Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

In search of the best DFT functional for dealing with organic anionic species

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Suplementary Information

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Chart S1. Representation of compounds 1-40 with negative electron affinities (*EA*s)

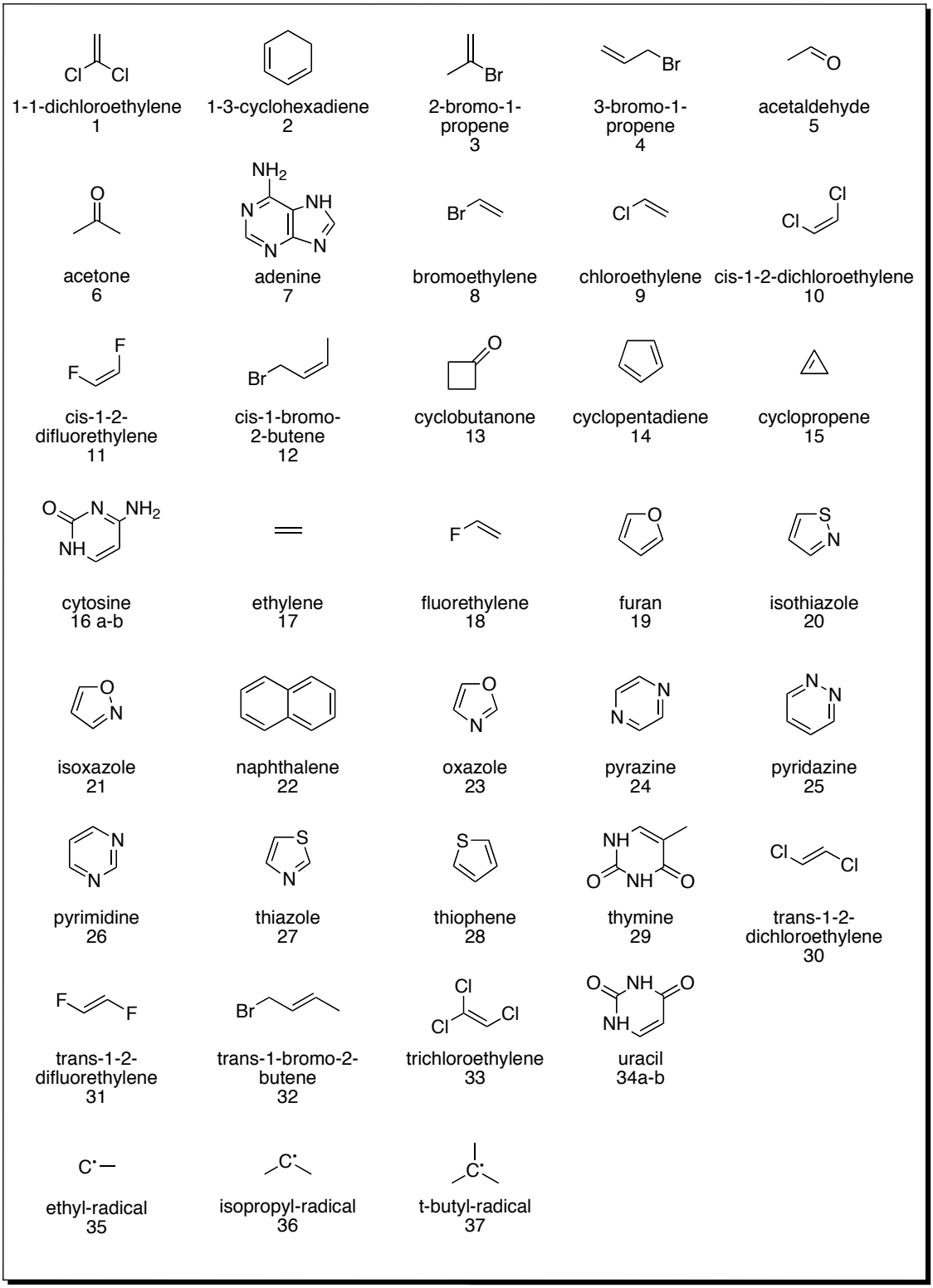

Chart S2. Representation of compounds 38-61 with negative *EA*s

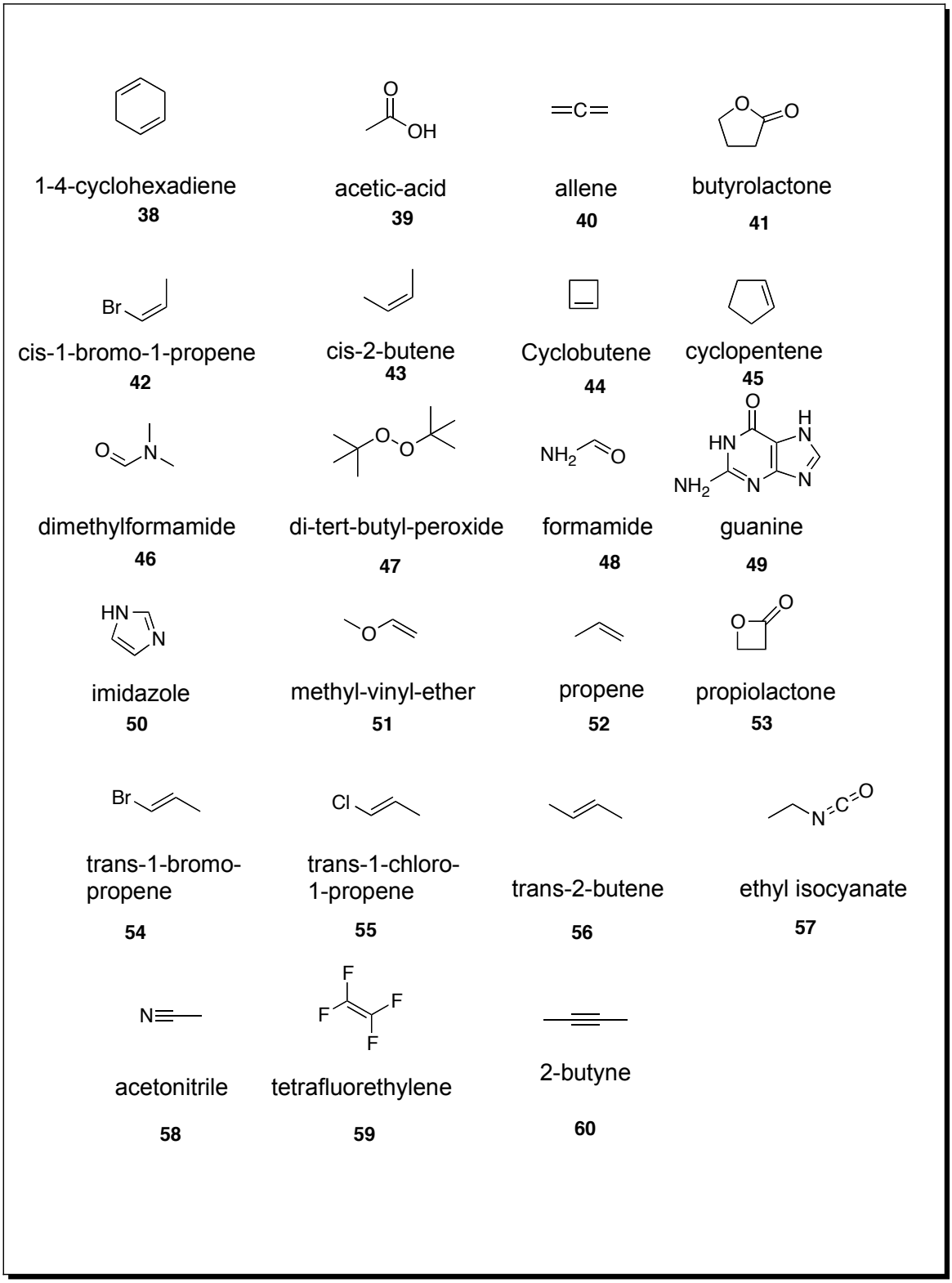

Table S1. List of experimental *EA*s of compounds 1-37 in chart S1, and their experimental references

	molecule	*EA* Exp	Reference
1	1-1-dichloroethylene	-0.76	[1]
2	1-3-cyclohexadiene	-0.8	[2]
3	2-bromo-1-propene	-1.31	[3]
4	3-bromo-1-propene	-0.6	[3]
5	acetaldehyde	-1.19	[4]
6	acetone	-1.51	[4]
7	adenine	-0.54	[5]
8	bromoethylene	-1.17	[3]
9	chloroethylene	-1.28	[1]
10	cis-1-2-dichloroethylene	-1.11	[1]
11	cis-1-2-difluorethylene	-2.18	[6]
12	cis-1-bromo-2-butene	-0.68	[3]
13	cyclobutanone	-1	[3]
14	cyclopentadiene	-1.19	[7]
15	cyclopropene	-1.73	[8]
16	cytosine (vertical)	-0.32	[5]
	(adiabatic)	-0.06	
17	ethylene	-1.78	[2]
18	fluorethylene	-1.91	[6]
19	furan	-1.76	[4]
20	isothiazole	-0.63	[3]
21	isoxazole	-1.09	[3]
22	naphthalene	-0.19	[4]
23	oxazole	-1.44	[3]
24	pyrazine	-0.07	[9]
25	pyridazine	-0.32	[9]
26	pyrimidine	-0.25	[9]
27	thiazole	-0.8	[3]
28	thiophene	-1.17	[4]
29	thymine	-0.29	[5]
30	trans-1-2-dichloroethylene	-0.80	[1]
31	trans-1-2-difluorethylene	-1.84	[6]
32	trans-1-bromo-2-butene	-0.68	[3]
33	trichloroethylene	-0.59	[1]
34	uracil (vertical)	-0.22;-0.19	[5], [10]
	(adiabatic)	0.15	
35	ethyl-radical (adiabatic)	-0.26	[11]
36	isopropyl-radical (adiabatic)	-0.32	[11]
37	t-butyl-radical (adiabatic)	-0.16	[11]

Table S2. List of experimental *EA*s of compounds 38-61 in chart S2, and their experimental references

	Molecule	EA exp. (ev)	Reference
38	1-4-cyclohexadiene	-1.75	[2]
39	acetic-acid	-1.8	[12]
40	allene	-1.90	[13]
41	butyrolactone	-1.98	[14]
42	cis-1-bromo-1-propene	-1.49	[3]
43	cis-2-butene	-2.22	[2]
44	Cyclobutene	-2	[8]
45	cyclopentene	-2.14	[8]
46	dimethylformamide	-2.4	[12]
47	di-tert-butyl-peroxide	-2	[15]
48	formamide	-2.05	[16]
49	guanine	-1.4	[5], [10]
50	imidazole	-2.13	[3]
51	methyl-vinyl-ether	-2.3	[17]
52	propene	-1.99	[2]
53	propiolactone	-1.9	[18]
54	trans-1-bromo-propene	-1.3	[3]
55	trans-1-chloro-1-propene	-1.49	[19]
56	trans-2-butene	-2.1	[4]
57	ethyl isocyanate	-2.63	[20]
58	acetonitrile	-2.84	[4]
59	tetrafluorethylene	-3	[6]
60	2-butyne	-3.34	[21]

Reference list for compounds in Tables S1-S2

1. Burrow, P.D. "Temporary Σ and Π anions of the chloroethylenes and chlorofluoroethylenes." *Chemical Physics Letters*, 1981, **82** (2), p. 270.
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15. Modelli, A. y Galasso, V. "Dissociative Electron Attachment to Di-tert-butylperoxide, Artemisinin, and β-Artemether." *The Journal of Physical Chemistry A*, 2007, **111** (32), p. 7787.
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Chart S3a. Representation of compounds 1-62 employed in the calculation of Redox Potentials.

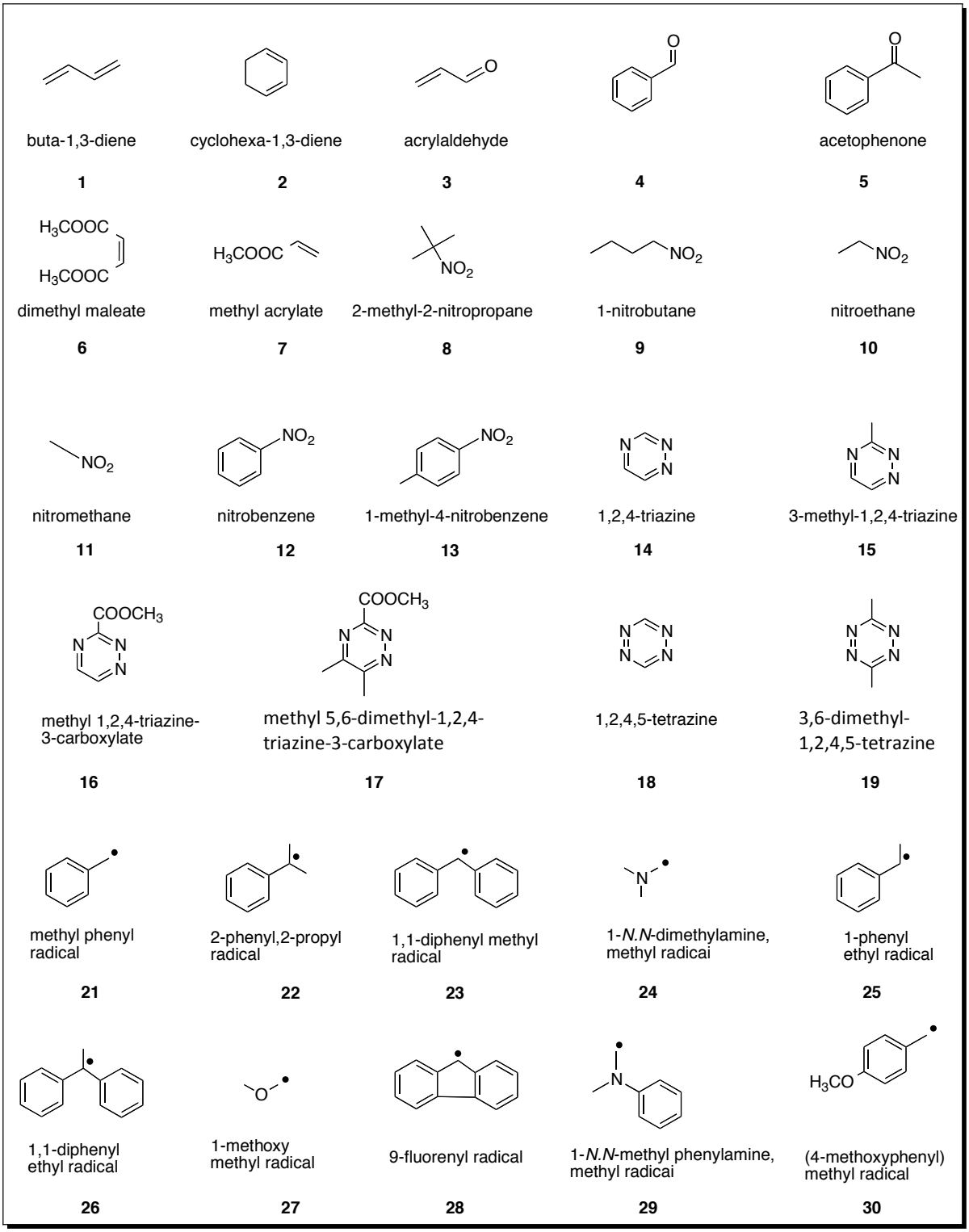
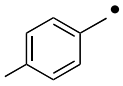
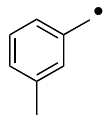


Chart S3b. Representation of compounds 1-62 employed in the calculation of Redox Potentials.



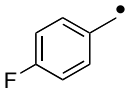
(4-methylphenyl) methyl radical

31



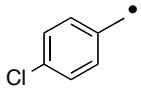
(3-methylphenyl) methyl radical

32



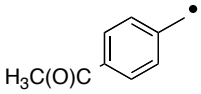
(4-fluorophenyl) methyl radical

33



(4-chlorophenyl) methyl radical

34



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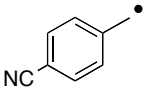

(4-cyanophenyl) methyl radical

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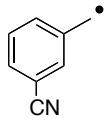

(3-cyanophenyl) methyl radical

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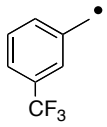
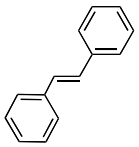


(3-trifluoromethyl-phenyl) methyl radical

38



(*E*)-1,2-diphenylethene

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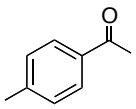
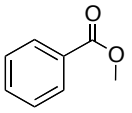


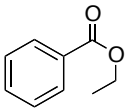
1-(*p*-tolyl)ethanone

41



methyl benzoate

42



ethyl benzoate

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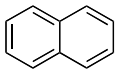

naphthalene

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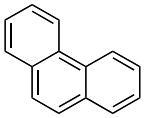

phenanthrene

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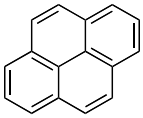
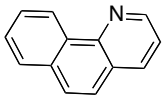


pyrene

46

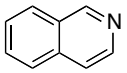
pyrimidine

47



benzo[*h*]quinoline

48

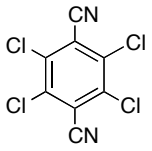


isoquinoline

49

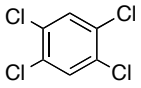
pyridine

50



2,3,5,6-tetrachloro terephthalonitrile

52



1,2,4,5-tetrachloro benzene

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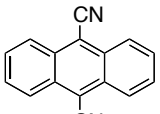
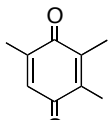


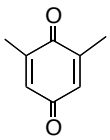
9,10 dicyano anthracene

54



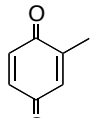
2,3,5-trimethyl cyclohexa-2,5-diene-1,4-dione

57



2,6-dimethyl cyclohexa-2,5-diene-1,4-dione

58



2-methyl cyclohexa-2,5-diene-1,4-dione

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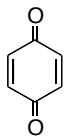
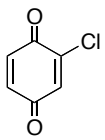


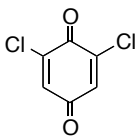
benzoquinone

60



2-chloro benzoquinone

61



2,6-dichloro benzoquinone

62

Table S3. List of experimental Reduction Potentials of compounds 1-62 in charts S-3ab, and their experimental references

	Molecule	Redox-potential (V)	Reference
1	buta-1,3-diene	-2.56	[1]
2	cyclohexa-1,3-diene	-2.71	[1]
3	acrylaldehyde	-1.19	[2]
4	benzaldehyde	-1.38	[2]
5	acetophenone	-1.55	[2]
6	dimethyl maleate	-1.29	[3]
7	methyl acrilate	-1.86	[3]
8	2-methyl-2-nitropropane	-1.545	[4]
9	1-nitrobutane	-1.43	[4]
10	nitroethane	-1.4	[4]
11	nitromethane	-1.385	[4]
12	nitrobenzene	-0.95	[4]
13	1-methyl-4-nitrobenzene	-0.97	[4]
14	1,2,4-triazine	-1.39	[5]
15	3-methyl-1,2,4-triazine	-1.46	[5]
16	methyl 1,2,4-triazine-3-carboxylate	-1.18	[5]
17	methyl 5,6-dimethyl-1,2,4-triazine-3-carboxylate	-1.42	[5]
18	1,2,4,5-tetrazine	-0.63	[5]
19	3,6-dimethyl-1,2,4,5-tetrazine	-0.79	[5]
21	methyl phenyl radical	-1.21	[6]
22	2-phenyl,2-propyl radical	-1.49	[7]
23	1,1.diphenyl methyl radical	-0.9	[6]
24	1-N.N-dimethylamine, methyl radical	-1.76	[7]
25	1-phenyl ethyl radical	-1.36	[7]
26	1,1-diphenyl ethyl radical	-1.1	[7]
27	1-methoxy methyl radical	-1.06	[7]
28	9 fluorenyl radical	-0.52	[7]
29	1-N.N-methyl phenylamine, methyl radicai	-1.79	[7]
30	(4-methoxyphenyl) methyl radical	-1.51	[8]
31	(4-methylphenyl) methyl radical	-1.38	[8]
32	(3-methylphenyl) methyl radical	-1.26	[8]
33	(4-fluorophenyl) methyl radical	-1.26	[8]
34	(4-chlorophenyl) methyl radical	-1.16	[8]
35	(4-acetylphenyl) methyl radical	-0.47	[8]
36	(4-cyanophenyl) methyl radical	-0.53	[8]
37	(3-cyanophenyl) methyl radical	-0.87	[8]
38	(3-trifluoromethyl-phenyl) methyl radical	-0.96	[9]
40	(E)-1,2-diphenylethene	-1.96	[10]
41	1-(p-tolyl)ethanone	-1.96	[10]
42	methyl benzoate	-2.13	[10]
43	ethyl benzoate	-2.16	[10]
44	naphthalene	-2.42	[11]

45	phenanthrene	-2.38	[11]
46	pyrene	-1.98	[11]
47	pyrimidine	-2.1	[12]
48	benzo[h]quinoline	-1.968	[12]
49	isoquinoline	-1.98	[12]
50	pyridine	-2.396	[12]
52	2,3,5,6-tetrachloro terephthalonitrile	-0.71	[13]
53	1,2,4,5-tetrachloro benzene	-0.5	[13]
54	9,10 dicyano anthracene	-0.65	[13]
57	2,3,5-trimethyl cyclohexa-2,5-diene-1,4-dione	-0.51	[13]
58	2,6-dimethyl cyclohexa-2,5-diene-1,4-dione	-0.39	[13]
59	2-methyl cyclohexa-2,5-diene-1,4-dione	-0.34	[13]
60	benzoquinone	-0.23	[13]
61	2-chloro benzoquinone	-0.1	[13]
62	2,6-dichloro benzoquinone	0.06	[13]

Reference list of compounds in Tables S-3

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Table S4. References for the DFT and *ab initio* methods employed in this article.

Functional	Reference
BLYP	1-3.
BPW91	1, 4-8
PW91	4-8
B97D	9
B3PW91	4-8, 10
B3LYP	2, 3, 10
B3LYP-D	2, 3, 10, 9, 11
CAM-B3LYP	12
LC-BLYP	1-3, 13
BHandHLYP	1-3, 14
ω-B97	15
ω-B97X	15
ω-B97XD	16
PBE0	17-19
LC- ωPBE	20-22
TPSS	23
TPSSh	23
M06	24
M06-2X	25, 26
M06-L	27
M06-HF	25, 26
B2PLYP	28
mPW2PLYP	29
HF	30-32
MP2	33-37

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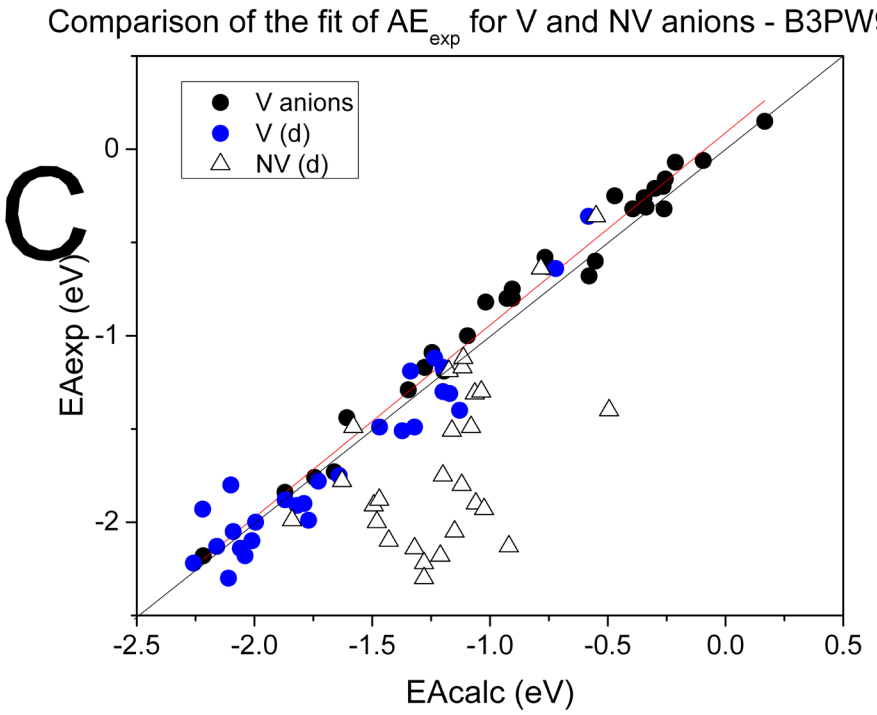
The references were taken from the following webpages, accessed on November 2015.

http://www.gaussian.com/g_tech/g_ur/k_dft.htm
http://www.gaussian.com/g_tech/g_ur/k_mp.htm
http://www.gaussian.com/g_tech/g_ur/k_hf.htm

Figures S0 –Comparision of the fit of experimental EAs with V and NV anions. Calculated with B3PW91 functional.
Circles represent V states and triangles NV states. Black circles represent the EAs of compounds for which only a V state was found, whereas blue circles represent compounds for which two states were found (V and NV). The energies for the compounds were two states were found are included in the table in the next page.



Energies of the molecules for which two anionic states were found, included in Figure S0 for the B3PW91 Functional with the folloe¡wing basis at 6-311+G(2df,p) t the geometries obtained with 6-31+G* basis set.

For finding the V and NV states three procedures were employed:

1) Use of a V guess (i.e. B3LYP in water) for compounds that gave NV states.

2) Use of a NV guess (TPSS or BLYP in gas phase

3) Use the procedure published in reference 27 and 28. Solvation and extrapolation, those energies are marked in red.

