1.52	*V*	-414.9764	-415.0024	0.826
(adiabatic)	Heptane	1.92	*V*	-414.9800	-415.0156	1.086
	Ciclohexane	2.02	*V*	-414.9808	-415.0182	1.136
	Benzene	2.25	*V*	-414.9823	-415.0232	1.231
	Ethyl Ether	*4.34*	*V*	-414.9900	-415.0457	1.634
	Chloroform	4.90	*V*	-414.9911	-415.0487	1.685
	Chlorobenzene	5.62	*V*	-414.9922	-415.0515	1.733
	Tetrahydrofuran	7.58	*V*	-414.9943	-415.0568	1.820
	Dichloroethane	10.36	*V*	-414.9960	-415.0610	1.886
	Acetone	20.70	*V*	-414.9984	-415.0667	1.978
	Ethanol	24.55	*V*	-414.9988	-415.0678	1.997
	Acetonitrile	36.64	*V*	-414.9998	-415.0695	2.014
	Dimethylsulfoxide	46.70	*V*	-414.9998	-415.0719	2.081
	Water	78.39	*V*	-415.0004	-415.0733	2.103
	EA experimental /eV		0.17			
	EA Linear extrap./eV		0.16			
	R^2		0.9985			

3.4. Table S4. ΔE vs (1/ε) extrapolation details for the N anions on Table 2

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	N	-233.4959	-233.4714	-0.6675
1,4-cyclohexadiene	Kripton	1.52	N	-233.4960	-233.4737	-0.6080
	Heptane	1.92	V	-233.4965	-233.4668	-0.8079
	Ciclohexane	2.02	V	-233.4966	-233.4688	-0.7574
	Benzene	2.25	V	-233.4968	-233.4728	-0.6554
	Ether	4.34	V	-233.4979	-233.4904	-0.2043
	Chloroform	4.9	V	-233.4981	-233.4927	-0.1470
	Dichloroethane	5.62	V	-233.4982	-233.4949	-0.0909
	THF	7.58	V	-233.4986	-233.4989	0.0093
	Chlorobenzene	10.36	V	-233.4988	-233.5020	0.0870
	Acetone	20.7	V	-233.4992	-233.5063	0.1939
	Ethanol	24.55	V	-233.4993	-233.5070	0.2111
	Acetonitrile	36.64	V	-233.4994	-233.5082	0.2412
	DMSO	46.7	V	-233.4994	-233.5088	0.2540
	EA experimental./eV		-1.75			
	EA Linear extrap./eV		-1.84			
	R^2		0.9996			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-196.6070	-196.5827	-0.662
2-methyl-2-butene	Krypton	1.52	*N*	-196.6071	-196.5851	-0.599
	Heptane	1.92	*N*	-196.6072	-196.5931	-0.385
	Ciclohexane	2.02	*N*	-196.6073	-196.5947	-0.343
	Benzene	2.25	*N*	-196.6073	-196.5976	-0.265
	Ethyl Ether	4.34	*N*	-196.6077	-196.6112	0.096
	Chloroform	4.90	*N*	-196.6078	-196.6131	0.145
	Chlorobenzene	5.62	*V*	-196.6078	-196.5984	-0.256
	Tetrahydrofuran	7.58	*V*	-196.6079	-196.6022	-0.157
	Dichloroethane	10.36	*V*	-196.6080	-196.6051	-0.080
	Acetone	20.70	*V*	-196.6082	-196.6093	0.030
	Ethanol	24.55	*V*	-196.6082	-196.6100	0.048
	Acetonitrile	36.64	*V*	-196.6082	-196.6112	0.080
	Dimethylsulfoxide	46.70	*V*	-196.6083	-196.6117	0.093
	Water	78.39	*V*	-196.6083	-196.6126	0.117
	EA experimental./eV		-2.24			
	EA Linear extrap./eV		-2.11			
	R^2		0.9996			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-229.1785	-229.1587	-0.539
acetic acid	Krypton	1.52	*V*	-229.1790	-229.1616	-0.473
	Heptane	1.92	*V*	-229.1807	-229.1715	-0.251
	Ciclohexane	2.02	*V*	-229.1811	-229.1511	-0.815
	Benzene	2.25	*V*	-229.1818	-229.1561	-0.700
	Ethyl Ether	4.34	*V*	-229.1855	-229.1790	-0.175
	Chloroform	4.9	*V*	-229.1860	-229.1821	-0.105
	Chlorobenzene	5.62	*V*	-229.1865	-229.1851	-0.039
	Tetrahydrofuran	7.58	*V*	-229.1875	-229.1905	0.082
	Dichloroethane	10.36	*V*	-229.1883	-229.1948	0.176
	Acetone	20.7	*V*	-229.1895	-229.2007	0.306
	Ethanol	24.55	*V*	-229.1897	-229.2017	0.327
	Acetonitrile	36.64	*V*	-229.1900	-229.2034	0.364
	Dimethylsulfoxide	45.6	*V*	-229.1902	-229.2041	0.378
	Water	78.39	*V*	-229.1904	-229.2054	0.407
	EA experimental./eV		-1.80			
	EA Linear extrap./eV		-2.15			
	R^2		0.9996			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-193.2283	-193.2027	-0.696
Acetone	Krypton	1.52	*V*	-193.2285	-193.2062	-0.608
	Heptane	1.92	*V*	-193.2294	-193.2182	-0.304
	Ciclohexane	2.02	*V*	-193.2296	-193.2207	-0.243
	Benzene	2.25	*V*	-193.2300	-193.2252	-0.129
	Ethyl Ether	4.34	*V*	-193.2318	-193.2461	0.387
	Chloroform	4.90	*V*	-193.2321	-193.2489	0.456
	Chlorobenzene	5.62	*V*	-193.2324	-193.2515	0.521
	Tetrahydrofuran	7.58	*V*	-193.2329	-193.2565	0.641
	Dichloroethane	10.36	*V*	-193.2333	-193.2603	0.734
	Acetone	20.70	*V*	-193.2340	-193.2658	0.865
	Ethanol	24.55	*V*	-193.2341	-193.2667	0.889
	Acetonitrile	36.64	*V*	-193.2343	-193.2683	0.926
	Dimethylsulfoxide	46.70	*V*	-193.2343	-193.2688	0.938
	Water	78.39	*V*	-193.2345	-193.2704	0.975
	EA experimental /eV		-1.51			
	EA Linear extrap./eV		-1.46			
	R^2		0.9988			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-77.3616	-77.3062	-1.509
Acetylene	Krypton	1.52	*N*	-77.3618	-77.3094	-1.426
	Heptane	1.92	*N*	-77.3626	-77.3209	-1.135
	Ciclohexane	2.02	*V*	-77.3628	-77.3232	-1.078
	Benzene	2.25	*V*	-77.3631	-77.3276	-0.967
	Ethyl Ether	4.34	*V*	-77.3648	-77.3483	-0.447
	Chloroform	4.90	*V*	-77.3650	-77.3511	-0.378
	Chlorobenzene	5.62	*V*	-77.3652	-77.3539	-0.309
	Tetrahydrofuran	7.58	*V*	-77.3657	-77.3589	-0.185
	Dichloroethane	10.36	*V*	-77.3660	-77.3628	-0.087
	Acetone	20.70	*V*	-77.3665	-77.3683	0.049
	Ethanol	24.55	*V*	-77.3666	-77.3692	0.071
	Acetonitrile	36.64	*V*	-77.3668	-77.3708	0.109
	Dimethylsulfoxide	46.70	*V*	-77.3668	-77.3715	0.127
	Water	78.39	*V*	-77.3669	-77.3724	0.150
	EA experimental /eV		-2.60			
	EA Linear extrap./eV		-2.40			
	R^2		0.9984			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-116.7023	-116.6671	-0.957
Allene	Krypton	1.52	*V*	-116.7023	-116.6701	-0.876
	Heptane	1.92	*V*	-116.7026	-116.6806	-0.601
	Ciclohexane	2.02	*V*	-116.7027	-116.6826	-0.547
	Benzene	2.25	*V*	-116.7028	-116.6864	-0.446
	Ethyl Ether	4.34	*V*	-116.7035	-116.7035	0.000
	Chloroform	4.90	*V*	-116.7036	-116.7057	0.058
	Chlorobenzene	5.62	*V*	-116.7037	-116.7078	0.113
	Tetrahydrofuran	7.58	*V*	-116.7039	-116.7117	0.212
	Dichloroethane	10.36	*V*	-116.7040	-116.7146	0.289
	Acetone	20.70	*V*	-116.7042	-116.7187	0.394
	Ethanol	24.55	*V*	-116.7043	-116.7194	0.411
	Acetonitrile	36.64	*V*	-116.7043	-116.7205	0.441
	Dimethylsulfoxide	46.70	*V*	-116.7043	-116.7210	0.453
	Water	78.39	*V*	-116.7044	-116.7219	0.476
	EA experimental /eV		-1.88			
	EA Linear extrap./eV		-1.60			
	R^2		0.9998			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-267.2526	-267.2319	-0.562
Butyrolactone	Krypton	1.52	*N*	-267.2530	-267.2346	-0.500
	Heptane	1.92	*N*	-267.2544	-267.2438	-0.289
	Ciclohexane	2.02	*V*	-267.2547	-267.2311	-0.643
	Benzene	2.25	*V*	-267.2553	-267.2354	-0.543
	Ethyl Ether	4.34	*V*	-267.2582	-267.2564	-0.050
	Chloroform	4.90	*V*	-267.2586	-267.2593	0.018
	Chlorobenzene	5.62	*V*	-267.2590	-267.2622	0.087
	Tetrahydrofuran	7.58	*V*	-267.2598	-267.2675	0.210
	Dichloroethane	10.36	*V*	-267.2605	-267.2718	0.308
	Acetone	20.70	*V*	-267.2614	-267.2777	0.444
	Ethanol	24.55	*V*	-267.2615	-267.2786	0.466
	Acetonitrile	36.64	*V*	-267.2618	-267.2803	0.505
	Dimethylsulfoxide	46.70	*V*	-267.2619	-267.2811	0.522
	Water	78.39	*V*	-267.2621	-267.2822	0.548
	EA experimental /eV		-1.93			
	EA Linear extrap./eV		-1.93			
	R^2		0.9969			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2691.4980	-2691.4568	-1.120
***cis*-1-bromo-**	Krypton	1.52	*V*	-2691.4980	-2691.4601	-1.032
-1-propene	Heptane	1.92	*V*	-2691.4979	-2691.4710	-0.731
	Ciclohexane	2.02	*V*	-2691.4978	-2691.4732	-0.668
	Benzene	2.25	*V*	-2691.4977	-2691.4772	-0.557
	Ethyl Ether	4.34	*V*	-2691.4974	-2691.4953	-0.056
	Chloroform	4.90	*V*	-2691.4971	-2691.4976	0.014
	Chlorobenzene	5.62	*V*	-2691.4969	-2691.4999	0.083
	Tetrahydrofuran	7.58	*V*	-2691.4967	-2691.5040	0.198
	Dichloroethane	10.36	*V*	-2691.4966	-2691.5072	0.289
	Acetone	20.70	*V*	-2691.4956	-2691.5116	0.435
	Ethanol	24.55	*V*	-2691.4954	-2691.5123	0.460
	Acetonitrile	36.64	*V*	-2691.4953	-2691.5135	0.497
	Dimethylsulfoxide	46.70	*V*	-2691.4948	-2691.5140	0.523
	Water	78.39	*V*	-2691.4947	-2691.5150	0.553
	EA experimental /eV		-1.49			
	EA Linear extrap./eV		-1.88			
	R^2		0.9979			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-277.1577	-277.1339	-0.65
cis 1,2-difluor-	Krypton	1.52	*V*	-277.1579	-277.1123	-1.24
ethylene	Heptane	1.92	*V*	-277.1587	-277.1241	-0.94
	Ciclohexane	2.02	*V*	-277.1589	-277.1265	-0.88
	Benzene	2.25	*V*	-277.1592	-277.1308	-0.77
	Ethyl Ether	4.34	*V*	-277.1610	-277.1502	-0.29
	Chloroform	4.9	*V*	-277.1612	-277.1527	-0.23
	Chlorobenzene	5.62	*V*	-277.1615	-277.1551	-0.17
	Tetrahydrofuran	7.58	*V*	-277.1619	-277.1595	-0.07
	Dichloroethane	10.36	*V*	-277.1623	-277.1628	0.01
	Acetone	20.7	*V*	-277.1629	-277.1675	0.13
	Ethanol	24.55	*V*	-277.1630	-277.1682	0.14
	Acetonitrile	36.64	*V*	-277.1631	-277.1695	0.17
	Dimethylsulfoxide	46.7	*V*	-277.1632	-277.1701	0.19
	Water	78.39	*V*	-277.1633	-277.1711	0.21
	EA experimental /eV		-2.18			
	EA Linear extrap./eV		-2.02			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-157.2782	-157.2521	-0.711
***cis*-2-butene**	Krypton	1.52	*N*	-157.2783	-157.2546	-0.645
	Heptane	1.92	*N*	-157.2785	-157.2631	-0.419
	Ciclohexane	2.02	*N*	-157.2786	-157.2648	-0.376
	Benzene	2.25	*N*	-157.2787	-157.2679	-0.294
	Ethyl Ether	4.34	*V*	-157.2792	-157.2610	-0.494
	Chloroform	4.90	*V*	-157.2793	-157.2634	-0.431
	Chlorobenzene	5.62	*V*	-157.2793	-157.2658	-0.369
	Tetrahydrofuran	7.58	*V*	-157.2795	-157.2700	-0.258
	Dichloroethane	10.36	*V*	-157.2796	-157.2733	-0.172
	Acetone	20.70	*V*	-157.2798	-157.2779	-0.052
	Ethanol	24.55	*V*	-157.2798	-157.2787	-0.032
	Acetonitrile	36.64	*V*	-157.2799	-157.2800	0.002
	Dimethylsulfoxide	46.70	*V*	-157.2799	-157.2815	0.044
	Water	78.39	*V*	-157.2800	-157.2815	0.042
	EA experimental /eV		-2.22			
	EA Linear extrap./eV		-2.42			
	R^2		0.9983			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-156.0249	-155.9895	-0.964
Cyclobutene	Krypton	1.52	*N*	-156.0250	-155.9919	-0.900
	Heptane	1.92	*V*	-156.0253	-155.9896	-0.971
	Ciclohexane	2.02	*V*	-156.0253	-155.9918	-0.911
	Benzene	2.25	*V*	-156.0254	-155.9961	-0.799
	Ethyl Ether	4.34	*V*	-156.0261	-156.0151	-0.297
	Chloroform	4.90	*V*	-156.0262	-156.0176	-0.233
	Chlorobenzene	5.62	*V*	-156.0262	-156.0200	-0.170
	Tetrahydrofuran	7.58	*V*	-156.0264	-156.0243	-0.057
	Dichloroethane	10.36	*V*	-156.0266	-156.0277	0.030
	Acetone	20.70	*V*	-156.0268	-156.0323	0.150
	Ethanol	24.55	*V*	-156.0268	-156.0330	0.170
	Acetonitrile	36.64	*V*	-156.0269	-156.0344	0.204
	Dimethylsulfoxide	46.70	*V*	-156.0269	-156.0349	0.218
	Water	78.39	*V*	-156.0269	-156.0358	0.242
	EA experimental /eV		-2.00			
	EA Linear extrap./eV		-2.12			
	R^2		0.9997			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-195.3910	-195.3612	-0.809
Cyclopentene	Krypton	1.52	*N*	-195.3910	-195.3636	-0.747
	Heptane	1.92	*N*	-195.3913	-195.3716	-0.537
	Ciclohexane	2.02	*N*	-195.3914	-195.3732	-0.496
	Benzene	2.25	*N*	-195.3915	-195.3761	-0.420
	Ethyl Ether	4.34	*N*	-195.3921	-195.3891	-0.082
	Chloroform	4.90	*N*	-195.3922	-195.3909	-0.037
	Chlorobenzene	5.62	*N*	-195.3923	-195.3927	0.010
	Tetrahydrofuran	7.58	*V*	-195.3925	-195.3833	-0.251
	Dichloroethane	10.36	*V*	-195.3927	-195.3866	-0.165
	Acetone	20.70	*V*	-195.3929	-195.3912	-0.045
	Ethanol	24.55	*V*	-195.3929	-195.3920	-0.026
	Acetonitrile	36.64	*V*	-195.3930	-195.3933	0.008
	Dimethylsulfoxide	46.70	*V*	-195.3930	-195.3938	0.023
	Water	78.39	*V*	-195.3930	-195.3948	0.046
	EA experimental /eV		-2.14			
	EA Linear extrap./eV		-2.42			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.4300	*N*	-466.2256	-466.2009	-0.67
Di-tert-butyl-	Krypton	1.5190	*N*	-466.2257	-466.2027	-0.63
peroxide	Heptane	1.9200	*N*	-466.2261	-466.2093	-0.46
	Ciclohexane	2.0230	*N*	-466.2262	-466.2104	-0.43
	Benzene	2.2470	*N*	-466.2264	-466.2128	-0.37
	Ethyl Ether	4.3350	*N*	-466.2275	-466.2236	-0.11
	Chloroform	4.9000	*N*	-466.2278	-466.2250	-0.08
	Chlorobenzene	5.6210	*N*	-466.2278	-466.2265	-0.04
	Tetrahydrofuran	7.5800	*N*	-466.2283	-466.2290	0.02
	Dichloroethane	10.3600	*N*	-466.2285	-466.2311	0.07
	Acetone	20.7000	*N*	-466.2291	-466.2341	0.13
	Ethanol	24.5500	*V*	-466.2295	-466.2307	0.03
	Acetonitrile	36.6400	*V*	-466.2297	-466.2318	0.06
	EA experimental /ε	-2.00				
	EA Linear extrap./ε	-1.80				
	R^2	0.9951				
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-342.5282	-342.5073	-0.569
Ethylene	Krypton	1.52	*N*	-342.5290	-342.5097	-0.526
Carbonate	Heptane	1.92	*N*	-342.5315	-342.5176	-0.378
	Ciclohexane	2.02	*N*	-342.5322	-342.5192	-0.353
	Benzene	2.25	*N*	-342.5334	-342.5221	-0.307
	Ethyl Ether	4.34	*N*	-342.5390	-342.5209	-0.494
	Chloroform	4.90	*N*	-342.5401	-342.5232	-0.458
	Chlorobenzene	5.62	*N*	-342.5407	-342.5259	-0.404
	Tetrahydrofuran	7.58	*V*	-342.5425	-342.5309	-0.314
	Dichloroethane	10.36	*V*	-342.5438	-342.5356	-0.221
	Acetone	20.70	*V*	-342.5457	-342.5429	-0.076
	Ethanol	24.55	*V*	-342.5462	-342.5441	-0.058
	Acetonitrile	36.64	*V*	-342.5469	-342.5462	-0.017
	Dimethylsulfoxide	46.70	*V*	-342.5468	-342.5472	0.012
	EA experimental /eV		-2.93			
	EA Linear extrap./eV		-2.85			
	R^2		0.9979			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-177.8940	-177.8534	-1.103
Fluorethylene	Krypton	1.52	*V*	-177.8941	-177.8570	-1.010
	Heptane	1.92	*V*	-177.8946	-177.8691	-0.694
	Ciclohexane	2.02	*V*	-177.8947	-177.8715	-0.633
	Benzene	2.25	*V*	-177.8950	-177.8759	-0.518
	Ethyl Ether	4.34	*V*	-177.8960	-177.8955	-0.014
	Chloroform	4.90	*V*	-177.8962	-177.8981	0.050
	Chlorobenzene	5.62	*V*	-177.8964	-177.9004	0.111
	Tetrahydrofuran	7.58	*V*	-177.8967	-177.9049	0.223