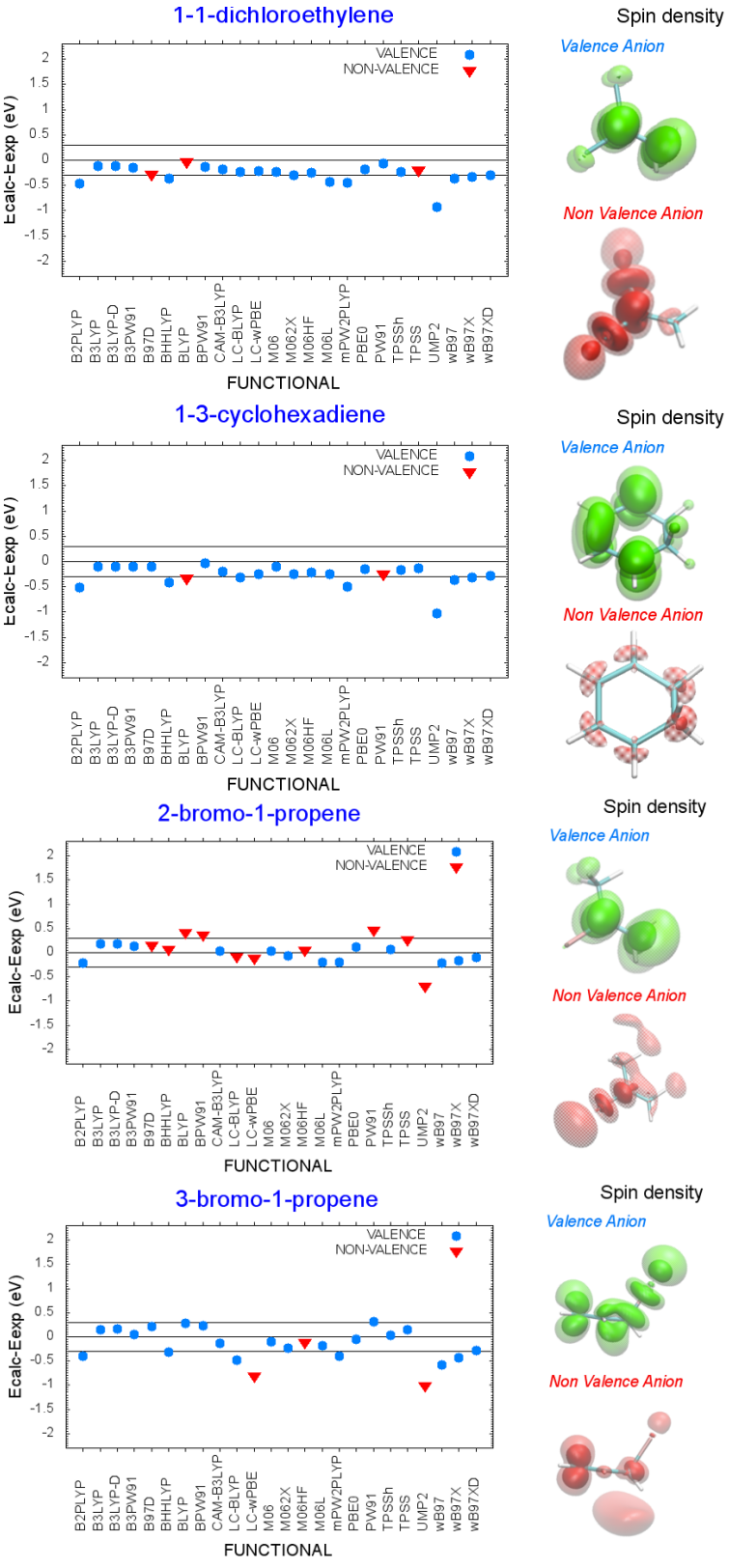
molecule	B3PW91/6-31+G*		B3PW91/6-311+G(2df,p) -SP					
	E-neutral	E-anion	E-neutral	E-anion		EA exp	Calculated Eas	
				V State	Nstate		V State	N State
2-bromo-1-propene	-2688.9769	-2688.9317	-2691.4307	-2691.3876	-2691.3915	-1.31	-1.17	-1.06
acetaldehyde	-153.7777	-153.7259	-153.8251	-153.7760	-153.7819	-1.19	-1.34	-1.18
acetone	-193.0904	-193.0351	-193.1483	-193.0979	-193.1073	-1.51	-1.37	-1.16
bromoethylene	-2649.6643	-2649.6175	-2652.1118	-2652.0677	-2652.0708	-1.17	-1.20	-1.12
cis-1-2-dichloroethylene	-997.6476	-997.5970	-997.7333	-997.6879	-997.6923	-1.12	-1.23	-1.11
cytosine-vertical	-394.7970	-394.7726	-394.9182	-394.8968	-394.8980	-0.36	-0.58	-0.55
ethylene	-78.5597	-78.4934	-78.5838	-78.5203	-78.5240	-1.78	-1.73	-1.63
fluorethylene	-177.7651	-177.6957	-177.8206	-177.7537	-177.7657	-1.91	-1.82	-1.49
cis-1-2-difluorethylene	-276.9595	-276.8833	-277.0466	-276.9652	-277.0022	-2.18	-2.04	-1.21
adenine	-467.1617	-467.1320	-467.2954	-467.2689	-467.2666	-0.64	-0.72	-0.78
trans-1-bromo-propene	-2688.9737	-2688.9328	-2691.4289	-2691.3848	-2691.3908	-1.3	-1.20	-1.04
guanine	-542.3704	-542.3510	-542.5324	-542.4909	-542.5143	-1.4	-1.13	-0.49
trans-1-chloro-1-propene	-577.4123	-577.3495	-577.4774	-577.4288	-577.4189	-1.49	-1.32	-1.58
cis-1-bromo-1-propene	-2688.9736	-2688.9287	-2691.4294	-2691.3754	-2691.3897	-1.49	-1.47	-1.08
1-4-cyclohexadiene	-233.3388	-233.2758	-233.4022	-233.3420	-233.3580	-1.75	-1.64	-1.20
acetic acid	-229.0066	-228.9614	-229.0834	-229.0062	-229.0423	-1.8	-2.10	-1.12
allene	-116.6146	-116.5592	-116.6491	-116.5803	-116.5951	-1.88	-1.87	-1.47
propiolactone	-267.0646	-267.0215	-267.1455	-267.0797	-267.1067	-1.9	-1.79	-1.06
butirolactone	-306.3905	-306.3465	-306.4818	-306.4002	-306.4441	-1.93	-2.22	-1.03
propene	-117.8666	-117.8043	-117.9012	-117.8361	-117.8336	-1.99	-1.77	-1.84
cyclobutene	-155.9220	-155.8632	-155.9643	-155.8910	-155.9098	-2	-2.00	-1.48
formamide	-169.8351	-169.7902	-169.8930	-169.8162	-169.8509	-2.05	-2.09	-1.15
transbutene	-157.1725	-157.1170	-157.2175	-157.1436	-157.1649	-2.1	-2.01	-1.43
imidazole	-226.1403	-226.1017	-226.2058	-226.1265	-226.1720	-2.13	-2.16	-0.92
cyclopentene	-195.2629	-195.2025	-195.3158	-195.2401	-195.2664	-2.14	-2.06	-1.32
cis-2-butene	-157.1690	-157.1122	-157.2139	-157.1309	-157.1668	-2.22	-2.26	-1.28
methylvynilether	-193.0434	-192.9880	-193.1036	-193.0261	-193.0565	-2.3	-2.11	-1.28

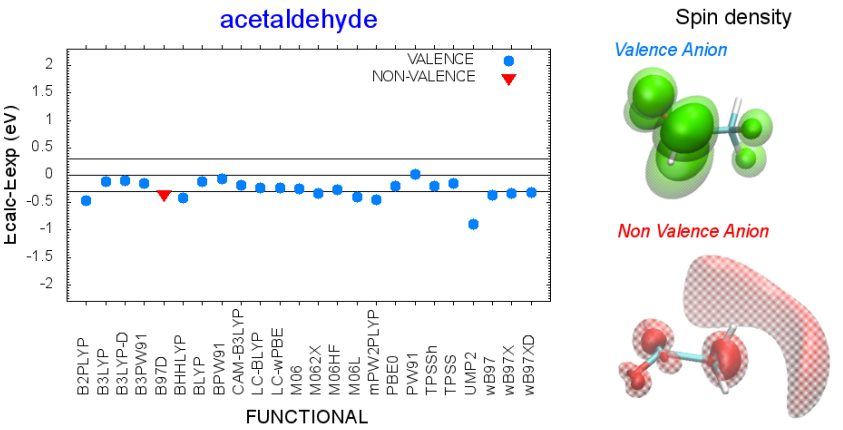
Table S5. Results of the calculations of the *EAs* of compounds from chart S-1 with different DFT functionals.

Functional	MAD (eV)[a]	V ratio[b]	Range (eV) [c]	Slope[d]	*y*-intercept[d]	R^2
BLYP	0.11	0.45	0.60	0.960	0.020	0.90
BPW91	0.09	0.65	0.49	1.006	0.005	0.95
PW91	0.12	0.48	0.49	0.971	-0.105	0.94
B97D	0.12	0.56	0.53	0.962	0.029	0.97
B3PW91	0.10	0.90	0.36	1.043	0.094	0.97
B3LYP	0.10	0.95	0.52	1.073	0.078	0.96
B3LYP-D	0.09	0.90	0.43	1.046	0.047	0.97
CAM-B3LYP	0.12	0.90	0.32	1.050	0.164	0.98
LC-BLYP	0.20	0.85	0.54	1.000	0.199	0.97
BHandHLYP	0.31	0.87	0.34	1.029	0.341	0.98
ω-B97	0.27	0.92	0.57	0.922	0.181	0.97
ω-B97X	0.29	0.95	0.41	1.003	0.290	0.92
ω-B97XD	0.20	0.95	0.32	0.980	0.180	0.98
PBE0	0.12	0.95	0.38	1.056	0.153	0.98
LC- ωPBE	0.17	0.87	0.50	0.963	0.119	0.98
TPSS	0.11	0.52	0.47	0.980	0.063	0.95
TPSSh	0.15	0.87	0.39	0.963	0.235	0.97
M06	0.11	0.80	0.32	0.967	0.066	0.97
M06-2X	0.18	0.90	0.37	0.981	0.160	0.98
M06-L	0.27	0.87	0.40	0.963	0.235	0.97
M06-HF	0.16	0.82	0.47	0.922	0.048	0.97
B2PLYP	0.38	0.95	0.47	1.063	0.482	0.97
mPW2PLYP	0.38	0.95	0.44	1.073	0.482	0.97
HF	0.60	0.83	1.14	1.031	1.106	0.96
MP2	0.89	0.87	1.02	0.957	0.810	0.86
CCSD	0.75	0.94	0.43	0.996	0.740	0.96
CCSD(T)	0.74	0.94	0.62	0.959	0.666	0.94

[a]MAD of the calculated *vs.* experimental *EA* values for V anions. [b] V state anions over total number of compounds.[c] Difference between the biggest and smallest deviation to measure the dispersion of the calculated values. [d] Results of the plots of calculated *vs.* experimental *EAs*. All the extrapolations are included in the supporting information, figures S2.1 to S2.24. The rows are colored grouping the functionals, from top to bottom: pure GGA (white), hybrid GGA(light grey), meta-GGA (grey), double hybrids (dark grey) and *ab initio* (white).

Figures S1.1 to S1.36. Residuals of the predicted vs calculated EA for each DFT functional. The spin density of the two anionic states is represented on the right.




acetaldehyde
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
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UMP2
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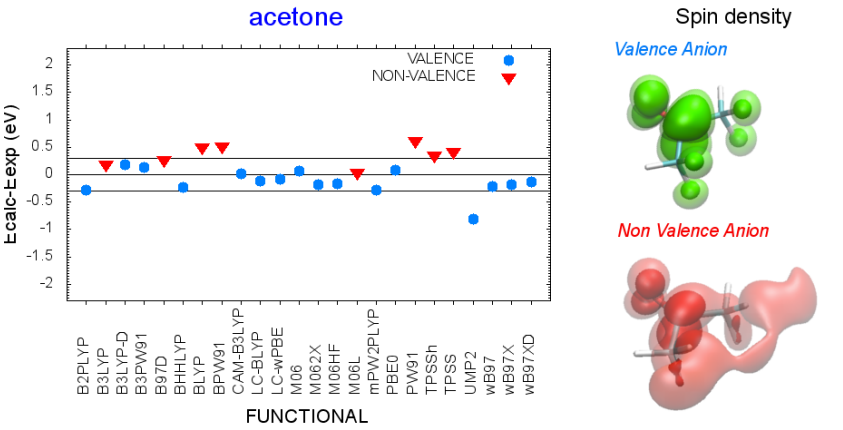
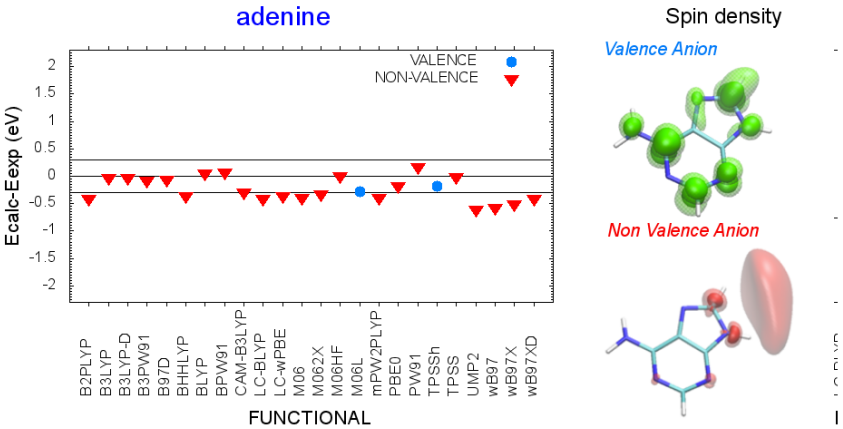
wB97X
wB97XD


acetone
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL


adenine
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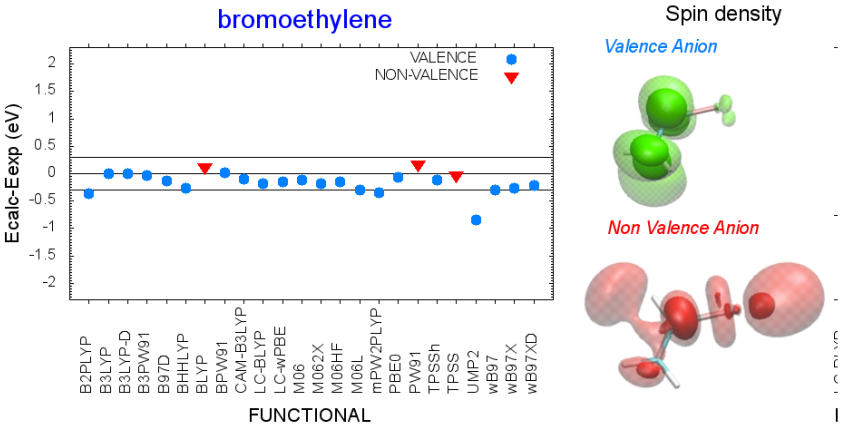
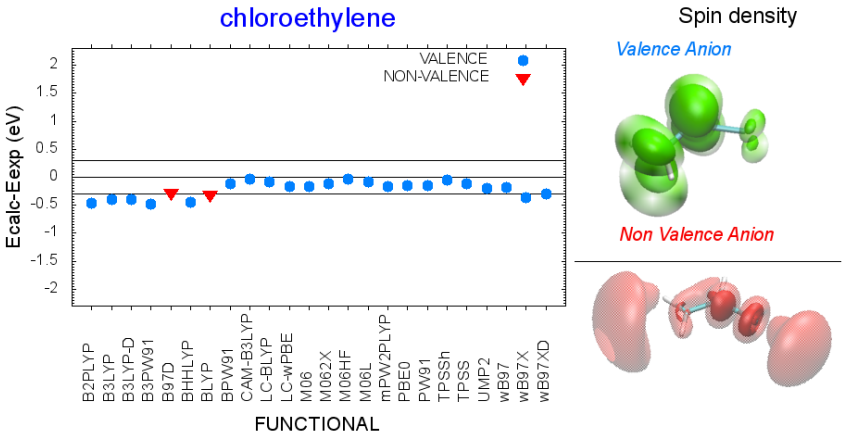
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL


bromoethylene
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL


chloroethylene
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
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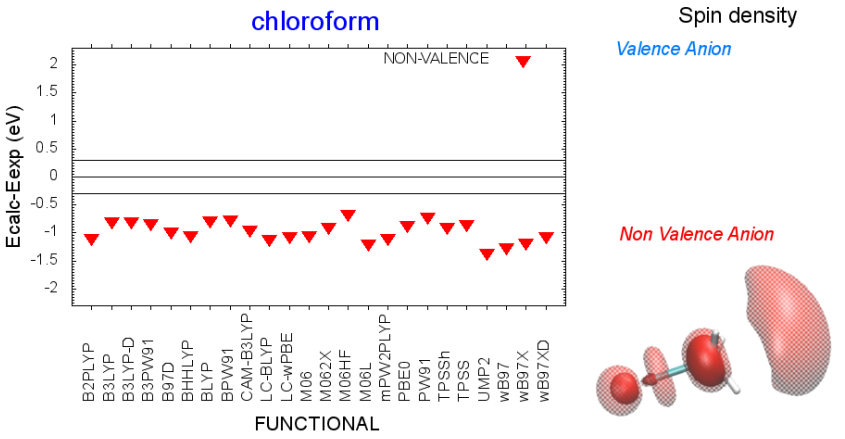
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL


chloroform
Spin density
Valence Anion
Non Valence Anion
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
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PW91
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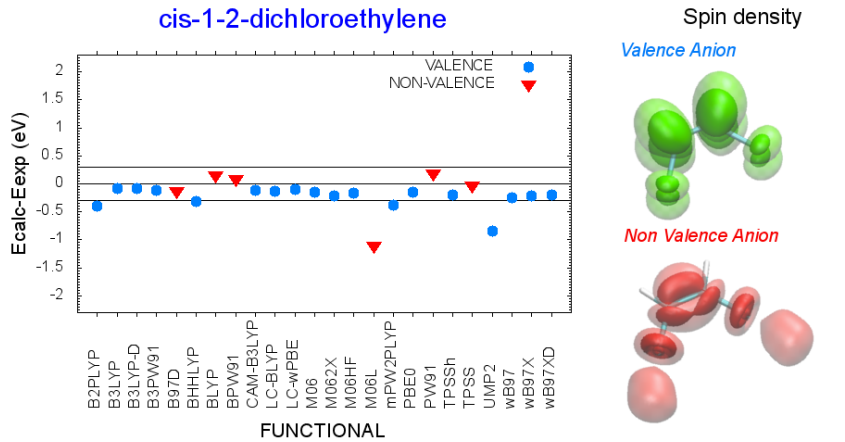
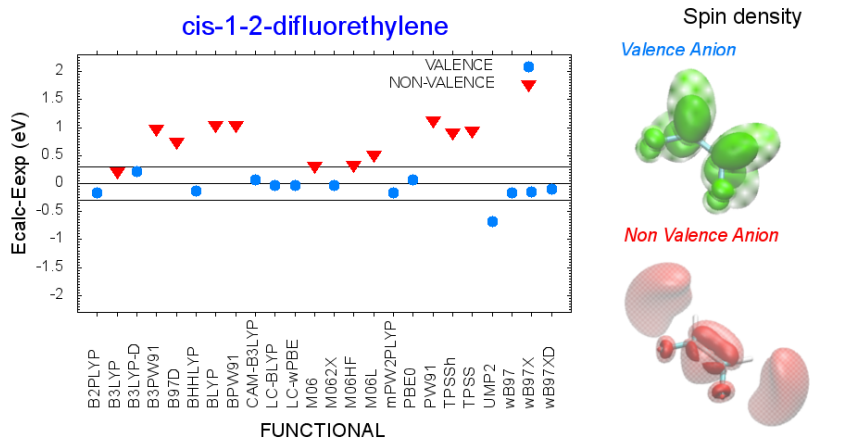
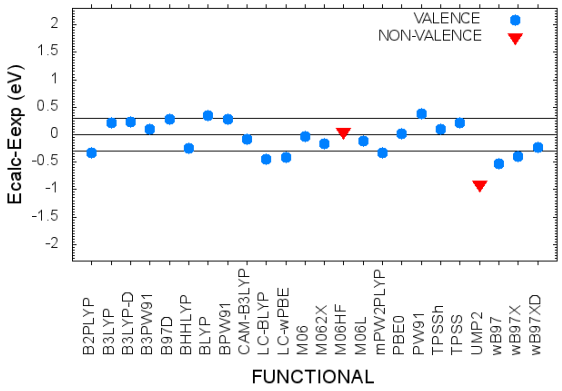
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

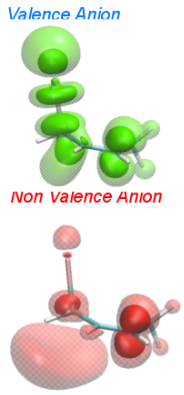

cis-1-2-dichloroethylene
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL


cis-1-2-difluorethylene
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

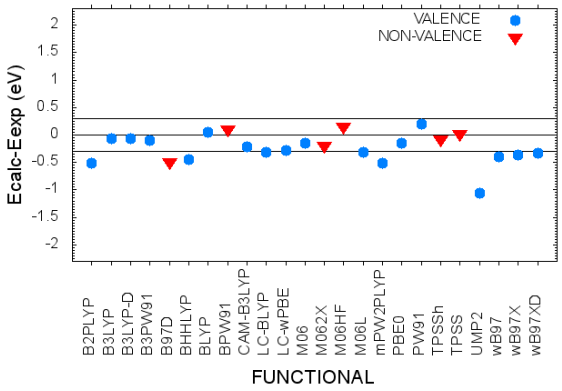
cis-1-bromo-2-butene



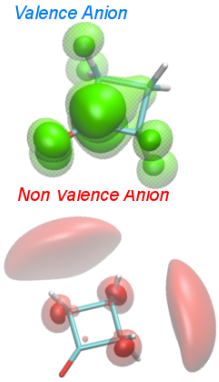
Spin density



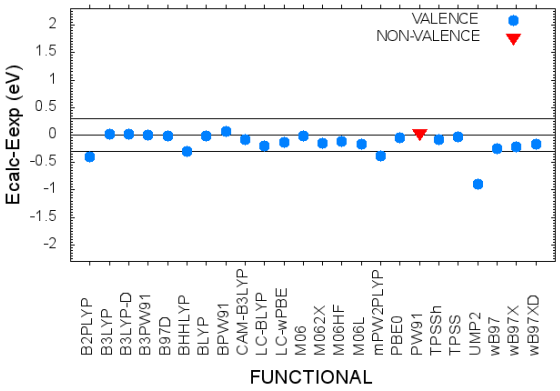
cyclobutanone



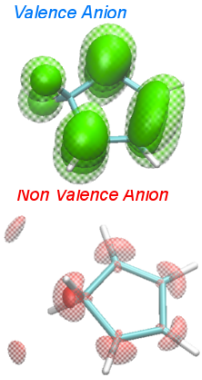
Spin density



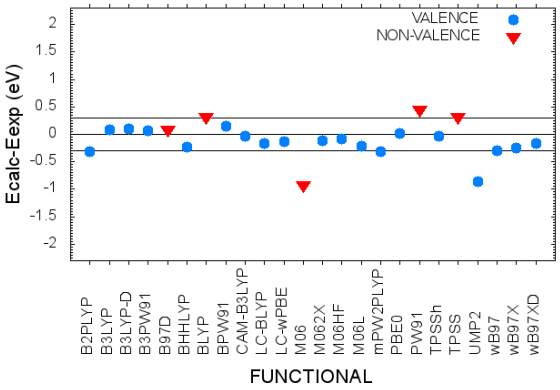
cyclopentadiene



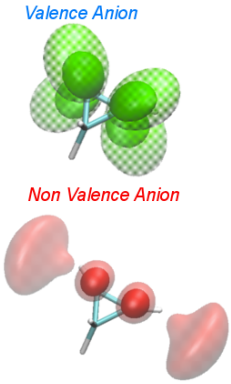
Spin density

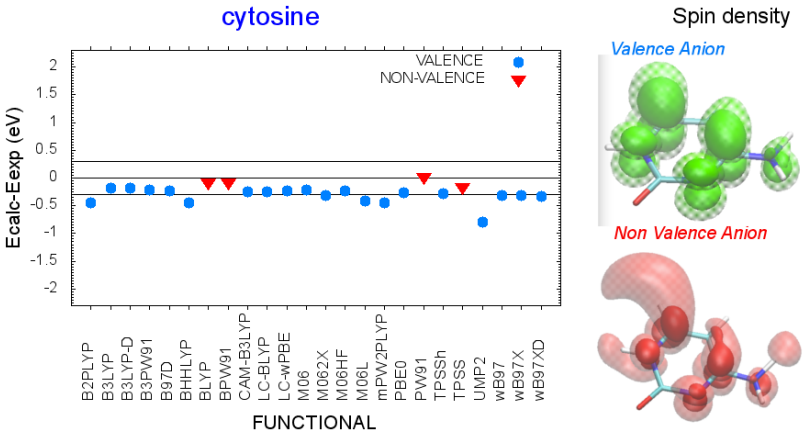


cyclopropene

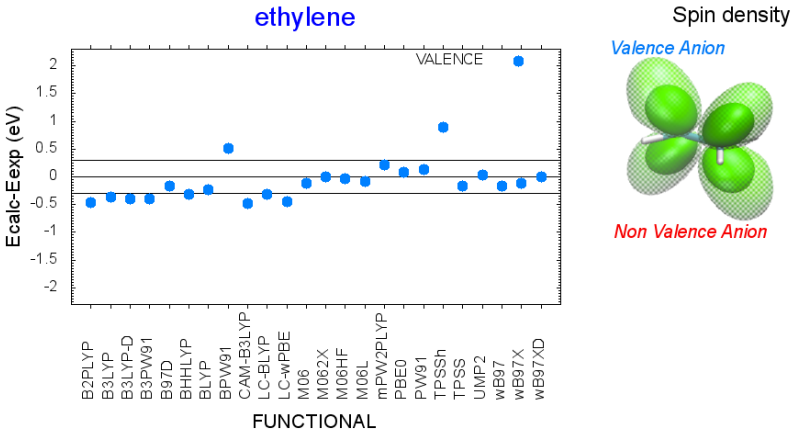


Spin density

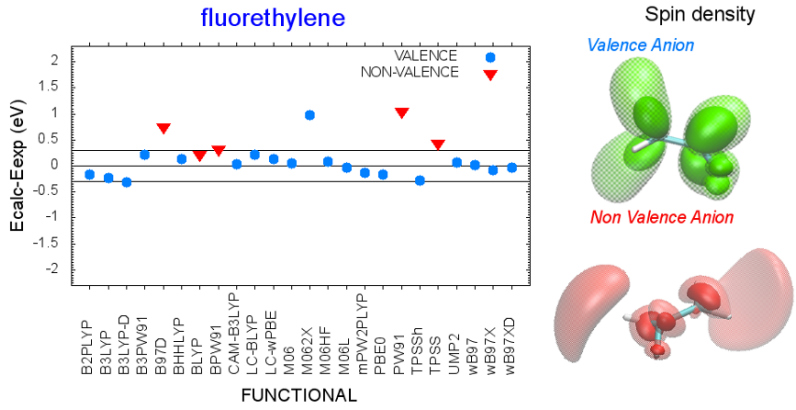



cytosine
VALENCE
NON-VALENCE
Ecalc-Exp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

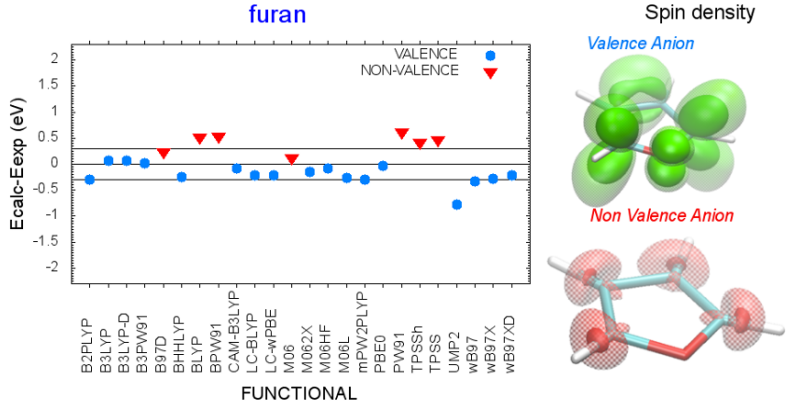
Spin density
Valence Anion
Non Valence Anion


ethylene
VALENCE
Ecalc-Exp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

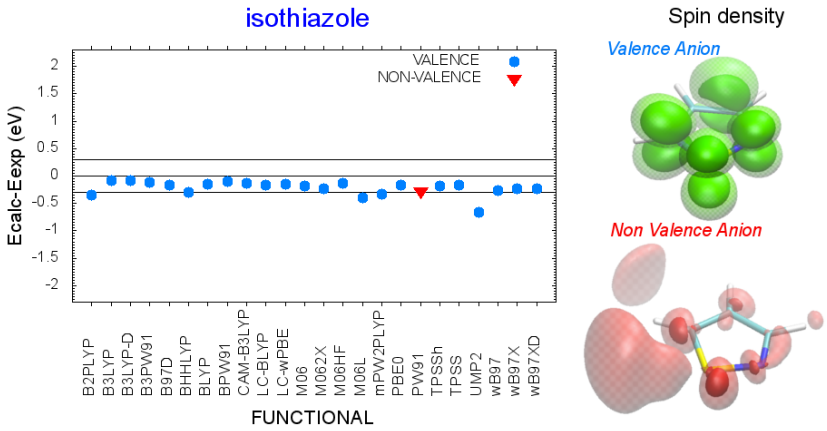
Spin density
Valence Anion
Non Valence Anion

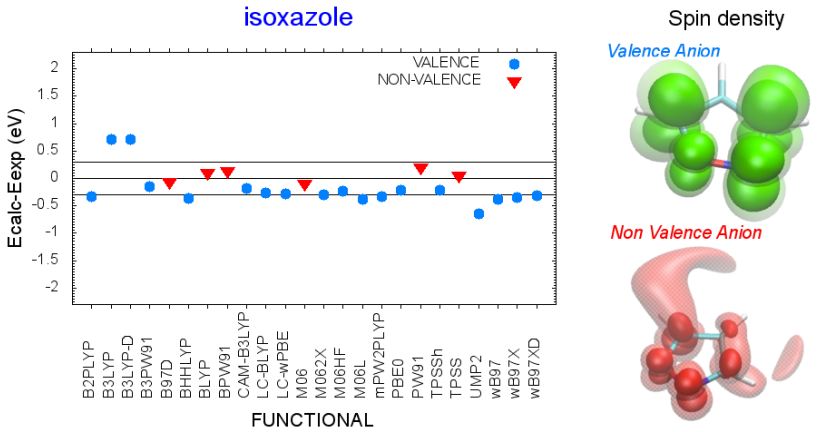

fluorethylene
VALENCE
NON-VALENCE
Ecalc-Exp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

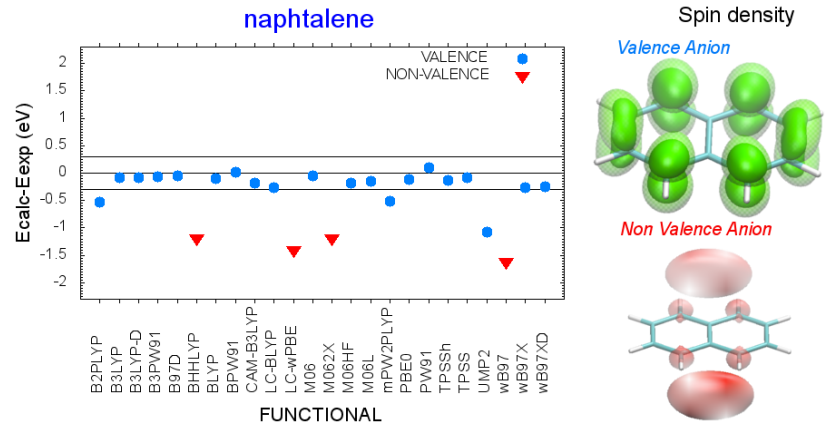
Spin density
Valence Anion
Non Valence Anion

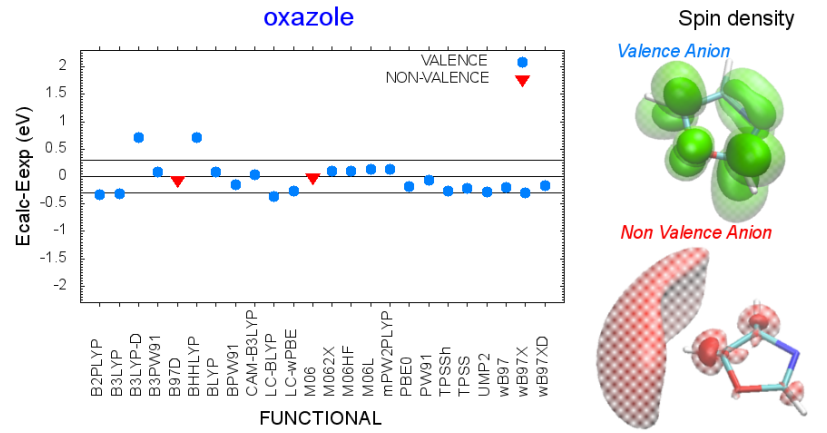

furan
VALENCE
NON-VALENCE
Ecalc-Exp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

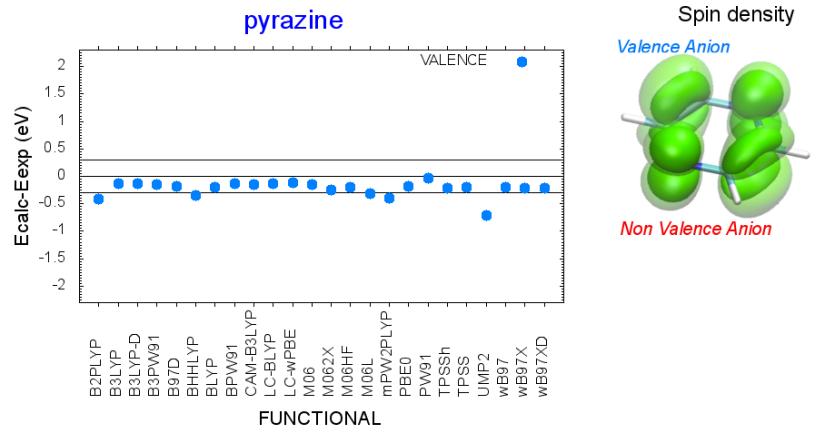
Spin density
Valence Anion
Non Valence Anion

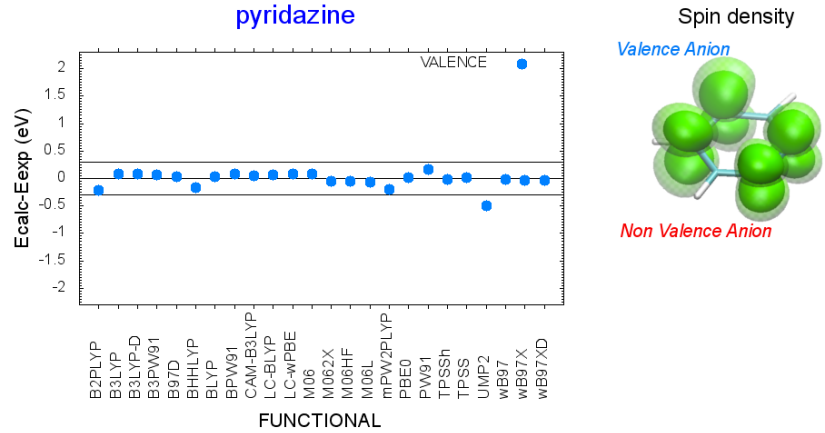

isothiazole
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD

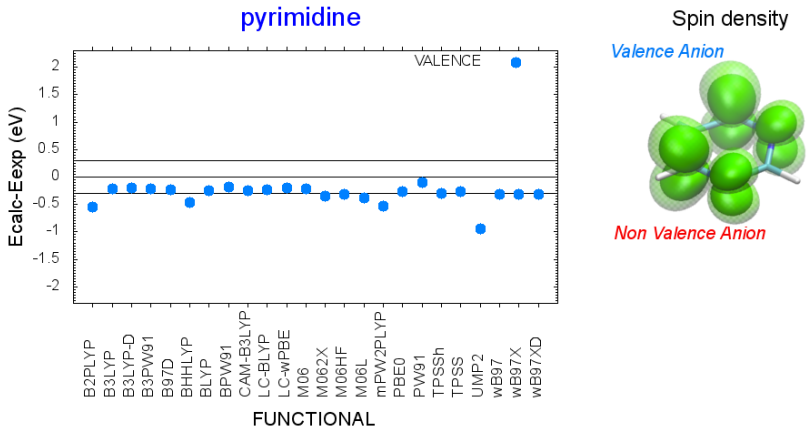

isoxazole
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD

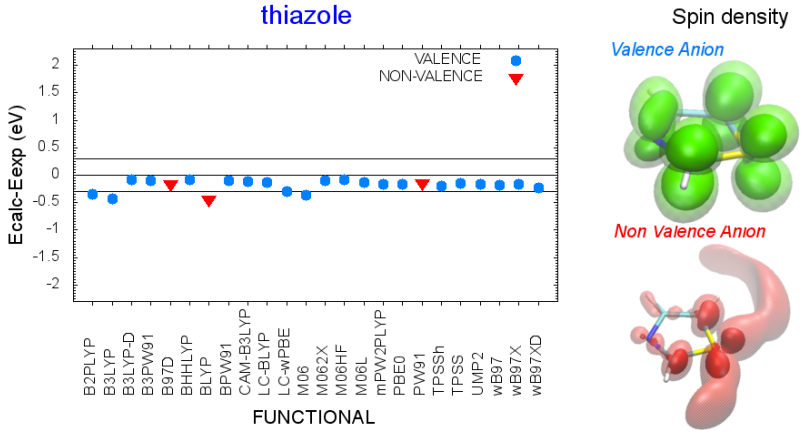

naphtalene
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD

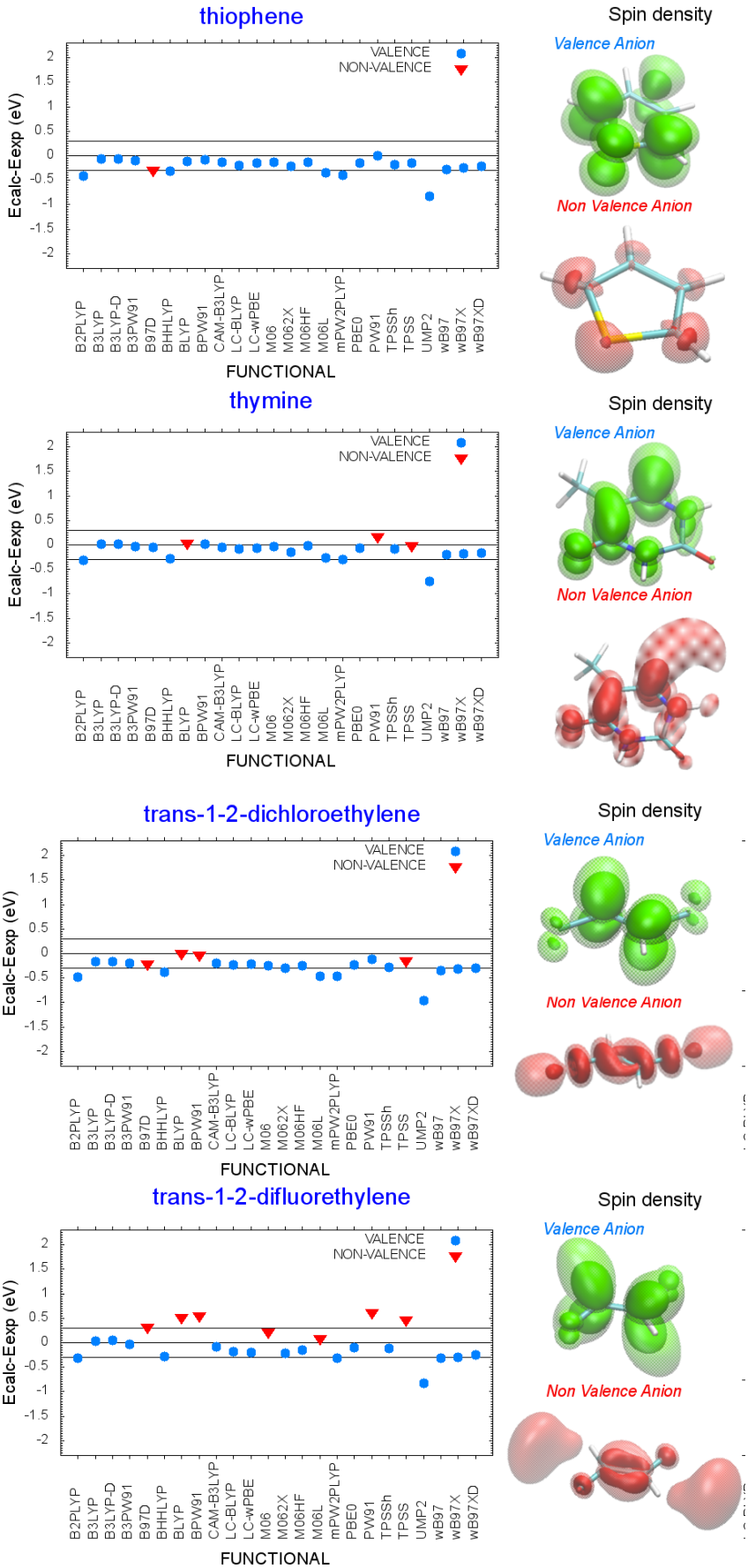

oxazole
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD

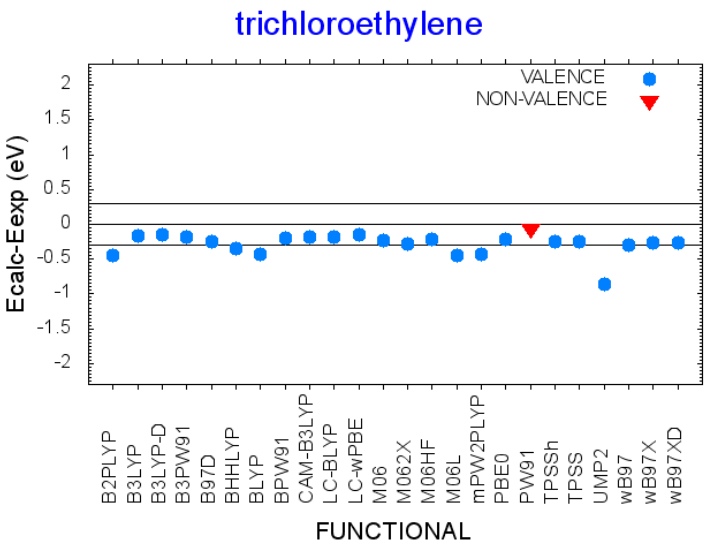

pyrazine
VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL
Spin density
Valence Anion
Non Valence Anion

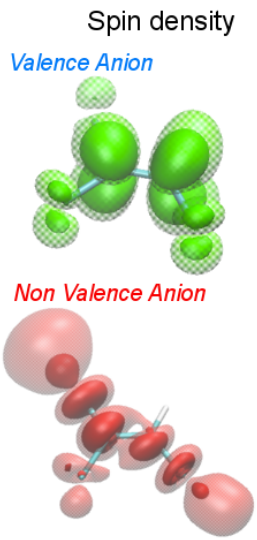

pyridazine
VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL
Spin density
Valence Anion
Non Valence Anion

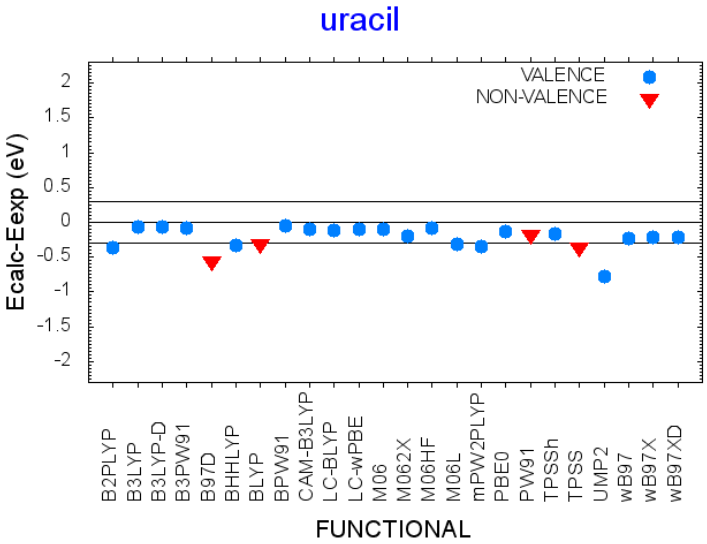

pyrimidine
VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL
Spin density
Valence Anion
Non Valence Anion

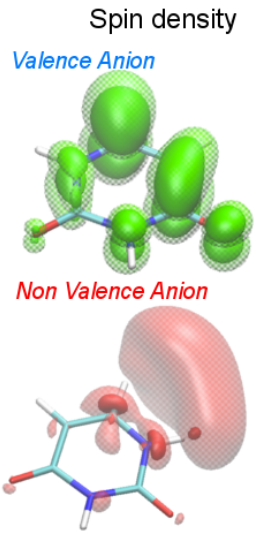

thiazole
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL
Spin density
Valence Anion
Non Valence Anion


thiophene
Spin density
Valence Anion
Non Valence Anion
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
FUNCTIONAL
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
thymine
Spin density
Valence Anion
Non Valence Anion
trans-1-2-dichloroethylene
Spin density
Valence Anion
Non Valence Anion
trans-1-2-difluorethylene
Spin density
Valence Anion
Non Valence Anion


trichloroethylene
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

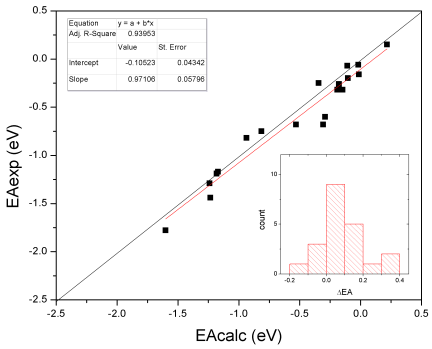

Spin density
Valence Anion
Non Valence Anion


uracil
VALENCE
NON-VALENCE
Ecalc-Eexp (eV)
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
B2PLYP
B3LYP
B3LYP-D
B3PW91
B97D
BHHLYP
BLYP
BPW91
CAM-B3LYP
LC-BLYP
LC-wPBE
M06
M062X
M06HF
M06L
mPW2PLYP
PBE0
PW91
TPSSh
TPSS
UMP2
wB97
wB97X
wB97XD
FUNCTIONAL

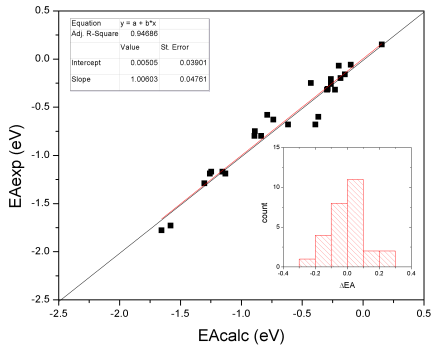

Spin density
Valence Anion
Non Valence Anion

Figures S2.1 to S2.24. Plots of the correlation between the predicted and experimental *EA* values for the different functionals. The black line shows the ideal correlation, the red one represents the linear fit of the data. The residuals are presented in the inset.

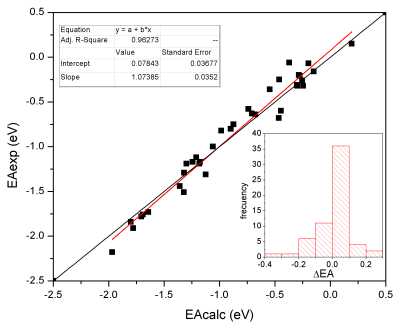
PW91



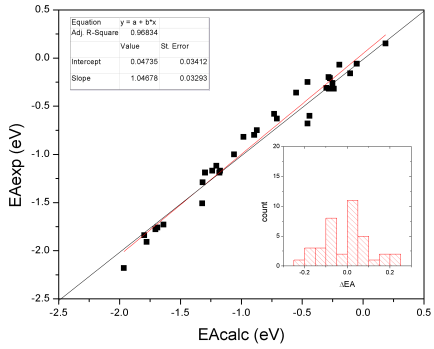
BPW91



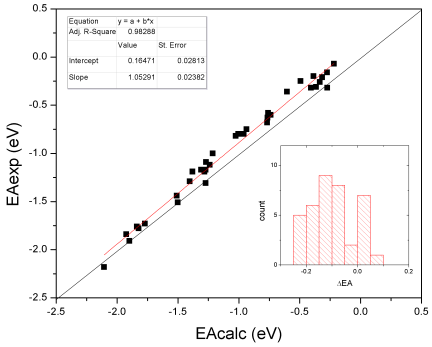
B3LYP



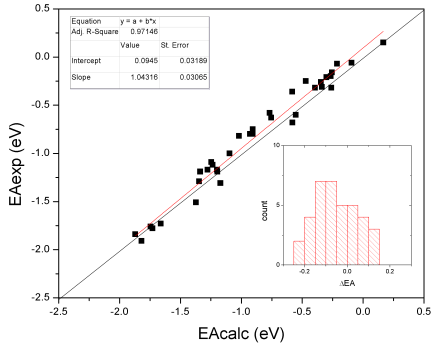
B3LYP-D



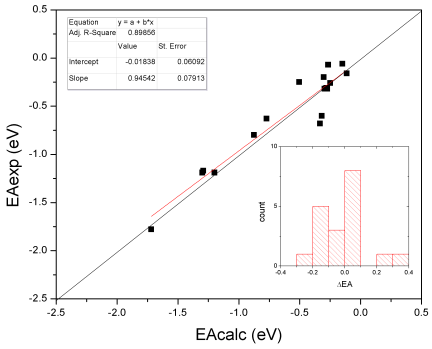
CAM-B3LYP



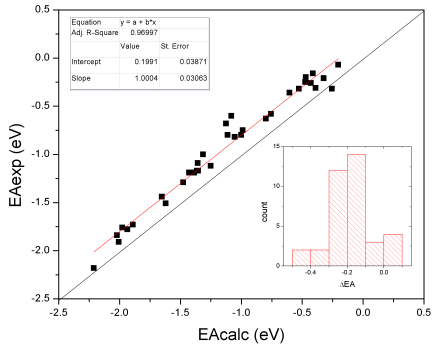
B3PW91



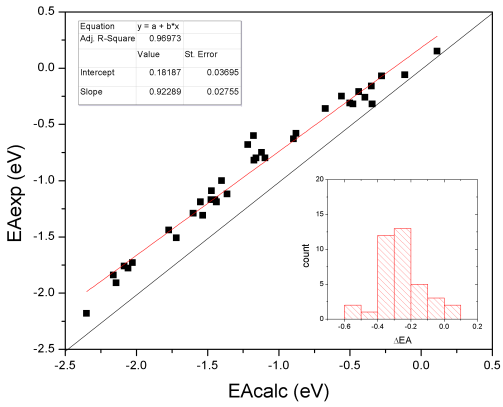
BLYP



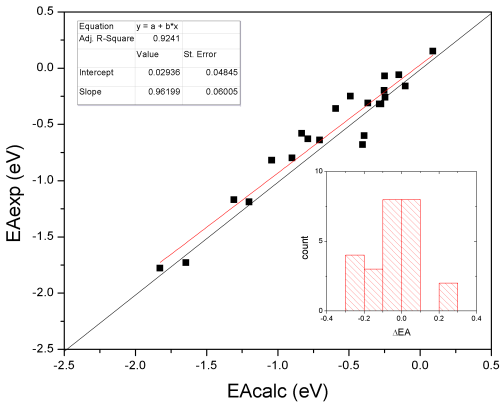
LC-BLYP



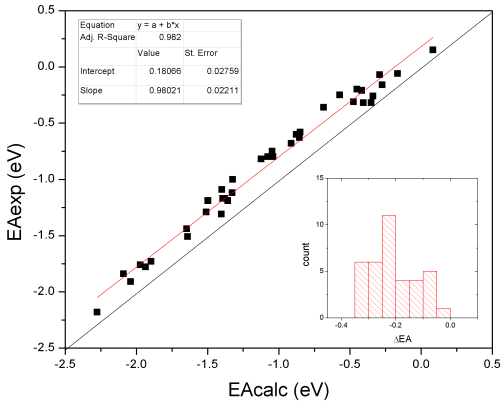
ωB97



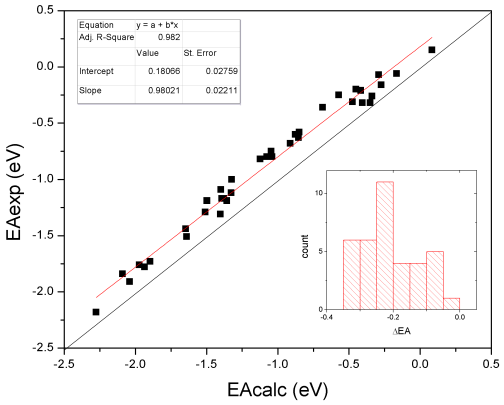
B97-D



ωB97-D



ωB97X-D



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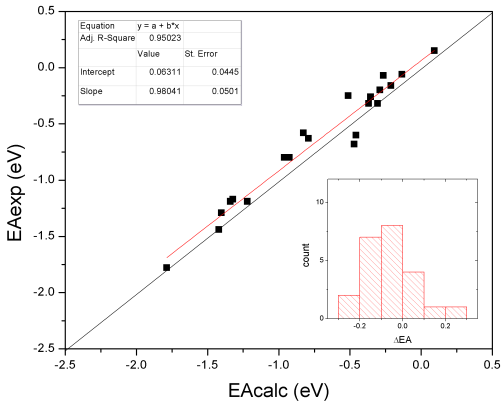
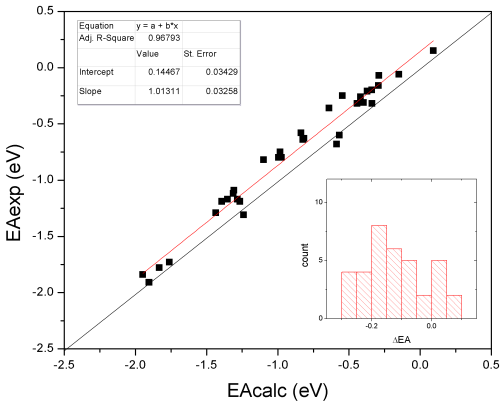


TPSSh



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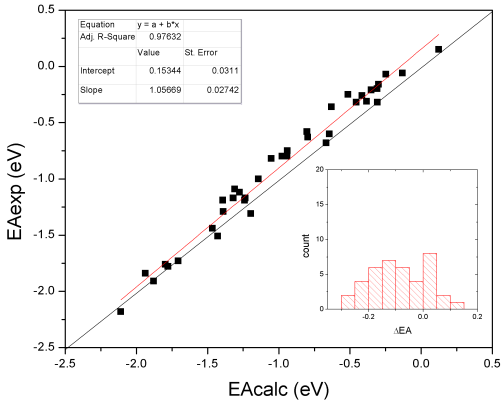
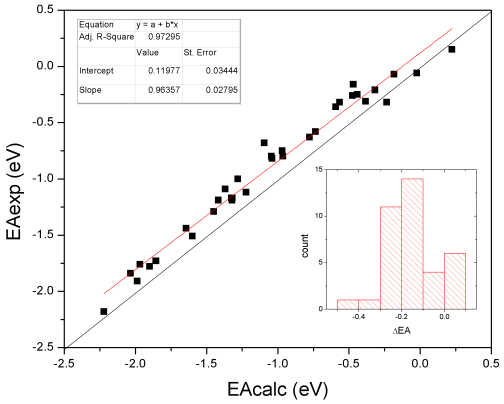
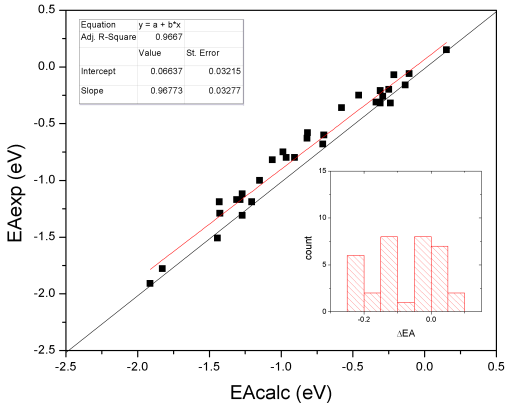


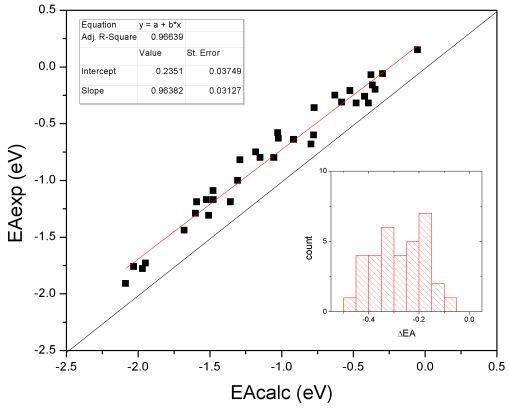
LC-ωPBE



M06



M06-L



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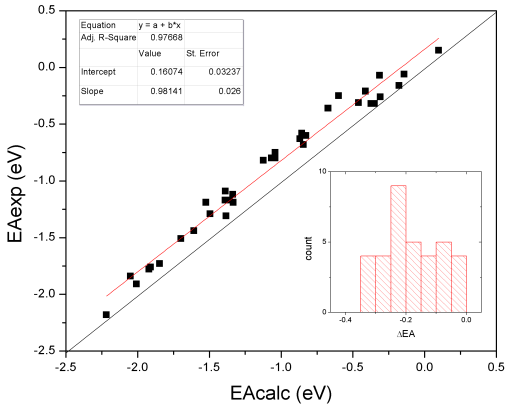

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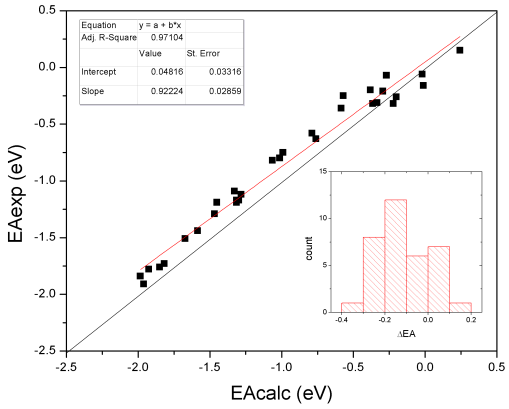

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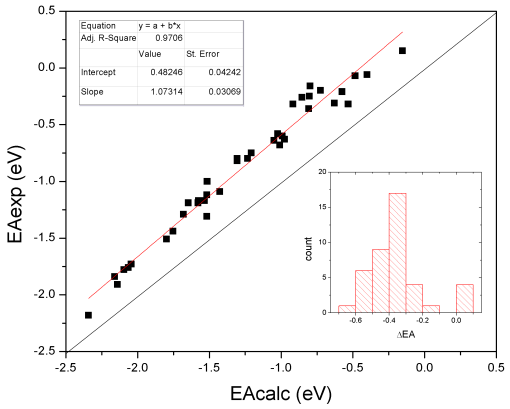