	Dichloroethane	10.36	*V*	-177.8969	-177.9082	0.308
	Acetone	20.70	*V*	-177.8972	-177.9129	0.425
	Ethanol	24.55	*V*	-177.8973	-177.9136	0.443
	Acetonitrile	36.64	*V*	-177.8974	-177.9149	0.476
	Dimethylsulfoxide	46.70	*V*	-177.8975	-177.9155	0.490
	Water	78.39	*V*	-177.8975	-177.9163	0.511
	EA experimental /eV		-1.91			
	EA Linealr extrap./eV		-1.82			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-169.9662	-169.9421	-0.655
Formamide	Krypton	1.52	*N*	-169.9668	-169.9450	-0.592
	Heptane	1.92	*V*	-169.9690	-169.9328	-0.986
	Ciclohexane	2.02	*V*	-169.9695	-169.9355	-0.924
	Benzene	2.25	*V*	-169.9704	-169.9407	-0.809
	Ethyl Ether	4.34	*V*	-169.9751	-169.9645	-0.288
	Chloroform	4.90	*V*	-169.9757	-169.9676	-0.221
	Chlorobenzene	5.62	*V*	-169.9764	-169.9707	-0.155
	Tetrahydrofuran	7.58	*V*	-169.9777	-169.9763	-0.037
	Dichloroethane	10.36	*V*	-169.9787	-169.9807	0.055
	Acetone	20.70	*V*	-169.9802	-169.9868	0.181
	Ethanol	24.55	*V*	-169.9804	-169.9878	0.201
	Acetonitrile	36.64	*V*	-169.9808	-169.9895	0.237
	Dimethylsulfoxide	46.70	*V*	-169.9810	-169.9903	0.252
	Water	78.39	*V*	-169.9813	-169.9915	0.277
	EA experimental /eV		-2.05			
	EA Linear extrap./eV		-2.19			
	R^2		0.9996			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-230.1023	-230.0630	-1.070
Furan	Krypton	1.52	*V*	-230.1026	-230.0664	-0.983
	Heptane	1.92	*V*	-230.1033	-230.0781	-0.687
	Ciclohexane	2.02	*V*	-230.1035	-230.0804	-0.629
	Benzene	2.25	*V*	-230.1038	-230.0847	-0.521
	Ethyl Ether	4.34	*V*	-230.1055	-230.1041	-0.039
	Chloroform	4.90	*V*	-230.1058	-230.1066	0.023
	Chlorobenzene	5.62	*V*	-230.1060	-230.1091	0.083
	Tetrahydrofuran	7.58	*V*	-230.1065	-230.1135	0.191
	Dichloroethane	10.36	*V*	-230.1069	-230.1170	0.275
	Acetone	20.70	*V*	-230.1074	-230.1218	0.390
	Ethanol	24.55	*V*	-230.1075	-230.1225	0.409
	Acetonitrile	36.64	*V*	-230.1077	-230.1239	0.441
	Dimethylsulfoxide	46.70	*V*	-230.1078	-230.1245	0.455
	Water	78.39	*V*	-230.1079	-230.1255	0.479
	EA experimental /eV		-1.76			
	EA Linear extrap./eV		-1.75			
	R^2		0.9997			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Ciclohexane	2.02	*N*	-542.7610	-542.7620	0.028
Guanine	Benzene	2.25	*V*	-542.7634	-542.7620	-0.037
	Ethyl Ether	4.34	*V*	-542.7752	-542.7925	0.472
	Chloroform	4.90	*V*	-542.7772	-542.7968	0.532
	Chlorobenzene	5.62	*V*	-542.7787	-542.8009	0.604
	Tetrahydrofuran	7.58	*V*	-542.7823	-542.8086	0.716
	Dichloroethane	10.36	*V*	-542.7851	-542.8148	0.808
	Acetone	20.70	*V*	-542.7891	-542.8235	0.935
	Ethanol	24.55	*V*	-542.7898	-542.8250	0.958
	Acetonitrile	36.64	*V*	-542.7910	-542.8275	0.995
	Dimethylsulfoxide	46.70	*V*	-542.7915	-542.8286	1.009
	Water	78.39	*V*	-542.7934	-542.8308	1.017
	EA experimental /eV		-1.40			
	EA Linear extrap./eV		-1.41			
	R^2		0.9992			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-226.2987	-226.2504	-1.316
Imidazole	Krypton	1.52	*N*	-226.2993	-226.2535	-1.246
	Heptane	1.92	*N*	-226.3015	-226.2650	-0.994
	Ciclohexane	2.02	*N*	-226.3020	-226.2673	-0.944
	Benzene	2.25	*V*	-226.3029	-226.2717	-0.849
	Ethyl Ether	4.34	*V*	-226.3075	-226.2931	-0.394
	Chloroform	4.90	*V*	-226.3083	-226.2959	-0.336
	Chlorobenzene	5.62	*V*	-226.3089	-226.2990	-0.272
	Tetrahydrofuran	7.58	*V*	-226.3103	-226.3043	-0.163
	Dichloroethane	10.36	*V*	-226.3114	-226.3085	-0.077
	Acetone	20.70	*V*	-226.3129	-226.3146	0.045
	Ethanol	24.55	*V*	-226.3131	-226.3155	0.063
	Acetonitrile	36.64	*V*	-226.3136	-226.3172	0.098
	Dimethylsulfoxide	46.70	*V*	-226.3138	-226.3181	0.117
	Water	78.39	*V*	-226.3145	-226.3190	0.122
	EA experimental /eV		-2.13			
	EA Linear extrap./eV		-2.15			
	R^2		0.9981			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-193.1857	-193.1530	-0.89
methyl vinyl ether	Krypton	1.52	*N*	-193.1859	-193.1551	-0.84
	Heptane	1.92	*V*	-193.1868	-193.1508	-0.98
	Ciclohexane	2.02	*V*	-193.1870	-193.1533	-0.92
	Benzene	2.25	*V*	-193.1874	-193.1578	-0.8
	Ethyl Ether	4.34	*V*	-193.1893	-193.1800	-0.25
	Chloroform	4.9	*V*	-193.1896	-193.1829	-0.18
	Chlorobenzene	5.62	*V*	-193.1899	-193.1860	-0.11
	Tetrahydrofuran	7.58	*V*	-193.1904	-193.1913	0.02
	Dichloroethane	10.36	*V*	-193.1909	-193.1956	0.13
	Acetone	20.7	*V*	-193.1916	-193.2016	0.27
	Ethanol	24.55	*V*	-193.1917	-193.2025	0.29
	Acetonitrile	36.64	*V*	-193.1919	-193.2043	0.34
	Dimethylsulfoxide	45.6	*V*	-193.1919	-193.2052	0.36
	Water	78.39	*V*	-193.1922	-193.2060	0.38
	EA experimental /eV		-2.30			
	EA Linear extrap./eV		-2.30			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-117.9512	-117.9076	-1.188
Propene	Krypton	1.52	*V*	-117.9513	-117.9109	-1.100
	Heptane	1.92	*V*	-117.9515	-117.9222	-0.799
	Ciclohexane	2.02	*V*	-117.9516	-117.9244	-0.741
	Benzene	2.25	*V*	-117.9517	-117.9285	-0.630
	Ethyl Ether	4.34	*V*	-117.9522	-117.9472	-0.137
	Chloroform	4.90	*V*	-117.9523	-117.9496	-0.073
	Chlorobenzene	5.62	*V*	-117.9523	-117.9519	-0.011
	Tetrahydrofuran	7.58	*V*	-117.9525	-117.9561	0.100
	Dichloroethane	10.36	*V*	-117.9526	-117.9594	0.186
	Acetone	20.70	*V*	-117.9528	-117.9640	0.305
	Ethanol	24.55	*V*	-117.9528	-117.9647	0.324
	Acetonitrile	36.64	*V*	-117.9528	-117.9660	0.358
	Dimethylsulfoxide	46.70	*V*	-117.9529	-117.9665	0.372
	Water	78.39	*V*	-117.9529	-117.9674	0.395
	EA experimental /eV		-1.99			
	EA Linear extrap./eV		-1.90			
	R^2		0.9996			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-116.7000	-116.6684	-0.860
Propyne	Krypton	1.52	*N*	-116.7002	-116.6704	-0.813
	Heptane	1.92	*N*	-116.7010	-116.6773	-0.643
	Ciclohexane	2.02	*N*	-116.7011	-116.6787	-0.611
	Benzene	2.25	*N*	-116.7015	-116.6813	-0.548
	Ethyl Ether	4.34	*N*	-116.7030	-116.6941	-0.243
	Chloroform	4.9	*V*	-116.7033	-116.6785	-0.674
	Chlorobenzene	5.62	*V*	-116.7035	-116.6810	-0.610
	Tetrahydrofuran	7.58	*V*	-116.7039	-116.6854	-0.503
	Dichloroethane	10.36	*V*	-116.7042	-116.6890	-0.415
	Acetone	20.7	*V*	-116.7047	-116.6941	-0.290
	Ethanol	24.55	*V*	-116.7048	-116.6949	-0.270
	Dimethylsulfoxide	45.6	*V*	-116.7050	-116.6971	-0.216
	Water	78.39	*V*	-116.7052	-116.6979	-0.198
	EA experimental /eV		-2.80			
	EA Linear extrap./eV		-2.67			
	R^2		0.9997			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-267.2526	-267.2319	-0.562
Propiolactone	Krypton	1.52	*N*	-267.2530	-267.2346	-0.500
	Heptane	1.92	*N*	-267.2544	-267.2438	-0.289
	Ciclohexane	2.02	*V*	-267.2547	-267.2311	-0.643
	Benzene	2.25	*V*	-267.2553	-267.2354	-0.543
	Ethyl Ether	4.34	*V*	-267.2582	-267.2564	-0.050
	Chloroform	4.90	*V*	-267.2586	-267.2593	0.018
	Chlorobenzene	5.62	*V*	-267.2590	-267.2622	0.087
	Tetrahydrofuran	7.58	*V*	-267.2598	-267.2675	0.210
	Dichloroethane	10.36	*V*	-267.2605	-267.2718	0.308
	Acetone	20.70	*V*	-267.2614	-267.2777	0.444
	Ethanol	24.55	*V*	-267.2615	-267.2786	0.466
	Acetonitrile	36.64	*V*	-267.2618	-267.2803	0.505
	Dimethylsulfoxide	46.70	*V*	-267.2619	-267.2811	0.522
	Water	78.39	*V*	-267.2621	-267.2822	0.548
	EA experimental /eV		-1.90			
	EA Linear extrap./eV		-1.93			
	R^2		0.9969			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	N	-210.2441	-210.2229	-0.578
Pyrrole	Kripton	1.52	N	-210.2445	-210.2253	-0.523
	Ciclohexane	2.02	N	-210.2462	-210.2350	-0.304
	Benzene	2.25	N	-210.2468	-210.2381	-0.238
	Ether	4.34	V	-210.2500	-210.2285	-0.586
	Chloroform	4.9	V	-210.2505	-210.2311	-0.529
	Chlorobenzene	5.62	V	-210.2509	-210.2336	-0.472
	Tetrahydrofuran	7.58	V	-210.2518	-210.2382	-0.371
	Dichloroethane	10.36	V	-210.2526	-210.2419	-0.291
	Acetone	20.7	V	-210.2537	-210.2478	-0.159
	Dimethylsulfoxide	46.7	V	-210.2543	-210.2499	-0.119
	Water	78.39	V	-210.2546	-210.2510	-0.098
	EA experimental /eV		-2.38			
	EA Linear extrap./eV		-2.21			
	R^2		0.9985			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Ciclohexane	2.02	*N*	-235.9296	-235.9127	-0.458
Tetramethyl	Benzene	2.25	*N*	-235.9297	-235.9152	-0.396
ethylene	Ethyl Ether	4.34	*V*	-235.9303	-235.9061	-0.657
	Chloroform	4.9	*V*	-235.9303	-235.9083	-0.600
	Chlorobenzene	5.62	*V*	-235.9304	-235.9110	-0.529
	Tetrahydrofuran	7.58	*V*	-235.9306	-235.9153	-0.415
	Dichloroethane	10.36	*V*	-235.9307	-235.9188	-0.324
	Acetone	20.7	*V*	-235.9308	-235.9236	-0.196
	Ethanol	24.55	*V*	-235.9309	-235.9245	-0.173
	Acetonitrile	36.64	*V*	-235.9309	-235.9260	-0.134
	EA experimental /eV		-2.27			
	EA Linear extrap./eV		-2.65			
	R^2		0.9994			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-2691.4944	-2691.4629	-0.859
***trans*-1-bromo-**	Krypton	1.52	*V*	-2691.4946	-2691.4660	-0.777
-1-propene	Heptane	1.92	*V*	-2691.4951	-2691.4768	-0.496
	Ciclohexane	2.02	*V*	-2691.4952	-2691.4789	-0.441
	Benzene	2.25	*V*	-2691.4954	-2691.4829	-0.339
	Ethyl Ether	4.34	*V*	-2691.4964	-2691.5008	0.119
	Chloroform	4.90	*V*	-2691.4966	-2691.5031	0.178
	Chlorobenzene	5.62	*V*	-2691.4967	-2691.5054	0.235
	Tetrahydrofuran	7.58	*V*	-2691.4970	-2691.5094	0.338
	Dichloroethane	10.36	*V*	-2691.4973	-2691.5126	0.417
	Acetone	20.70	*V*	-2691.4976	-2691.5170	0.528
	Ethanol	24.55	*V*	-2691.4977	-2691.5177	0.545
	Acetonitrile	36.64	*V*	-2691.4978	-2691.5190	0.575
	Dimethylsulfoxide	46.70	*V*	-2691.4979	-2691.5195	0.587
	Water	78.39	*V*	-2691.4979	-2691.5204	0.613
	EA experimental /eV		-1.30			
	EA Linear extrap./eV		-1.52			
	R^2		0.9997			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-577.5800	-577.5452	-0.948
***trans*-1-chloro-**	Krypton	1.52	*V*	-577.5802	-577.5484	-0.863
-1-propene	Heptane	1.92	*V*	-577.5806	-577.5595	-0.575
	Ciclohexane	2.02	*V*	-577.5808	-577.5617	-0.519
	Benzene	2.25	*V*	-577.5810	-577.5658	-0.414
	Ethyl Ether	4.34	*V*	-577.5820	-577.5841	0.057
	Chloroform	4.90	*V*	-577.5822	-577.5864	0.117
	Chlorobenzene	5.62	*V*	-577.5823	-577.5888	0.176
	Tetrahydrofuran	7.58	*V*	-577.5826	-577.5929	0.281
	Dichloroethane	10.36	*V*	-577.5828	-577.5962	0.363
	Acetone	20.70	*V*	-577.5832	-577.6006	0.475
	Ethanol	24.55	*V*	-577.5832	-577.6014	0.494
	Acetonitrile	36.64	*V*	-577.5833	-577.6027	0.526
	Dimethylsulfoxide	46.70	*V*	-577.5834	-577.6032	0.539
	Water	78.39	*V*	-577.5835	-577.6042	0.563
	EA experimental /eV		-1.49			
	EA Linear extrap./eV		-1.63			
	R^2		0.9997			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*V*	-277.1561	-277.1137	-1.153
***Trans*-1,2-**	Krypton	1.52	*V*	-277.1563	-277.1173	-1.063
-difluorethylene	Heptane	1.92	*V*	-277.1571	-277.1292	-0.759
	Ciclohexane	2.02	*V*	-277.1572	-277.1315	-0.699
	Benzene	2.25	*V*	-277.1575	-277.1359	-0.589
	Ethyl Ether	4.34	*V*	-277.1590	-277.1553	-0.101
	Chloroform	4.90	*V*	-277.1592	-277.1577	-0.039
	Chlorobenzene	5.62	*V*	-277.1594	-277.1601	0.021
	Tetrahydrofuran	7.58	*V*	-277.1598	-277.1645	0.127
	Dichloroethane	10.36	*V*	-277.1601	-277.1678	0.210
	Acetone	20.70	*V*	-277.1606	-277.1724	0.322
	Ethanol	24.55	*V*	-277.1606	-277.1731	0.340
	Acetonitrile	36.64	*V*	-277.1608	-277.1744	0.372
	Water	78.39	*V*	-277.1609	-277.1758	0.407
	EA experimental /eV		-1.84			
	EA Linear extrap./eV		-1.85			
	R^2		0.9999			
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-157.2818	-157.2477	-0.930
***trans*-2-butene**	Krypton	1.52	*N*	-157.2819	-157.2501	-0.865
	Heptane	1.92	*V*	-157.2821	-157.2410	-1.120
	Ciclohexane	2.02	*V*	-157.2822	-157.2430	-1.065
	Benzene	2.25	*V*	-157.2823	-157.2469	-0.962
	Ethyl Ether	4.34	*V*	-157.2828	-157.2644	-0.498
	Chloroform	4.90	*V*	-157.2828	-157.2667	-0.438
	Chlorobenzene	5.62	*V*	-157.2829	-157.2690	-0.379
	Tetrahydrofuran	7.58	*V*	-157.2831	-157.2730	-0.273
	Dichloroethane	10.36	*V*	-157.2832	-157.2762	-0.190
	Acetone	20.70	*V*	-157.2834	-157.2806	-0.075
	Ethanol	24.55	*V*	-157.2834	-157.2813	-0.056
	Acetonitrile	36.64	*V*	-157.2834	-157.2826	-0.023
	Dimethylsulfoxide	46.70	*V*	-157.2835	-157.2831	-0.010
	Water	78.39	*V*	-157.2835	-157.2841	0.016
Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Ciclohexane	2.02	*N*	-376.4294	-376.4123	-0.466
trifluorethylene	Benzene	2.25	*N*	-376.4298	-376.4152	-0.395
	Ethyl Ether	4.34	*V*	-376.4316	-376.4144	-0.466
	Chloroform	4.9	*V*	-376.4319	-376.4168	-0.412
	Chlorobenzene	5.62	*V*	-376.4321	-376.4192	-0.351
	Tetrahydrofuran	7.58	*V*	-376.4327	-376.4234	-0.253
	Dichloroethane	10.36	*V*	-376.4331	-376.4267	-0.175
	Acetone	20.7	*V*	-376.4337	-376.4312	-0.068
	Ethanol	24.55	*V*	-376.4339	-376.4319	-0.054
	Acetonitrile	36.64	*V*	-376.4341	-376.4332	-0.024
	Dimethylsulfoxide	46.7	*V*	-376.4341	-376.4339	-0.006
	Water	78.39	*V*	-376.4349	-376.4344	-0.012
	EA experimental /eV		-2.40			
	EA Linear extrap./eV		-2.15			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
acetonitrile	Argon	1.43	*N*	-132.8044	-132.7906	-0.376
	Krypton	1.51	*N*	-132.8047	-132.7934	-0.308
	Heptane	1.92	*N*	-132.8058	-132.8030	-0.077
	Ciclohexane	2.02	*N*	-132.8061	-132.8049	-0.033
	Benzene	2.24	*N*	-132.8065	-132.8084	0.050
	Ethyl Ether	4.33	*N*	-132.8087	-132.8237	0.406
	Chloroform	4.90	*N*	-132.8090	-132.8256	0.450
	Tetrahydrofuran	7.58	*N*	-132.8099	-132.8308	0.569
	Acetone	20.70	*N*	-132.8110	-132.8370	0.707
	Ethanol	24.55	*N*	-132.8111	-132.8376	0.720
	Acetonitrile	36.64	*N*	-132.8113	-132.8386	0.742
	Water	78.39	*N*	-132.8115	-132.8397	0.767