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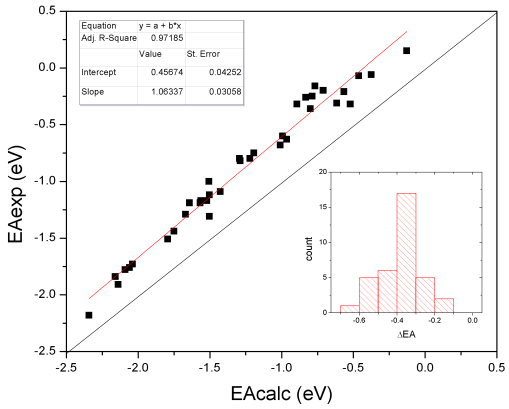
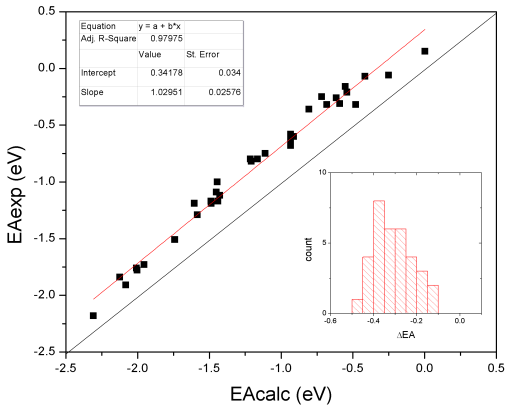
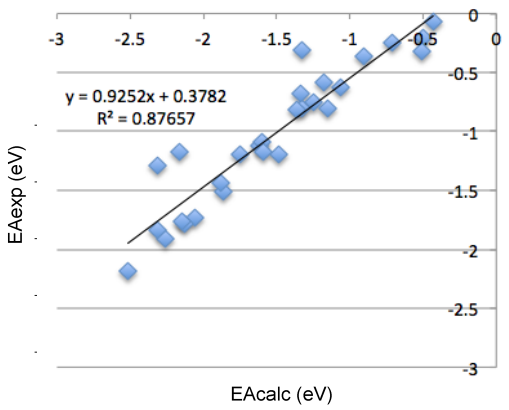
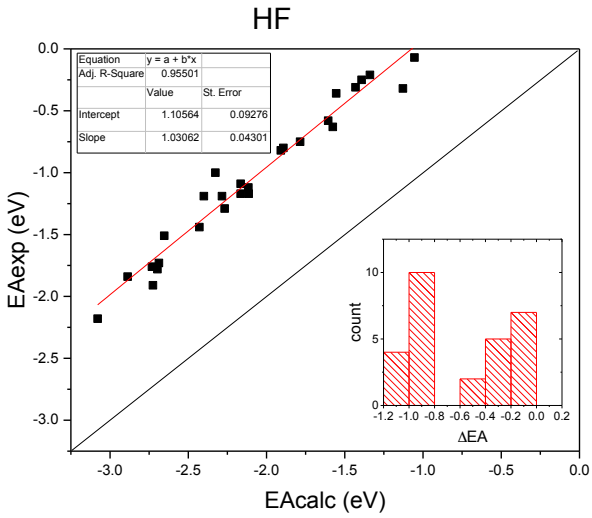


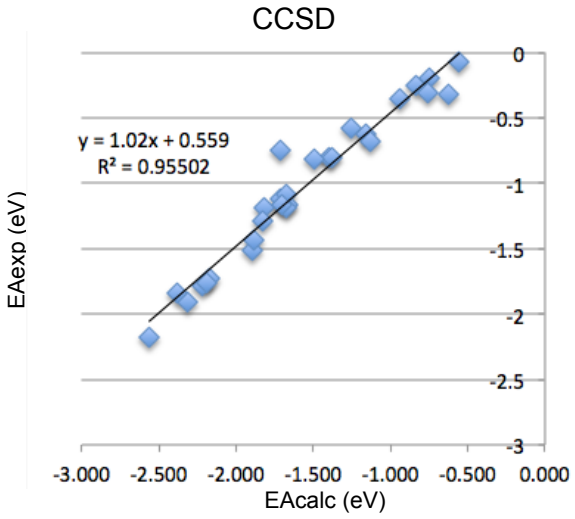
BHandHLYP

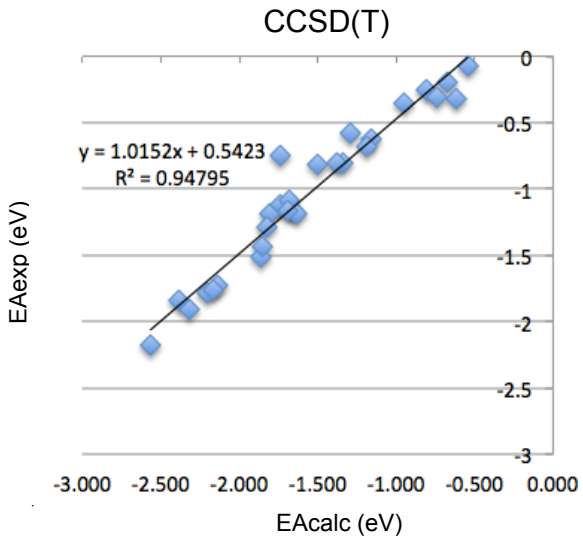


MP2




HF
Equation y = a + b*x
Adj. R-Square 0.95501
Value St. Error
Intercept 1.10564 0.09276
Slope 1.03062 0.04301
EAexp (eV)
EAcalc (eV)
count
ΔEA


CCSD
y = 1.02x + 0.559
R² = 0.95502
EAexp (eV)
EAcalc (eV)


CCSD(T)
y = 1.0152x + 0.5423
R² = 0.94795
EAexp (eV)
EAcalc (eV)

Tables S6.1-26. Detailed values of the energies employed for computing the EAs in table 1 for each DFT method employed.

BLYP Functional	Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1 1-1-dichloroethylene	-997.7116749	-997.6813361	-997.8042336	-997.7754804	-0.78	-0.75	0.669	N
2 1-3-cyclohexadiene	-233.2989248	-233.2619734	-233.3681109	-233.326427	-1.13	-0.8	0.968	N
3 2-bromo-1-propene	-2688.97739	-2688.94076	-2691.430373	-2691.397309	-0.90	-1.31	0.774	N
4 3-bromo-1-propene	-2688.972098	-2688.958418	-2691.427836	-2691.416124	-0.32	-0.6	0.282	V
5 acetaldehyde	-153.7860289	-153.7356261	-153.836764	-153.7889908	-1.30	-1.19	0.336	V
6 acetone	-193.0847696	-193.041415	-193.1472825	-193.1098976	-1.02	-1.51	0.712	N
7 adenine	-467.204073	-467.179225	-467.3449515	-467.3232027	-0.59	-0.64	0.773	N
8 bromoethylene	-2649.67849	-2649.638256	-2652.124094	-2652.085079	-1.06	-1.17	0.674	N
9 chloroethylene	-538.1316641	-538.0799393	-538.1909997	-538.1441431	-1.28	-1.29	0.688	N
chloroform	-500.0623224	-500.016384	-500.1096543	-500.0680767	-1.13	-0.35	0.628	N
10 cis-1-2-dichloroethylene	-997.7144036	-997.6762053	-997.8063141	-997.7708342	-0.97	-1.12	0.783	N
11 cis-1-2-difluorethylene	-277.0220141	-276.9777547	-277.1136792	-277.0717768	-1.14	-2.18	0.888	N
12 cis-1-bromo-2-butene	-2728.265118	-2728.250742	-2730.730847	-2730.718612	-0.33	-0.68	0.328	V
13 cyclobutanone	-231.1447687	-231.1054782	-231.215949	-231.1811941	-0.95	-1	0.549	N
14 cyclopentadiene	-194.0083808	-193.9614814	-194.0663115	-194.0222426	-1.20	-1.19	0.244	V
15 cyclopropene	-116.5638928	-116.5096184	-116.6006913	-116.5489144	-1.41	-1.73	0.902	N
16 cytosine-vertical	-394.8390658	-394.8199291	-394.9670558	-394.9505438	-0.45	-0.36	0.755	N
17 ethylene	-78.54420611	-78.47858925	-78.57126245	-78.5080821	-1.72	-1.78	0.401	V
18 fluorethylene	-177.7887305	-177.7285402	-177.8478889	-177.7932551	-1.49	-1.91	0.946	N
19 furan	-229.9525748	-229.9005605	-230.0241914	-229.9786122	-1.24	-1.76	1.039	N
20 isothiazole	-568.9735786	-568.9426559	-569.0615286	-569.0331985	-0.77	-0.63	0.324	V
21 isoxazole	-245.982683	-245.9422142	-246.0576976	-246.0214165	-0.99	-1.09	0.744	N
22 naphtalene	-385.7286925	-385.7141393	-385.836269	-385.8251597	-0.30	-0.2	0.271	V
23 oxazole	-246.0144347	-245.9635861	-246.0901232	-246.040976	-1.34	-1.44	0.502	N
24 pyrazine	-264.2394555	-264.226928	-264.3149879	-264.3052181	-0.27	-0.07	0.307	V
25 pyridazine	-264.2115243	-264.1982228	-264.2871093	-264.2762715	-0.29	-0.32	0.290	V
26 pyrimidine	-264.2452112	-264.224058	-264.3207614	-264.3022581	-0.50	-0.25	0.304	V
27 thiazole	-568.9793337	-568.9435689	-569.064175	-569.0320426	-0.87	-0.8	0.589	V
28 thiophene	-552.9209526	-552.8704031	-553.0023591	-552.9549018	-1.29	-1.17	0.319	V
29 thymine	-454.030509	-454.0177639	-454.1755495	-454.1652242	-0.28	-0.31	0.595	V
30 trans-1-2-dichloroethylene	-997.7141543	-997.6833092	-997.8059997	-997.7761232	-0.81	-0.82	0.605	N
31 trans-1-2-difluorethylene	-277.0211711	-276.971717	-277.1122704	-277.063486	-1.33	-1.84	0.857	N
33 trichloroethylene	-1457.291848	-1457.268123	-1457.41709	-1457.37989	-1.01	-0.58		
34 uracil-vertical	-414.7375146	-414.71655	-414.8713902	-414.8523394	-0.52	-0.21	1.022	N
16 cytosine - adiabatic	-394.8390658	-394.8293516	-394.9670558	-394.9572759	-0.15	-0.06	0.312	V
34 uracil - adiabatic	-414.7375146	-414.7160492	-414.8713876	-414.8523394	-0.52	0.15	1.022	N
36 ethyl-radical	-79.10428466	-79.09088068	-79.13071208	-79.11969576	-0.25	-0.26	0.158	V
36 isopropyl-radical	-118.3981001	-118.383971	-118.4362994	-118.4240435	-0.27	-0.32	0.236	V
37 t-butyl-radical	-157.691678	-157.6837263	-157.741179	-157.7342518	-0.11	-0.16	0.271	V

BPW91 Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7701478	-997.7364074	-997.85858	-997.8259605	-0.88762	-0.75	0.36578	V
2	1-3-cyclohexadiene	-233.3880257	-233.3532782	-233.4518859	-233.4211668	-0.835912	-0.8	0.24831	V
3	2-bromo-1-propene	-2689.179635	-2689.141181	-2691.628772	-2691.594242	-0.939606	-1.31	0.76252	N
4	3-bromo-1-propene	-2689.172784	-2689.157084	-2691.624679	-2691.611186	-0.367179	-0.6	0.29931	V
5	acetaldehyde	-153.8189703	-153.7634623	-153.8668393	-153.8206234	-1.257599	-1.19	0.34037	V
6	acetone	-193.1367978	-193.093847	-193.1954509	-193.1587976	-0.997387	-1.51	0.71743	N
7	adenine	-467.3053616	-467.2809829	-467.4399695	-467.4190346	-0.569667	-0.64	0.74343	N
8	bromoethylene	-2649.861675	-2649.816605	-2652.30428	-2652.261903	-1.15314	-1.17	0.41766	V
9	chloroethylene	-538.1760589	-538.1242238	-538.2320405	-538.1841453	-1.303295	-1.29	0.38595	V
	chloroform	-500.0999653	-500.0545911	-500.1449089	-500.1040728	-1.111208	-0.35	0.67424	N
10	cis-1-2-dichloroethylene	-997.7730065	-997.7318266	-997.8607199	-997.8228768	-1.029763	-1.12	0.81813	N
11	cis-1-2-difluorethylene	-277.0383432	-276.9932985	-277.1263233	-277.0843035	-1.143417	-2.18	0.9243	N
12	cis-1-bromo-2-butene	-2728.484954	-2728.468272	-2730.945961	-2730.931597	-0.390859	-0.68	0.32582	V
13	cyclobutanone	-231.2110001	-231.1732214	-231.2777285	-231.2447791	-0.896598	-1	0.55781	N
14	cyclopentadiene	-194.0796937	-194.0347926	-194.1334954	-194.0920022	-1.129086	-1.19	0.2258	V
15	cyclopropene	-116.6079811	-116.5471975	-116.6418636	-116.5838175	-1.579516	-1.73	0.42818	V
16	cytosine-vertical	-394.9166858	-394.8972596	-395.0386975	-395.0222396	-0.44784	-0.36	0.73142	N
17	ethylene	-78.57473394	-78.51113758	-78.59933844	-78.53855262	-1.654067	-1.78	0.40107	V
18	fluorethylene	-177.8121277	-177.7532477	-177.8682496	-177.8153847	-1.438526	-1.91	0.93229	N
19	furan	-230.0064432	-229.9537989	-230.0740924	-230.0290429	-1.22586	-1.76	1.04661	N
20	isothiazole	-569.0346453	-569.004733	-569.1193289	-569.0922564	-0.736681	-0.63	0.31255	V
21	isoxazole	-246.0284767	-245.9883498	-246.0999788	-246.0647186	-0.959479	-1.09	0.78228	N
22	naphtalene	-385.8514068	-385.8407329	-385.9513165	-385.9445499	-0.184129	-0.2	0.2501	V
23	oxazole	-246.0606935	-246.0109131	-246.1328059	-246.0847583	-1.307442	-1.44	0.5273	N
24	pyrazine	-264.3006043	-264.2903986	-264.3716499	-264.3643764	-0.197924	-0.07	0.28692	V
25	pyridazine	-264.2729303	-264.2618765	-264.3439822	-264.3355502	-0.229448	-0.32	0.27537	V
26	pyrimidine	-264.3066316	-264.2881123	-264.3777235	-264.3620129	-0.427508	-0.25	0.28467	V
27	thiazole	-569.0410879	-569.0056131	-569.1225027	-569.0897599	-0.890977	-0.8	0.29	V
28	thiophene	-552.9907508	-552.9414858	-553.0682882	-553.0224781	-1.246557	-1.17	0.30106	V
29	thymine	-454.1177202	-454.104244	-454.2558453	-454.2452178	-0.289189	-0.31	0.36458	V
30	trans-1-2-dichloroethylene	-997.7724034	-997.7394451	-997.8600597	-997.8285775	-0.856674	-0.82	0.66599	N
31	trans-1-2-difluorethylene	-277.0372781	-276.989153	-277.1247023	-277.0774112	-1.286858	-1.84	0.89477	N
32	trans-1-bromo-2-butene	-2727.207523	-2727.18272	-2729.667404	-2729.644794	-0.615242	-0.68	0.4795	V
33	trichloroethylene	-1457.36446	-1457.337564	-1457.484788	-1457.455921	-0.785496	-0.58	0.32144	V
34	uracil-vertical	-414.8056771	-414.7927895	-414.9333442	-414.9236491	-0.263818	-0.21	0.29556	V
16	cytosine - adiabatic	-394.9166858	-394.9087245	-395.0386975	-395.0309137	-0.100818	-0.06	0.28995	V
34	uracil - adiabatic	-414.8056771	-414.8043901	-414.9333442	-414.932951	0.155295	0.15	0.25574	V
36	ethyl-radical	-79.14310747	-79.12860505	-79.16726904	-79.15565524	-0.263923	-0.26	0.14642	V
36	isopropyl-radical	-118.455801	-118.4403035	-118.4908035	-118.4776295	-0.294509	-0.32	0.21702	V
37	t-butyl-radical	-157.7681641	-157.7583034	-157.8137324	-157.8052687	-0.149091	-0.16	0.2498	V

PW91 Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.6980874	-997.6642187	-997.787519	-997.7576124	-0.814	-0.75	0.363	V
2	1-3-cyclohexadiene	-233.3185922	-233.2875207	-233.3825057	-233.3438338	-1.052	-0.8	0.968	N
3	2-bromo-1-propene	-2689.106954	-2689.071649	-2691.555931	-2691.524601	-0.853	-1.31	0.809	N
4	3-bromo-1-propene	-2689.099764	-2689.087069	-2691.551519	-2691.540831	-0.291	-0.6	0.299	V
5	acetaldehyde	-153.777104	-153.7245956	-153.8251068	-153.7816897	-1.181	-1.19	0.333	V
6	acetone	-193.0834709	-193.0440134	-193.1422731	-193.1091057	-0.903	-1.51	0.712	N
7	adenine	-467.196323	-467.175537	-467.331816	-467.3142136	-0.479	-0.64	0.763	N
8	bromoethylene	-2649.800317	-2649.762338	-2652.242819	-2652.206157	-0.998	-1.17	0.702	N
9	chloroethylene	-538.1254072	-538.0725354	-538.181908	-538.1363342	-1.240	-1.29	0.377	V
	chloroform	-500.058884	-500.015177	-500.1042438	-500.065347	-1.058	-0.35	0.662	N
10	cis-1-2-dichloroethylene	-997.7009116	-997.6634633	-997.789626	-997.7553096	-0.934	-1.12	0.829	N
11	cis-1-2-difluorethylene	-276.9822989	-276.9411055	-277.0704625	-277.0319214	-1.049	-2.18	0.910	N
12	cis-1-bromo-2-butene	-2728.400496	-2728.387022	-2730.861292	-2730.850037	-0.306	-0.68	0.340	V
13	cyclobutanone	-231.1485324	-231.1139314	-231.215373	-231.1856222	-0.810	-1	0.546	N
14	cyclopentadiene	-194.0213436	-193.9686942	-194.0751758	-194.0324607	-1.162	-1.19	0.972	N
15	cyclopropene	-116.5693675	-116.5193118	-116.6033113	-116.5560358	-1.286	-1.73	0.897	N
16	cytosine-vertical	-394.8249363	-394.8095762	-394.9477345	-394.9350952	-0.344	-0.36	0.744	N
17	ethylene	-78.54577168	-78.48410264	-78.57037267	-78.51152854	-1.601	-1.78	0.386	V
18	fluorethylene	-177.7696971	-177.7134105	-177.8259237	-177.775382	-1.375	-1.91	0.934	N
19	furan	-229.94742	-229.898283	-230.0152737	-229.9733629	-1.140	-1.76	1.044	N
20	isothiazole	-568.9662569	-568.9393558	-569.0515218	-569.017927	-0.914	-0.63	1.008	N
21	isoxazole	-245.9686257	-245.9314346	-246.0404473	-246.0078784	-0.886	-1.09	0.786	N
22	naphtalene	-385.745707	-385.7382435	-385.8460328	-385.8422438	-0.103	-0.2	0.260	V
23	oxazole	-246.001115	-245.9540952	-246.0735417	-246.028241	-1.233	-1.44	0.516	V
24	pyrazine	-264.2319824	-264.2251515	-264.3034378	-264.2994322	-0.109	-0.07	0.298	V
25	pyridazine	-264.2041036	-264.196215	-264.2755865	-264.2701732	-0.147	-0.32	0.283	V
26	pyrimidine	-264.2379773	-264.2226375	-264.3094597	-264.2968343	-0.344	-0.25	0.294	V
27	thiazole	-568.9728122	-568.9351318	-569.054761	-569.0190022	-0.973	-0.8	1.104	N
28	thiophene	-552.922933	-552.8766144	-553.000918	-552.957922	-1.170	-1.17	0.308	V
29	thymine	-454.0137211	-454.00597	-454.1525795	-454.1472289	-0.146	-0.31	0.597	N
30	trans-1-2-dichloroethylene	-997.6999946	-997.6697263	-997.788684	-997.754267	-0.937	-0.82	0.335	V
31	trans-1-2-difluorethylene	-276.9811522	-276.9355035	-277.0687924	-277.0238633	-1.223	-1.84	0.879	N
32	trans-1-bromo-2-butene	-2727.125115	-2727.103677	-2729.58491	-2729.565447	-0.530	-0.68	0.465	V
33	trichloroethylene	-1457.270989	-1457.246653	-1457.39278	-1457.36926	-0.640	-0.58	0.627	N
34	uracil-vertical	-414.7129115	-414.6966039	-414.841358	-414.8270826	-0.388	-0.21	1.023	N
16	cytosine - adiabatic	-394.8249363	-394.8201176	-394.9477345	-394.9429451	-0.018	-0.06	0.312	V
34	uracil - adiabatic	-414.7129115	-414.7166451	-414.841358	-414.8451238	0.218	0.15	0.289	V
36	ethyl-radical	-79.11249425	-79.10112235	-79.13656919	-79.12820732	-0.177	-0.26	0.153	V
36	isopropyl-radical	-118.4136004	-118.4019335	-118.4485774	-118.439378	-0.190	-0.32	0.226	V
37	t-butyl-radical	-157.7147972	-157.7099405	-157.7603531	-157.7570077	-0.013	-0.16	0.259	V

B97D Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7470705	-997.7053334	-997.8339686	-997.7961955	-1.028	-0.75	0.610	N
2	1-3-cyclohexadiene	-233.2484972	-233.2115374	-233.3136341	-233.2806229	-0.898	-0.8	0.240	V
3	2-bromo-1-propene	-2690.253182	-2690.206561	-2692.704464	-2692.661542	-1.168	-1.31	0.663	N
4	3-bromo-1-propene	-2690.246984	-2690.230069	-2692.700991	-2692.686549	-0.393	-0.6	0.227	V
5	acetaldehyde	-153.738598	-153.685486	-153.7874757	-153.730684	-1.545	-1.19	0.922	N
6	acetone	-193.0353552	-192.983719	-193.0953249	-193.0493928	-1.250	-1.51	0.647	N
7	adenine	-467.0079818	-466.9790125	-467.1437349	-467.1178158	-0.705	-0.64	0.621	V
8	bromoethylene	-2650.955896	-2650.907206	-2653.400424	-2653.352402	-1.307	-1.17	0.344	V
9	chloroethylene	-538.1440616	-538.0869483	-538.1996661	-538.1407794	-1.602	-1.29	0.898	N
	chloroform	-500.0935743	-500.0399896	-500.1379598	-500.0893533	-1.323	-0.35	0.644	N
10	cis-1-2-dichloroethylene	-997.7499649	-997.6961896	-997.8362225	-997.7900061	-1.258	-1.12	0.662	N
11	cis-1-2-difluorethylene	-276.9127964	-276.8563128	-277.0017723	-276.9491277	-1.433	-2.18	0.929	N
12	cis-1-bromo-2-butene	-2729.538957	-2729.521505	-2732.002252	-2731.987406	-0.404	-0.68	0.243	V
13	cyclobutanone	-231.0791926	-231.0351682	-231.1472321	-231.0925364	-1.488	-1	0.983	N
14	cyclopentadiene	-193.9585782	-193.911044	-194.0133589	-193.9692087	-1.201	-1.19	0.213	V
15	cyclopropene	-116.5391771	-116.470854	-116.5737736	-116.5133109	-1.645	-1.73	0.820	V
16	cytosine-vertical	-394.6798709	-394.6551458	-394.8032505	-394.7814857	-0.592	-0.36	0.537	V
17	ethylene	-78.53380166	-78.46381119	-78.55905772	-78.49188664	-1.828	-1.78	0.361	V
18	fluorethylene	-177.728782	-177.6607411	-177.7857308	-177.7235245	-1.693	-1.91	0.837	N
19	furan	-229.867337	-229.8015688	-229.9361927	-229.8800373	-1.528	-1.76	1.046	N
20	isothiazole	-568.9207531	-568.8888298	-569.0053293	-568.9763889	-0.788	-0.63	0.292	V
21	isoxazole	-245.8787707	-245.831047	-245.9513349	-245.9086759	-1.161	-1.09	0.691	N
22	naphtalene	-385.6046256	-385.5917425	-385.7067887	-385.6975329	-0.252	-0.2	0.257	V
23	oxazole	-245.9118158	-245.8555233	-245.9849315	-245.9316952	-1.449	-1.44	1.073	N
24	pyrazine	-264.1343328	-264.1222739	-264.2064548	-264.1973053	-0.249	-0.07	0.279	V
25	pyridazine	-264.1066605	-264.0936877	-264.1787987	-264.1682991	-0.286	-0.32	0.272	V
26	pyrimidine	-264.1405687	-264.1198616	-264.2126872	-264.1947361	-0.488	-0.25	0.277	V
27	thiazole	-568.92704	-568.8896834	-569.0084429	-568.9624022	-1.253	-0.8	0.876	N
28	thiophene	-552.8866556	-552.8350569	-552.9643429	-552.9104055	-1.468	-1.17	1.080	N
29	thymine	-453.8536405	-453.8372876	-453.9937544	-453.980285	-0.367	-0.31	0.335	V
30	trans-1-2-dichloroethylene	-997.7494517	-997.7087295	-997.8356779	-997.7973842	-1.042	-0.82	0.607	V
31	trans-1-2-difluorethylene	-276.9117179	-276.8542766	-277.0001442	-276.9442359	-1.521	-1.84	0.901	N
32	trans-1-bromo-2-butene	-2728.196181	-2728.249823	-2730.658173	-2730.713385	1.502	-0.68	0.178	V
33	trichloroethylene	-1457.350308	-1457.317693	-1457.467999	-1457.437455	-0.831	-0.58	0.547	V
34	uracil-vertical	-414.561868	-414.5300947	-414.6912579	-414.662626	-0.779	-0.21	1.035	N
16	cytosine - adiabatic	-394.6798709	-394.670384	-394.8032505	-394.7935154	-0.149	-0.06	0.283	V
34	uracil - adiabatic	-414.561868	-414.5609397	-414.6912579	-414.6901111	0.091	0.15	0.261	V
36	ethyl-radical	-79.1031844	-79.0895424	-79.12789801	-79.11692187	-0.245	-0.26	0.154	V
36	isopropyl-radical	-118.3947346	-118.3804143	-118.430725	-118.4183781	-0.274	-0.32	0.228	V
37	t-butyl-radical	-157.6872321	-157.6797063	-157.7341485	-157.7275953	-0.104	-0.16	0.264	V

B3PW91 Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.6443767	-997.6072266	-997.73083	-997.6975594	-0.905	-0.75	0.351	V
2	1-3-cyclohexadiene	-233.3394864	-233.3023766	-233.401899	-233.3686359	-0.905	-0.8	0.250	V
3	2-bromo-1-propene	-2688.976886	-2688.931743	-2691.430664	-2691.387643	-1.171	-1.31	0.490	V
4	3-bromo-1-propene	-2688.970175	-2688.947923	-2691.426699	-2691.406396	-0.552	-0.6	0.314	V
5	acetaldehyde	-153.7777238	-153.725886	-153.8251098	-153.7759669	-1.337	-1.19	0.306	V
6	acetone	-193.0904264	-193.0351146	-193.148308	-193.0978714	-1.372	-1.51	0.431	V
7	adenine	-467.1617164	-467.131953	-467.29541	-467.268903	-0.721	-0.64	0.812	N
8	bromoethylene	-2649.664252	-2649.617513	-2652.11181	-2652.067738	-1.199	-1.17	0.388	V
9	chloroethylene	-538.1057838	-538.0525016	-538.1605101	-538.1110237	-1.347	-1.29	0.371	V
	chloroform	-500.0431544	-499.9931303	-500.0870568	-500.0436032	-1.182	-0.35	0.721	N
10	cis-1-2-dichloroethylene	-997.6475797	-997.5969636	-997.7332555	-997.6878789	-1.235	-1.12	0.262	V
11	cis-1-2-difluorethylene	-276.9595227	-276.8833496	-277.0466394	-277.002156	-1.210	-2.18	0.961	N
12	cis-1-bromo-2-butene	-2728.276694	-2728.253386	-2730.741982	-2730.720696	-0.579	-0.68	0.347	V
13	cyclobutanone	-231.1530675	-231.1078379	-231.2185356	-231.1782713	-1.096	-1	0.321	V
14	cyclopentadiene	-194.0358458	-193.988687	-194.0885879	-194.0446462	-1.196	-1.19	0.231	V
15	cyclopropene	-116.5800136	-116.5163001	-116.6134474	-116.5524052	-1.661	-1.73	0.419	V
16	cytosine-vertical	-394.7970116	-394.7726434	-394.9182182	-394.8968404	-0.582	-0.36	0.325	V
17	ethylene	-78.55967872	-78.4933635	-78.58382015	-78.52028559	-1.729	-1.78	0.392	V
18	fluorethylene	-177.7651208	-177.6956804	-177.8205614	-177.7537136	-1.819	-1.91	0.451	V
19	furan	-229.941817	-229.87538	-230.0086324	-229.9445174	-1.745	-1.76	0.502	V
20	isothiazole	-568.9336479	-568.9033684	-569.0167943	-568.9890971	-0.754	-0.63	0.316	V
21	isoxazole	-245.9491859	-245.9009419	-246.0201717	-245.9743823	-1.246	-1.09	0.345	V
22	naphtalene	-385.755253	-385.7418086	-385.8535889	-385.8438597	-0.265	-0.2	0.265	V
23	oxazole	-245.9849363	-245.9315148	-246.0564635	-246.0047212	-1.408	-1.44	0.531	N
24	pyrazine	-264.2223939	-264.2118023	-264.2927846	-264.2849632	-0.213	-0.07	0.290	V
25	pyridazine	-264.1931077	-264.1811195	-264.2635399	-264.2539603	-0.261	-0.32	0.280	V
26	pyrimidine	-264.229183	-264.2092844	-264.2996606	-264.282392	-0.470	-0.25	0.287	V
27	thiazole	-568.9406844	-568.9041869	-569.020429	-568.9863196	-0.928	-0.8	0.293	V
28	thiophene	-552.9026873	-552.8525402	-552.978205	-552.9312591	-1.277	-1.17	0.300	V
29	thymine	-453.983207	-453.968075	-454.1203052	-454.107899	-0.338	-0.31	0.361	V
30	trans-1-2-dichloroethylene	-997.64693	-997.6048718	-997.7325587	-997.695158	-1.018	-0.82	0.315	V
31	trans-1-2-difluorethylene	-276.9584676	-276.8879781	-277.044988	-276.9762515	-1.870	-1.84	0.485	V
33	trichloroethylene	-1457.183429	-1457.150267	-1457.301017	-1457.272856	-0.766	-0.58	0.303	V
34	uracil-vertical	-414.6765829	-414.6625526	-414.8033977	-414.7923822	-0.300	-0.21	0.302	V
16	cytosine - adiabatic	-394.7970116	-394.7900803	-394.9182182	-394.9108813	-0.094	-0.06	0.288	V
34	uracil - adiabatic	-414.6765829	-414.6760748	-414.8033977	-414.8033714	0.167	0.15	0.263	V
36	ethyl-radical	-79.13277908	-79.1154228	-79.15633472	-79.14188858	-0.345	-0.26	0.137	V
36	isopropyl-radical	-118.4397155	-118.4206883	-118.4737502	-118.4570532	-0.394	-0.32	0.197	V
37	t-butyl-radical	-157.7464762	-157.7326784	-157.7908283	-157.7785094	-0.256	-0.16	0.240	V

B3LYP Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)				
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Anion typ
1	1-1-dichloroethylene	-997.7811016	-997.7452589	-997.8702483	-997.8381578	-0.873	-0.75	V
2	1-3-cyclohexadiene	-233.4288202	-233.3923704	-233.4949888	-233.4619957	-0.898	-0.8	V
3	2-bromo-1-propene	-2689.039052	-2688.995775	-2691.495386	-2691.454082	-1.124	-1.31	V
4	3-bromo-1-propene	-2689.033474	-2689.015281	-2691.492576	-2691.476209	-0.445	-0.6	V
5	acetaldehyde	-153.8397469	-153.7893253	-153.8890697	-153.8413626	-1.298	-1.19	V
6	acetone	-193.1662535	-193.1129022	-193.226748	-193.1781885	-1.321	-1.51	V
7	adenine	-467.3398754	-467.3119387	-467.4778555	-467.4530435	-0.675	-0.64	V
8	bromoethylene	-2649.712635	-2649.66696	-2652.162208	-2652.119022	-1.175	-1.17	V
9	chloroethylene	-538.191031	-538.1389561	-538.2480309	-538.1995292	-1.320	-1.29	V
	chloroform	-500.1115215	-500.0633954	-500.1569244	-500.1148178	-1.146	-0.35	N
10	cis-1-2-dichloroethylene	-997.7842508	-997.7348136	-997.872669	-997.828225	-1.209	-1.12	V
11	cis-1-2-difluorethylene	-277.0666446	-276.9931336	-277.1563426	-277.0840152	-1.968	-2.18	V
12	cis-1-bromo-2-butene	-2728.353724	-2728.334685	-2730.822156	-2730.80507	-0.465	-0.68	V
13	cyclobutanone	-231.2396391	-231.195847	-231.3081285	-231.269202	-1.059	-1	V
14	cyclopentadiene	-194.1103278	-194.0640873	-194.1659493	-194.122558	-1.181	-1.19	V
15	cyclopropene	-116.6248416	-116.5620536	-116.6603061	-116.5999414	-1.643	-1.73	V
16	cytosine-vertical	-394.9497539	-394.9265586	-395.0751564	-395.0550449	-0.547	-0.36	V
17	ethylene	-78.59326802	-78.52805782	-78.61915249	-78.55647637	-1.706	-1.78	V
18	fluorethylene	-177.835485	-177.7677856	-177.8930856	-177.8277227	-1.779	-1.91	V
19	furan	-230.0314372	-229.9671086	-230.1010496	-230.0388945	-1.691	-1.76	V
20	isothiazole	-569.0497938	-569.0212687	-569.1350715	-569.1090372	-0.708	-0.63	V
21	isoxazole	-246.0090936	-245.992186	-246.079732	-246.0656951	-0.382	-1.09	V
22	naphtalene	-385.9069275	-385.8930833	-386.0107062	-386.0002951	-0.283	-0.2	V
23	oxazole	-246.08119	-246.0296165	-246.1551908	-246.1053105	-1.357	-1.44	V
24	pyrazine	-264.3285538	-264.3186129	-264.4020601	-264.3948241	-0.197	-0.07	V
25	pyridazine	-264.2989167	-264.2875903	-264.3725015	-264.3635401	-0.244	-0.32	V
26	pyrimidine	-264.3350994	-264.3155753	-264.4086815	-264.3917447	-0.461	-0.25	V
27	thiazole	-569.0563243	-569.0209631	-569.1383117	-569.1053065	-0.898	-0.8	V
28	thiophene	-553.0113615	-552.9627815	-553.0894735	-553.0438306	-1.242	-1.17	V
29	thymine	-454.1581073	-454.1444372	-454.3000606	-454.289007	-0.301	-0.31	V
30	trans-1-2-dichloroethylene	-997.7838515	-997.7432723	-997.872217	-997.8360726	-0.984	-0.82	V
31	trans-1-2-difluorethylene	-277.0657441	-276.9979222	-277.1548707	-277.0887299	-1.800	-1.84	V
33	trichloroethylene	-1457.371621	-1457.339594	-1457.492335	-1457.465185	-0.739	-0.58	V
34	uracil-vertical	-414.8376589	-414.8246207	-414.9688674	-414.9587832	-0.274	-0.21	V
16	cytosine - adiabatic	-394.9497539	-394.9438889	-395.0751564	-395.0575439	-0.370	-0.06	V
34	uracil - adiabatic	-414.8376589	-414.838269	-414.9688674	-414.9697796	0.193	0.15	V
36	ethyl-radical	-79.16285056	-79.14924525	-79.18794158	-79.17690165	-0.253	-0.26	V
36	isopropyl-radical	-118.4837306	-118.4685772	-118.5199287	-118.506799	-0.298	-0.32	V
37	t-butyl-radical	-157.8044905	-157.7949439	-157.8514994	-157.8432166	-0.150	-0.16	V

B3LYP-D Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7810955	-997.7479784	-997.8728452	-997.8408332	-0.871	-0.75	0.351	V
2	1-3-cyclohexadiene	-233.4287934	-233.4039166	-233.5063134	-233.4734499	-0.894	-0.8	0.271	V
3	2-bromo-1-propene	-2689.039026	-2689.001973	-2691.50158	-2691.460242	-1.125	-1.31	0.505	N
4	3-bromo-1-propene	-2689.033436	-2689.021426	-2691.498394	-2691.482279	-0.439	-0.6	0.304	V
5	acetaldehyde	-153.8397395	-153.7919526	-153.8916217	-153.8439642	-1.297	-1.19	0.308	V
6	acetone	-193.1662094	-193.1189623	-193.2327589	-193.1842195	-1.321	-1.51	0.436	V
7	adenine	-467.3398558	-467.3232395	-467.4890858	-467.4643274	-0.674	-0.64	0.816	N
8	bromoethylene	-2649.712626	-2649.669461	-2652.164629	-2652.121497	-1.174	-1.17	0.392	V
9	chloroethylene	-538.1910258	-538.1411121	-538.2500813	-538.2016504	-1.318	-1.29	0.370	V
	chloroform	-500.1115113	-500.0650833	-500.1581478	-500.1163016	-1.139	-0.35	0.678	N
10	cis-1-2-dichloroethylene	-997.7842387	-997.7376569	-997.875264	-997.8310055	-1.204	-1.12	0.267	V
11	cis-1-2-difluorethylene	-277.0666416	-276.995192	-277.1582345	-277.0860516	-1.964	-2.18	0.493	V
12	cis-1-bromo-2-butene	-2728.353595	-2728.345205	-2730.832184	-2730.815456	-0.455	-0.68	0.338	V
13	cyclobutanone	-231.2396276	-231.2038644	-231.3160674	-231.2771789	-1.058	-1	0.340	V
14	cyclopentadiene	-194.1103231	-194.0703606	-194.1721228	-194.1287847	-1.179	-1.19	0.245	V
15	cyclopropene	-116.6248294	-116.5653172	-116.663353	-116.6031228	-1.639	-1.73	0.423	V
16	cytosine-vertical	-394.9497334	-394.9355515	-395.0841969	-395.0640072	-0.549	-0.36	0.380	V
17	ethylene	-78.59326433	-78.52976714	-78.62078395	-78.55814712	-1.704	-1.78	0.393	V
18	fluorethylene	-177.8354793	-177.7696431	-177.8948354	-177.8295548	-1.776	-1.91	0.440	V
19	furan	-230.0314349	-229.9707818	-230.1045851	-230.042526	-1.689	-1.76	0.486	V
20	isothiazole	-569.0497902	-569.0243194	-569.1379963	-569.1120363	-0.706	-0.63	0.325	V
22	naphtalene	-385.9069115	-385.9094508	-386.0269242	-386.0165648	-0.282	-0.2	0.282	V
23	oxazole	-246.0811881	-246.0322622	-246.1577419	-246.107929	-1.355	-1.44	0.510	N
24	pyrazine	-264.3285479	-264.3235997	-264.4068855	-264.3997469	-0.194	-0.07	0.305	V
25	pyridazine	-264.29891	-264.2928681	-264.3775253	-264.3687373	-0.239	-0.32	0.292	V
26	pyrimidine	-264.3350931	-264.3206657	-264.4135046	-264.3967598	-0.456	-0.25	0.301	V
27	thiazole	-569.0563194	-569.0239928	-569.1410658	-569.108276	-0.892	-0.8	0.301	V
28	thiophene	-553.0113567	-552.9668182	-553.093276	-553.0477987	-1.238	-1.17	0.311	V
29	thymine	-454.1580875	-454.1570062	-454.3125699	-454.3015556	-0.300	-0.31	0.379	V
30	trans-1-2-dichloroethylene	-997.7838467	-997.7459886	-997.8747917	-997.8387551	-0.981	-0.82	0.324	V
31	trans-1-2-difluorethylene	-277.0657402	-276.9999567	-277.1567506	-277.0907466	-1.796	-1.84	0.474	V
33	trichloroethylene	-1457.371608	-1457.343156	-1457.49551	-1457.46867	-0.730	-0.58	0.306	V
34	uracil-vertical	-414.8376549	-414.8329255	-414.9770349	-414.9670422	-0.272	-0.21	0.313	V
16	cytosine - adiabatic	-394.9497334	-394.9438579	-395.0841969	-395.07764	-0.051	-0.06	0.300	V
34	uracil - adiabatic	-414.8376549	-414.8382605	-414.9770349	-414.9780436	0.185	0.15	0.269	V
36	ethyl-radical	-79.16284098	-79.14923286	-79.19043014	-79.17941657	-0.250	-0.26	0.142	V
36	isopropyl-radical	-118.4836895	-118.4685062	-118.5253344	-118.5128295	-0.280	-0.32	0.214	V
37	t-butyl-radical	-157.8044332	-157.7947747	-157.8612763	-157.8545956	-0.105	-0.16	0.253	V

CAM-B3LYP Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7307533	-997.6925607	-997.8212028	-997.7867714	-0.937	-0.75	0.315	V
2	1-3-cyclohexadiene	-233.2824101	-233.24188	-233.349345	-233.3124578	-1.004	-0.8	0.255	V
3	2-bromo-1-propene	-2689.056913	-2689.007979	-2691.515779	-2691.469026	-1.272	-1.31	0.438	V
4	3-bromo-1-propene	-2689.050558	-2689.021552	-2691.512207	-2691.485113	-0.737	-0.6	0.300	V
5	acetaldehyde	-153.7636082	-153.7097811	-153.8135896	-153.7628805	-1.380	-1.19	0.258	V
6	acetone	-193.0653773	-193.0060045	-193.1265758	-193.0714028	-1.501	-1.51	0.309	V
7	adenine	-467.1195088	-467.0817475	-467.2606049	-467.2263906	-0.931	-0.64	1.175	N
8	bromoethylene	-2649.755554	-2649.706001	-2652.207641	-2652.160903	-1.272	-1.17	0.334	V
9	chloroethylene	-538.1377231	-538.0824685	-538.1954322	-538.1439062	-1.402	-1.29	0.331	V
	chloroform	-500.0802613	-500.0246606	-500.1260936	-500.0787138	-1.289	-0.35	0.712	N
10	cis-1-2-dichloroethylene	-997.7338873	-997.6833802	-997.8235489	-997.7780503	-1.238	-1.12	0.247	V
11	cis-1-2-difluorethylene	-276.9763015	-276.8972971	-277.0672425	-276.9898192	-2.107	-2.18	0.405	V
12	cis-1-bromo-2-butene	-2728.345374	-2728.315187	-2730.816335	-2730.788138	-0.767	-0.68	0.333	V
13	cyclobutanone	-231.1197775	-231.0703774	-231.1888681	-231.1442407	-1.214	-1	0.257	V
14	cyclopentadiene	-193.9889746	-193.9389168	-194.0453117	-193.9982362	-1.281	-1.19	0.231	V
15	cyclopropene	-116.5489298	-116.4812851	-116.584905	-116.51985	-1.770	-1.73	0.380	V
16	cytosine-vertical	-394.7692442	-394.7439072	-394.8973238	-394.8751105	-0.604	-0.36	0.324	V
17	ethylene	-78.53714187	-78.46739294	-78.56320229	-78.49624448	-1.822	-1.78	0.350	V
18	fluorethylene	-177.7623638	-177.6899833	-177.8206864	-177.7508975	-1.899	-1.91	0.392	V
19	furan	-229.9160806	-229.8460328	-229.9867296	-229.9192345	-1.837	-1.76	0.435	V
20	isothiazole	-568.948823	-568.9181804	-569.0359067	-569.0078627	-0.763	-0.63	0.314	V
21	isoxazole	-245.9311239	-245.8817822	-246.0058905	-245.9592544	-1.269	-1.09	0.319	V
22	naphtalene	-385.6735278	-385.6557461	-385.7791839	-385.7650252	-0.385	-0.2	0.281	V
23	oxazole	-245.9685612	-245.9110722	-246.0439124	-245.9884285	-1.510	-1.44	0.454	V
24	pyrazine	-264.1889808	-264.1779781	-264.2641011	-264.2560769	-0.218	-0.07	0.297	V
25	pyridazine	-264.1588032	-264.1462281	-264.233976	-264.2239664	-0.272	-0.32	0.288	V
26	pyrimidine	-264.1961547	-264.1752316	-264.2714021	-264.2532899	-0.493	-0.25	0.293	V
27	thiazole	-568.9557629	-568.9181758	-569.0393873	-569.0041188	-0.960	-0.8	0.294	V
28	thiophene	-552.9089506	-552.8578428	-552.9882711	-552.9401903	-1.308	-1.17	0.294	V
29	thymine	-453.9557239	-453.9394175	-454.1005127	-454.0870863	-0.365	-0.31	0.354	V
30	trans-1-2-dichloroethylene	-997.7333459	-997.691198	-997.8229514	-997.7853099	-1.024	-0.82	0.295	V
31	trans-1-2-difluorethylene	-276.9754711	-276.9025759	-277.0658324	-276.9950961	-1.925	-1.84	0.393	V
32	trans-1-bromo-2-butene	-2727.002249	-2727.05467	-2729.471864	-2729.526015	1.474	-0.68	0.179	V
33	trichloroethylene	-1457.324145	-1457.291619	-1457.446714	-1457.418856	-0.758	-0.58	0.281	V
34	uracil-vertical	-414.6602571	-414.6455728	-414.7941933	-414.7826135	-0.315	-0.21	0.307	V
16	cytosine - adiabatic	-394.7692442	-394.7407363	-394.8973238	-394.8705442	-0.715	-0.06	1.096	N
34	uracil - adiabatic	-414.6602571	-414.6386015	-414.7941933	-414.7738144	-0.516	0.15	1.015	N
36	ethyl-radical	-79.10560373	-79.08898283	-79.13067101	-79.11689242	-0.334	-0.26	0.135	V
36	isopropyl-radical	-118.4010773	-118.3819533	-118.4372601	-118.420392	-0.407	-0.32	0.190	V
37	t-butyl-radical	-157.6967055	-157.6824317	-157.7437747	-157.7311009	-0.274	-0.16	0.233	V

LC-BLYP Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-996.9891372	-996.9488125	-997.0845987	-997.0483126	-0.987	-0.75	0.280	V
2	1-3-cyclohexadiene	-232.6826238	-232.6376875	-232.7509887	-232.7101259	-1.112	-0.8	0.244	V
3	2-bromo-1-propene	-2688.24961	-2688.193562	-2690.702979	-2690.652008	-1.387	-1.31	0.984	N
4	3-bromo-1-propene	-2688.241926	-2688.199936	-2690.698227	-2690.658507	-1.081	-0.6	0.289	V
5	acetaldehyde	-153.441335	-153.3851689	-153.4926685	-153.4401511	-1.429	-1.19	0.216	V
6	acetone	-192.6430343	-192.5796054	-192.7056734	-192.6461435	-1.620	-1.51	0.205	V
7	adenine	-466.113352	-466.0707293	-466.2601476	-466.2212842	-1.058	-0.64	1.183	N
8	bromoethylene	-2649.048641	-2648.995411	-2651.495277	-2651.445503	-1.354	-1.17	0.284	V
9	chloroethylene	-537.6610891	-537.6026272	-537.7214403	-537.6671715	-1.477	-1.29	0.287	V
	chloroform	-499.7006191	-499.6376363	-499.7484391	-499.6946738	-1.463	-0.35	0.751	N
10	cis-1-2-dichloroethylene	-996.9921657	-996.9409117	-997.0867936	-997.0407962	-1.252	-1.12	0.229	V
11	cis-1-2-difluorethylene	-276.5261342	-276.4424678	-276.6201263	-276.5388547	-2.212	-2.18	0.322	V
12	cis-1-bromo-2-butene	-2727.435883	-2727.392311	-2729.90146	-2729.860096	-1.126	-0.68	0.323	V
13	cyclobutanone	-230.6057947	-230.5524477	-230.6763051	-230.627992	-1.315	-1	0.206	V
14	cyclopentadiene	-193.4899415	-193.4356354	-193.5475668	-193.4965987	-1.387	-1.19	0.218	V
15	cyclopropene	-116.245674	-116.1731896	-116.2825856	-116.2131086	-1.891	-1.73	0.333	V
16	cytosine-vertical	-393.9490835	-393.9233814	-394.0821761	-394.0600045	-0.603	-0.36	0.315	V
17	ethylene	-78.32579268	-78.25136039	-78.3522259	-78.28110223	-1.935	-1.78	0.304	V
18	fluorethylene	-177.4318327	-177.3549936	-177.491875	-177.4181448	-2.006	-1.91	0.338	V
19	furan	-229.4080638	-229.3321544	-229.4807912	-229.408114	-1.978	-1.76	0.381	V
20	isothiazole	-568.284367	-568.2521262	-568.3760125	-568.3466999	-0.798	-0.63	0.305	V
21	isoxazole	-245.4159812	-245.3628703	-245.4933475	-245.4435013	-1.356	-1.09	0.291	V
22	naphtalene	-384.6891381	-384.6677155	-384.7979443	-384.7806843	-0.470	-0.2	0.281	V
23	oxazole	-245.4556684	-245.3923575	-245.5336919	-245.4729956	-1.652	-1.44	0.390	V
24	pyrazine	-263.5802395	-263.5692439	-263.6582804	-263.6508213	-0.203	-0.07	0.289	V
25	pyridazine	-263.5494423	-263.5370102	-263.6274272	-263.6180609	-0.255	-0.32	0.284	V
26	pyrimidine	-263.5882346	-263.5675251	-263.6665032	-263.6490881	-0.474	-0.25	0.286	V
27	thiazole	-568.2918761	-568.2525802	-568.3798173	-568.3430224	-1.001	-0.8	0.288	V
28	thiophene	-552.2508168	-552.1973748	-552.3337658	-552.2836526	-1.364	-1.17	0.280	V
29	thymine	-453.0302304	-453.0125516	-453.1806264	-453.166307	-0.390	-0.31	0.341	V
30	trans-1-2-dichloroethylene	-996.9914352	-996.9478862	-997.0859601	-997.0472509	-1.053	-0.82	0.268	V
31	trans-1-2-difluorethylene	-276.5253845	-276.4480804	-276.6188171	-276.5445531	-2.021	-1.84	0.325	V
32	trans-1-bromo-2-butene	-2726.092653	-2726.143405	-2728.55722	-2728.610148	1.440	-0.68	0.176	V
33	trichloroethylene	-1456.317365	-1456.284901	-1456.447274	-1456.419481	-0.756	-0.58	0.253	V
34	uracil-vertical	-413.8350761	-413.8196656	-413.9744694	-413.9625942	-0.323	-0.21	0.305	V
16	cytosine - adiabatic	-393.9490835	-393.9151015	-394.0821761	-394.050004	-0.827	-0.06	1.090	N
34	uracil - adiabatic	-413.8350761	-413.8092098	-413.9744694	-413.9498948	-0.604	0.15	1.032	N
36	ethyl-radical	-78.89304127	-78.8727952	-78.91797803	-78.9011044	-0.428	-0.26	0.124	V
36	isopropyl-radical	-118.0873684	-118.0637838	-118.1234745	-118.1026597	-0.525	-0.32	0.172	V
37	t-butyl-radical	-157.2822672	-157.2627275	-157.3293622	-157.312007	-0.412	-0.16	0.211	V

BHand-HLYP Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.6995407	-997.655439	-997.7858368	-997.7450292	-1.110	-0.75	0.340	V
2	1-3-cyclohexadiene	-233.2747953	-233.2270112	-233.3394039	-233.2947949	-1.214	-0.8	0.277	V
3	2-bromo-1-propene	-2688.899854	-2688.84942	-2691.369693	-2691.324026	-1.243	-1.31	0.988	N
4	3-bromo-1-propene	-2688.894733	-2688.859871	-2691.367257	-2691.333752	-0.912	-0.6	0.360	V
5	acetaldehyde	-153.7451098	-153.6834675	-153.7941052	-153.7351215	-1.605	-1.19	0.267	V
6	acetone	-193.0451381	-192.9773633	-193.1050315	-193.0410603	-1.741	-1.51	0.346	V
7	adenine	-467.0633768	-467.0228641	-467.2010709	-467.1640946	-1.006	-0.64	1.218	N
8	bromoethylene	-2649.600315	-2649.545004	-2652.063625	-2652.010728	-1.439	-1.17	0.368	V
9	chloroethylene	-538.1212335	-538.0597468	-538.1765113	-538.1183282	-1.583	-1.29	0.359	V
	chloroform	-500.0652574	-500.0054735	-500.1092935	-500.0584049	-1.385	-0.35	0.752	N
10	cis-1-2-dichloroethylene	-997.7031004	-997.6461123	-997.7885949	-997.7361706	-1.427	-1.12	0.255	V
11	cis-1-2-difluorethylene	-276.9404151	-276.8545705	-277.0293929	-276.9446047	-2.307	-2.18	0.486	V
12	cis-1-bromo-2-butene	-2728.187775	-2728.15206	-2730.669293	-2730.635034	-0.932	-0.68	0.414	V
13	cyclobutanone	-231.0974072	-231.0400034	-231.164671	-231.1115944	-1.444	-1	0.267	V
14	cyclopentadiene	-193.981999	-193.9247718	-194.0364838	-193.9818295	-1.487	-1.19	0.256	V
15	cyclopropene	-116.5430483	-116.4689038	-116.5780631	-116.5062154	-1.955	-1.73	0.421	V
16	cytosine-vertical	-394.7191078	-394.6870045	-394.8441562	-394.8145558	-0.805	-0.36	0.339	V
17	ethylene	-78.53485525	-78.45879673	-78.56021021	-78.4865905	-2.003	-1.78	0.390	V
18	fluorethylene	-177.7430473	-177.6643125	-177.8000223	-177.7235289	-2.081	-1.91	0.441	V
19	furan	-229.8926483	-229.816764	-229.9615353	-229.8877303	-2.008	-1.76	0.496	V
20	isothiazole	-568.9215531	-568.8851184	-569.0051215	-568.9708183	-0.933	-0.63	0.333	V
21	isoxazole	-245.8965139	-245.8409279	-245.9697069	-245.916346	-1.452	-1.09	0.344	V
22	naphtalene	-385.6646237	-385.6106984	-385.7665754	-385.7151987	-1.398	-0.2	1.187	N
23	oxazole	-245.9365907	-245.8724836	-246.0102918	-245.947705	-1.703	-1.44	0.531	N
24	pyrazine	-264.1654816	-264.1477981	-264.2384837	-264.2232585	-0.414	-0.07	0.311	V
25	pyridazine	-264.1339773	-264.1143128	-264.2070916	-264.1894777	-0.479	-0.32	0.299	V
26	pyrimidine	-264.1733138	-264.144649	-264.2464574	-264.2200968	-0.717	-0.25	0.306	V
27	thiazole	-568.9287856	-568.884114	-569.0089952	-568.966212	-1.164	-0.8	0.309	V
28	thiophene	-552.8913171	-552.8340028	-552.9670117	-552.9123082	-1.489	-1.17	0.318	V
29	thymine	-453.8980383	-453.8739855	-454.0394173	-454.0177116	-0.591	-0.31	0.376	V
30	trans-1-2-dichloroethylene	-997.7026808	-997.6542722	-997.7881593	-997.7438058	-1.207	-0.82	0.306	V
31	trans-1-2-difluorethylene	-276.9394947	-276.8597848	-277.027864	-276.9498238	-2.124	-1.84	0.448	V
32	trans-1-bromo-2-butene	-2726.8484	-2726.896163	-2729.328287	-2729.3775	1.339	-0.68	0.184	V
33	trichloroethylene	-1457.278556	-1457.240136	-1457.395255	-1457.360977	-0.933	-0.58	0.288	V
34	uracil-vertical	-414.604567	-414.5821162	-414.7352937	-414.7154478	-0.540	-0.21	0.323	V
16	cytosine - adiabatic	-394.7191078	-394.7076031	-394.8441562	-394.8312081	-0.251	-0.06	0.302	V
34	uracil - adiabatic	-414.604567	-414.598571	-414.7352937	-414.7290084	0.002	0.15	0.279	V
36	ethyl-radical	-79.10535228	-79.07867175	-79.12984151	-79.10566172	-0.615	-0.26	0.138	V
36	isopropyl-radical	-118.3988403	-118.3698082	-118.4340586	-118.4069891	-0.680	-0.32	0.194	V
37	t-butyl-radical	-157.6923984	-157.6681219	-157.7382301	-157.7152161	-0.552	-0.16	0.241	V