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-475.5379	-475.5124	-0.696
tetrafluorethylene	Heptane	1.92	*N*	-475.5388	-475.5231	-0.429
	Ciclohexane	2.02	*N*	-475.5391	-475.5247	-0.392
	Benzene	2.25	*N*	-475.5395	-475.5277	-0.321
	Ethyl Ether	4.34	*N*	-475.5413	-475.5410	-0.007
	Chlorobenzene	5.62	*N*	-475.5418	-475.5444	0.070
	Tetrahydrofuran	7.58	*N*	-475.5424	-475.5473	0.132
	Dichloroethane	10.36	*N*	-475.5429	-475.5496	0.182
	Acetone	20.70	*N*	-475.5436	-475.5527	0.247
	Ethanol	24.55	*N*	-475.5438	-475.5532	0.254
	Acetonitrile	36.64	*N*	-475.5441	-475.5540	0.272
	Water	78.39	*N*	-475.5450	-475.5551	0.274

3.5. ΔE vs. 1/ε profiles obtained for some compounds on tables 1 and 2

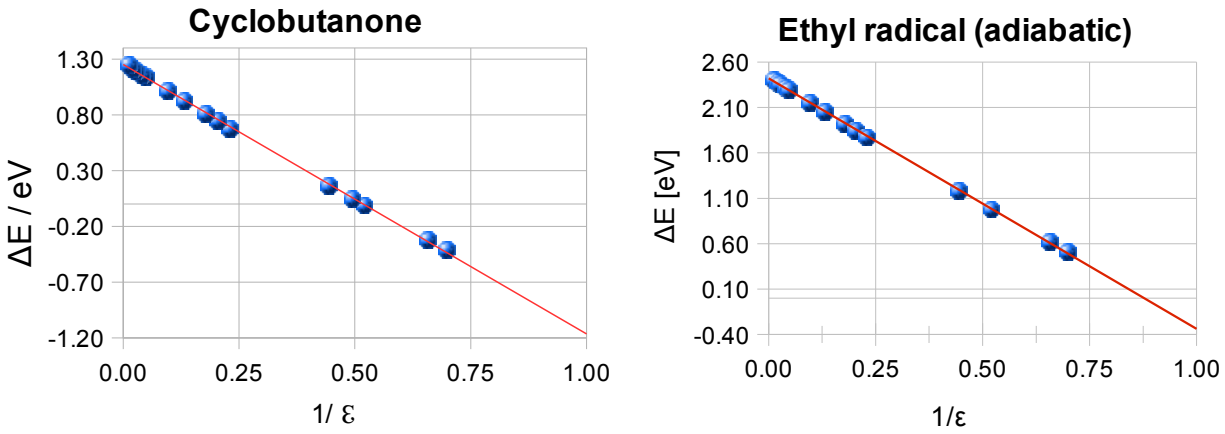


Figure S1. ΔE vs. 1/ ε profiles obtained for the compounds on table 1, cyclobutanone and ethyl radical.

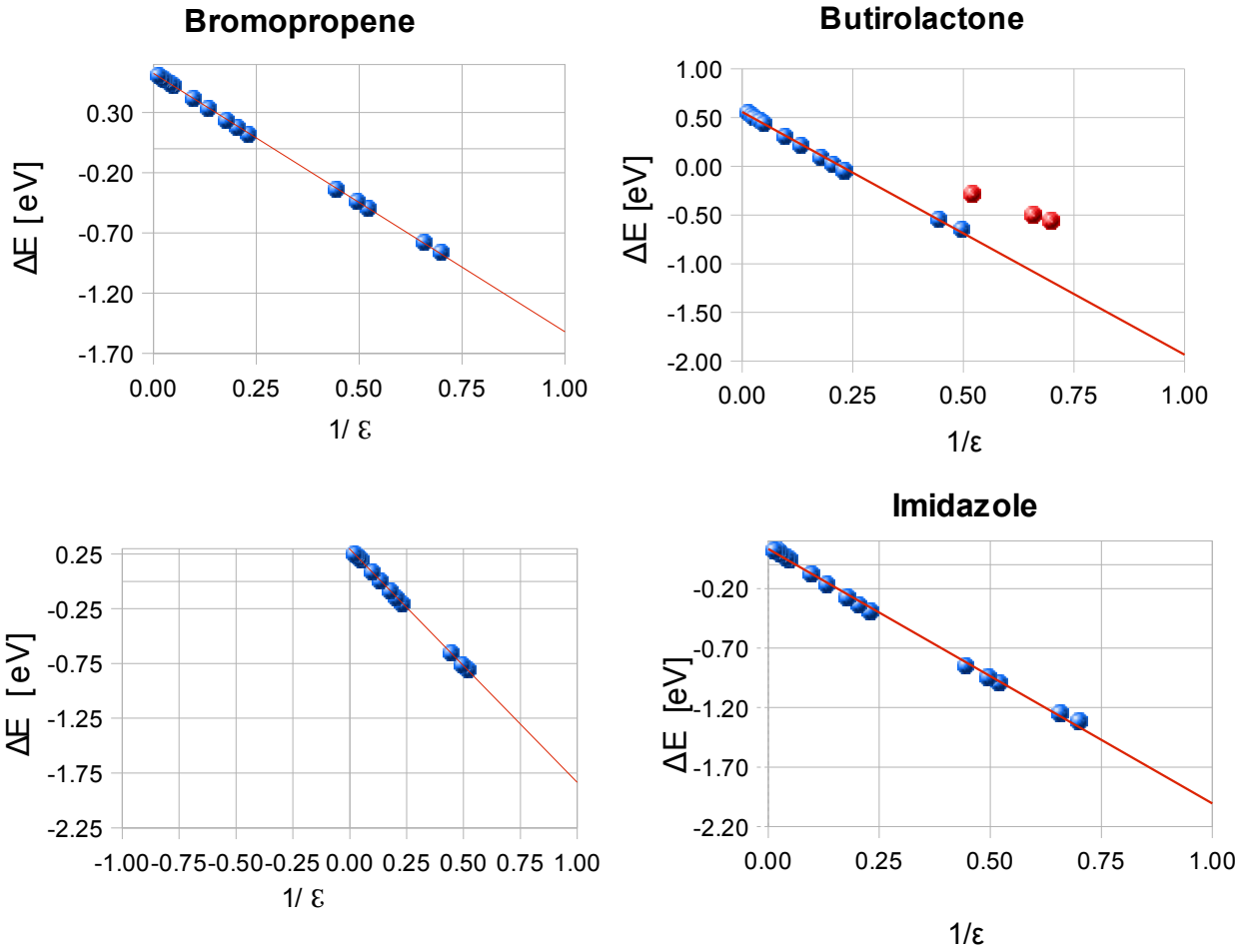


Figure S2. ΔE vs. 1/ ε profiles obtained for the compounds of table 2, bromopropene, butirolactone, 1,4-cyclohexadiene, and imidazol. ● Valence anion. ● Non valence anion.

Part 4. Comparison of the results obtained with different functionals and basis sets

4.1. **Table S5.** Electron affinities obtained with the 6-311+G(2df,p) and Aug-CC-pVTZ basis sets

Species	B3LYP/6-311+G(2df,p)			B3LYP/Aug-CC-pVTZ				Experimental[a,b]
	calc. eq. 1	anion type gas phase	extrapol. eq. 9	calc. eq. 1	anion type gas phase	extrapol. eq. 9	anion type solvent	
Acetone	*-1.05*	*N*	*-1.46*	-0.33	*N*	-1.20	*V*	-1.51
Adenine	-0.74	*V*	-0.79	-0.17	*V*	-0.86	*V*	-0.64
cyclobutene	-1.42	*N*	-2.12	-0.51	*N*	-2.10	*V*	-2.00
cyclopentadiene	-1.19	*V*	-1.22	-0.47	*V*	-1.34	*V*	-1.18
cyclopropene	-1.64	*V*	-1.70	-0.60	*N*	-1.67	*V*	-1.73
Cytosine	-0.55	*V*	-0.56	-0.03	*V*	-0.57	*V*	-0.36
Ethylene	-1.71	*V*	-1.75	-0.72	*N*	-1.71	*V*	-1.78
Fluorethylene	-1.45	*N*	-1.82	-0.66	*N*	-1.82	*V*	-1.91
Formamide	-1.18	*N*	-2.18	-0.26	*N*	-2.23	*V*	-2.05
Furan	-1.23	*N*	-1.75	-0.47	*N*	-1.71	*V*	-1.76
Propene	-1.33	*N*	-1.90	-0.48	*N*	-1.66	*V*	-1.99
Thiophene	-1.24	*V*	-1.29	-0.45	*N*	-1.28	*V*	-1.17
Thymine	-0.30	*V*	-0.34	-0.23	*V*	-0.48	*V*	-0.31
***trans*-1-bromo-1-propene**	-0.30	*N*	-1.51	-0.39	*N*	-1.59	*V*	-1.30
***trans*-1-chloro-1-propene**	-1.14	*N*	-1.62	-0.42	*N*	-1.57	*V*	-1.49
uracil	-0.27	*V*	-0.26	-0.04	*N*	-0.27	*V*	-0.21
1,4-cyclohexadiene	-1.10	*N*	-1.84	-0.40	*N*	-0.60	*N*	-1.75
Imidazole	-0.90	*N*	-2.15	-0.23	*N*	-0.32	*N*	-2.13
Propiolactone	-1.01	*N*	-1.93	-0.26	*N*	-1.29	*N*	-1.90
***trans*-2-butene**	-1.40	*N*	-2.20	-0.5	*N*	-0.67	*N*	-2.10

a) The esa are expressed in eV. b) For experimental references see main text reference 25

4.2. **Table S6.** Gas phase calculation details for the compounds on Table S5

Species	B3LYP/Aug-CC-pVDZ			B3LYP/Aug.CC-pVTZ//B3LYP/Aug-CC-pVDZ		
	E(neutral)	ZPE	E(anion)	E(neutral)	E(anion)	Anion type gas phase
Acetone	-193.18162	0.08286	-193.16641	*-193.23586*	-193.22381	*N*
Adenine	-467.38951	0.11145	-467.38046	-467.49578	-467.48947	*V*
cyclobutene	-155.98954	0.08572	-155.96617	-156.03247	-156.01369	*N*
cyclopentadiene	-194.12391	0.09174	-210.18191	-194.17552	-194.15843	*V*
cyclopropene	-116.63192	0.05544	-116.60649	-116.66601	-116.64412	*N*
Cytosine	-394.99614	0.09774	-394.99287	-395.09115	-395.09016	*V*
Ethylene	-78.59836	0.05085	-78.57190	-78.62374	-78.59725	*N*
Fluorethylene	-177.84980	0.04377	-177.82540	-177.84976	-177.82534	*N*
Formamide	-169.92537	0.04526	-169.91211	-169.97007	-169.96061	*N*
Furan	-230.05171	0.06955	-230.03035	-230.11138	-230.09420	*N*
Propene	-117.92087	0.08322	-117.89810	-117.95675	-117.93900	*N*
Thiophene	-553.04370	0.06623	-553.02293	-553.09979	-553.08315	*N*
Thymine	-454.20670	0.11441	-454.19621	-454.31773	-454.30932	*V*
***trans*-1-bromo-1-propene**	-2691.47850	0.06986	-2691.46092	-2691.58539	-2691.57124	*N*
***trans*-1-chloro-1-propene**	-577.54207	0.07040	-577.52285	-577.59119	-577.57576	*N*
uracil	-414.88426	0.08682	-414.87397	-414.98453	-414.98311	*N*
1,4-cyclohexadiene	-233.44477	0.12135	-233.42653	-233.50681	-233.49195	*N*
Imidazole	-226.25004	0.07101	-226.23844	-226.30493	-226.29653	*N*
Propiolactone	-267.19291	0.06817	-267.17995	-267.26135	-267.25171	*N*
***trans*-2-butene**	-157.24248	0.10704	-157.22002	-157.29031	-157.27205	*N*