ωB97 Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7300556	-997.6846679	-997.8181293	-997.7769435	-1.121	-0.75	0.265	V
2	1-3-cyclohexadiene	-233.3761554	-233.3298265	-233.4375762	-233.3949683	-1.159	-0.8	0.225	V
3	2-bromo-1-propene	-2689.132578	-2689.073336	-2691.584259	-2691.527911	-1.533	-1.31	0.332	V
4	3-bromo-1-propene	-2689.12479	-2689.079439	-2691.579248	-2691.536027	-1.176	-0.6	0.256	V
5	acetaldehyde	-153.8059014	-153.7459624	-153.8532804	-153.7963143	-1.550	-1.19	0.206	V
6	acetone	-193.1258062	-193.0594861	-193.1835731	-193.1203978	-1.719	-1.51	0.190	V
7	adenine	-467.2640841	-467.2140531	-467.3944082	-467.349499	-1.222	-0.64	1.194	N
8	bromoethylene	-2649.812989	-2649.755253	-2652.258672	-2652.204482	-1.475	-1.17	0.267	V
9	chloroethylene	-538.1508439	-538.0876585	-538.2064152	-538.1476109	-1.600	-1.29	0.269	V
	chloroform	-500.0804711	-500.0117551	-500.1254238	-500.0663204	-1.608	-0.35	0.773	N
10	cis-1-2-dichloroethylene	-997.7331633	-997.6780866	-997.8204312	-997.7703813	-1.362	-1.12	0.222	V
11	cis-1-2-difluorethylene	-277.017351	-276.9286632	-277.1059805	-277.0196238	-2.350	-2.18	0.303	V
12	cis-1-bromo-2-butene	-2728.437788	-2728.391064	-2730.900699	-2730.855968	-1.217	-0.68	0.273	V
13	cyclobutanone	-231.1989931	-231.1432642	-231.2642853	-231.2128195	-1.400	-1	0.211	V
14	cyclopentadiene	-194.0640381	-194.0080157	-194.1161692	-194.0633521	-1.437	-1.19	0.199	V
15	cyclopropene	-116.5983294	-116.5205773	-116.632172	-116.557648	-2.028	-1.73	0.310	V
16	cytosine-vertical	-394.8829681	-394.8553574	-395.0020379	-394.9773352	-0.672	-0.36	0.302	V
17	ethylene	-78.56466405	-78.48543511	-78.58889674	-78.5132969	-2.057	-1.78	0.282	V
18	fluorethylene	-177.7967263	-177.7148085	-177.852983	-177.7742921	-2.141	-1.91	0.311	V
19	furan	-229.9836191	-229.9034461	-230.0500975	-229.973465	-2.085	-1.76	0.346	V
20	isothiazole	-568.9902046	-568.9549029	-569.0730201	-569.0401091	-0.896	-0.63	0.286	V
21	isoxazole	-246.0002406	-245.9431769	-246.070482	-246.0164003	-1.472	-1.09	0.273	V
22	naphtalene	-385.8156089	-385.7441631	-385.9124626	-385.8455195	-1.822	-0.2	1.158	N
23	oxazole	-246.0363046	-245.9684708	-246.1070865	-246.0419309	-1.773	-1.44	0.358	V
24	pyrazine	-264.2718729	-264.2587865	-264.3408028	-264.3306333	-0.277	-0.07	0.277	V
25	pyridazine	-264.2436361	-264.2285032	-264.3126059	-264.3000114	-0.343	-0.32	0.268	V
26	pyrimidine	-264.2800638	-264.256723	-264.3490803	-264.3285386	-0.559	-0.25	0.271	V
27	thiazole	-568.9980609	-568.9558132	-569.0777341	-569.0374625	-1.096	-0.8	0.274	V
28	thiophene	-552.9521849	-552.8959288	-553.02764	-552.9744057	-1.449	-1.17	0.262	V
29	thymine	-454.0853996	-454.0643554	-454.2209502	-454.2025563	-0.501	-0.31	0.318	V
30	trans-1-2-dichloroethylene	-997.7321085	-997.6842394	-997.81929	-997.7761542	-1.174	-0.82	0.257	V
31	trans-1-2-difluorethylene	-277.0165401	-276.9342121	-277.1045719	-277.0251435	-2.161	-1.84	0.307	V
32	trans-1-bromo-2-butene	-2727.089092	-2727.137147	-2729.551793	-2729.601355	1.349	-0.68	0.170	V
33	trichloroethylene	-1457.309579	-1457.272886	-1457.429533	-1457.397269	-0.878	-0.58	0.246	V
34	uracil-vertical	-414.7716662	-414.752748	-414.8969944	-414.8808898	-0.438	-0.21	0.293	V
16	cytosine - adiabatic	-394.8829681	-394.8758932	-395.0020379	-394.9942262	-0.114	-0.06	0.280	V
34	uracil - adiabatic	-414.7716662	-414.7693384	-414.8969944	-414.8950725	0.113	0.15	0.259	V
36	ethyl-radical	-79.13532538	-79.11681753	-79.15909315	-79.14341741	-0.394	-0.26	0.122	V
36	isopropyl-radical	-118.4488612	-118.4275117	-118.4828432	-118.4635874	-0.478	-0.32	0.166	V
37	t-butyl-radical	-157.7628192	-157.7459226	-157.8068808	-157.7915602	-0.348	-0.16	0.206	V

ωB97X Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7237109	-997.679925	-997.8108356	-997.7711602	-1.080	-0.75	0.276	V
2	1-3-cyclohexadiene	-233.3609457	-233.3161237	-233.4219084	-233.3808074	-1.118	-0.8	0.231	V
3	2-bromo-1-propene	-2688.99362	-2688.936575	-2691.451869	-2691.397502	-1.479	-1.31	0.347	V
4	3-bromo-1-propene	-2688.986416	-2688.946228	-2691.4474	-2691.40925	-1.038	-0.6	0.255	V
5	acetaldehyde	-153.7939851	-153.73495	-153.8408303	-153.7848666	-1.523	-1.19	0.222	V
6	acetone	-193.1110306	-193.0453591	-193.1680852	-193.1059116	-1.692	-1.51	0.206	V
7	adenine	-467.2229435	-467.1755348	-467.3531747	-467.3106567	-1.157	-0.64	1.183	N
8	bromoethylene	-2649.676925	-2649.621191	-2652.129351	-2652.076866	-1.428	-1.17	0.281	V
9	chloroethylene	-538.1463449	-538.0850365	-538.2013212	-538.1441757	-1.555	-1.29	0.282	V
	chloroform	-500.0784608	-500.0134472	-500.1227235	-500.0667537	-1.523	-0.35	0.757	N
10	cis-1-2-dichloroethylene	-997.726891	-997.6726879	-997.8132151	-997.7641301	-1.336	-1.12	0.228	V
11	cis-1-2-difluorethylene	-276.9978148	-276.9101702	-277.0851008	-276.9994578	-2.330	-2.18	0.333	V
12	cis-1-bromo-2-butene	-2728.296575	-2728.255021	-2730.765912	-2730.726366	-1.076	-0.68	0.274	V
13	cyclobutanone	-231.1797119	-231.1248183	-231.244116	-231.1937224	-1.371	-1	0.214	V
14	cyclopentadiene	-194.0519808	-193.9974531	-194.1037408	-194.0523466	-1.399	-1.19	0.206	V
15	cyclopropene	-116.5889393	-116.5134168	-116.6223367	-116.549804	-1.974	-1.73	0.326	V
16	cytosine-vertical	-394.8489057	-394.8208722	-394.9675774	-394.9425285	-0.682	-0.36	0.306	V
17	ethylene	-78.56173029	-78.48480112	-78.58571082	-78.51202895	-2.005	-1.78	0.297	V
18	fluorethylene	-177.7854015	-177.7052649	-177.8408664	-177.76362	-2.102	-1.91	0.333	V
19	furan	-229.96719	-229.8889809	-230.0330455	-229.9580142	-2.042	-1.76	0.367	V
20	isothiazole	-568.9800233	-568.9455635	-569.0622404	-569.0303027	-0.869	-0.63	0.292	V
21	isoxazole	-245.9792574	-245.9234812	-246.0490476	-245.99617	-1.439	-1.09	0.281	V
22	naphtalene	-385.792292	-385.771367	-385.8884813	-385.8712322	-0.469	-0.2	0.265	V
23	oxazole	-246.01598	-245.9501263	-246.0863198	-246.0229255	-1.725	-1.44	0.382	V
24	pyrazine	-264.2520558	-264.2387084	-264.3208176	-264.3104791	-0.281	-0.07	0.282	V
25	pyridazine	-264.2229708	-264.207653	-264.2917732	-264.2790352	-0.347	-0.32	0.272	V
26	pyrimidine	-264.2598197	-264.2362185	-264.328693	-264.3079404	-0.565	-0.25	0.275	V
27	thiazole	-568.9875154	-568.9462291	-569.0664302	-569.0272804	-1.065	-0.8	0.278	V
28	thiophene	-552.9451402	-552.8900139	-553.0197789	-552.9677295	-1.416	-1.17	0.268	V
29	thymine	-454.0457619	-454.0251457	-454.1804398	-454.1625492	-0.487	-0.31	0.327	V
30	trans-1-2-dichloroethylene	-997.7259629	-997.6792106	-997.8121844	-997.7702489	-1.141	-0.82	0.265	V
31	trans-1-2-difluorethylene	-276.9969424	-276.9156613	-277.0836169	-277.00493	-2.141	-1.84	0.331	V
32	trans-1-bromo-2-butene	-2726.947941	-2726.997628	-2729.416821	-2729.467935	1.391	-0.68	0.172	V
33	trichloroethylene	-1457.301449	-1457.265472	-1457.420106	-1457.388784	-0.852	-0.58	0.252	V
34	uracil-vertical	-414.7349857	-414.7165581	-414.8596299	-414.8440653	-0.424	-0.21	0.295	V
16	cytosine - adiabatic	-394.8489057	-394.8106244	-394.9675774	-394.9316182	-0.975	-0.06	1.085	V
34	uracil - adiabatic	-414.7349857	-414.7041857	-414.8596299	-414.830908	-0.761	0.15	1.037	V
36	ethyl-radical	-79.13193017	-79.11440301	-79.15519274	-79.1405461	-0.364	-0.26	0.127	V
36	isopropyl-radical	-118.4426822	-118.4221431	-118.4761056	-118.4578094	-0.444	-0.32	0.176	V
37	t-butyl-radical	-157.7537375	-157.7378202	-157.797147	-157.7829293	-0.311	-0.16	0.218	V

ωB97XD Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7176412	-997.6753295	-997.8045061	-997.7660893	-1.045	-0.75	0.299	V
2	1-3-cyclohexadiene	-233.347485	-233.3040129	-233.4091106	-233.3695503	-1.076	-0.8	0.236	V
3	2-bromo-1-propene	-2689.018931	-2688.964931	-2691.476841	-2691.425263	-1.404	-1.31	0.391	V
4	3-bromo-1-propene	-2689.01235	-2688.978344	-2691.472837	-2691.440652	-0.876	-0.6	0.266	V
5	acetaldehyde	-153.7851076	-153.7271799	-153.8320274	-153.7770041	-1.497	-1.19	0.251	V
6	acetone	-193.100222	-193.0358508	-193.1573947	-193.0971215	-1.640	-1.51	0.273	V
7	adenine	-467.1825962	-467.1390134	-467.314439	-467.2754327	-1.061	-0.64	1.172	N
8	bromoethylene	-2649.704179	-2649.650712	-2652.156167	-2652.105508	-1.379	-1.17	0.313	V
9	chloroethylene	-538.142695	-538.0833117	-538.1974702	-538.1420271	-1.509	-1.29	0.310	V
	chloroform	-500.0788173	-500.0186275	-500.1227217	-500.0710445	-1.406	-0.35	0.742	N
10	cis-1-2-dichloroethylene	-997.7208606	-997.6671561	-997.8069568	-997.7582183	-1.326	-1.12	0.237	V
11	cis-1-2-difluorethylene	-276.9810141	-276.8957351	-277.0679202	-276.9842988	-2.275	-2.18	0.391	V
12	cis-1-bromo-2-butene	-2728.321228	-2728.285816	-2730.790265	-2730.756753	-0.912	-0.68	0.287	V
13	cyclobutanone	-231.1649526	-231.1113936	-231.2297441	-231.181094	-1.324	-1	0.252	V
14	cyclopentadiene	-194.0400504	-193.9869379	-194.0923734	-194.0425235	-1.356	-1.19	0.213	V
15	cyclopropene	-116.5797746	-116.5072278	-116.6132951	-116.5436071	-1.896	-1.73	0.356	V
16	cytosine-vertical	-394.8172813	-394.7892245	-394.9367566	-394.9115996	-0.685	-0.36	0.308	V
17	ethylene	-78.56009727	-78.48586131	-78.58395428	-78.51282107	-1.936	-1.78	0.328	V
18	fluorethylene	-177.7760927	-177.6984065	-177.8313204	-177.7563656	-2.040	-1.91	0.375	V
19	furan	-229.9507183	-229.875365	-230.0167915	-229.9443125	-1.972	-1.76	0.408	V
20	isothiazole	-568.9672428	-568.9334115	-569.0501437	-569.0187709	-0.854	-0.63	0.297	V
21	isoxazole	-245.9590838	-245.9049621	-246.0293007	-245.9778646	-1.400	-1.09	0.303	V
22	naphtalene	-385.7657066	-385.7453508	-385.8630185	-385.8464773	-0.450	-0.2	0.264	V
23	oxazole	-245.9960814	-245.933495	-246.0668255	-246.0063551	-1.645	-1.44	0.431	V
24	pyrazine	-264.2311544	-264.2175249	-264.3006409	-264.2899781	-0.290	-0.07	0.281	V
25	pyridazine	-264.2013855	-264.1859434	-264.2709559	-264.258066	-0.351	-0.32	0.273	V
26	pyrimidine	-264.2384634	-264.2146815	-264.3080739	-264.287096	-0.571	-0.25	0.278	V
27	thiazole	-568.9742133	-568.9338573	-569.053717	-569.0155194	-1.039	-0.8	0.280	V
28	thiophene	-552.9347413	-552.8804336	-553.0099456	-552.9587467	-1.393	-1.17	0.275	V
29	thymine	-454.0101967	-453.9900927	-454.1456857	-454.1282442	-0.475	-0.31	0.337	V
30	trans-1-2-dichloroethylene	-997.7202226	-997.6743479	-997.8061831	-997.7649107	-1.123	-0.82	0.280	V
31	trans-1-2-difluorethylene	-276.9800413	-276.9010031	-277.0663433	-276.9895154	-2.091	-1.84	0.379	V
32	trans-1-bromo-2-butene	-2726.970364	-2727.02021	-2729.438704	-2729.489959	1.395	-0.68	0.172	V
33	trichloroethylene	-1457.293013	-1457.257247	-1457.411402	-1457.380204	-0.849	-0.58	0.267	V
34	uracil-vertical	-414.7009521	-414.6828534	-414.8262966	-414.810974	-0.417	-0.21	0.296	V
16	cytosine - adiabatic	-394.8172813	-394.8083455	-394.9367566	-394.9270313	-0.165	-0.06	0.281	V
34	uracil - adiabatic	-414.7009521	-414.6978469	-414.8262966	-414.8232325	0.085	0.15	0.260	V
36	ethyl-radical	-79.13078361	-79.1139315	-79.15393185	-79.14016183	-0.336	-0.26	0.133	V
36	isopropyl-radical	-118.4397355	-118.4199431	-118.4732157	-118.4559573	-0.405	-0.32	0.184	V
37	t-butyl-radical	-157.7493119	-157.7341174	-157.7929561	-157.7796164	-0.272	-0.16	0.225	V

PBE0 Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.3559481	-997.3177705	-997.4413475	-997.4068228	-0.939	-0.75	0.351	V
2	1-3-cyclohexadiene	-233.1390123	-233.1008574	-233.1995879	-233.164996	-0.941	-0.8	0.258	V
3	2-bromo-1-propene	-2688.556532	-2688.510557	-2691.013561	-2690.969625	-1.196	-1.31	0.492	V
4	3-bromo-1-propene	-2688.549424	-2688.524042	-2691.009225	-2690.985555	-0.644	-0.6	0.332	V
5	acetaldehyde	-153.6567588	-153.6028866	-153.7032258	-153.6520451	-1.393	-1.19	0.299	V
6	acetone	-192.9345504	-192.8774034	-192.9912365	-192.9387155	-1.429	-1.51	0.424	V
7	adenine	-466.8202661	-466.7865293	-466.9519095	-466.921721	-0.821	-0.64	1.188	N
8	bromoethylene	-2649.27876	-2649.230795	-2651.729868	-2651.684478	-1.235	-1.17	0.384	V
9	chloroethylene	-537.9236826	-537.8690005	-537.97756	-537.9265079	-1.389	-1.29	0.369	V
	chloroform	-499.8900458	-499.837846	-499.9334679	-499.8888555	-1.214	-0.35	0.735	N
10	cis-1-2-dichloroethylene	-997.3592088	-997.3074085	-997.4437946	-997.3969389	-1.275	-1.12	0.264	V
11	cis-1-2-difluorethylene	-276.7810321	-276.7023958	-276.8669588	-276.7894351	-2.110	-2.18	0.510	V
12	cis-1-bromo-2-butene	-2727.820985	-2727.794638	-2730.289185	-2730.264657	-0.667	-0.68	0.378	V
13	cyclobutanone	-230.9704322	-230.9236093	-231.0343998	-230.9924213	-1.142	-1	0.320	V
14	cyclopentadiene	-193.8702133	-193.8216736	-193.9215838	-193.8760039	-1.240	-1.19	0.234	V
15	cyclopropene	-116.4771155	-116.4118327	-116.5097578	-116.4470635	-1.706	-1.73	0.413	V
16	cytosine-vertical	-394.5091621	-394.4832999	-394.628412	-394.6052728	-0.630	-0.36	0.331	V
17	ethylene	-78.48408197	-78.41603664	-78.50757715	-78.44223832	-1.778	-1.78	0.385	V
18	fluorethylene	-177.6380826	-177.5665629	-177.6926211	-177.6235987	-1.878	-1.91	0.449	V
19	furan	-229.7655817	-229.6974034	-229.8311355	-229.7651303	-1.796	-1.76	0.508	V
20	isothiazole	-568.6966324	-568.6650733	-568.778427	-568.7491923	-0.796	-0.63	0.324	V
21	isoxazole	-245.7679675	-245.7176143	-245.8378631	-245.7897644	-1.309	-1.09	0.349	V
22	naphtalene	-385.441746	-385.4270242	-385.537389	-385.526058	-0.308	-0.2	0.272	V
23	oxazole	-245.8041972	-245.7488317	-245.8745952	-245.8207633	-1.465	-1.44	0.541	V
24	pyrazine	-264.018384	-264.0068206	-264.0873264	-264.0782498	-0.247	-0.07	0.297	V
25	pyridazine	-263.9890436	-263.9756679	-264.0580538	-264.0467913	-0.306	-0.32	0.286	V
26	pyrimidine	-264.0253919	-264.0041815	-264.0944258	-264.0755776	-0.513	-0.25	0.293	V
27	thiazole	-568.7039578	-568.6659678	-568.7823094	-568.7464362	-0.976	-0.8	0.299	V
28	thiophene	-552.6708208	-552.6193736	-552.7447825	-552.6962869	-1.320	-1.17	0.305	V
29	thymine	-453.6546969	-453.6381089	-453.7893477	-453.7752867	-0.383	-0.31	0.370	V
30	trans-1-2-dichloroethylene	-997.3582948	-997.3152528	-997.4428761	-997.404213	-1.052	-0.82	0.318	V
31	trans-1-2-difluorethylene	-276.779878	-276.7070292	-276.8652169	-276.7940244	-1.937	-1.84	0.485	V
32	trans-1-bromo-2-butene	-2726.476447	-2726.524664	-2728.944015	-2728.993558	1.348	-0.68	0.186	V
33	trichloroethylene	-1456.788715	-1456.754652	-1456.905003	-1456.875564	-0.801	-0.58	0.307	V
34	uracil-vertical	-414.3829194	-414.3672612	-414.5075404	-414.4946675	-0.350	-0.21	0.309	V
16	cytosine - adiabatic	-394.5091621	-394.5011632	-394.628412	-394.6197781	-0.132	-0.06	0.295	V
34	uracil - adiabatic	-414.3829194	-414.3810396	-414.5075404	-414.5059724	0.125	0.15	0.269	V
36	ethyl-radical	-79.05476642	-79.03504728	-79.07773323	-79.06082389	-0.414	-0.26	0.138	V
36	isopropyl-radical	-118.3265977	-118.3054897	-118.3597101	-118.3408492	-0.456	-0.32	0.202	V
37	t-butyl-radical	-157.5985418	-157.5833455	-157.641674	-157.6278928	-0.299	-0.16	0.244	V

LC-ωPBE Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.4399242	-997.400564	-997.5278613	-997.4922736	-0.968	-0.75	0.273	V
2	1-3-cyclohexadiene	-233.2621991	-233.2196841	-233.3226834	-233.2842693	-1.045	-0.8	0.222	V
3	2-bromo-1-propene	-2688.572237	-2688.514064	-2691.023909	-2690.971507	-1.426	-1.31	0.969	N
4	3-bromo-1-propene	-2688.564463	-2688.508677	-2691.018937	-2690.966899	-1.416	-0.6	0.859	N
5	acetaldehyde	-153.7380304	-153.6825587	-153.7848831	-153.7328101	-1.417	-1.19	0.213	V
6	acetone	-193.0410336	-192.9785963	-193.0979968	-193.0392122	-1.600	-1.51	0.193	V
7	adenine	-467.0209737	-466.9802564	-467.1548209	-467.1182243	-0.996	-0.64	1.180	N
8	bromoethylene	-2649.269764	-2649.217937	-2651.715691	-2651.667222	-1.319	-1.17	0.275	V
9	chloroethylene	-537.9891277	-537.9317933	-538.0441666	-537.9908869	-1.450	-1.29	0.282	V
	chloroform	-499.9438813	-499.8835801	-499.9882744	-499.9367435	-1.402	-0.35	0.795	N
10	cis-1-2-dichloroethylene	-997.4429758	-997.3931789	-997.5300813	-997.4851918	-1.222	-1.12	0.221	V
11	cis-1-2-difluorethylene	-276.9004565	-276.8167026	-276.9875144	-276.9058951	-2.221	-2.18	0.326	V
12	cis-1-bromo-2-butene	-2727.860386	-2727.818005	-2730.323064	-2730.282859	-1.094	-0.68	0.292	V
13	cyclobutanone	-231.0930432	-231.0411149	-231.1569453	-231.1099071	-1.280	-1	0.195	V
14	cyclopentadiene	-193.9687775	-193.9168572	-194.0201175	-193.9715693	-1.321	-1.19	0.198	V
15	cyclopropene	-116.5409714	-116.4697126	-116.5737015	-116.5055168	-1.855	-1.73	0.322	V
16	cytosine-vertical	-394.6851941	-394.6603374	-394.8065596	-394.7848192	-0.592	-0.36	0.297	V
17	ethylene	-78.53113045	-78.45794706	-78.55444642	-78.48465732	-1.899	-1.78	0.298	V
18	fluorethylene	-177.7214686	-177.6453947	-177.7764984	-177.7034818	-1.987	-1.91	0.343	V
19	furan	-229.8732606	-229.7977923	-229.9390541	-229.8667441	-1.968	-1.76	0.369	V
20	isothiazole	-568.7898184	-568.7586367	-568.8740068	-568.8454525	-0.777	-0.63	0.287	V
21	isoxazole	-245.8786889	-245.8253201	-245.9491891	-245.8988631	-1.369	-1.09	0.275	V
22	naphtalene	-385.6061737	-385.5433633	-385.7021166	-385.6428332	-1.613	-0.2	1.158	N
23	oxazole	-245.9159154	-245.8532363	-245.9870327	-245.9266776	-1.642	-1.44	0.385	V
24	pyrazine	-264.1317648	-264.1218736	-264.2016178	-264.1949076	-0.183	-0.07	0.273	V
25	pyridazine	-264.1026537	-264.0913894	-264.1723834	-264.1637817	-0.234	-0.32	0.265	V
26	pyrimidine	-264.1396451	-264.1205694	-264.209751	-264.1935554	-0.441	-0.25	0.267	V
27	thiazole	-568.7975286	-568.7599907	-568.8782403	-568.8428333	-0.963	-0.8	0.272	V
28	thiophene	-552.761589	-552.7096837	-552.8371981	-552.7885217	-1.325	-1.17	0.260	V
29	thymine	-453.8622579	-453.8451732	-453.999211	-453.98515	-0.383	-0.31	0.319	V
30	trans-1-2-dichloroethylene	-997.4422862	-997.3996028	-997.5293672	-997.4911882	-1.039	-0.82	0.255	V
31	trans-1-2-difluorethylene	-276.8996288	-276.8221353	-276.9860997	-276.9113777	-2.033	-1.84	0.323	V
32	trans-1-bromo-2-butene	-2726.499102	-2726.549859	-2728.961506	-2729.014135	1.432	-0.68	0.167	V
33	trichloroethylene	-1456.890949	-1456.859765	-1457.011163	-1456.984169	-0.735	-0.58	0.245	V
34	uracil-vertical	-414.5656479	-414.5508821	-414.6926179	-414.6809847	-0.317	-0.21	0.290	V
16	cytosine - adiabatic	-394.6851941	-394.6812538	-394.8065596	-394.8020813	-0.022	-0.06	0.276	V
34	uracil - adiabatic	-414.5656479	-414.5675503	-414.6926179	-414.6949129	0.225	0.15	0.256	V
36	ethyl-radical	-79.10998418	-79.08789933	-79.13241368	-79.11369047	-0.475	-0.26	0.120	V
36	isopropyl-radical	-118.406218	-118.3810112	-118.4385935	-118.4161428	-0.565	-0.32	0.162	V
37	t-butyl-radical	-157.7026263	-157.680858	-157.744954	-157.7252086	-0.469	-0.16	0.197	V

M06L Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7269182	-997.6798166	-997.8105491	-997.7671925	-1.179794	-0.75	0.32573	V
2	1-3-cyclohexadiene	-233.3803022	-233.3377888	-233.4491219	-233.4104242	-1.05302	-0.8	0.21785	V
3	2-bromo-1-propene	-2688.827642	-2688.769594	-2691.333741	-2691.278346	-1.507387	-1.31	0.36075	V
4	3-bromo-1-propene	-2688.818787	-2688.787258	-2691.32733	-2691.298771	-0.777119	-0.6	0.31489	V
5	acetaldehyde	-153.8119021	-153.7514413	-153.8612814	-153.8027646	-1.592324	-1.19	0.30542	V
6	acetone	-193.1307583	-193.0708654	-193.1919992	-193.1375735	-1.480997	-1.51	0.65293	N
7	adenine	-467.2865834	-467.2494348	-467.4138499	-467.3801834	-0.91611	-0.64	0.39049	V
8	bromoethylene	-2649.508587	-2649.451163	-2652.00689	-2651.952693	-1.474759	-1.17	0.33552	V
9	chloroethylene	-538.1509127	-538.088327	-538.2060635	-538.1473022	-1.598976	-1.29	0.34706	V
	chloroform	-500.0770505	-500.0159922	-500.1213659	-500.0647237	-1.541312	-0.35	0.70594	N
11	cis-1-2-difluorethylene	-277.0217074	-276.9542451	-277.1086737	-277.0475144	-1.664229	-2.18	0.96983	N
12	cis-1-bromo-2-butene	-2728.132591	-2728.100774	-2730.65132	-2730.622117	-0.794668	-0.68	0.33073	V
13	cyclobutanone	-231.2030904	-231.1520022	-231.2722576	-231.2242546	-1.306228	-1	0.20949	V
14	cyclopentadiene	-194.0705842	-194.0174522	-194.1284433	-194.0786145	-1.35591	-1.19	0.19778	V
15	cyclopropene	-116.6055826	-116.531842	-116.6439394	-116.5723361	-1.948425	-1.73	0.40814	V
16	cytosine-vertical	-394.9013796	-394.8692492	-395.0171245	-394.9887426	-0.772311	-0.36	0.30628	V
17	ethylene	-78.56843258	-78.49337701	-78.59655355	-78.52418922	-1.969134	-1.78	0.37643	V
18	fluorethylene	-177.8002273	-177.7207153	-177.8575645	-177.7808894	-2.086436	-1.91	0.43853	V
19	furan	-229.9927517	-229.9152046	-230.0623391	-229.9877218	-2.030441	-1.76	0.47699	V
20	isothiazole	-569.0077614	-568.9680178	-569.0892516	-569.0516835	-1.022282	-0.63	0.27757	V
21	isoxazole	-246.0114427	-245.9544442	-246.0823456	-246.0280507	-1.477438	-1.09	0.32808	V
22	naphtalene	-385.8424271	-385.825836	-385.9461954	-385.9334283	-0.34741	-0.2	0.24946	V
23	oxazole	-246.0459367	-245.9819022	-246.1178671	-246.0561631	-1.679051	-1.44	0.49748	V
24	pyrazine	-264.2879425	-264.270565	-264.3583076	-264.3444644	-0.376691	-0.07	0.25812	V
25	pyridazine	-264.2587602	-264.2413167	-264.3289973	-264.3145268	-0.393763	-0.32	0.25252	V
26	pyrimidine	-264.2944844	-264.2682085	-264.3648884	-264.3418193	-0.627742	-0.25	0.25433	V
27	thiazole	-569.0130902	-568.9692235	-569.0918569	-569.0496231	-1.149239	-0.8	0.26877	V
28	thiophene	-552.9648149	-552.906109	-553.0414596	-552.9854413	-1.524338	-1.17	0.27295	V
29	thymine	-454.1034084	-454.0789548	-454.237072	-454.2157133	-0.581199	-0.31	0.31482	V
30	trans-1-2-dichloroethylene	-997.7285576	-997.6765751	-997.811175	-997.7637758	-1.289797	-0.82	0.28544	V
31	trans-1-2-difluorethylene	-277.0198958	-276.9542055	-277.1063334	-277.0416763	-1.75941	-1.84	0.92336	N
32	trans-1-bromo-2-butene	-2726.790038	-2726.834336	-2729.306523	-2729.352194	1.242783	-0.68	0.17069	V
33	trichloroethylene	-1457.303461	-1457.261309	-1457.415154	-1457.377417	-1.026862	-0.58	0.28407	V
34	uracil-vertical	-414.7902931	-414.7674182	-414.9119215	-414.8926927	-0.523243	-0.21	0.27071	V
16	cytosine - adiabatic	-394.9013796	-394.8865392	-395.0171245	-395.0023898	-0.294917	-0.06	0.26341	V
34	uracil - adiabatic	-414.7902931	-414.7806659	-414.9119215	-414.9035544	-0.051974	0.15	0.24177	V
36	ethyl-radical	-79.13837793	-79.12034123	-79.16672547	-79.14998187	-0.420389	-0.26	0.13728	V
36	isopropyl-radical	-118.451638	-118.4321232	-118.4923171	-118.4727429	-0.479274	-0.32	0.19209	V
37	t-butyl-radical	-157.7653844	-157.7506538	-157.8180215	-157.802174	-0.367054	-0.16	0.23416	V