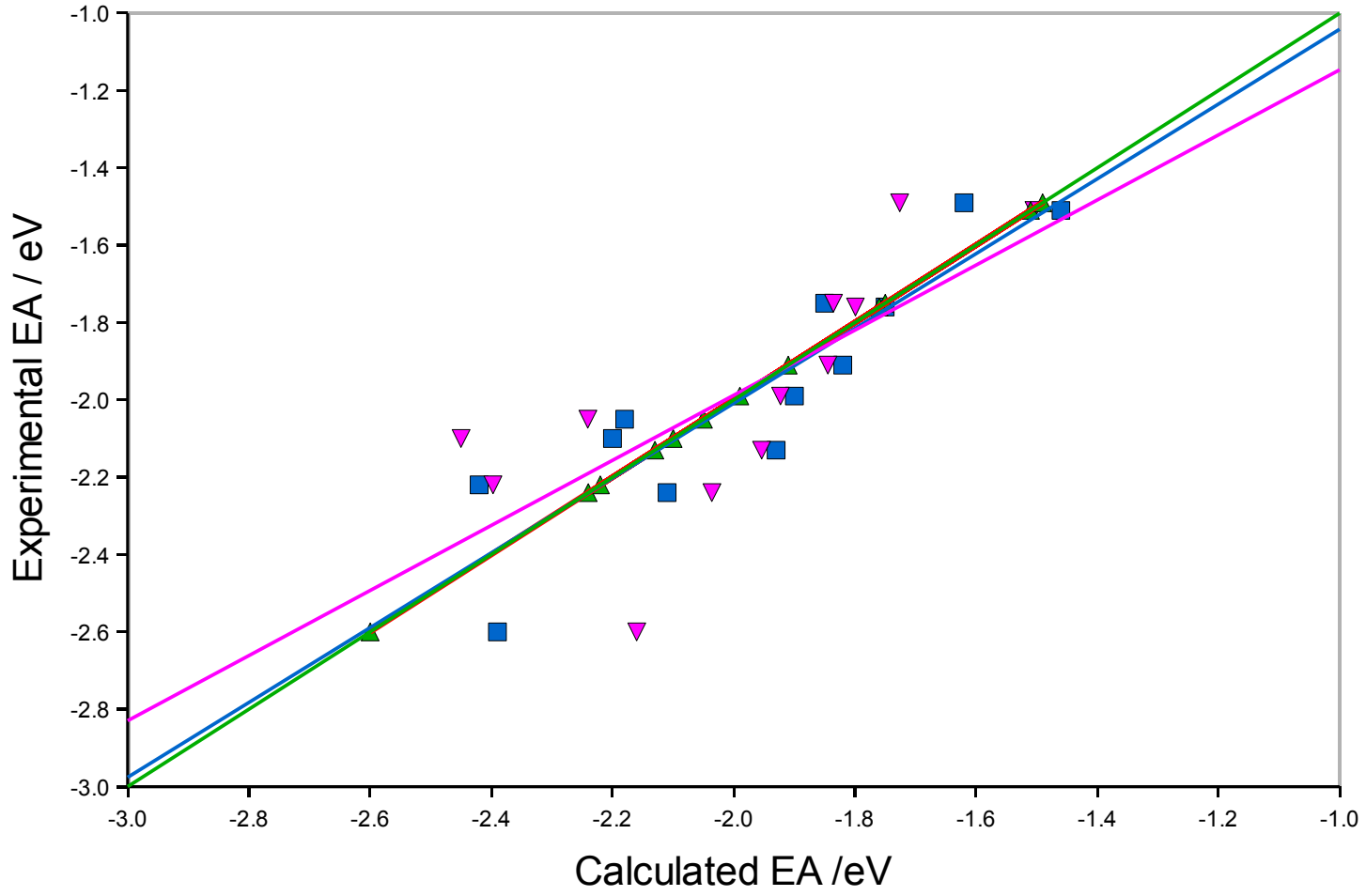
All energies in Hartree

4.3. Table S7. Comparison between B3PW91, B1B95 and B3LYP functionals. Electron affinities obtained with the three functionals with 6-311+G(2df,p) basis sets

Functional	B3LYP (main text		**B3PW91**				**B1B95**				Experimental[b]
Species	calc.	extrapol.	anion type	calc.	extrapol.	anion type	anion type	calc.	extrapol.	anion type	
	eq. 1	eq. 9	gas phase	eq. 1	eq. 9	after	gas phase	eq. 1	eq. 9	after	
2-methyl-2-butene	-1.12	-2.11	N	-1.22	-2.04	V	N	-1.26	-2.06	V	-2.24
acetone	-1.05	-1.46	V	-1.37	-1.50	V	N	-1.18	-1.66	V	-1.51
1,4-cyclohexadiene	-1.10	-1.85	N	-1.20	-1.84	V	N	-1.24	-2.02	V	-1.75
cis-2-butene	-1.19	-2.42	N	-1.28	-2.40	V	N	-1.32	-2.56	V	-2.22
Fluorethylene	-1.45	-1.82	V	-1.61	-1.84	V	N	-1.76	-2.02	V	-1.91
Formamide	-1.11	-2.18	N	-0.62	-2.24	V	N	-1.25	-2.38	V	-2.05
Furan	-1.23	-1.75	N	-1.29	-1.80	V	N	-1.32	-1.96	V	-1.76
Imidazol	-0.90	-1.93	N	-0.92	-1.95	V	N	-1.04	-2.07	V	-2.13
Propene	-1.33	-1.90	V	-1.84	-1.92	V	V	-1.99	-2.08	V	-1.99
trans-2-butene	-1.40	-2.20	N	-1.43	-2.45	V	N	-1.54	-2.34	V	-2.10
cyclopropene	-1.14	-1.62	V	-1.66	-1.73	V	V	-1.84	-1.90	V	-1.49
acetylene	-1.33	-2.39	N	-1.31	-2.16	V	N	-1.48	-2.34	V	-2.60

a) B3PW91 and B1B95/6-311+G(2df,p); all energies in eV. b) as in main text.

Figure S3. Comparison between the correlations obtained with three functionals for a subset of 12 compounds: B3LYP (blue, $y = 0.97x$-0.07); B3PW91 (pink, $y = 0.84x - 0.31$) and B1B95 (green, $y = 0.98x + 0.09$) and an ideal prediction (red, $y = x$)



4.4. Table S8. Gas phase calculation details for the compounds on Table S7 with the B3PW91 and B1B95 functionals.

functional			B3PW91				
	Species	Anion	6-31+G*			6-311+G(2df,p)//B3LYP/6-31+G*	
		type	E(neutral)	ZPE	E(anion)	E(neutral)	E(anion)
26	**1,4-ciclohexadiene**	*N*	-233.33878	0.12258	-233.28335	-233.40224	-233.35805
27	**2-methyl-2-butene**	*N*	-196.47321	0.13586	-196.42081	-196.52856	-196.48374
28	**Acetone**	*V*	-193.09044	0.08416	-193.04105	-193.14831	-193.09774
33	**cis-2-butene**	*N*	-157.17046	0.10852	-157.11369	-157.21554	-157.16844
37	**Fluorethylene**	*N*	-177.76512	0.04421	-177.70355	-177.82057	-177.76570
38	**Formamide**	*N*	-169.83508	0.04569	-169.79023	-169.89300	-169.85089
39	**Furan**	*N*	-229.94182	0.07036	-229.88654	-230.00864	-229.96140
41	**Imidazole**	*N*	-226.14031	0.07157	-226.10171	-226.20583	-226.17200
42	**Propene**	*V*	-117.86659	0.08003	-117.79512	-117.90116	-117.83361
48	**trans-2-butene**	*N*	-157.17251	0.10837	-157.11688	-157.21735	-157.16487
11	**Cyclopropene**	*V*	-116.58001	0.05625	-116.49658	-116.59089	-116.55448
29	**acetylene**	*N*	-77.29636	0.02688	-77.24406	-77.32161	-77.27347

functional			B1B95				
	Species	Anion	6-31+G*			6-311+G(2df,p)//B3LYP/6-31+G*	
		type	E(neutral)	ZPE	E(anion)	E(neutral)	E(anion)
26	**1,4-ciclohexadiene**	*N*	-233.30016	0.12276	-233.24152	-233.36220	-233.31683
27	**2-methyl-2-butene**	*N*	-196.41956	0.13588	-196.36321	-196.47345	-196.42709
28	**Acetone**	*N*	-193.06908	0.08427	-193.01627	-193.12617	-193.06953
33	**cis-2-butene**	*N*	-157.12761	0.10851	-157.06721	-157.17145	-157.12309
37	**Fluorethylene**	*N*	-177.76907	0.04430	-177.70150	-177.82411	-177.76633
38	**Formamide**	*N*	-169.83501	0.04575	-169.78620	-169.89237	-169.84628
39	**Furan**	*N*	-229.93885	0.07058	-229.88061	-230.00531	-229.95693
41	**Imidazole**	*N*	-226.13549	0.07181	-226.09242	-226.20052	-226.16244
42	**Propene**	*V*	-117.83471	0.08016	-117.75726	-117.86835	-117.79499
48	**trans-2-butene**	*N*	-157.12948	0.10857	-157.06876	-157.17300	-157.11638
11	**Cyclopropene**	*V*	-116.56472	0.05644	-116.49459	-116.59748	-116.52978
29	**acetylene**	*N*	-77.29031	0.02696	-77.23136	-77.31513	-77.26084

All energies in Hartree

Part 5. TD-DFT Calculation details and summary of results obtained with the PBE0 functional

5.1. Table S9. TD-DFT calculation details for the compounds on Table 3 with the B3LYP functional

	Species	Anion Type	B3LYP/6-311+G(2df,p)//B3LYP/6-31+G* E(neutral)	E(anion)	Root Nº [a]	Calc.EA [eV]	Exp. EA [eV]
26	**1,4-Cyclohexadiene**	N	-233.4951	-233.4548	3	-1.63	-1.75
27	**2-methyl-2-butene**	N	-196.6068	-196.5657	3	-1.77	-2.24
28	**acetic acid**	N	-229.1754	-229.1379	2	-1.76	-1.80
29	**Acetone**	N	-193.2267	-193.1882	1	-1.07	-1.51
30	**Acetylene**	N	-77.3602	-77.3115	2	-2.02	-2.60
31	**Allene**	N	-116.7017	-116.6515	2	-1.57	-1.88
32	**Butyrolactone**	N	-306.6008	-306.5656	3	-1.62	-1.93
33	***cis*-1-bromo-1-propene**	N	-2691.4952	-2691.4580	2	-1.48	-1.49
34	**cis-1,2-difluorethylene**	N	-277.1563	-277.1144	1	-1.84	-2.18
35	***cis*-2-butene**	N	-157.2778	-157.2341	3	-1.94	-2.22
36	**Cyclobutene**	N	-156.0244	-155.9721	3	-1.86	-2.00
37	**Cyclopentene**	N	-195.3905	-195.3443	5	-1.97	-2.14
38	**di-tert-butil-peroxide**	N	-466.2245	-466.1880	7	-1.97	-2.00
39	**Ethylene Carbonate**	N	-342.5234	-342.4911	4	-2.16	-2.93
40	**Fluorethylene**	N	-177.8931	-177.8355	1	-1.74	-1.91
41	**Formamide**	N	-169.9624	-169.9215	2	-1.91	-2.05
42	**Furan**	N	-230.1010	-230.0560	1	-1.58	-1.76
43	**Guanine**	N	-542.7433	-542.7286	2	-0.83	-1.40
44	**Imidazole**	N	-226.2950	-226.2620	2	-1.76	-2.13
45	**Propene**	N	-117.9509	-117.9020	1	-1.70	-1.99
46	**propine**	N	-116.6987	-116.6550	5	-2.67	-2.80
47	**Propiolactone**	N	-267.2501	-267.2128	1	-1.43	-1.90
48	**Pyrrole**	N	-210.2417	-210.2060	4	-2.09	-2.38
49	**tetramethylethyelene**	N	-235.9288	-235.8889	5	-2.04	-2.27
50	***trans*-1-bromo-1-propene**	N	-2691.4935	-2691.4592	2	-1.31	-1.30
51	***trans*-1-chloro-1-propene**	N	-577.5792	-577.5373	1	-1.31	-1.49
52	***trans*-1,2-difluorethylene**	N	-277.1563	-277.1144	1	-1.42	-1.84
53	***trans*-2-butene**	N	-157.2815	-157.2301	3	-2.02	-2.10
54	**trifluorethylene**	N	-376.4265	-376.3837	2	-1.96	-2.40
55	**vinyl ether**	N	-193.1841	-193.1381	1	-1.59	-2.30
56	**2-butine**	N	-156.0349	-155.9925	8	-3.24	-3.43
57	**acetonitrile**	N	-132.8024	-132.7701	4	-2.42	-2.82
58	**dimethylformamide**	N	-248.6018	-248.5665	5	-2.31	-2.40
59	**ethyl isocyanate**	N	-247.3955	-247.3642	8	-2.94	-2.63
60	**tetrafluoroethylene**	N	-475.6918	-475.6504	4	-2.95	-3.00

All energies in Hartrees

5.2. Table S10. TD-DFT calculation details for the compounds on Table 3 with the PBE0 functional

	Species	*Anion Type*	PBE1/6-311+G(2df,p)//PBE/6-31+G* E(neutral)	E(anion)	Root Nº [a]	Calc.EA [eV]	Exp. EA [eV]
18	**oxazole**	*N*	-245.8746	-245.8300	1	-1.34	-1.44
26	**1,4-Cyclohexadiene**	*N*	-233.1999	-233.1560	4	-1.76	-1.75
27	**2-methyl-2-butene**	*N*	-196.3466	-196.3020	3	-1.82	-2.24
28	**acetic acid**	*N*	-228.9166	-228.8752	2	-1.79	-1.80
29	**Acetone** [b]	*V*	-192.9912	-192.9387	-	-1.43	-1.51
30	**Acetylene**	*N*	-77.2517	-77.2018	2	-2.12	-2.60
31	**Allene**	*N*	-116.5431	-116.4835	2	-1.62	-1.88
32	**Butyrolactone**	*N*	-266.9508	-266.9118	2	-1.61	-1.93
33	***cis*-1-bromo-1-propene**	*N*	-2691.01	-2690.9501	3	-1.58	-1.49
34	**cis-1,2-difluorethylene**	*N*	-276.8670	-276.8219	2	-2.03	-2.18
35	***cis*-2-butene**	*N*	-157.0670	-157.0199	4	-2.08	-2.22
36	**Cyclobutene**	*N*	-155.8260	-155.7491	3	-2.01	-2.00
37	**Cyclopentene**	*N*	-195.1428	-195.0935	5	-2.12	-2.14
38	**di-tert-butil-peroxide**	*N*	-465.6581	-465.6168	8	-2.31	-2.00
39	**Ethylene Carbonate**	*N*	-342.1495	-342.1152	5	-2.40	-2.93
40	**Fluorethylene**	*N*	-177.6926	-177.6370	1	-1.78	-1.91
41	**Formamide**	*N*	-169.7671	-169.7242	2	-2.09	-2.05
42	**Furan**	*N*	-229.8311	-229.7837	3	-1.75	-1.76
43	**Guanine**	*N*	-542.1435	-542.1252	2	-1.03	-1.40
44	**Imidazole**	*N*	-226.0303	-225.9961	2	-1.89	-2.13
45	**Propene**	*N*	-117.7895	-117.7203	2	-1.79	-1.99
46	**propyne**	*N*	-116.5404	-116.4944	5	-3.13	-2.80
47	**Propiolactone**	*N*	-266.9508	-266.9118	2	-1.61	-1.90
48	**Pyrrole**	*N*	-209.9880	-209.9507	4	-2.20	-2.38
49	**tetramethylethylene**	*N*	-235.6198	-235.5755	7	-2.04	-2.27
50	***trans*-1-bromo-1-propene**	*N*	-2691.0115	-2690.9727	3	-1.65	-1.30
51	***trans*-1-chloro-1-propene**	*N*	-577.2590	-577.1991	1	-1.44	-1.49
52	***trans*-1,2-difluorethylene**	*N*	-276.8652	-276.8120	2	-2.01	-1.84
53	***trans*-2-butene**	*N*	-157.0704	-157.0168	3	-2.02	-2.10
54	**trifluorethylene**	*N*	-376.0495	-376.0031	2	-2.14	-2.40
55	**Methyl vinyl ether**	*N*	-192.9459	-192.8983	1	-1.81	-2.30
56	**2-butyne**	*N*	-155.8268	-155.7814	8	-3.62	-3.43
57	**acetonitrile**	*N*	-132.6335	-132.5991	4	-2.57	-2.82
58	**dimethylformamide**	*N*	-248.3054	-248.2674	6	-2.44	-2.40
59	**ethyl isocyanate**	*N*	-247.1029	-247.0678	9	-2.94	-2.63
60	**tetrafluoroethylene**	*N*	-475.2270	-475.1807	4	-3.02	-3.00

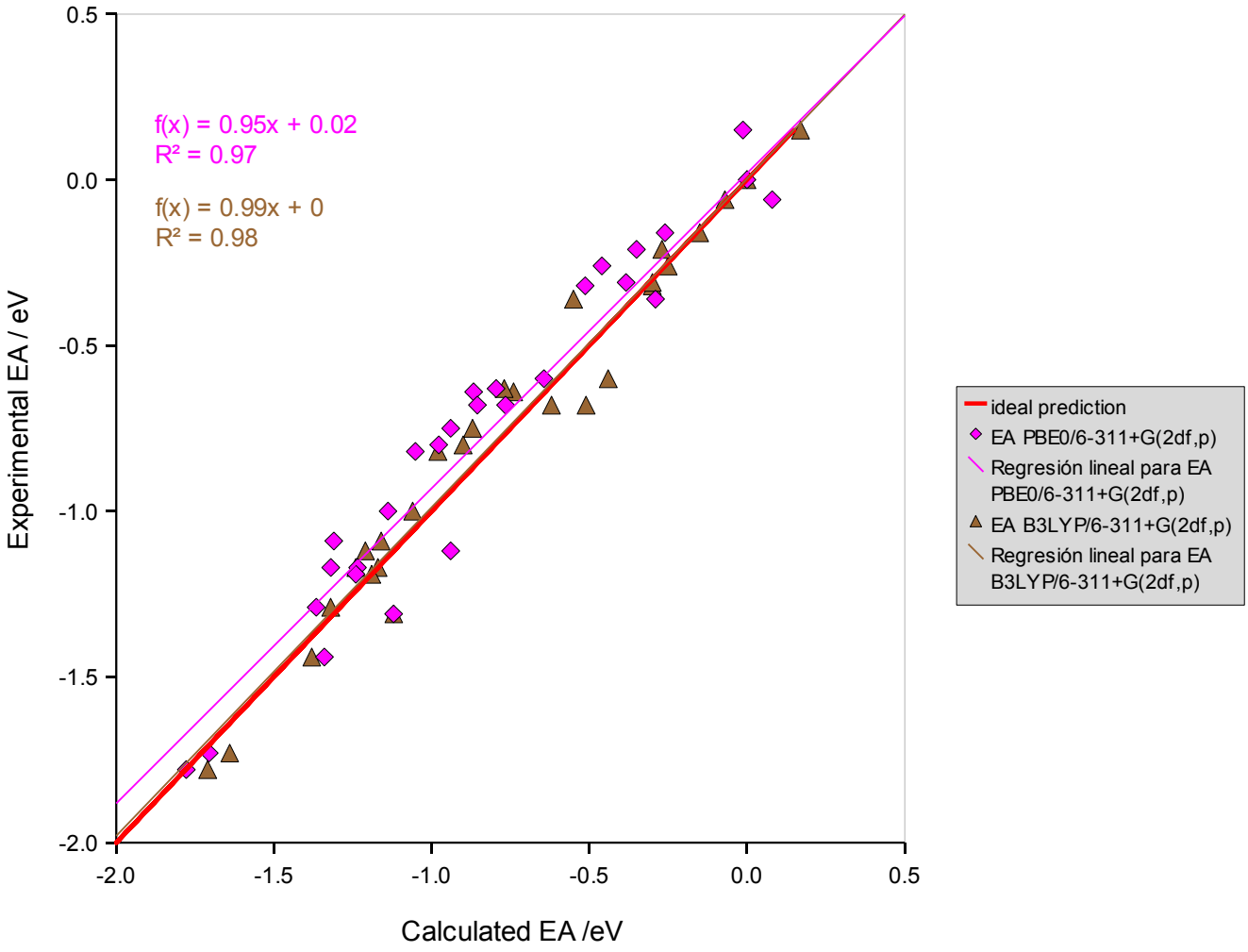
All energies in Hartrees

[a] First Valence excited state found with TD-DFT used for the estimation of the EA.

[b] The Valence anion was the ground state, TD-DFT was not used for calculating the EA of this compound

5.3. Comparison of results obtained with B3LYP and PBE0 functionals for compounds with valence anion ground state (compounds on main text table1)

Figure S4. Comparison between the correlations of calculated EA vs. experimental EA obtained for compounds on Table 1 (main text) with PBE0 and B3LYP : B3LYP (pink, $y = 0.95x + 0.02$) and PBE0 (light brown, $y = 0.99\,x + 0.01$) and an ideal prediction (red, $y = x$)

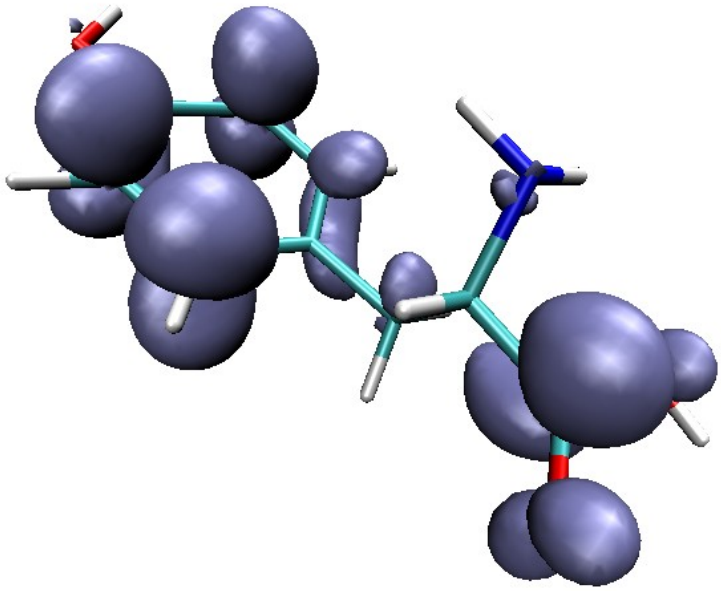


Part 6. Prediction of EAs

6-1 Table S11. Gas phase calculation details for the compounds on Table 4 (main text)

	Species	Anion Type	B3LYP/6-311+G(2df,p)//B3LYP/6-31+G*		
			E(neutral)	E(anion)	ZPE*
61	**α-L-Alanine**	N	-323.8700	-323.8353	0.1081
62	**α-L-Glycine**	N	-284.5422	-284.5076	0.0798
63	**α-L-Tyrosine**	N	-630.2370	-630.2176	0.1935
64	**Ascorbic Acid**	N	-685.0242	-685.0083	0.1505
65	**β-Alanine**	N	-323.8697	-323.8332	0.1088
66	**carbonyl fluoride**	N	-313.1333	-313.0942	0.0139
67	**Succinic Acid**	N	-457.1429	-457.1145	0.1056
68	**Urea**	N	-225.3585	-225.3244	0.0616
All energies in Hartrees. ZPE were obtained at the B3LYP/6-31+G* level.					

Figure S5. Spin densitie of the anions of the α-L-tyrosine, the figure was made with an isodensity value of 0.0020 a.u..



6-2 Table S12. ΔE vs (1/ε) extrapolation details for the compounds on Table 4 (main text)

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-323.8746	-323.8540	-0.56
α-L-alanine	Krypton	1.52	*N*	-323.8753	-323.8567	-0.50
	Heptane	1.92	*N*	-323.8778	-323.8663	-0.31
	Ciclohexane	2.02	*N*	-323.8784	-323.8682	-0.28
	Benzene	2.25	*N*	-323.8795	-323.8719	-0.21
	Ethyl Ether	4.34	*N*	-323.8849	-323.8909	0.16
	Chloroform	4.9	*V*	-323.8857	-323.8937	0.22
	Chlorobenzene	5.62	*V*	-323.8865	-323.8967	0.28
	Tetrahydrofuran	7.58	*V*	-323.8880	-323.9021	0.38
	Dichloroethane	10.36	*V*	-323.8892	-323.9065	0.47
	Acetone	20.7	*V*	-323.8911	-323.9130	0.59
	Ethanol	24.55	*V*	-323.8916	-323.9141	0.61
	Acetonitrile	36.64	*V*	-323.8921	-323.9160	0.65
	EA Linear extrap./eV		-1.73			
	R^2		0.9993			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-685.0317	-685.0313	-0.01
Ascorbic Acid	Krypton	1.52	*N*	-685.0329	-685.0346	0.05
Vitamin C	Heptane	1.92	*N*	-685.0371	-685.0465	0.25
	Ciclohexane	2.02	*N*	-685.0382	-685.0490	0.30
	Ethyl Ether	4.34	*V*	-685.0495	-685.0780	0.78
	Chloroform	4.9	*V*	-685.0508	-685.0815	0.83
	Chlorobenzene	5.62	*V*	-685.0524	-685.0850	0.89
	Tetrahydrofuran	7.58	*V*	-685.0547	-685.0913	1.00
	Dichloroethane	10.36	*V*	-685.0570	-685.0965	1.08
	Acetone	20.7	*V*	-685.0602	-685.1040	1.19
	Ethanol	24.55	*V*	-685.0611	-685.1055	1.21
	Acetonitrile	36.64	*V*	-685.0621	-685.1077	1.24
	Dimethylsulfoxide	46.7	*V*	-685.0620	-685.1082	1.26
	EA Linear extrap./eV		-0.99			
	R^2		0.9998			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
	Argon	1.43	*N*	-323.8743	-323.8510	-0.63
β-Alanine	Krypton	1.52	*N*	-323.8741	-323.8536	-0.56
	Heptane	1.92	*N*	-323.8774	-323.8627	-0.40
	Ciclohexane	2.02	*N*	-323.8780	-323.8644	-0.37
	Benzene	2.25	*N*	-323.8790	-323.8679	-0.30
	Ethyl Ether	4.34	*V*	-323.8844	-323.8863	0.05
	Chloroform	4.9	*V*	-323.8853	-323.8891	0.10
	Chlorobenzene	5.62	*V*	-323.8860	-323.8921	0.17
	Dichloroethane	10.36	*V*	-323.8888	-323.9025	0.37
	Acetone	20.7	*V*	-323.8906	-323.9093	0.51
	Ethanol	24.55	*V*	-323.8910	-323.9104	0.53
	Acetonitrile	36.64	*V*	-323.8915	-323.9124	0.57
	Water	78.39	*V*	-323.8928	-323.9149	0.60
	EA Linear extrap./eV		-1.94			
	R^2		0.9989			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
Carbonyl fluoride	Argon	1.43	*V*	-313.1341	-313.0966	-1.02
	Krypton	1.52	*V*	-313.1342	-313.1005	-0.92
	Heptane	1.92	*V*	-313.1347	-313.1143	-0.56
	Ciclohexane	2.02	*V*	-313.1348	-313.1171	-0.48
	Benzene	2.25	*V*	-313.1350	-313.1223	-0.35
	Ethyl Ether	4.34	*V*	-313.1360	-313.1454	0.26
	Chloroform	4.9	*V*	-313.1361	-313.1483	0.33
	Chlorobenzene	5.62	*V*	-313.1363	-313.1512	0.41
	Tetrahydrofuran	7.58	*V*	-313.1365	-313.1563	0.54
	Dichloroethane	10.36	*V*	-313.1368	-313.1602	0.64
	Acetone	20.7	*V*	-313.1371	-313.1655	0.77
	Ethanol	24.55	*V*	-313.1371	-313.1663	0.79
	Dimethylsulfoxide	46.7	*V*	-313.1373	-313.1685	0.85
	Water	78.39	*V*	-313.1374	-313.1695	0.87
	EA Linear extrap./eV		-1.92			
	R^2		1.0000			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
α-L-Glycine	Argon	1.43	*N*	-284.5464	-284.5284	-0.49
	Krypton	1.52	*N*	-284.5470	-284.5313	-0.43
	Heptane	1.92	*N*	-284.5495	-284.5414	-0.22
	Ciclohexane	2.02	*N*	-284.5500	-284.5434	-0.18
	Benzene	2.25	*N*	-284.5510	-284.5471	-0.11
	Ethyl Ether	4.34	*V*	-284.5561	-284.5503	-0.16
	Chloroform	4.9	*V*	-284.5568	-284.5534	-0.09
	Chlorobenzene	5.62	*V*	-284.5576	-284.5564	-0.03
	Tetrahydrofuran	7.58	*V*	-284.5590	-284.5619	0.08
	Dichloroethane	10.36	*V*	-284.5601	-284.5662	0.17
	Acetone	20.7	*V*	-284.5617	-284.5723	0.29
	Ethanol	24.55	*V*	-284.5620	-284.5733	0.31
	Acetonitrile	36.64	*V*	-284.5625	-284.5750	0.34
	Water	78.39	*V*	-284.5631	-284.5771	0.38
	EA Linear extrap./eV		-2.05			
	R^2		0.9999			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
Succinic Acid	Argon	1.43	*N*	-457.1487	-457.1342	-0.40
	Ciclohexane	2.02	*N*	-457.1536	-457.1486	-0.14
	Benzene	2.25	*N*	-457.1550	-457.1523	-0.07
	Ethyl Ether	4.34	*V*	-457.1620	-457.1672	0.14
	Chloroform	4.9	*V*	-457.1630	-457.1703	0.20
	Chlorobenzene	5.62	*V*	-457.1640	-457.1732	0.25
	Dichloroethane	10.36	*V*	-457.1675	-457.1828	0.42
	Acetone	20.7	*V*	-457.1698	-457.1887	0.52
	Ethanol	24.55	*V*	-457.1701	-457.1887	0.50
	Acetonitrile	36.64	*V*	-457.1708	-457.1914	0.56
	Water	78.39	*V*	-457.1717	-457.1936	0.60
	EA Linear extrap./eV		-1.43			
	R^2		0.9967			

Species	Media	ε	type	*E*(neutral)	*E*(anion)	ΔE / eV
α-L-Tyrosine	Argon	1.43	*N*	-630.2435	-630.2372	-0.17
	Krypton	1.52	*N*	-630.2446	-630.2402	-0.12
	Heptane	1.92	*N*	-630.2483	-630.2508	0.07
	Ciclohexane	2.02	*N*	-630.2492	-630.2532	0.11
	Benzene	2.25	*N*	-630.2508	-630.2574	0.18
	Ethyl Ether	4.34	*V*	-630.2592	-630.2780	0.51
	Chloroform	4.9	*V*	-630.2605	-630.2809	0.56
	Chlorobenzene	5.62	*V*	-630.2617	-630.2836	0.60
	Tetrahydrofuran	7.58	*V*	-630.2641	-630.2888	0.67
	Dichloroethane	10.36	*V*	-630.2661	-630.2930	0.73
	Acetone	20.7	*V*	-630.2690	-630.2990	0.81
	Ethanol	24.55	*V*	-630.2696	-630.3000	0.83
	Dimethylsulfoxide	46.7	*V*	-630.2706	-630.3023	0.86
	Water	78.39	*V*	-630.2718	-630.3041	0.88
	EA Linear extrap./eV		-0.78			
	R^2		0.9998			

Part 7. XYZ Coordinates

List of XZY coordinates of the optimized geometries at the B3LYP/6-31+G* level of theory.

Compounds of table 1

1,1-dicholoroethylene

C	0.000000	0.000000	0.424331
C	0.000000	0.000000	1.755535
Cl	1.466514	0.000000	-0.520397
Cl	-1.466514	0.000000	-0.520397
H	-0.933552	0.000000	2.307153
H	0.933552	0.000000	2.307153

2-bromo-1-propene

C	-0.754206	-0.404361	-1.829334
C	-0.782092	-0.200964	-0.513357
Br	0.845907	0.196496	0.423497
C	-1.992703	-0.247261	0.368158
H	-1.679247	-0.629299	-2.355523
H	0.158099	-0.356632	-2.413557
H	-1.881658	-1.010853	1.147300
H	-2.146995	0.713660	0.873377
H	-2.882938	-0.478725	-0.226786

3-bromo-1-propene

C	-1.080650	-1.011539	-2.299309
C	-1.083193	-1.044432	-0.962238
C	0.158939	-1.059269	-0.145479
Br	0.429452	0.706348	0.761983
H	-2.005577	-1.005746	-2.869628
H	-2.024474	-1.041752	-0.414496
H	-0.154110	-0.994135	-2.870140
H	1.056040	-1.210052	-0.746078
H	0.126741	-1.779044	0.673115

Adenine

N	-1.007247	-0.001424	-1.638847
C	-1.007862	0.000589	-0.299143
C	0.113073	0.004153	0.538716
C	1.367402	0.005998	-0.108225
N	1.401984	-0.001743	-1.452512
C	0.237666	-0.003200	-2.125690
N	-0.256531	-0.000812	1.875041
C	-1.567700	-0.005789	1.843998
N	-2.083465	-0.004460	0.562299
N	2.538727	0.040613	0.577407
H	0.327195	-0.008126	-3.209227
H	-3.058143	-0.007416	0.293029
H	-2.212655	-0.010631	2.713099
H	3.397768	-0.102052	0.064968
H	2.536076	-0.107502	1.576472

Bromoethylene

C	1.094238	0.000000	-1.843221
C	1.090113	0.000000	-0.514336
H	2.044073	0.000000	-2.372709
H	1.986242	0.000000	0.095740

H	0.183702	0.000000	-2.434488
Br	-0.494861	0.000000	0.538766

Chloroethylene

C	-0.747423	0.000000	-1.494215
C	-0.747294	0.000000	-0.164293
H	0.167252	0.000000	-2.078947
H	-1.695020	0.000000	-2.025858
H	-1.644914	0.000000	0.444503
Cl	0.714175	0.000000	0.800668

cis-1-bromo-2-butene

C	-2.109721	1.044360	-1.648316
C	-2.063533	1.138679	-0.150057
C	-0.981158	1.082435	0.643852
C	0.423061	0.949457	0.179788
Br	1.064833	-0.955087	0.284951
H	-3.032350	1.253754	0.337186
H	-1.121374	1.118721	1.722745
H	1.124446	1.490829	0.814181
H	0.577186	1.229959	-0.860130
H	-2.561517	1.946308	-2.083177
H	-1.126258	0.900463	-2.103569
H	-2.741195	0.198419	-1.952125

cis-1,2-dichloroethylene

C	0.961157	0.000000	-0.666673
C	0.961157	0.000000	0.666673
H	1.895844	0.000000	-1.216310
Cl	-0.450752	0.000000	-1.672693
Cl	-0.450752	0.000000	1.672693
H	1.895844	0.000000	1.216310

cyclobutanone

C	-0.910078	-0.343885	-1.117393
C	-1.111871	0.161162	0.346756
C	0.416122	0.158551	0.510050
C	0.639629	-0.348764	-0.923638
O	1.156717	0.446566	1.417310
H	1.207489	0.346942	-1.552646
H	1.128816	-1.329101	-0.968835
H	-1.623959	-0.530065	1.026764
H	-1.565830	1.152702	0.459858
H	-1.261676	0.353096	-1.882697
H	-1.341394	-1.328485	-1.315574

cyclopentadiene

C	-0.978666	0.000000	-0.754212
C	-1.059467	0.000000	0.595450
C	0.333475	0.000000	1.172676
C	1.214160	0.000000	-0.051200
C	0.435351	0.000000	-1.156417
H	-1.964188	0.000000	1.193598
H	2.298247	0.000000	-0.018668
H	0.780629	0.000000	-2.185688
H	-1.813921	0.000000	-1.447720
H	0.515057	0.879273	1.810347
H	0.515057	-0.879273	1.810347

cyclopropene

C	-0.475840	0.666900	-0.038231
C	-0.527405	-0.626566	0.036760
C	0.862921	-0.035000	0.001283
H	1.464589	-0.004688	0.914888
H	1.463549	-0.111572	-0.910427
H	-1.107023	-1.536487	0.090191
H	-0.979163	1.620947	-0.093664

cytosine
Neutral

C	-1.117194	-0.002827	-1.125609
C	-1.117194	-0.002827	0.315847
N	-0.021628	-0.002827	1.053926
C	1.214334	0.004834	0.460014
N	1.230080	0.004092	-0.967084
C	0.104770	-0.000210	-1.724579
N	-2.308670	0.027573	0.978436
O	2.286410	0.008291	1.050315
H	2.151271	0.005911	-1.387962
H	0.238874	0.001899	-2.801901
H	-2.032303	0.003587	-1.705563
H	-3.173387	-0.175653	0.500040
H	-2.282501	-0.097767	1.981876