M06 Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.6538852	-997.6137022	-997.7360128	-997.6997796	-0.986	-0.75	0.316	V
2	1-3-cyclohexadiene	-233.2319569	-233.1935106	-233.2935592	-233.2602701	-0.906	-0.8	0.247	V
3	2-bromo-1-propene	-2688.773776	-2688.724533	-2691.259053	-2691.212371	-1.270	-1.31	0.412	V
4	3-bromo-1-propene	-2688.76623	-2688.738505	-2691.25373	-2691.227949	-0.702	-0.6	0.299	V
5	acetaldehyde	-153.7383178	-153.6823736	-153.7834814	-153.7309177	-1.430	-1.19	0.277	V
6	acetone	-193.0318624	-192.973609	-193.0873692	-193.0343593	-1.442	-1.51	0.375	V
7	adenine	-467.0387947	-466.9956261	-467.1638162	-467.1255015	-1.043	-0.64	1.154	N
8	bromoethylene	-2649.479751	-2649.42982	-2651.958862	-2651.91162	-1.286	-1.17	0.344	V
9	chloroethylene	-538.0885254	-538.0319986	-538.1409268	-538.0885159	-1.426	-1.29	0.327	V
	chloroform	-500.0387912	-499.9811629	-500.0805826	-500.0293225	-1.395	-0.35	0.692	N
11	cis-1-2-difluorethylene	-276.943781	-276.8724683	-277.0243902	-276.9557974	-1.867	-2.18	1.039	N
12	cis-1-bromo-2-butene	-2728.053824	-2728.02552	-2730.549954	-2730.523935	-0.708	-0.68	0.317	V
13	cyclobutanone	-231.0806494	-231.0322861	-231.1433063	-231.1010624	-1.150	-1	0.319	V
14	cyclopentadiene	-193.9469176	-193.8982779	-193.9987454	-193.9545137	-1.204	-1.19	0.222	V
15	cyclopropene	-116.5312909	-116.4678396	-116.5652658	-116.4678396	-2.651	-1.73	0.854	N
16	cytosine-vertical	-394.70588	-394.6808798	-394.8184548	-394.7972042	-0.578	-0.36	0.326	V
17	ethylene	-78.51711079	-78.44634367	-78.54130662	-78.47418337	-1.827	-1.78	0.356	V
18	fluorethylene	-177.7356279	-177.6620665	-177.787777	-177.7174812	-1.913	-1.91	0.413	V
19	furan	-229.8737711	-229.8063695	-229.9379615	-229.8774025	-1.648	-1.76	1.081	N
20	isothiazole	-568.8936373	-568.8609514	-568.9730814	-568.9429741	-0.819	-0.63	0.308	V
21	isoxazole	-245.8867922	-245.8370995	-245.9535773	-245.9100158	-1.185	-1.09	0.728	N
22	naphtalene	-385.594317	-385.5803391	-385.6895536	-385.6804328	-0.248	-0.2	0.268	V
23	oxazole	-245.926301	-245.8689493	-245.9942955	-245.9422105	-1.417	-1.44	1.087	N
24	pyrazine	-264.1365392	-264.1246085	-264.2035845	-264.1957696	-0.213	-0.07	0.283	V
25	pyridazine	-264.1055609	-264.093244	-264.1720487	-264.1633544	-0.237	-0.32	0.277	V
26	pyrimidine	-264.1439749	-264.1232599	-264.2109218	-264.1940765	-0.458	-0.25	0.281	V
27	thiazole	-568.8995313	-568.8619511	-568.9757241	-568.9402977	-0.964	-0.8	0.286	V
28	thiophene	-552.8521895	-552.8009534	-552.9250317	-552.8769283	-1.309	-1.17	0.294	V
29	thymine	-453.8862395	-453.8705472	-454.0149338	-454.0025428	-0.337	-0.31	0.349	V
30	trans-1-2-dichloroethylene	-997.6552456	-997.6121556	-997.7363148	-997.697363	-1.060	-0.82	0.302	V
31	trans-1-2-difluorethylene	-276.9424934	-276.8806753	-277.0225527	-276.9627218	-1.628	-1.84	0.924	N
32	trans-1-bromo-2-butene	-2726.717479	-2726.763223	-2729.21217	-2729.259647	1.292	-0.68	0.184	V
33	trichloroethylene	-1457.21931	-1457.18537	-1457.330543	-1457.300609	-0.815	-0.58	0.295	V
34	uracil-vertical	-414.5982088	-414.5834499	-414.7164077	-414.7050682	-0.309	-0.21	0.297	V
16	cytosine - adiabatic	-394.70588	-394.6982591	-394.8184548	-394.8107618	-0.107	-0.06	0.285	V
34	uracil - adiabatic	-414.5982088	-414.5973371	-414.7164077	-414.7158828	0.153	0.15	0.260	V
36	ethyl-radical	-79.08500774	-79.06998666	-79.10880917	-79.0969471	-0.290	-0.26	0.132	V
36	isopropyl-radical	-118.3725065	-118.356222	-118.4072004	-118.3937635	-0.309	-0.32	0.191	V
37	t-butyl-radical	-157.6607947	-157.6509067	-157.7061166	-157.6988036	-0.135	-0.16	0.232	V

M06-HF Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.6989459	-997.6579009	-997.8250736	-997.788684	-0.990	-0.75	0.340	V
2	1-3-cyclohexadiene	-233.355382	-233.3136562	-233.4252179	-233.3880059	-1.013	-0.8	0.275	V
3	2-bromo-1-propene	-2689.373102	-2689.32277	-2691.706529	-2691.660507	-1.252	-1.31	0.782	N
4	3-bromo-1-propene	-2689.367478	-2689.338505	-2691.704525	-2691.678012	-0.721	-0.6	0.923	N
5	acetaldehyde	-153.7680346	-153.7110308	-153.825311	-153.7719516	-1.452	-1.19	0.270	V
6	acetone	-193.0790049	-193.0128408	-193.1471787	-193.0857404	-1.672	-1.51	0.204	V
7	adenine	-467.2190329	-467.1936843	-467.3816094	-467.3578487	-0.647	-0.64	1.295	N
8	bromoethylene	-2650.06133	-2650.009947	-2652.387799	-2652.339549	-1.313	-1.17	0.365	V
9	chloroethylene	-538.1318612	-538.0734885	-538.2067882	-538.1528502	-1.468	-1.29	0.374	V
	chloroform	-500.0580603	-500.0125863	-500.1210995	-500.0838231	-1.014	-0.35	0.838	N
11	cis-1-2-difluorethylene	-276.9697204	-276.8989607	-277.0769753	-277.0093066	-1.841	-2.18	1.060	N
12	cis-1-bromo-2-butene	-2728.671477	-2728.64336	-2731.01856	-2730.995324	-0.632	-0.68	0.980	N
13	cyclobutanone	-231.1485312	-231.1098838	-231.2262398	-231.1950513	-0.849	-1	1.001	N
14	cyclopentadiene	-194.0511479	-193.998893	-194.1091714	-194.060898	-1.314	-1.19	0.241	V
15	cyclopropene	-116.5875355	-116.5177239	-116.6232725	-116.5564818	-1.817	-1.73	0.415	V
16	cytosine-vertical	-394.8226753	-394.797527	-394.9717005	-394.9502159	-0.585	-0.36	0.352	V
17	ethylene	-78.55775332	-78.48383861	-78.58205542	-78.51128147	-1.926	-1.78	0.380	V
18	fluorethylene	-177.7697513	-177.6943685	-177.8353675	-177.7632933	-1.961	-1.91	0.408	V
19	furan	-229.9653005	-229.8944554	-230.0425621	-229.9745783	-1.850	-1.76	0.528	V
20	isothiazole	-568.9659309	-568.9347633	-569.0747667	-569.0468503	-0.760	-0.63	0.318	V
21	isoxazole	-245.9665247	-245.9143422	-246.0518773	-246.0030431	-1.329	-1.09	0.313	V
22	naphtalene	-385.804321	-385.7869425	-385.9188374	-385.9048116	-0.382	-0.2	0.295	V
23	oxazole	-246.0102457	-245.9504864	-246.0960379	-246.0377937	-1.585	-1.44	0.539	V
24	pyrazine	-264.2515154	-264.2398132	-264.3379814	-264.3281163	-0.268	-0.07	0.306	V
25	pyridazine	-264.2191032	-264.2038331	-264.3053713	-264.2919611	-0.365	-0.32	0.297	V
26	pyrimidine	-264.2588227	-264.2361171	-264.3457068	-264.3247386	-0.571	-0.25	0.309	V
27	thiazole	-568.9758835	-568.9356355	-569.080858	-569.0436363	-1.013	-0.8	0.307	V
28	thiophene	-552.9369031	-552.884433	-553.0340468	-552.9863506	-1.298	-1.17	0.292	V
29	thymine	-454.0040134	-453.9875605	-454.1742866	-454.1620276	-0.334	-0.31	0.383	V
30	trans-1-2-dichloroethylene	-997.7009327	-997.6555714	-997.827129	-997.7880595	-1.063	-0.82	0.306	V
31	trans-1-2-difluorethylene	-276.9698187	-276.8938397	-277.0766479	-277.003735	-1.984	-1.84	0.414	V
32	trans-1-bromo-2-butene	-2727.327374	-2727.37983	-2729.674651	-2729.72933	1.488	-0.68	0.186	V
33	trichloroethylene	-1457.265721	-1457.230043	-1457.443295	-1457.414357	-0.787	-0.58	0.286	V
34	uracil-vertical	-414.6972764	-414.6825379	-414.8562456	-414.8454789	-0.293	-0.21	0.342	V
16	cytosine - adiabatic	-394.8226753	-394.8176679	-394.9717005	-394.9667967	-0.019	-0.06	0.319	V
34	uracil - adiabatic	-414.6972764	-414.6994473	-414.8562456	-414.8596045	0.243	0.15	0.294	V
36	ethyl-radical	-79.11468549	-79.10099238	-79.13906747	-79.12950533	-0.201	-0.26	0.131	V
36	isopropyl-radical	-118.4174583	-118.4042145	-118.4534588	-118.4431968	-0.221	-0.32	0.174	V
37	t-butyl-radical	-157.7222572	-157.7161441	-157.7693264	-157.7656933	-0.012	-0.16	0.213	V

M06-2X Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.6766663	-997.6347749	-997.7744968	-997.7362412	-1.041	-0.75	0.335	V
2	1-3-cyclohexadiene	-233.3092365	-233.2679278	-233.3771826	-233.3388924	-1.042	-0.8	0.247	V
3	2-bromo-1-propene	-2689.04301	-2688.990372	-2691.453272	-2691.402421	-1.384	-1.31	0.530	V
4	3-bromo-1-propene	-2689.035641	-2689.003818	-2691.448859	-2691.41847	-0.827	-0.6	0.287	V
5	acetaldehyde	-153.7601173	-153.7019857	-153.8114906	-153.7554968	-1.524	-1.19	0.292	V
6	acetone	-193.0653188	-192.9999201	-193.1279855	-193.0655767	-1.698	-1.51	0.371	V
7	adenine	-467.155771	-467.1172868	-467.3000125	-467.2644251	-0.968	-0.64	1.197	N
8	bromoethylene	-2649.737626	-2649.685199	-2652.140901	-2652.090969	-1.359	-1.17	0.362	V
9	chloroethylene	-538.1123352	-538.0540335	-538.1738773	-538.1189558	-1.494	-1.29	0.359	V
	chloroform	-500.0472651	-499.9920005	-500.097032	-500.0514436	-1.241	-0.35	0.750	N
11	cis-1-2-difluorethylene	-276.9560644	-276.8733273	-277.0506925	-276.9692127	-2.217	-2.18	0.474	V
12	cis-1-bromo-2-butene	-2728.334358	-2728.301876	-2730.757023	-2730.726025	-0.844	-0.68	0.315	V
13	cyclobutanone	-231.1271331	-231.0778455	-231.1985135	-231.1541909	-1.206	-1	0.782	N
14	cyclopentadiene	-194.0118631	-193.9603898	-194.0691176	-194.0201201	-1.333	-1.19	0.224	V
15	cyclopropene	-116.5669192	-116.497173	-116.6035421	-116.5356577	-1.847	-1.73	0.418	V
16	cytosine-vertical	-394.7848317	-394.756864	-394.9157035	-394.8910085	-0.672	-0.36	0.320	V
17	ethylene	-78.54128311	-78.46881953	-78.56739377	-78.49683781	-1.920	-1.78	0.384	V
18	fluorethylene	-177.7542539	-177.6783191	-177.814512	-177.7407067	-2.008	-1.91	0.419	V
19	furan	-229.9309525	-229.8585393	-230.0031891	-229.9330164	-1.909	-1.76	0.491	V
20	isothiazole	-568.9376146	-568.9031968	-569.0294034	-568.9975106	-0.868	-0.63	0.301	V
21	isoxazole	-245.9403907	-245.8867663	-246.0173468	-245.9663572	-1.387	-1.09	0.316	V
22	naphtalene	-385.7297858	-385.675885	-385.8377516	-385.7864674	-1.396	-0.2	1.163	N
23	oxazole	-245.9802197	-245.9194782	-246.0576384	-245.9985616	-1.608	-1.44	0.517	V
24	pyrazine	-264.2116925	-264.1976006	-264.2886797	-264.277184	-0.313	-0.07	0.284	V
25	pyridazine	-264.1807388	-264.1647992	-264.2578291	-264.2441368	-0.373	-0.32	0.276	V
26	pyrimidine	-264.2186952	-264.194307	-264.295902	-264.2738781	-0.599	-0.25	0.283	V
27	thiazole	-568.9451454	-568.9036896	-569.0334554	-568.9942333	-1.067	-0.8	0.285	V
28	thiophene	-552.901767	-552.8476031	-552.9854218	-552.9343295	-1.390	-1.17	0.284	V
29	thymine	-453.9683341	-453.9483467	-454.1169854	-454.1000806	-0.460	-0.31	0.349	V
30	trans-1-2-dichloroethylene	-997.6785139	-997.6324178	-997.775673	-997.7343826	-1.124	-0.82	0.298	V
31	trans-1-2-difluorethylene	-276.9552735	-276.8780546	-277.0493496	-276.9740273	-2.050	-1.84	0.460	V
32	trans-1-bromo-2-butene	-2726.992357	-2727.043449	-2729.414152	-2729.466574	1.426	-0.68	0.175	V
33	trichloroethylene	-1457.24111	-1457.20466	-1457.374845	-1457.343418	-0.855	-0.58	0.282	V
34	uracil-vertical	-414.6686385	-414.6500615	-414.8061281	-414.7910245	-0.411	-0.21	0.304	V
16	cytosine - adiabatic	-394.7848317	-394.7761263	-394.9157035	-394.906912	-0.142	-0.06	0.287	V
34	uracil - adiabatic	-414.6686385	-414.6650861	-414.8061281	-414.8037446	0.099	0.15	0.265	V
36	ethyl-radical	-79.10456908	-79.09021515	-79.1300925	-79.11738241	-0.308	-0.26	0.131	V
36	isopropyl-radical	-118.4030009	-118.3877861	-118.4398441	-118.4252362	-0.349	-0.32	0.180	V
37	t-butyl-radical	-157.7025309	-157.6939464	-157.7503735	-157.7414588	-0.178	-0.16	0.225	V

TPSS Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.8078078	-997.7702837	-997.8955092	-997.8605611	-0.951	-0.75	0.707	N
2	1-3-cyclohexadiene	-233.4669889	-233.4293621	-233.5306185	-233.4966398	-0.925	-0.8	0.252	V
3	2-bromo-1-propene	-2688.929183	-2688.886404	-2691.391513	-2691.353002	-1.048	-1.31	0.783	N
4	3-bromo-1-propene	-2688.923268	-2688.9046	-2691.388338	-2691.371549	-0.457	-0.6	0.289	V
5	acetaldehyde	-153.8588703	-153.7998424	-153.9070061	-153.8577994	-1.339	-1.19	0.319	V
6	acetone	-193.1908178	-193.1439026	-193.2495331	-193.2094005	-1.092	-1.51	0.748	N
7	adenine	-467.4195489	-467.3920315	-467.5548417	-467.5304703	-0.663	-0.64	0.757	N
8	bromoethylene	-2649.596882	-2649.54854	-2652.052793	-2652.008614	-1.202	-1.17	0.822	N
9	chloroethylene	-538.2095416	-538.1544491	-538.2650919	-538.2135761	-1.402	-1.29	0.376	V
	chloroform	-500.122712	-500.0735342	-500.1672143	-500.1232078	-1.197	-0.35	0.691	N
10	cis-1-2-dichloroethylene	-997.8109524	-997.7650197	-997.8980443	-997.8554865	-1.158	-1.12	0.854	N
11	cis-1-2-difluorethylene	-277.0931275	-277.0446753	-277.1805333	-277.1353603	-1.229	-2.18	0.948	N
12	cis-1-bromo-2-butene	-2728.24969	-2728.23038	-2730.723765	-2730.706493	-0.470	-0.68	0.321	V
13	cyclobutanone	-231.2757626	-231.2347286	-231.3426186	-231.3064688	-0.984	-1	0.558	N
14	cyclopentadiene	-194.1443359	-194.0964119	-194.1981233	-194.1532747	-1.220	-1.19	0.225	V
15	cyclopropene	-116.6482643	-116.5933086	-116.6820367	-116.6299821	-1.416	-1.73	0.984	N
16	cytosine-vertical	-395.0087198	-394.9868321	-395.1310376	-395.1117859	-0.524	-0.36	0.690	N
17	ethylene	-78.60383906	-78.53569511	-78.62821277	-78.56254707	-1.787	-1.78	0.393	V
18	fluorethylene	-177.8539411	-177.7915568	-177.9096603	-177.853796	-1.520	-1.91	1.005	N
19	furan	-230.07091	-230.0143373	-230.1389219	-230.0911482	-1.300	-1.76	1.066	N
20	isothiazole	-569.0924441	-569.0607908	-569.1764435	-569.1473628	-0.791	-0.63	0.306	V
21	isoxazole	-246.0913447	-246.0479085	-246.1635814	-246.1251655	-1.045	-1.09	0.806	N
22	naphtalene	-385.9756661	-385.961655	-386.0761539	-386.065513	-0.290	-0.2	0.257	V
23	oxazole	-246.1236414	-246.0700597	-246.1963713	-246.1441765	-1.420	-1.44	0.523	V
24	pyrazine	-264.3746223	-264.3624752	-264.4462845	-264.4365776	-0.264	-0.07	0.284	V
25	pyridazine	-264.3467271	-264.33341	-264.4184133	-264.4072024	-0.305	-0.32	0.273	V
26	pyrimidine	-264.3807706	-264.359678	-264.4524844	-264.433694	-0.511	-0.25	0.282	V
27	thiazole	-569.0983669	-569.0606641	-569.1791794	-569.1438918	-0.960	-0.8	0.286	V
28	thiophene	-553.0497454	-552.9949314	-553.1263715	-553.0777953	-1.322	-1.17	0.293	V
29	thymine	-454.2246749	-454.2107261	-454.363398	-454.351653	-0.320	-0.31	0.596	N
30	trans-1-2-dichloroethylene	-997.8104234	-997.773176	-997.8974483	-997.8616058	-0.975	-0.82	0.668	N
31	trans-1-2-difluorethylene	-277.0920922	-277.0404056	-277.178896	-277.1280491	-1.384	-1.84	0.910	N
32	trans-1-bromo-2-butene	-2726.969368	-2726.94083	-2729.442609	-2729.416037	-0.723	-0.68	0.503	N
33	trichloroethylene	-1457.406723	-1457.375993	-1457.526148	-1457.495773	-0.827	-0.58	0.305	V
34	uracil-vertical	-414.8983095	-414.8832529	-415.0266729	-415.0058323	-0.567	-0.21	1.053	N
16	cytosine - adiabatic	-395.0087198	-395.0000809	-395.1310376	-395.1219149	-0.134	-0.06	0.288	V
34	uracil - adiabatic	-414.8983095	-414.897715	-415.0266807	-415.0257366	0.094	0.15	0.271	V
36	ethyl-radical	-79.17455056	-79.15699548	-79.19839661	-79.18346432	-0.354	-0.26	0.145	V
36	isopropyl-radical	-118.5011218	-118.4829716	-118.5356706	-118.5197291	-0.368	-0.32	0.214	V
37	t-butyl-radical	-157.8276407	-157.8154026	-157.872688	-157.8617746	-0.212	-0.16	0.248	V

TPSSh Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.7872385	-997.7473675	-997.8740258	-997.8378783	-0.984	-0.75	0.345	V
2	1-3-cyclohexadiene	-233.4448166	-233.4055079	-233.5076781	-233.4719374	-0.973	-0.8	0.251	V
3	2-bromo-1-propene	-2688.919767	-2688.872164	-2691.38421	-2691.338648	-1.240	-1.31	0.477	V
4	3-bromo-1-propene	-2688.913777	-2688.891165	-2691.380948	-2691.360096	-0.567	-0.6	0.298	V
5	acetaldehyde	-153.8410747	-153.7873821	-153.8889361	-153.8377268	-1.393	-1.19	0.307	V
6	acetone	-193.1701683	-193.119898	-193.2284882	-193.1855126	-1.169	-1.51	0.816	N
7	adenine	-467.3630736	-467.3304615	-467.4978434	-467.4675873	-0.823	-0.64	0.443	V
8	bromoethylene	-2649.590418	-2649.540806	-2652.048579	-2652.001421	-1.283	-1.17	0.384	V
9	chloroethylene	-538.1952962	-538.1390228	-538.2502464	-538.197494	-1.435	-1.29	0.369	V
	chloroform	-500.1136975	-500.0617646	-500.1577672	-500.111864	-1.249	-0.35	0.723	N
10	cis-1-2-dichloroethylene	-997.7905459	-997.7373488	-997.8766736	-997.8284673	-1.312	-1.12	0.257	V
11	cis-1-2-difluorethylene	-277.0627542	-277.0121901	-277.1497638	-277.1028762	-1.276	-2.18	0.966	N
12	cis-1-bromo-2-butene	-2728.23711	-2728.213669	-2730.713121	-2730.691574	-0.586	-0.68	0.333	V
13	cyclobutanone	-231.2511517	-231.2064277	-231.3173504	-231.2775631	-1.083	-1	0.555	N
14	cyclopentadiene	-194.1248743	-194.0753484	-194.1781017	-194.1315695	-1.266	-1.19	0.226	V
15	cyclopropene	-116.6355343	-116.5683419	-116.6690684	-116.6043534	-1.761	-1.73	0.415	V
16	cytosine-vertical	-394.9611328	-394.9350759	-395.0829727	-395.0594847	-0.639	-0.36	0.341	V
17	ethylene	-78.59578289	-78.52598163	-78.61992059	-78.5526145	-1.831	-1.78	0.389	V
18	fluorethylene	-177.8346998	-177.7623275	-177.890105	-177.8201333	-1.904	-1.91	0.450	V
19	furan	-230.0440699	-229.9749428	-230.1116083	-230.0623462	-1.340	-1.76	1.074	N
20	isothiazole	-569.0645188	-569.0321054	-569.147871	-569.117897	-0.816	-0.63	0.307	V
21	isoxazole	-246.0589474	-246.0087496	-246.1308514	-246.0827962	-1.308	-1.09	0.332	V
22	naphtalene	-385.9353347	-385.9195598	-386.0348016	-386.0223285	-0.339	-0.2	0.263	V
23	oxazole	-246.0930017	-246.0370792	-246.1653795	-246.1108251	-1.485	-1.44	0.527	N
24	pyrazine	-264.342609	-264.3295998	-264.4138241	-264.4031801	-0.290	-0.07	0.286	V
25	pyridazine	-264.3139655	-264.299544	-264.385234	-264.3728239	-0.338	-0.32	0.275	V
26	pyrimidine	-264.3491386	-264.3268506	-264.420428	-264.4003634	-0.546	-0.25	0.282	V
27	thiazole	-569.0708309	-569.0320351	-569.1509401	-569.114388	-0.995	-0.8	0.287	V
28	thiophene	-553.0266306	-552.9738557	-553.1023891	-553.0527043	-1.352	-1.17	0.294	V
29	thymine	-454.1709239	-454.1538639	-454.3090248	-454.2943951	-0.398	-0.31	0.357	V
30	trans-1-2-dichloroethylene	-997.789967	-997.7451272	-997.8760369	-997.8356282	-1.100	-0.82	0.306	V
31	trans-1-2-difluorethylene	-277.0616993	-276.9886036	-277.1481006	-277.0764929	-1.949	-1.84	0.479	V
32	trans-1-bromo-2-butene	-2726.891764	-2726.939831	-2729.366891	-2729.416358	1.346	-0.68	0.181	V
33	trichloroethylene	-1457.379913	-1457.344323	-1457.49807	-1457.467363	-0.836	-0.58	0.297	V
34	uracil-vertical	-414.8475512	-414.8312336	-414.9753544	-414.9616958	-0.372	-0.21	0.295	V
16	cytosine - adiabatic	-394.9611328	-394.9523357	-395.0829727	-395.0734317	-0.149	-0.06	0.285	V
34	uracil - adiabatic	-414.8475512	-414.8445207	-414.9753544	-414.9724963	0.094	0.15	0.258	V
36	ethyl-radical	-79.16829666	-79.14846116	-79.19188571	-79.17468828	-0.418	-0.26	0.137	V
36	isopropyl-radical	-118.4917865	-118.4709851	-118.5259129	-118.5072971	-0.442	-0.32	0.202	V
37	t-butyl-radical	-157.8152472	-157.8000785	-157.8597637	-157.8459143	-0.293	-0.16	0.242	V