Optimized Anion

C	-1.129611	-0.025173	-1.113356
C	-1.129611	-0.025173	0.272582
N	-0.011308	-0.025173	1.063067
C	1.197912	0.042105	0.456102
N	1.241526	0.192221	-0.954117
C	0.116341	-0.039379	-1.787415
N	-2.348295	-0.027828	1.016994
O	2.296438	0.002168	1.052520
H	2.166089	0.020788	-1.325877
H	0.222041	0.278314	-2.823048
H	-2.059452	-0.036969	-1.678842
H	-3.058208	-0.622160	0.596167
H	-2.145613	-0.346141	1.962359

ethyl radical
Neutral

C	-0.060838	-0.692711	0.007584
C	0.048066	0.794612	-0.010273
H	0.092183	1.362891	0.915228
H	0.226656	1.330787	-0.938745
H	-0.521417	-1.078885	-0.910768
H	0.929212	-1.178014	0.087761
H	-0.650001	-1.048185	0.862661

Optimized Anion

C	-0.688405	0.000003	0.068601
C	0.819903	-0.000004	-0.206589
H	1.304875	0.893353	0.235175
H	1.304866	-0.893366	0.235175
H	-1.174774	-0.878287	-0.390982
H	-1.049189	0.000005	1.139546
H	-1.174765	0.878299	-0.390982

ethylene

C	0.000000	0.000000	-0.667301
C	0.000000	0.000000	0.667301
H	0.923951	0.000000	-1.241095
H	-0.923951	0.000000	-1.241095
H	-0.923951	0.000000	1.241095
H	0.923951	0.000000	1.241095

isopropil radical
Neutral

C	1.300156	-0.198373	0.003054
C	0.000000	0.535303	-0.045419
C	-1.300156	-0.198373	0.003055
H	0.000000	1.612880	0.103380
H	2.149516	0.455567	-0.225218
H	1.491047	-0.639569	0.999587
H	1.316958	-1.038107	-0.708127
H	-2.149517	0.455568	-0.225211
H	-1.316960	-1.038103	-0.708133
H	-1.491043	-0.639576	0.999585

Neutral in acetone

C	1.298517	-0.198986	0.000208
C	0.000015	0.539641	-0.002309
C	-1.298532	-0.198919	0.000627
H	0.000050	1.628331	0.000370
H	2.158650	0.479364	-0.019704
H	1.402200	-0.842811	0.891390
H	1.385923	-0.876040	-0.867325
H	-2.158688	0.479683	0.003386
H	-1.396320	-0.858766	-0.879181
H	-1.391817	-0.860176	0.879909

Neutral in THF

C	1.269082	-0.196774	-0.000127
C	0.000076	0.525556	-0.000210
C	-1.269092	-0.196844	0.000017
H	-0.000206	1.618565	0.000218
H	2.140426	0.502263	-0.023949
H	1.354620	-0.834905	0.917247
H	1.335280	-0.872700	-0.891513
H	-2.140438	0.502637	0.002940
H	-1.346414	-0.851502	-0.906257
H	-1.343666	-0.855989	0.903236

Anion

C	1.246097	-0.203186	0.048882
C	0.000000	0.591292	-0.293485
C	-1.246097	-0.203186	0.048882
H	0.000000	1.530826	0.292504
H	2.163393	0.401718	-0.040323
H	1.257546	-0.647964	1.098304
H	1.385795	-1.073925	-0.617071
H	-2.163393	0.401718	-0.040323
H	-1.385795	-1.073925	-0.617071
H	-1.257546	-0.647964	1.098304

Anion in acetone

C	0.039449	-0.204481	1.247800
C	0.040250	0.678960	-0.000011
C	0.039608	-0.204522	-1.247771

H	-0.912520	1.246646	-0.000041
H	-0.103642	0.374046	2.173835
H	-0.755950	-0.998872	1.244652
H	0.989624	-0.751691	1.370210
H	-0.103971	0.374025	-2.173728
H	0.989928	-0.751379	-1.370485
H	-0.755571	-0.999126	-1.244462

Anion in THF

C	1.246116	-0.206151	0.049497
C	0.000000	0.603365	-0.303402
C	-1.246116	-0.206151	0.049497
H	0.000000	1.505942	0.341324
H	2.171838	0.383271	-0.044487
H	1.242813	-0.625809	1.094926
H	1.372332	-1.083619	-0.607876
H	-2.171838	0.383271	-0.044487
H	-1.372332	-1.083619	-0.607876
H	-1.242813	-0.625809	1.094926

isothiazole

C	-1.160004	0.000000	-0.434135
C	-1.098625	0.000000	0.936725
C	0.261528	0.000000	1.367358
N	1.191662	0.000000	0.430603
S	0.440686	0.000000	-1.072935
H	-2.036945	0.000000	-1.069609
H	-1.957978	0.000000	1.597729
H	0.584916	0.000000	2.404932

oxazole

C	-0.947203	0.000000	-0.621330
C	-0.897421	0.000000	0.726951
N	0.431812	0.000000	1.131138
C	1.100663	0.000000	0.030670
O	0.338876	0.000000	-1.088485
H	-1.731153	0.000000	-1.356759
H	-1.708166	0.000000	1.435815
H	2.169394	0.000000	-0.106893

t-butil radical
Neutral

C	0.242345	1.468358	0.014339
C	0.000046	-0.000061	-0.159758
C	1.150128	-0.944237	0.016118
C	-1.392393	-0.524077	0.017617
H	-0.556981	2.069923	-0.437823
H	0.284429	1.756254	1.083725
H	1.196918	1.779832	-0.429320
H	0.945019	-1.924954	-0.432565
H	2.072953	-0.550822	-0.429629
H	1.372431	-1.129187	1.085961
H	-2.140255	0.146815	-0.424755
H	-1.515385	-1.517483	-0.433299
H	-1.659883	-0.630280	1.087815

Anion

C	0.242345	1.468358	0.014339
C	0.000000	0.000000	-0.159758
C	1.150128	-0.944237	0.016118

C	-1.392393	-0.524077	0.017617
H	-0.556981	2.069923	-0.437823
H	0.284429	1.756254	1.083725
H	1.196918	1.779832	-0.429320
H	0.945019	-1.924954	-0.432565
H	2.072953	-0.550822	-0.429629
H	1.372431	-1.129187	1.085961
H	-2.140255	0.146815	-0.424755
H	-1.515385	-1.517483	-0.433299
H	-1.659883	-0.630280	1.087815

thiazole

C	-1.175963	0.000000	-0.326081
C	-0.985673	0.000000	1.021687
N	0.320766	0.000000	1.439164
C	1.126959	0.000000	0.423578
S	0.347847	0.000000	-1.126453
H	-2.103289	0.000000	-0.875070
H	-1.776261	0.000000	1.758732
H	2.204886	0.000000	0.502751

thiophene

C	-1.069456	0.000000	-0.996562
C	-1.187464	0.000000	0.368885
S	0.365492	0.000000	1.143428
C	1.181268	0.000000	-0.388269
C	0.293141	0.000000	-1.432111
H	-2.091594	0.000000	0.963697
H	2.262776	0.000000	-0.428159
H	0.597589	0.000000	-2.473647
H	-1.921578	0.000000	-1.668406

thymine

C	-0.936155	0.034786	-0.838790
C	-0.926819	-0.106009	0.622672
N	0.353024	-0.099154	1.208685
C	1.579349	0.022636	0.576281
N	1.461942	0.149763	-0.801267
C	0.254536	0.154806	-1.472311
O	-1.923284	-0.223038	1.324974
O	2.653337	0.019582	1.157903
C	-2.263234	0.036497	-1.542560
H	0.384970	-0.195072	2.218970
H	2.336204	0.241392	-1.301880
H	0.330641	0.263075	-2.549814
H	-2.898104	0.852688	-1.178813
H	-2.135639	0.149478	-2.624205
H	-2.809322	-0.894470	-1.350948

trans-1-bromo-2-butene

C	1.013488	-0.941658	-1.764565
C	0.894848	-0.908599	-0.429851
C	2.307571	-0.923152	-2.522889
H	1.783521	-0.834057	0.196864
H	0.103974	-0.994652	-2.366985
C	-0.412122	-0.948574	0.270441
H	-0.415700	-1.609232	1.137681
Br	-0.885268	0.848923	1.037274
H	-1.242596	-1.192901	-0.391914
H	2.413733	-1.819929	-3.148271

H	2.348267	-0.059214	-3.200524
H	3.170455	-0.870428	-1.850249

trans-1,2-dichloroethylene

C	0.000337	0.000000	-0.665602
C	-0.000337	0.000000	0.665602
H	0.898209	0.000000	-1.272286
Cl	-1.484014	0.000000	-1.580345
H	-0.898209	0.000000	1.272286
Cl	1.484014	0.000000	1.580345

uracil

Neutral

C	-0.311907	0.000000	1.300436
O	-0.222524	0.000000	2.519819
N	0.853145	0.000000	0.502283
C	0.939674	0.000000	-0.879701
N	-0.305895	0.000000	-1.505094
C	-1.501576	0.000000	-0.822177
C	-1.550835	0.000000	0.528894
H	1.739086	0.000000	0.998469
O	1.989534	0.000000	-1.501242
H	-0.278742	0.000000	-2.516519
H	-2.390694	0.000000	-1.444014
H	-2.488622	0.000000	1.068407

Anion

C	1.306648	0.341238	0.003711
O	2.297251	1.121228	0.038024
N	-0.000413	0.978724	-0.056867
C	-1.226039	0.359937	0.004944
N	-1.170240	-1.007213	0.080465
C	0.027925	-1.775770	-0.106303
C	1.254016	-1.059838	-0.000207
H	-0.001277	1.989300	-0.027021
O	-2.303930	0.986775	-0.009037
H	-2.065723	-1.449088	-0.071437
H	-0.054774	-2.797347	0.261666
H	2.194478	-1.600861	0.026835

Compounds of table 2

1,4-ciclohexadiene

C	-1.181390	-0.026124	-0.793065
C	-1.325896	0.014781	0.707210
C	0.001132	0.039282	1.422594
C	1.181390	0.026124	0.793065
C	1.325896	-0.014781	-0.707210
C	-0.001132	-0.039282	-1.422594
H	-2.102280	-0.045490	-1.375120
H	1.918917	0.850074	-1.049242
H	0.028010	-0.069239	-2.511379
H	-1.918917	-0.850074	1.049242
H	-1.925154	0.892928	1.001118
H	-0.028010	0.069239	2.511379
H	2.102280	0.045490	1.375120
H	1.925154	-0.892928	-1.001118

2-methyl-2-butene

C	-0.169586	-0.008279	0.435233

C	-0.185112	0.027466	1.943809
C	0.971188	0.102758	-0.265620
C	-1.510857	-0.176383	-0.251646
C	1.065710	0.075957	-1.772233
H	1.905463	0.221602	0.283221
H	-2.328977	-0.250496	0.473032
H	-1.734230	0.669130	-0.916930
H	-1.537048	-1.081985	-0.873409
H	-0.810257	0.853006	2.314252
H	-0.613180	-0.897175	2.357751
H	0.821198	0.151091	2.358661
H	2.102403	0.184372	-2.107005
H	0.681909	-0.865185	-2.191645
H	0.484660	0.886523	-2.235181

acetic acid

C	0.044500	0.000000	-1.401337
C	0.113955	0.000000	0.102906
O	1.125595	0.000000	0.771863
O	-1.125313	0.000000	0.662616
H	-1.001447	0.000000	1.631179
H	1.053741	0.000000	-1.814443
H	-0.502642	-0.882314	-1.750988
H	-0.502642	0.882314	-1.750988

acetone

C	-0.170344	0.023269	-1.421520
C	-0.154694	-0.002642	0.097433
C	1.208896	-0.005526	0.767161
O	-1.185697	-0.020255	0.746978
H	-1.199599	0.022692	-1.787125
H	0.351801	0.914507	-1.793397
H	0.363564	-0.847602	-1.823656
H	1.094352	-0.024844	1.853259
H	1.791689	-0.877646	0.443225
H	1.780562	0.884465	0.473341

acetylene

C	0.000000	0.000000	-0.603804
C	0.000000	0.000000	0.603804
H	0.000000	0.000000	-1.671377
H	0.000000	0.000000	1.671377

allene

C	0.000005	0.000014	-0.000001
C	0.047212	0.125088	1.302613
C	-0.047203	-0.125061	-1.302615
H	0.872776	0.635896	1.794246
H	-0.737323	-0.277468	1.940295
H	-0.528960	0.624185	-1.927696
H	0.393427	-0.982854	-1.806819

butyrolactone

C	-1.079298	0.191197	-1.055936
O	-1.079334	-0.114796	0.357682
C	0.187124	-0.071935	0.866048
C	1.170615	0.227758	-0.261711
C	0.361334	-0.059713	-1.531862
O	0.418927	-0.246407	2.035827
H	-1.825708	-0.451175	-1.527728

H	-1.380917	1.238808	-1.176011
H	2.075601	-0.372392	-0.142721
H	1.460942	1.283950	-0.184317
H	0.631856	0.572604	-2.382447
H	0.482824	-1.106016	-1.834083

cis-1-bromo-1-propene

C	-1.097393	0.000730	0.166499
C	-1.071801	0.001240	1.499133
C	0.122460	0.001046	2.403004
Br	0.430495	-0.000728	-0.969697
H	-2.051210	0.002298	1.980410
H	-2.017497	0.001200	-0.405383
H	0.117224	0.888107	3.050401
H	0.106541	-0.875499	3.064241
H	1.058009	-0.008730	1.837919

cis-1,2-difluorethylene

C	-0.439969	-0.654226	0.399787
C	-0.423739	0.674039	0.385039
F	0.427775	1.377771	-0.388707
F	0.392554	-1.396541	-0.356702
H	-1.115961	-1.237027	1.014041
H	-1.084749	1.287076	0.985680

cis-2-butene

C	-0.681637	-0.000685	-0.673410
C	-0.685123	-0.001891	0.667403
C	0.522218	-0.000413	1.564096
H	-1.650271	-0.004168	1.175730
H	-1.646209	-0.002053	-1.180525
C	0.542009	0.002421	-1.562886
H	0.522537	0.879796	2.222307
H	0.525864	-0.881789	2.220732
H	1.461072	0.001864	1.001264
H	0.256744	0.002828	-2.619886
H	1.171063	0.886578	-1.394631
H	1.174399	-0.879652	-1.396211

cyclobutene

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.520221
C	1.339283	0.000000	1.622286
C	1.569652	0.000000	0.119621
H	2.062512	0.890677	-0.290091
H	2.062512	-0.890677	-0.290091
H	-0.807275	0.000000	2.249113
H	-0.425082	0.890677	-0.479667
H	-0.425082	-0.890676	-0.479666
H	2.026781	0.000000	2.465092

cyclopentene

C	-1.079217	-0.136263	-0.677058
C	-0.966004	0.058556	0.820095
C	0.308557	0.084765	1.227505
C	1.276089	-0.087008	0.075713
C	0.372481	0.109329	-1.172575
H	-1.832464	0.124844	1.473738
H	0.632337	0.176636	2.261489
H	1.727865	-1.091270	0.099535

H	2.109718	0.626547	0.105809
H	0.652403	-0.544129	-2.005670
H	0.463539	1.143743	-1.525176
H	-1.422579	-1.157233	-0.907147
H	-1.802261	0.544584	-1.144654

di-tert-butyl peroxide

C	0.696976	1.207199	1.157559
C	0.628311	1.088267	2.686220
C	2.152249	1.187192	0.670646
O	0.005244	0.009083	0.737390
C	-0.047986	2.457499	0.670646
H	-0.035116	2.520914	-0.420699
H	-1.091809	2.433410	1.003623
H	0.424029	3.360845	1.075186
H	2.200734	1.230046	-0.420699
H	2.698563	2.047642	1.075186
H	2.653300	0.271171	1.003623
H	-0.411505	1.065516	3.029720
H	1.128516	0.176385	3.029720
H	1.125608	1.949610	3.146231
O	-0.005244	-0.009083	-0.737390
C	-0.696976	-1.207199	-1.157559
C	-0.628311	-1.088267	-2.686220
C	0.047986	-2.457499	-0.670646
C	-2.152249	-1.187192	-0.670646
H	-1.125608	-1.949610	-3.146231
H	-1.128516	-0.176385	-3.029720
H	0.411505	-1.065516	-3.029720
H	-2.698563	-2.047642	-1.075186
H	-2.200734	-1.230046	0.420699
H	-2.653300	-0.271171	-1.003623
H	-0.424029	-3.360845	-1.075186
H	1.091809	-2.433410	-1.003623
H	0.035116	-2.520914	0.420699

ethylene carbonate

C	-1.252004	-0.255571	-0.809820
C	-1.297375	-0.287495	0.723052
O	-0.019598	0.261334	1.089106
C	0.832665	0.177374	0.028340
O	0.159371	-0.231559	-1.084349
O	2.002160	0.426498	0.068144
H	-1.368456	-1.304155	1.124471
H	-2.079932	0.337714	1.156303
H	-1.704530	0.649551	-1.229060
H	-1.682267	-1.139134	-1.284350

fluorethylene

C	-0.402382	0.000000	-1.131582
C	-0.394094	0.000000	0.194241
F	0.763389	0.000000	0.904519
H	0.517132	0.000000	-1.708013
H	-1.350044	0.000000	-1.658790
H	-1.258737	0.000000	0.850176

formamide

N	-0.233254	0.216948	-1.050354
C	-0.301475	0.012102	0.294207
O	0.644880	-0.290701	1.000983

H	-1.323734	0.150038	0.695263
H	0.655605	0.117501	-1.525216
H	-1.049253	0.466953	-1.590659

furan

C	-0.957505	0.000000	-0.722894
C	-0.957505	0.000000	0.639717
O	0.322651	0.000000	1.114832
C	1.151168	0.000000	0.029431
C	0.423402	0.000000	-1.122552
H	-1.734755	0.000000	1.388857
H	2.208387	0.000000	0.247645
H	0.814572	0.000000	-2.130903
H	-1.826767	0.000000	-1.366455

guanine

N	-2.284659	-0.094091	0.442420
C	-2.148604	-0.100098	1.743856
N	-0.823287	-0.047655	2.143781
C	-0.067319	-0.007071	1.001549
C	-0.992288	-0.035538	-0.044043
C	-0.503785	-0.014352	-1.398221
O	-1.092690	-0.043551	-2.467573
N	0.933566	0.042554	-1.392476
C	1.743972	0.075982	-0.286062
N	1.288376	0.061292	0.944589
N	3.104754	0.070183	-0.507958
H	-0.463611	-0.042733	3.088950
H	-2.957365	-0.140126	2.461366
H	3.449989	0.546128	-1.332479
H	3.646387	0.257921	0.327372
H	1.343012	-0.012299	-2.319592

imidazole

C	0.636448	-0.986072	0.000000
N	-0.742328	-0.986303	0.000000
C	-1.092607	0.282767	0.000000
N	0.000000	1.106769	0.000000
C	1.121491	0.300558	0.000000
H	1.197904	-1.910411	0.000000
H	-2.106021	0.661442	0.000000
H	-0.010579	2.117291	0.000000
H	2.123001	0.704891	0.000000

methyl vinyl ether

C	0.615248	-0.107734	0.337804
C	0.931913	-0.889613	1.373591
H	1.350525	0.524881	-0.161869
H	1.950607	-0.908025	1.743103
H	0.189881	-1.514248	1.861489
O	-0.647960	-0.041857	-0.171474
C	-0.822251	0.838860	-1.275946
H	-1.874500	0.774741	-1.558984
H	-0.583913	1.874380	-0.997498
H	-0.198386	0.534044	-2.127133

propene

C	-0.433698	0.152445	-0.116442
C	-0.535642	-0.163611	1.178525
C	0.812561	0.024417	-0.946885

H	-1.314843	0.536847	-0.633645
H	-1.469272	-0.047112	1.723284
H	0.312462	-0.550919	1.741422
H	0.650900	-0.647861	-1.800685
H	1.111346	0.996275	-1.363161
H	1.650083	-0.366737	-0.358400

propiolactone

C	-1.028717	0.000000	-0.980662
O	-0.955646	0.000000	0.490225
C	0.421121	0.000000	0.465684
O	1.171978	0.000000	1.396383
C	0.506667	0.000000	-1.062208
H	0.974201	0.894354	-1.482345
H	0.974200	-0.894355	-1.482345
H	-1.536737	-0.900082	-1.332526
H	-1.536737	0.900082	-1.332526

propyne

C	0.581028	-1.024334	0.398074
H	0.601441	-1.065630	1.493733
H	1.617779	-1.053364	0.041851
H	0.076927	-1.929043	0.037554
C	-0.101934	0.179707	-0.069837
C	-0.667418	1.176638	-0.457262
H	-1.166199	2.055974	-0.798987

pyrrole

C	-0.919519	0.000000	-0.730917
N	-0.919520	0.000000	0.645603
C	0.375185	0.000000	1.113107
C	1.216332	0.000000	0.017814
C	0.396338	0.000000	-1.150089
H	-1.844689	0.000000	-1.289787
H	0.586626	0.000000	2.173093
H	2.297892	0.000000	0.051331
H	-1.745325	0.000000	1.225407
H	0.732120	0.000000	-2.178752

tetramethylethylene

C	0.772046	1.337223	1.196141
H	0.782352	1.355074	2.290570
H	1.817149	1.387269	0.858014
C	0.061654	0.106787	0.663446
H	0.292835	2.267332	0.858014
C	-0.061654	-0.106787	-0.663446
C	-0.505599	-0.875723	1.671064
C	-0.772046	-1.337223	-1.196141
C	0.505599	0.875723	-1.671064
H	-0.318599	-0.551830	2.699812
H	-1.592552	-0.998255	1.558845
H	-0.068238	-1.878318	1.558845
H	0.318599	0.551830	-2.699812
H	0.068238	1.878318	-1.558845
H	1.592552	0.998255	-1.558845
H	-0.782352	-1.355074	-2.290570
H	-0.292835	-2.267332	-0.858014
H	-1.817149	-1.387269	-0.858014

trans-1-bromo-1-propene

C	-0.296317	-0.000928	-0.687942
Br	-0.295751	-0.000341	1.212486
C	0.804730	0.001052	-1.435767
C	0.758148	0.001052	-2.938692
H	-1.301120	-0.003093	-1.096897
H	1.784226	0.003034	-0.960268
H	1.264105	0.886795	-3.345649
H	1.275402	-0.877933	-3.345980
H	-0.270691	-0.005393	-3.313803

trans-1-chloro-1-propene

C	0.321379	0.000000	-0.319846
C	0.303895	0.000000	1.012521
C	1.548702	0.000000	1.855696
H	-0.653895	0.000000	1.531114
Cl	-1.131147	0.000000	-1.303722
H	1.227768	0.000000	-0.916700
H	1.578121	0.882369	2.508554
H	1.578121	-0.882369	2.508554
H	2.455532	0.000000	1.241529

trans-1,2-difluorethylene

C	0.007844	-0.662614	0.000000
C	-0.009677	0.664414	-0.000115
F	1.157188	1.353516	0.013699
H	0.892433	-1.288475	0.010565
F	-1.155969	-1.355180	-0.013684
H	-0.892403	1.292655	-0.010564

trans-2-butene

C	-0.016421	-0.000473	-0.668988
C	0.016421	0.000473	0.668988
C	1.263688	-0.001040	1.508750
H	-0.929898	0.002506	1.215528
C	-1.263688	0.001040	-1.508750
H	0.929898	-0.002506	-1.215528
H	1.304710	0.880663	2.163427
H	1.301684	-0.881898	2.164746
H	2.166801	-0.003056	0.887549
H	-2.166801	0.003056	-0.887549
H	-1.301684	0.881898	-2.164746
H	-1.304710	-0.880663	-2.163427

trifluorethylene

C	0.245657	0.000000	-0.957578
C	0.224491	0.000000	0.369481
F	1.332061	0.000000	1.106993
F	-0.867418	0.000000	1.118382
F	-0.906183	0.000000	-1.661575
H	1.152964	0.000000	-1.545622

2-butyne

C	0.964269	-1.711125	0.650664
H	0.990054	-1.761576	1.746360
H	2.000807	-1.744790	0.292591
H	0.458814	-2.615189	0.288801
C	0.282341	-0.501022	0.190516
C	-0.282341	0.501022	-0.190516
C	-0.964269	1.711125	-0.650664
H	-0.990269	1.761455	-1.746361

H	-2.000733	1.744910	-0.292387
H	-0.458673	2.615192	-0.289004

acetonitrile

C	0.552985	-0.968563	0.391022
H	0.560170	-0.984538	1.485634
H	1.587411	-0.984507	0.032983
H	0.042815	-1.867476	0.030236
C	-0.131208	0.229813	-0.092778
N	-0.674437	1.181289	-0.476902

dimethyl formamide

C	-0.135078	-0.546385	-0.922402
N	0.237889	0.048495	0.246683
C	1.540863	-0.186605	0.842047
C	-0.669724	0.948260	0.941621
H	-0.889797	0.569277	1.948349
H	-1.595789	1.015533	0.368524
H	-0.223806	1.947341	1.033972
H	2.112752	-0.878372	0.216543
H	1.439868	-0.625272	1.843895
H	2.105691	0.751195	0.930397
H	0.657557	-1.200865	-1.331339
O	-1.211007	-0.401240	-1.488090

ethyl isocyanate

C	-0.620570	0.000000	-1.222051
N	-0.252678	0.000000	-0.075272
C	0.961163	0.000000	0.720090
C	0.633216	0.000000	2.210876
H	1.555754	-0.885626	0.462625
H	1.555754	0.885626	0.462625
H	1.560274	0.000000	2.795372
H	0.051826	0.887528	2.481684
H	0.051826	-0.887528	2.481684
O	-1.106192	0.000000	-2.301322

tetrafluoroethylene

C	-0.020970	0.000000	-0.662733
C	0.020970	0.000000	0.662733
F	1.151608	0.000000	1.356718
F	1.063534	0.000000	-1.426808
F	-1.151608	0.000000	-1.356718
F	-1.063534	0.000000	1.426808

Compounds of Table 3

List of the XYZ coordinates for the optimized structures
at the B3LYP/Aug-CC-pVDZ level

Acetone

C	-0.000535	-0.014180	0.001383
C	-0.001595	0.000031	1.518181
O	1.034919	-0.000197	2.156582
C	-1.355687	0.014543	2.201632
H	-1.230764	-0.076788	3.285416
H	-1.876903	0.956351	1.969857
H	-1.989631	-0.801326	1.823544
H	1.023579	0.076869	-0.374698
H	-0.442380	-0.955759	-0.359988

H	-0.623149	0.801989	-0.394470

Adenine

N	-1.008017	0.006260	-1.639703
C	-1.008848	-0.001374	-0.299738
C	0.113109	-0.016614	0.538437
C	1.368379	-0.024619	-0.108840
N	1.401715	-0.017284	-1.453969
C	0.237331	-0.002588	-2.126705
N	-0.257668	-0.020810	1.874991
C	-1.570107	-0.008407	1.844314
N	-2.085208	0.003726	0.562370
N	2.538421	-0.039300	0.575667
H	0.326101	0.002769	-3.214133
H	-3.059393	0.014332	0.294708
H	-2.216071	-0.007380	2.716318
H	3.407085	-0.044954	0.064356
H	2.539462	-0.045559	1.583315

Cyclobutene

C	-0.733443	-0.000804	-0.758021
C	-0.662105	-0.144604	0.808234
C	0.840574	0.022954	0.639964
C	0.779622	0.145818	-0.698264
H	-0.995084	-1.117698	1.197560
H	-1.173308	0.651967	1.368152
H	1.533672	0.296389	-1.472435
H	-1.108205	-0.889673	-1.286061
H	-1.286429	0.879992	-1.115467
H	1.662564	0.036576	1.357426

Cyclopenatadiene

C	-0.040342	-0.755070	-0.978447
C	-0.043610	0.596253	-1.057711
C	0.013734	1.172441	0.333109
C	0.050005	-0.050048	1.212822
C	0.017938	-1.157482	0.435070
H	-0.081036	1.195232	-1.965453
H	0.094816	-0.018772	2.299651
H	0.032370	-2.188981	0.785101
H	-0.074977	-1.447772	-1.818500
H	0.901506	1.811864	0.478775
H	-0.859033	1.811864	0.551363

Cyclopropne

C	-0.475269	0.668144	-0.038584
C	-0.527447	-0.627863	0.036961
C	0.866212	-0.034792	0.001389
H	1.466950	-0.005513	0.918860
H	1.465611	-0.112284	-0.914150
H	-1.111618	-1.538989	0.090468
H	-0.984309	1.623179	-0.093840

Cytosine

C	0.001282	-0.019234	0.001145
C	0.002245	-0.031340	1.442718
N	1.099194	-0.019936	2.181530
C	2.333686	0.004903	1.584681
N	2.348159	0.017120	0.159175
C	1.223660	0.005433	-0.598188

N	-1.185726	-0.056002	2.105192
O	3.405699	0.017167	2.173598
H	3.267899	0.035429	-0.262180
H	1.355136	0.016639	-1.679467
H	-0.916144	-0.029067	-0.581305
H	-2.067103	-0.066031	1.619523
H	-1.171599	-0.064256	3.114251

Ethylene

C	0.000000	0.000000	-0.667627
C	0.000000	0.000000	0.667627
H	0.928688	0.000000	-1.240795
H	-0.928688	0.000000	-1.240795
H	-0.928688	0.000000	1.240795
H	0.928688	0.000000	1.240795

Fluorethylene

C	0.176987	-1.131977	0.359088
C	0.173284	0.194754	0.351575
F	-0.338420	0.906022	-0.686619
H	-0.230410	-1.711791	-0.467479
H	0.598913	-1.654272	1.215132
H	0.558984	0.847815	1.134121

Formamide

N	-0.231614	0.216834	-1.051449
C	-0.300736	0.012094	0.293365
O	0.645427	-0.290392	0.998126
H	-1.327427	0.150875	0.694780
H	0.656671	0.117158	-1.524301
H	-1.049560	0.466240	-1.586302

Furan

C	-0.000439	0.000000	0.000155
C	0.000215	0.000000	1.364288
O	1.280824	0.000000	1.840027
C	2.109407	0.000000	0.753896
C	1.381323	0.000000	-0.399723
H	-0.784147	0.000000	2.111639
H	3.171695	0.000000	0.966765
H	1.776817	0.000000	-1.410272
H	-0.874479	0.000000	-0.643024

Propene

C	0.238586	1.217833	0.406121
C	0.231173	-0.119153	0.393506
C	-0.393192	-0.976451	-0.669296
H	0.715425	-0.653620	1.217808
H	0.712527	1.777714	1.212871
H	-0.229506	1.800481	-0.390672
H	0.357018	-1.634192	-1.135810
H	-1.165929	-1.634190	-0.241124
H	-0.856332	-0.367668	-1.457660

Thiophene

C	-0.000758	0.000000	-0.000242
C	-0.000758	0.000000	1.430761
C	1.264026	0.000000	1.960992
S	2.478052	0.000000	0.715260
C	1.264027	0.000000	-0.530473

H	1.560254	0.000000	3.006121
H	1.560256	0.000000	-1.575602
H	-0.903639	0.000000	-0.608955
H	-0.903640	0.000000	2.039472

Thymine

C	-0.936094	0.034551	-0.839041
C	-0.926492	-0.106389	0.622567
N	0.352299	-0.099542	1.209104
C	1.577627	0.022666	0.575859
N	1.461890	0.150126	-0.801015
C	0.255120	0.155122	-1.472914
O	-1.921965	-0.223739	1.323753
O	2.650427	0.019722	1.157728
C	-2.262332	0.036652	-1.542507
H	0.384723	-0.195584	2.218418
H	2.335741	0.241883	-1.300180
H	0.329589	0.263435	-2.554069
H	-2.896896	0.855805	-1.176427
H	-2.132474	0.148058	-2.626347
H	-2.809714	-0.895803	-1.346032

trans-1-bromo-1-propene

C	-0.307291	-0.001571	-0.689223
Br	-0.271935	-0.000683	1.222692
C	0.791746	0.001908	-1.442175
C	0.762670	0.001240	-2.944810
H	-1.323507	-0.005228	-1.081027
H	1.772208	0.005468	-0.959642
H	1.278624	0.887905	-3.344175
H	1.285448	-0.881712	-3.343514
H	-0.265231	-0.002855	-3.330639

trans-1-chloro-1-propene

C	0.324191	0.000000	-0.319733
C	0.306903	0.000000	1.012552
C	1.549088	0.000000	1.856668
H	-0.655777	0.000000	1.529515
Cl	-1.135812	0.000000	-1.300106
H	1.229736	0.000000	-0.925380
H	1.575822	0.884556	2.511437
H	1.575822	-0.884556	2.511437
H	2.458507	0.000000	1.241305

Uracil

C	-0.310928	0.000000	1.300091
O	-0.220357	0.000000	2.518091
N	0.854269	0.000000	0.502593
C	0.939362	0.000000	-0.878657
N	-0.305138	0.000000	-1.505260
C	-1.500323	0.000000	-0.822899
C	-1.550142	0.000000	0.529036
H	1.739561	0.000000	0.998128
O	1.988416	0.000000	-1.499865
H	-0.277278	0.000000	-2.515646
H	-2.394428	0.000000	-1.444321
H	-2.492368	0.000000	1.068273

1-4,cyclohexadiene

C	-1.180941	-0.026085	-0.791698

C	-1.326033	0.014783	0.707283
C	0.000246	0.039247	1.421460
C	1.180941	0.026085	0.791698
C	1.326033	-0.014783	-0.707283
C	-0.000246	-0.039247	-1.421460
H	-2.103044	-0.045577	-1.378172
H	1.921055	0.851315	-1.050420
H	0.025900	-0.069311	-2.513713
H	-1.921055	-0.851315	1.050420
H	-1.927301	0.894217	1.002225
H	-0.025900	0.069311	2.513713
H	2.103044	0.045577	1.378172
H	1.927301	-0.894217	-1.002225

Imidazole

C	-0.970655	0.000000	-0.661342
N	-1.005445	0.000000	0.717466
C	0.255162	0.000000	1.101416
N	1.105599	0.000000	0.029820
C	0.329731	0.000000	-1.112368
H	-1.881055	0.000000	-1.251853
H	0.609156	0.000000	2.126830
H	2.114461	0.000000	0.066509
H	0.761157	0.000000	-2.106159

Propiolactone

C	-1.030049	0.000000	-0.982338
O	-0.954984	0.000000	0.491835
C	0.424800	0.000000	0.465373
O	1.172846	0.000000	1.395625
C	0.505879	0.000000	-1.061701
H	0.974636	0.897423	-1.480169
H	0.974636	-0.897423	-1.480169
H	-1.538710	-0.903712	-1.334388
H	-1.538709	0.903712	-1.334388

trans-2-butene

C	0.000989	0.000000	0.001706
C	-0.000227	0.000000	1.503983
C	1.091745	0.000000	2.277757
C	1.090529	0.000000	3.780034
H	-0.984286	0.000000	1.987012
H	2.075804	0.000000	1.794728
H	-0.522623	-0.883390	-0.397103
H	-0.522623	0.883390	-0.397103
H	1.024504	0.000000	-0.397707
H	0.067014	0.000000	4.179447
H	1.614141	-0.883390	4.178843
H	1.614141	0.883390	4.178843

Compounds of Table S5
List of the XYZ coordinates for the optimized structures
at the B1B95/6-31+G* level

1,4-ciclohexadiene

C	-1.175539	-0.025925	-0.786620
C	-1.320508	0.014721	0.704335
C	-0.000965	0.039041	1.414146
C	1.175539	0.025925	0.786620
C	1.320508	-0.014721	-0.704335

C	0.000965	-0.039041	-1.414146
H	-2.093813	-0.045320	-1.370063
H	1.912182	0.848457	-1.045600
H	0.027498	-0.068969	-2.501533
H	-1.912182	-0.848457	1.045600
H	-1.918407	0.891161	0.997569
H	-0.027498	0.068969	2.501533
H	2.093813	0.045320	1.370063
H	1.918407	-0.891161	-0.997569

2-methyl-2-butene

C	0.154546	0.000000	-1.939098
C	0.158956	0.000000	-0.439057
C	1.506588	0.000000	0.235794
C	-0.973798	0.000000	0.276075
C	-1.024202	0.000000	1.776251
H	-1.923742	0.000000	-0.255899
H	2.323021	0.000000	-0.491586
H	1.635386	0.879691	0.878300
H	1.635386	-0.879691	0.878300
H	0.678348	0.879346	-2.335194
H	0.678348	-0.879346	-2.335194
H	-0.861875	0.000000	-2.342299
H	-2.052823	0.000000	2.144124
H	-0.522297	-0.879551	2.199827
H	-0.522297	0.879551	2.199827

Acetone

C	0.153477	-0.018713	-1.415145
C	0.154567	-0.000036	0.095200
O	1.188660	-0.000275	0.732109
C	-1.194727	0.018954	0.773827
H	-1.075034	-0.098252	1.851114
H	-1.697939	0.970739	0.568493
H	-1.841193	-0.772811	0.381151
H	1.169443	0.098230	-1.792967
H	-0.256642	-0.970286	-1.772342
H	-0.487820	0.773351	-1.815617

cis-2-butene

C	-0.972251	0.191892	-1.343384
C	-0.930467	-0.036767	0.134694
C	0.148527	-0.139912	0.918529
C	1.586872	-0.053010	0.515568
H	-1.904430	-0.127936	0.614661
H	-0.023082	-0.307656	1.981399
H	-1.495588	-0.628182	-1.849344
H	-1.525696	1.108557	-1.579662
H	0.020552	0.278495	-1.789597
H	2.091320	0.762711	1.047102
H	2.120710	-0.974154	0.778079
H	1.720130	0.114949	-0.555076

Fluorethylene

C	0.176876	-1.127507	0.358864
C	0.172187	0.194811	0.349350
F	-0.335202	0.900506	-0.680089
H	-0.228807	-1.703907	-0.464225
H	0.595893	-1.651001	1.209004
H	0.555349	0.846534	1.126745

Formamide

N	-0.232764	0.216073	-1.045358
C	-0.300125	0.012074	0.292739
O	0.642933	-0.289621	0.996431
H	-1.320901	0.149822	0.693279
H	0.653829	0.116851	-1.518934
H	-1.046298	0.465337	-1.584722

Furan

C	-0.952691	0.000000	-0.720619
C	-0.949573	0.000000	0.637478
O	0.320915	0.000000	1.108496
C	1.143089	0.000000	0.031615
C	0.420547	0.000000	-1.118069
H	-1.726353	0.000000	1.385535
H	2.199299	0.000000	0.249289
H	0.813984	0.000000	-2.124078
H	-1.822482	0.000000	-1.361147

Imidazole

C	-0.964166	0.000000	-0.656860
N	-1.001680	0.000000	0.712689
C	0.253016	0.000000	1.092578
N	1.100279	0.000000	0.028538
C	0.329209	0.000000	-1.107254
H	-1.871892	0.000000	-1.242826
H	0.605502	0.000000	2.114239
H	2.107868	0.000000	0.065559
H	0.759976	0.000000	-2.096344

Propene

C	0.237382	1.211479	0.404072
C	0.231664	-0.121275	0.394343
C	-0.391002	-0.972347	-0.665567
H	0.713551	-0.653493	1.214619
H	0.707746	1.773992	1.204731
H	-0.229574	1.788704	-0.390787
H	0.353908	-1.626239	-1.133799
H	-1.162658	-1.626237	-0.242862
H	-0.851239	-0.363870	-1.448990

trans-2-butene

C	-0.543290	0.000000	-1.881118
C	-0.544816	0.000000	-0.385343
C	0.544816	0.000000	0.385343
C	0.543290	0.000000	1.881118
H	-1.524058	0.000000	0.096299
H	1.524058	0.000000	-0.096299
H	-1.062978	-0.879542	-2.279341
H	-1.062978	0.879542	-2.279341
H	0.475354	0.000000	-2.279651
H	-0.475354	0.000000	2.279651
H	1.062978	-0.879542	2.279341
H	1.062978	0.879542	2.279341

Cyclopropene

C	-0.386012	0.682384	-0.025249
C	-0.452724	-0.669195	0.024810
C	0.877834	-0.019689	0.000019

H	1.279624	0.108386	1.019001
H	1.271268	-0.189959	-1.015613
H	-1.452438	-1.088041	0.043248
H	-1.333041	1.208614	-0.044114

Acetylene

C	0.000000	0.000000	-0.602954
C	0.000000	0.000000	0.602954
H	0.000000	0.000000	-1.670096
H	0.000000	0.000000	1.670096

List of the XYZ coordinates for the optimized structures
at the B3PW91/6-31+G* level

1,4-ciclohexadiene

C	-1.178701	-0.026010	-0.789285
C	-1.322784	0.014747	0.705550
C	-0.000511	0.039156	1.418256
C	1.178701	0.026010	0.789285
C	1.322784	-0.014747	-0.705550
C	0.000511	-0.039156	-1.418256
H	-2.098992	-0.045409	-1.372629
H	1.915883	0.849812	-1.047615
H	0.028250	-0.069124	-2.507262
H	-1.915883	-0.849812	1.047615
H	-1.922119	0.892599	0.999507
H	-0.028250	0.069124	2.507262
H	2.098992	0.045409	1.372629
H	1.922119	-0.892599	-0.999507

2-methyl-2-butene

C	0.166446	0.000000	-1.940426
C	0.166308	0.000000	-0.436449
C	1.517458	0.000000	0.240144
C	-0.973697	0.000000	0.272775
C	-1.049937	0.000000	1.775487
H	-1.919510	0.000000	-0.269854
H	2.334737	0.000000	-0.489034
H	1.648045	0.881213	0.882817
H	1.648045	-0.881213	0.882817
H	0.692292	0.880756	-2.336074
H	0.692292	-0.880756	-2.336074
H	-0.849944	0.000000	-2.348607
H	-2.088160	0.000000	2.121920
H	-0.558632	-0.881372	2.211453
H	-0.558632	0.881372	2.211453

Acetone

C	0.153869	-0.019137	-1.418426
C	0.155287	-0.000036	0.095643
O	1.191195	-0.000276	0.733671
C	-1.197480	0.019379	0.775654
H	-1.078670	-0.100441	1.854636
H	-1.700313	0.974038	0.572471
H	-1.846838	-0.771620	0.380895
H	1.170952	0.100420	-1.797798
H	-0.254159	-0.973585	-1.776253
H	-0.490590	0.772161	-1.820543

cis-2-butene

C	-0.976197	0.191596	-1.346938
C	-0.931943	-0.037667	0.134284
C	0.149392	-0.140188	0.919778
C	1.591461	-0.051785	0.518213
H	-1.907177	-0.129939	0.615428
H	-0.022871	-0.308571	1.984231
H	-1.500916	-0.630175	-1.853033
H	-1.531711	1.109493	-1.582829
H	0.017400	0.278916	-1.795741
H	2.095203	0.765750	1.051729
H	2.126793	-0.974016	0.782138
H	1.727001	0.116809	-0.553943

Fluorethylene

C	0.177106	-1.130236	0.359330
C	0.172416	0.194785	0.349814
F	-0.335716	0.903216	-0.681132
H	-0.228764	-1.708921	-0.464137
H	0.596816	-1.654340	1.210877
H	0.556256	0.847020	1.128586

Formamide

N	-0.233057	0.216498	-1.047614
C	-0.300546	0.012090	0.293157
O	0.643936	-0.290201	0.998776
H	-1.323185	0.150193	0.693788
H	0.654438	0.117287	-1.522361
H	-1.048071	0.466104	-1.587278

Furan

C	-0.954977	0.000000	-0.722459
C	-0.952441	0.000000	0.638956
O	0.321687	0.000000	1.111556
C	1.146440	0.000000	0.031490
C	0.421557	0.000000	-1.120855
H	-1.730071	0.000000	1.388249
H	2.204054	0.000000	0.249666
H	0.814699	0.000000	-2.128672
H	-1.825654	0.000000	-1.364477

Imidazole

C	-0.966888	0.000000	-0.658913
N	-1.003791	0.000000	0.714499
C	0.253979	0.000000	1.095637
N	1.102885	0.000000	0.028649
C	0.330009	0.000000	-1.110147
H	-1.876165	0.000000	-1.245220
H	0.606298	0.000000	2.118893
H	2.111732	0.000000	0.065272
H	0.761883	0.000000	-2.100448

Propene

C	0.238166	1.214618	0.405407
C	0.231605	-0.120893	0.394242
C	-0.391813	-0.975023	-0.666948
H	0.714213	-0.654101	1.215744
H	0.709812	1.776122	1.208248
H	-0.228608	1.795312	-0.389144
H	0.354790	-1.630589	-1.135010

H	-1.164146	-1.630587	-0.242681
H	-0.853811	-0.368365	-1.453368

trans-2-butene

C	-0.544323	0.000000	-1.885765
C	-0.545553	0.000000	-0.386741
C	0.545553	0.000000	0.386741
C	0.544323	0.000000	1.885765
H	-1.527014	0.000000	0.094057
H	1.527014	0.000000	-0.094057
H	-1.065564	-0.880994	-2.284379
H	-1.065564	0.880994	-2.284379
H	0.475269	0.000000	-2.286985
H	-0.475269	0.000000	2.286985
H	1.065564	-0.880994	2.284379
H	1.065564	0.880994	2.284379

Cyclopropene

C	-0.594612	0.557310	-0.076684
C	-0.554622	-0.765878	0.032379
C	0.770832	0.023791	-0.000478
H	1.374731	0.130176	0.911115
H	1.401336	-0.095626	-0.893150
H	-1.487128	-1.321167	0.056125
H	-1.106026	1.503894	-0.027204

Acetylene

C	0.000000	0.000000	-0.603791
C	0.000000	0.000000	0.603791
H	0.000000	0.000000	-1.672016
H	0.000000	0.000000	1.672016

List of the XYZ coordinates for the optimized structures
at the B3LYP/6-31+G* level of the compounds in Table 4.

α-L-Alanine

N	-1.644188	-0.874528	-0.379473
C	-0.220510	-0.761888	-0.172262
C	0.294826	0.673484	-0.225690
C	0.246510	-1.383725	1.143983
O	1.650106	0.784943	-0.241401
O	-0.354531	1.722720	-0.273999
H	-1.922964	-0.379941	-1.204466
H	-2.153587	-0.518578	0.405663
H	0.286623	-1.308439	-1.026308
H	1.357098	-1.289924	1.214585
H	-0.032495	-2.464175	1.174945
H	-0.216311	-0.868801	2.019295
H	1.901395	1.723015	-0.280378

Ascorbic Acid

C	-0.112667	0.412530	-0.922113
C	-0.091280	0.342349	0.580105
O	1.308983	0.306966	0.914050
C	2.076983	0.300368	-0.249860
C	1.149680	0.373362	-1.387609
O	3.279413	0.252140	-0.220268
C	-0.761964	-0.881833	1.243248
C	-2.154348	-1.189613	0.699441
O	-2.931276	-0.009969	0.424273

O	1.624616	0.428342	-2.656496
O	-1.229648	0.549721	-1.668578
O	-0.898562	-0.648782	2.644222
H	-0.515406	1.250373	1.027889
H	-2.078499	-1.709246	-0.258627
H	-0.017063	-0.486093	3.020355
H	-2.680154	-1.838758	1.408248
H	-0.120750	-1.757016	1.061669
H	0.876387	0.504978	-3.272203
H	-2.018264	0.575756	-1.079953
H	-3.130635	0.445732	1.258455

β-Alanine

C	-0.657809	-0.763140	-1.285874
C	-0.624424	-0.725330	0.242907
N	0.697812	-0.875711	-1.833734
H	-1.219124	-1.654666	-1.587787
H	-1.213328	0.114388	-1.656583
H	0.666644	-1.094808	-2.826926
H	1.183295	0.014136	-1.734724
H	-1.639277	-0.777219	0.659280
H	-0.080151	-1.595985	0.630180
C	0.035403	0.516937	0.796505
O	0.029482	0.529959	2.153515
O	0.523402	1.420279	0.145975
H	0.475161	1.351424	2.435556

Carbonyl Fluoride

C	0.126041	0.000000	-0.072770
F	-0.016398	0.000000	1.246229
O	1.147316	0.000000	-0.662403
F	-1.087465	0.000000	-0.608913

α-L-Glycine

N	1.974825	0.077629	-0.027643
C	0.755597	-0.671614	0.206555
C	-0.547328	0.088230	-0.026380
O	-1.629456	-0.693153	0.219176
O	-0.638876	1.242877	-0.385068
H	2.005683	0.419202	-0.986114
H	2.007077	0.902347	0.568231
H	0.741512	-1.563019	-0.432911
H	0.744434	-1.046489	1.237615
H	-2.425436	-0.152930	0.052765

Phosgene

C	0.063342	0.000000	0.492883
O	0.214633	0.000000	1.666408
Cl	1.390959	0.000000	-0.666332
Cl	-1.514319	0.000000	-0.291819

Succinic Acid

C	1.250346	0.000000	1.475173
O	1.088040	0.000000	2.822531
O	2.345488	0.000000	0.952200
H	1.979178	0.000000	3.220749
C	-0.080211	0.000000	0.759077
C	0.080211	0.000000	-0.759077

H	-0.654861	-0.870542	1.096985
H	-0.654861	0.870542	1.096985
C	-1.250346	0.000000	-1.475173
H	0.654861	0.870542	-1.096985
H	0.654861	-0.870542	-1.096985
O	-1.088040	0.000000	-2.822531
O	-2.345488	0.000000	-0.952200
H	-1.979178	0.000000	-3.220749

α-L-Tyrosine

C	3.313487	0.052025	0.084003
C	2.666979	-1.110676	-0.343281
C	1.301678	-1.074685	-0.644557
C	0.558217	0.106653	-0.529225
C	1.233252	1.263108	-0.100761
C	2.591805	1.245391	0.204558
C	-0.924310	0.139543	-0.825540
C	-1.797653	0.099009	0.473035
C	-3.252844	0.288508	0.073933
O	-3.820456	1.356691	-0.006840
O	4.649033	0.090891	0.394508
N	-1.646571	-1.087898	1.310585
O	-3.854096	-0.882793	-0.260139
H	-1.542908	0.973256	1.079991
H	-1.202057	-0.713748	-1.457008
H	-1.175773	1.052387	-1.381453
H	0.686344	2.199744	-0.010530
H	3.107468	2.143932	0.530062
H	3.223202	-2.040976	-0.447314
H	0.814049	-1.985205	-0.986372
H	5.044088	-0.785934	0.268513
H	-1.929031	-1.927090	0.807058
H	-0.670494	-1.200124	1.578288
H	-4.768409	-0.672528	-0.528547

Urea

C	0.000000	0.000000	0.138512
N	0.000000	1.163452	-0.598116
N	0.000000	-1.163452	-0.598116
O	0.000000	0.000000	1.365692
H	0.000000	2.031989	-0.085311
H	0.000000	1.197831	-1.606182
H	0.000000	-2.031989	-0.085311
H	0.000000	-1.197831	-1.606182