B2PLYP Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
	Molecule	E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.1921287	-997.1446834	-997.2773684	-997.2329945	-1.207	-0.75	0.334	V
2	1-3-cyclohexadiene	-232.8851492	-232.8341157	-232.9482386	-232.9002316	-1.306	-0.8	0.276	V
3	2-bromo-1-propene	-2688.236629	-2688.179182	-2690.706856	-2690.651095	-1.517	-1.31	0.505	V
4	3-bromo-1-propene	-2688.232044	-2688.194366	-2690.704801	-2690.668353	-0.992	-0.6	0.353	V
5	acetaldehyde	-153.5268525	-153.463726	-153.5749281	-153.5144133	-1.647	-1.19	0.250	V
6	acetone	-192.7571258	-192.6875573	-192.8159014	-192.7498225	-1.798	-1.51	0.294	V
7	adenine	-466.3954817	-466.3531975	-466.5304194	-466.4918657	-1.049	-0.64	1.211	N
8	bromoethylene	-2649.006946	-2648.948325	-2651.470746	-2651.414409	-1.533	-1.17	0.364	V
9	chloroethylene	-537.8001719	-537.7353359	-537.8546522	-537.7929354	-1.679	-1.29	0.358	V
	chloroform	-499.8003736	-499.7381489	-499.8440484	-499.7908838	-1.447	-0.35	0.763	N
11	cis-1-2-difluorethylene	-276.6264107	-276.5393038	-276.7141462	-276.6280585	-2.343	-2.18	0.446	V
12	cis-1-bromo-2-butene	-2727.455232	-2727.416812	-2729.936807	-2729.899712	-1.009	-0.68	0.393	V
13	cyclobutanone	-230.7515277	-230.6917098	-230.8174699	-230.7618097	-1.515	-1	0.242	V
14	cyclopentadiene	-193.6621897	-193.6017052	-193.7153936	-193.6573662	-1.579	-1.19	0.255	V
15	cyclopropene	-116.3505803	-116.2732686	-116.3847336	-116.3096037	-2.044	-1.73	0.420	V
16	cytosine-vertical	-394.1671124	-394.1351872	-394.2895889	-394.2599342	-0.807	-0.36	0.330	V
17	ethylene	-78.39993259	-78.32060628	-78.42469638	-78.34770069	-2.095	-1.78	0.392	V
18	fluorethylene	-177.5185105	-177.4377077	-177.5745399	-177.4959045	-2.140	-1.91	0.437	V
19	furan	-229.5584023	-229.4804737	-229.6259135	-229.5500321	-2.065	-1.76	0.475	V
20	isothiazole	-568.4838165	-568.446001	-568.5657171	-568.5298689	-0.975	-0.63	0.319	V
21	isoxazole	-245.555116	-245.5004522	-245.6267954	-245.5743454	-1.427	-1.09	0.313	V
22	naphtalene	-385.0464524	-385.0167615	-385.1457826	-385.1191465	-0.725	-0.2	0.308	V
23	oxazole	-245.5953964	-245.5295	-245.6677112	-245.6033106	-1.752	-1.44	0.497	V
24	pyrazine	-263.7751458	-263.7549937	-263.846475	-263.8287144	-0.483	-0.07	0.304	V
25	pyridazine	-263.7435518	-263.7220273	-263.8149193	-263.7953634	-0.532	-0.32	0.290	V
26	pyrimidine	-263.7830757	-263.751361	-263.8545917	-263.8250984	-0.803	-0.25	0.300	V
27	thiazole	-568.4912956	-568.4442342	-568.5700398	-568.5247521	-1.232	-0.8	0.302	V
28	thiophene	-552.4608655	-552.400479	-552.5351293	-552.4772259	-1.576	-1.17	0.314	V
29	thymine	-453.2696173	-453.2443151	-453.4081434	-453.385084	-0.627	-0.31	0.365	V
30	trans-1-2-dichloroethylene	-997.1954701	-997.1436759	-997.279944	-997.2319761	-1.305	-0.82	0.297	V
31	trans-1-2-difluorethylene	-276.6255047	-276.5445418	-276.7125807	-276.6332304	-2.159	-1.84	0.424	V
32	trans-1-bromo-2-butene	-2726.13095	-2726.170181	-2728.611371	-2728.651839	1.101	-0.68	0.185	V
33	trichloroethylene	-1456.584758	-1456.543286	-1456.700198	-1456.662579	-1.024	-0.58	0.278	V
34	uracil-vertical	-414.0460896	-414.0225247	-414.1741158	-414.153024	-0.574	-0.21	0.314	V
16	cytosine - adiabatic	-394.1671124	-394.1501732	-394.2895889	-394.2714162	-0.401	-0.06	0.304	V
34	uracil - adiabatic	-414.0460896	-414.0341752	-414.1741158	-414.1622024	-0.154	0.15	0.275	V
36	ethyl-radical	-78.96634553	-78.93097942	-78.99049556	-78.9574978	-0.854	-0.26	0.139	V
36	isopropyl-radical	-118.189999	-118.1522366	-118.2246878	-118.188824	-0.917	-0.32	0.197	V
37	t-butyl-radical	-157.4136394	-157.3804143	-157.4587856	-157.4267717	-0.797	-0.16	0.245	V

mPW2PLYP Functional		Basis set 6-31+G*		Basis set 6-311+G(2df,p)					
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	Rydberg contrib.	Anion typ
1	1-1-dichloroethylene	-997.2362861	-997.1894525	-997.3216676	-997.2778492	-1.192	-0.75	0.333	V
2	1-3-cyclohexadiene	-232.9115375	-232.861003	-232.9747555	-232.9272537	-1.293	-0.8	0.279	V
3	2-bromo-1-propene	-2688.297114	-2688.240195	-2690.768353	-2690.713101	-1.503	-1.31	0.502	V
4	3-bromo-1-propene	-2688.292467	-2688.254828	-2690.766234	-2690.729779	-0.992	-0.6	0.361	V
5	acetaldehyde	-153.5401691	-153.4772115	-153.5884124	-153.5280939	-1.641	-1.19	0.249	V
6	acetone	-192.7755133	-192.7061694	-192.8344751	-192.7685521	-1.794	-1.51	0.286	V
7	adenine	-466.4396306	-466.3980456	-466.5751347	-466.5372247	-1.032	-0.64	1.217	N
8	bromoethylene	-2649.062356	-2649.004204	-2651.527163	-2651.47128	-1.521	-1.17	0.360	V
9	chloroethylene	-537.8262526	-537.7618372	-537.8808199	-537.8195023	-1.669	-1.29	0.355	V
	chloroform	-499.8227857	-499.7608048	-499.8665151	-499.8136481	-1.439	-0.35	0.764	N
11	cis-1-2-difluorethylene	-276.6462187	-276.5590827	-276.7340799	-276.6479913	-2.343	-2.18	0.442	V
12	cis-1-bromo-2-butene	-2727.520679	-2727.48232	-2730.003271	-2729.966212	-1.008	-0.68	0.407	V
13	cyclobutanone	-230.7739498	-230.7144676	-230.8400499	-230.7847435	-1.505	-1	0.243	V
14	cyclopentadiene	-193.6833367	-193.6232834	-193.7366408	-193.6790531	-1.567	-1.19	0.256	V
15	cyclopropene	-116.3623466	-116.2852484	-116.3966002	-116.3216944	-2.038	-1.73	0.416	V
16	cytosine-vertical	-394.2032862	-394.1716778	-394.3262594	-394.2968794	-0.799	-0.36	0.333	V
17	ethylene	-78.40799569	-78.32884357	-78.43279554	-78.35599892	-2.090	-1.78	0.387	V
18	fluorethylene	-177.532468	-177.4517173	-177.5885949	-177.5100255	-2.138	-1.91	0.433	V
19	furan	-229.5799785	-229.5022316	-229.6476657	-229.5719939	-2.059	-1.76	0.473	V
20	isothiazole	-568.5170084	-568.4796711	-568.5991697	-568.5637573	-0.964	-0.63	0.323	V
21	isoxazole	-245.5764632	-245.5218369	-245.6484066	-245.5959771	-1.427	-1.09	0.316	V
22	naphtalene	-385.0885442	-385.0594382	-385.1881444	-385.162064	-0.710	-0.2	0.312	V
23	oxazole	-245.6170502	-245.5512594	-245.6896027	-245.6253104	-1.749	-1.44	0.498	V
24	pyrazine	-263.8002331	-263.780889	-263.8718543	-263.8548717	-0.462	-0.07	0.307	V
25	pyridazine	-263.7685293	-263.7474692	-263.8402105	-263.8210808	-0.521	-0.32	0.293	V
26	pyrimidine	-263.8082468	-263.7771745	-263.8800574	-263.8511775	-0.786	-0.25	0.302	V
27	thiazole	-568.5244951	-568.4779323	-568.6034491	-568.558602	-1.220	-0.8	0.305	V
28	thiophene	-552.494097	-552.4342569	-552.5684912	-552.5111028	-1.562	-1.17	0.315	V
29	thymine	-453.3111203	-453.2862813	-453.4501792	-453.4275503	-0.616	-0.31	0.367	V
30	trans-1-2-dichloroethylene	-997.2395519	-997.188449	-997.32417	-997.276808	-1.289	-0.82	0.298	V
31	trans-1-2-difluorethylene	-276.6452972	-276.5643096	-276.7325212	-276.6531787	-2.159	-1.84	0.422	V
32	trans-1-bromo-2-butene	-2726.19497	-2726.235607	-2728.676349	-2728.718208	1.139	-0.68	0.188	V
33	trichloroethylene	-1456.647006	-1456.606266	-1456.762637	-1456.725609	-1.008	-0.58	0.280	V
34	uracil-vertical	-414.0825235	-414.0593304	-414.2110726	-414.1903092	-0.565	-0.21	0.317	V
16	cytosine - adiabatic	-394.2032862	-394.1874096	-394.3262594	-394.3090312	-0.374	-0.06	0.307	V
34	uracil - adiabatic	-414.0825235	-414.0716545	-414.2110726	-414.2000733	-0.128	0.15	0.278	V
36	ethyl-radical	-78.97486795	-78.94031632	-78.99902905	-78.96688689	-0.831	-0.26	0.139	V
36	isopropyl-radical	-118.2034964	-118.16664	-118.238233	-118.2032946	-0.893	-0.32	0.198	V
37	t-butyl-radical	-157.4322333	-157.400108	-157.477453	-157.4465405	-0.768	-0.16	0.246	V

HF Method		Basis set 6-31+G*		Basis set 6-311+G(2df,p)						
Molecule		E-neutral	E-anion	E-neutra-ext	E-anion-ext	EA calc	EA exp	diff EA	Rydberg contrib.	Dipole Moment	Anion typ
1	1-1-dichloroethylene	-995.8288815	-995.7613682	-995.9135889	-995.8479847	-1.785181	-0.75	-0.285181	0.38168	3.8987	V
2	1-3-cyclohexadiene	-231.8385642	-231.7608783	-231.9020281	-231.8268453	-2.045828	-0.8	-0.445828	0.30832	2.4084	V
3	2-bromo-1-propene	-2686.402862	-2686.335566	-2688.896404	-2688.83533	-1.661899	-1.31	-0.351899	1.04774	5.0882	N
4	3-bromo-1-propene	-2686.400017	-2686.337881	-2688.895902	-2688.836407	-1.618953	-0.6	-0.418953	0.95496	5.183	N
5	acetaldehyde	-152.921121	-152.8308193	-152.9709184	-152.8827028	-2.400469	-1.19	-0.020469	0.24378	3.4927	V
6	acetone	-191.9676128	-191.8680595	-192.0283727	-191.930881	-2.652883	-1.51	-1.142883	0.19621	3.0351	V
7	adenine	-464.5341995	-464.4818194	-464.6727121	-464.6249475	-1.299741	-0.64	-0.019741	1.28487	14.6673	N
8	bromoethylene	-2647.357515	-2647.278232	-2649.844269	-2649.7666	-2.113466	-1.17	-0.943466	0.42033	5.413	V
9	chloroethylene	-536.9369135	-536.8514393	-536.9912729	-536.9079655	-2.266909	-1.29	-0.976909	0.42416	4.4214	V
	chloroform	-499.0941581	-499.0212712	-499.138291	-499.0755322	-1.707755	-0.35	-0.307755	0.8654	9.0017	N
10	cis-1-2-dichloroethylene	-995.8329044	-995.7518607	-995.9168404	-995.8390939	-2.11559	-1.12	-0.99559	0.24141	0.4333	V
11	cis-1-2-difluorethylene	-275.7366725	-275.6233925	-275.82582	-275.7126652	-3.079098	-2.18	-0.899098	0.63227	1.1112	V
12	cis-1-bromo-2-butene	-2725.438643	-2725.376329	-2727.943564	-2727.884898	-1.596382	-0.68	-0.236382	0.98823	4.8816	N
13	cyclobutanone	-229.8038534	-229.7147967	-229.8714667	-229.7859649	-2.326623	-1	-0.326623	0.2076	4.7535	V
14	cyclopentadiene	-192.7981832	-192.7123038	-192.8517517	-192.7677972	-2.284518	-1.19	-1.094518	0.30076	1.4817	V
15	cyclopropene	-115.8264127	-115.7260871	-115.8614303	-115.7626685	-2.687443	-1.73	-0.957443	0.49865	1.196	V
16	cytosine-vertical	-392.6285004	-392.569725	-392.7538093	-392.6966767	-1.554656	-0.36	-0.114656	0.35483	4.831	V
17	ethylene	-78.0358171	-77.93494115	-78.06086785	-77.96176084	-2.696839	-1.78	-0.916839	0.45676	0	V
18	fluorethylene	-176.8913644	-176.7893316	-176.9482127	-176.8480418	-2.725789	-1.91	-0.815789	0.59987	5.2014	V
19	furan	-228.6327874	-228.5312162	-228.7012867	-228.6009083	-2.731436	-1.76	-0.971436	0.66512	2.3362	V
20	isothiazole	-567.2866522	-567.2272147	-567.3692422	-567.3113203	-1.576136	-0.63	-0.316136	0.35506	2.13	V
21	isoxazole	-244.5954572	-244.5141769	-244.669303	-244.5897578	-2.164536	-1.09	-1.074536	0.36088	1.988	V
22	naphtalene	-383.3661149	-383.2938138	-383.464808	-383.3966018	-1.855984	-0.2	-0.055984	1.25427	0	N
23	oxazole	-244.640218	-244.5502581	-244.7144323	-244.6251789	-2.428708	-1.44	-0.988708	0.84679	3.3071	V
24	pyrazine	-262.6904796	-262.6495852	-262.7631862	-262.7244319	-1.05456	-0.07	-0.00456	0.33255	0	V
25	pyridazine	-262.6575432	-262.6145361	-262.7303957	-262.6889399	-1.128069	-0.32	-0.168069	0.31446	3.2607	V
26	pyrimidine	-262.7010159	-262.6480503	-262.7740181	-262.7228664	-1.391909	-0.25	-0.141909	0.31429	1.5269	V
27	thiazole	-567.2949552	-567.2241892	-567.3745265	-567.3049873	-1.892257	-0.8	-0.292257	0.32243	1.9451	V
28	thiophene	-551.296419	-551.2148768	-551.370216	-551.290669	-2.164586	-1.17	-0.994586	0.34678	0.2534	V
29	thymine	-451.5216518	-451.4672854	-451.663498	-451.610904	-1.431155	-0.31	-0.191155	0.39153	3.2923	V
30	trans-1-2-dichloroethylene	-995.8330399	-995.7600301	-995.9170426	-995.8469224	-1.908067	-0.82	-0.268067	0.28928	0	V
31	trans-1-2-difluorethylene	-275.7357602	-275.6287847	-275.8241653	-275.7180605	-2.88726	-1.84	-1.04726	0.55965	0.0102	V
32	trans-1-bromo-2-butene	-2724.149878	-2724.173684	-2726.653036	-2726.677943	0.677773	-0.68	0.677773	0.18973	11.6988	V
33	trichloroethylene	-1454.72172	-1454.66025	-1454.836261	-1454.777253	-1.605676	-0.58	-0.445676	0.26276	0.8032	V
34	uracil-vertical	-412.4826701	-412.4315088	-412.6135631	-412.5643576	-1.338949	-0.21	-0.078949	0.34874	3.9271	V
16	cytosine - adiabatic	-392.6285004	-392.5975915	-392.7538093	-392.7202654	-0.912775	-0.06	-0.852775	0.31458	5.4028	V
34	uracil - adiabatic	-412.4826701	-412.4535088	-412.6135631	-412.5831273	-0.828201	0.15	-0.978201	0.29999	4.608	V
36	ethyl-radical	-78.5991609	-78.5311056	-78.62386828	-78.55767099	-1.80132	-0.26	-1.54132	0.134	4.4247	V
36	isopropyl-radical	-117.6381703	-117.566915	-117.673563	-117.6037382	-1.900028	-0.32	-1.580028	0.18165	3.2134	V
37	t-butyl-radical	-156.6772284	-156.608749	-156.7233821	-156.6556404	-1.843346	-0.16	-1.683346	0.22788	1.6999	V

MP2/6-311+G(2d,p)//B3LYP/6-31+G*				Mp2-TZ		
Molecule		Neutral	Anion		EA exp	Anion typ
7	adenine	-466.2647	-466.2269	-1.029493	-0.64	N
12	cis-1-bromo-2-butene	-2728.68	-2728.638	-1.155588	-0.68	N
1	1-1-dichloroethylene	-996.5115	-996.4657	-1.247418	-0.75	V
2	1-3-cyclohexadiene	-232.7813	-232.739	-1.153188	-0.6	V
5	acetaldehyde	-153.4805	-153.4164	-1.745025	-1.19	V
6	acetone	-192.6941	-192.6257	-1.861435	-1.51	V
8	bromoethylene	-2649.839	-2649.759	-2.163317	-1.17	V
9	chloroethylene	-536.9857	-536.9006	-2.315997	-1.29	V
10	cis-1-2-dichloroethylene	-996.5126	-996.4532	-1.615165	-1.12	V
11	cis-1-2-difluorethylene	-276.5543	-276.4619	-2.514365	-2.18	V
14	cyclopentadiene	-193.5765	-193.522	-1.481321	-1.19	V
15	cyclopropene	-116.2966	-116.2209	-2.058548	-1.73	V
16	cytosine-vertical	-394.0583	-394.025	-0.905328	-0.36	V
17	ethylene	-78.36156	-78.28324	-2.131306	-1.78	V
18	fluorethylene	-177.4634	-177.3803	-2.262524	-1.91	V
19	furan	-229.481	-229.4022	-2.144147	-1.76	V
20	isothiazole	-568.1205	-568.0815	-1.061559	-0.63	V
21	isoxazole	-245.4865	-245.4276	-1.601796	-1.09	V
22	naphtalene	-384.8822	-384.8638	-0.498538	-0.2	V
23	oxazole	-245.524	-245.455	-1.878138	-1.44	V
24	pyrazine	-263.6818	-263.666	-0.431231	-0.07	V
25	pyridazine	-263.6519	-263.6331	-0.511053	-0.32	V
26	pyrimidine	-263.6875	-263.6615	-0.708697	-0.25	V
27	thiazole	-568.1248	-568.076	-1.327035	-0.6	V
28	thiophene	-552.0883	-552.03	-1.587872	-1.17	V
29	thymine	-568.1248	-568.076	-1.327035	-0.31	V
30	trans-1-2-dichloroethylene	-996.5116	-996.4614	-1.363711	-0.82	V
31	trans-1-2-difluorethylene	-276.5527	-276.4678	-2.311439	-1.84	V
32	trans-1-bromo-2-butene	-2727.342	-2727.391	1.335424	-0.68	V
33	trichloroethylene	-1455.583	-1455.54	-1.181569	-0.58	V
						0.935484

		6-311+G(2d,p	6-31+G*	i-311+G(2d,p	6-31+G*	6-311+G(2d,p)		
Molecule		MP2	CCSD	CCSD(T)	CCSD	CCSD(T)	EA exp	
7	adenine	-1.029	-1.157	-1.114	-1.029	-0.982	-0.64	N
12	cis-1-bromo-2-butene	-1.156	-1.240	-1.210	-1.086	-1.045	-0.68	N
1	1-1-dichloroethylene	-1.247	-1.640	-1.651	-1.717	-1.736	-0.75	V
2	1-3-cyclohexadiene	-1.153	-1.701	-1.665	-1.398	-1.344	-0.8	V
5	acetaldehyde	-1.745	-2.045	-2.042	-1.819	-1.806	-1.19	V
6	acetone	-1.861	-2.195	-2.182	-1.895	-1.868	-1.51	V
8	bromoethylene	-2.163	-1.886	-1.883	-1.667	-1.652	-1.17	V
9	chloroethylene	-2.316	-2.098	-2.102	-1.832	-1.825	-1.29	V
10	cis-1-2-dichloroethylene	-1.615	-2.046	-2.078	-1.717	-1.736	-1.12	V
11	cis-1-2-difluorethylene	-2.514	-2.730	-2.737	-2.563	-2.565	-2.18	V
14	cyclopentadiene	-1.481	-1.964	-1.939	-1.673	-1.630	-1.19	V
15	cyclopropene	-2.059	-2.391	-2.376	-2.169	-2.140	-1.73	V
16	cytosine-vertical	-0.905	-1.187	-1.212	-0.939	-0.946	-0.36	V
17	ethylene	-2.131	-2.462	-2.456	-2.225	-2.209	-1.78	V
18	fluorethylene	-2.263	-2.534	-2.537	-2.320	-2.315	-1.91	V
19	furan	-2.144	-2.382	-2.364	-2.193	-2.166	-1.76	V
20	isothiazole	-1.062	-1.392	-1.410	-1.157	-1.162	-0.63	V
21	isoxazole	-1.602	-1.905	-1.920	-1.680	-1.685	-1.09	V
22	naphtalene	-0.499	-1.069	-1.019	-0.752	-0.677	-0.2	V
23	oxazole	-1.878	-2.039	-2.016	-1.889	-1.856	-1.44	V
24	pyrazine	-0.431	-0.796	-0.800	-0.555	-0.545	-0.07	V
25	pyridazine	-0.511	-0.866	-0.874	-0.625	-0.615	-0.32	V
26	pyrimidine	-0.709	-1.076	-1.076	-0.831	-0.811	-0.25	V
27	thiazole	-1.327	-1.625	-1.638	-1.383	-1.378	-0.8	V
28	thiophene	-1.588	-1.972	-1.979	-1.702	-1.693	-1.17	V
29	thymine	-1.327	-0.993	-0.995	-0.755	-0.743	-0.31	V
30	trans-1-2-dichloroethylene	-1.364	-1.793	-1.816	-1.491	-1.502	-0.82	V
31	trans-1-2-difluorethylene	-2.311	-2.572	-2.581	-2.382	-2.385	-1.84	V
32	trans-1-bromo-2-butene	-1.335	-0.928	-0.972	-1.128	-1.190	-0.68	V
33	trichloroethylene	-1.182	-1.564	-1.608	-1.259	-1.289	-0.58	V

Figure S3. Plots of the fit of eq. 8 to get EAs by extrapolation method. Formamide was selected as an example. Red line corresponds to a linear fit, blue line corresponds to a quadratic fit

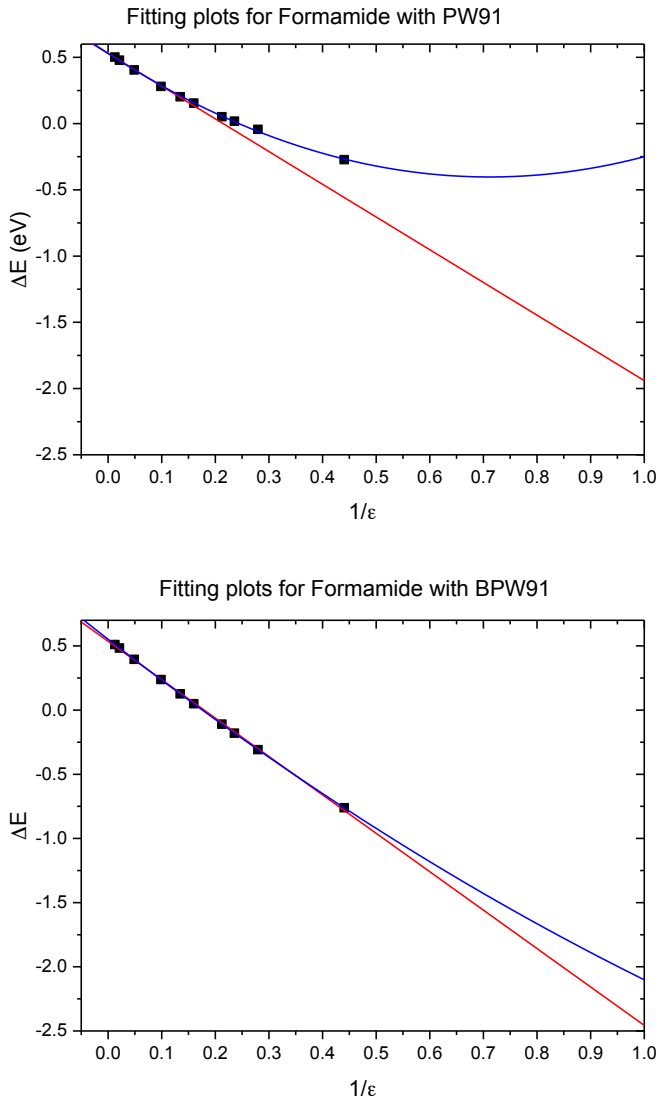


Table S7. Results of the calculations of the *EAs* of compounds from chart S-2 with different DFT functionals.

Functional	MAD (eV)[a]	V ratio[b]	ΔE *vs.* 1/ε Fitting	Limitting value
BLYP	0.16	0.43	linear	-2.1
BPW91	0.14	0.61	quadratic	-3.0
PW91	0.17	0.61	linear	-2.3
B97D	0.15	0.35	quadratic	-2.1
B3PW91	0.23	0.70	linear	-3.4
B3LYP	0.15	0.70	quadratic	-2.2
B3LYP-D	0.14	0.61	quadratic	-2.3
CAM-B3LYP	0.11	0.57	quadratic	-2.4
LC-BLYP	0.09	0.65	quadratic	-2.3
BHandHLYP	0.14	0.65	quadratic	-2.4
ω-B97	0.19	0.43	quadratic	-2.3
ω-B97X	0.13	0.56	quadratic	-2.3
ω-B97XD	0.11	0.56	quadratic	-2.3
PBE0	0.09	0.61	quadratic	-3.0
LC- ωPBE	0.10	0.65	quadratic	-2.8
TPSS	0.14	0.61	linear	-2.4
TPSSh	0.09	0.57	quadratic	-2.3
M06	0.13	0.57	quadratic	-2.2
M06-2X	0.12	0.65	quadratic	-2.3
M06-L	0.15	0.61	quadratic	-2.3
M06-HF	0.12	0.74	quadratic	-2.8

[a]MAD of the calculated *vs.* experimental *EA* values. The *EAs* obtained for V anions were employed for these calculations.
[b]V state anions over total number of compounds. All the calculated *EAs* are included in the SI, tables S-8.1 to S-8.21.

Tables S8.1-21. Detailed values of the energies employed for computing the EAs in table 2 for each DFT method employed. The values in red correspond to N anions or V anions with EAs with high deviation and are not considered for the computation of MAD.

	BLYP	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.10966	-1.54057	1	0.9998	0.190	0.241
49	guanine	-1.4	-0.95901	-1.56909	1	0.99836	0.441	0.169
55	transcloropropene	-1.49	-1.30744	-1.55288	1	0.9993	0.183	0.063
42	cis-bromopropeno	-1.49	-0.76128	-1.2596	1	0.99632	0.729	0.230
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	1	0.99989	0.111	0.169
39	acetic-acid	-1.8	-0.75343	-1.38328	1	0.99889	1.047	0.417
40	allene	-1.88	-1.45606	-1.76998	1	0.99883	0.424	0.110
53	propiolactone	-1.9	-0.68861	-1.7484	0.99967	0.99945	1.211	0.152
41	butirolactone	-1.93	-0.21465	-1.57286	1	0.99913	1.715	0.357
52	Propene	-1.99	-1.64558	-2.26678	1	0.99969	0.344	0.277
47	diterbutylperoxide	-2	0.77536	-1.69359	0.99998	0.99796	2.775	0.306
44	cyclobuteno	-2	-0.92046	-1.95654	0.9997	0.98696	1.080	0.043
48	formamide	-2.05	-0.73937	-1.38462	0.99906	0.99083	1.311	0.665
56	trasnbuteno	-2.1	-0.60028	-1.77517	0.99999	0.99786	1.500	0.325
50	imidazole	-2.13	--	-2.2565	--	--		0.127
45	cyclopenteno	-2.14	-1.0216	-1.67466	0.99968	0.99904	1.118	0.465
43	cis-2-buteno	-2.22	-1.16125	-1.25737	1	0.99974	1.059	0.963
51	methylvynilether	-2.3	-0.91887	-1.38045	0.99944	0.99423	1.381	0.920
46	dimethylformamide	-2.4	0.72057	-1.74274	--	0.99986	3.121	0.657

	BPW91	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.16678	-1.44789	1	0.99916	0.133	0.148
49	guanine	-1.4	-0.79619	-1.42035	1	0.9996	0.604	0.020
55	transcloropropene	-1.49	-1.29308	-1.55922	1	0.99928	0.197	0.069
42	cis-bromopropeno	-1.49	-1.42405	-1.67306	1	0.99937	0.066	0.183
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	0.99999	0.99898	0.111	0.169
39	acetic-acid	-1.8	-2.01646	-2.2261	1	0.99968	0.216	0.426
40	allene	-1.88	-1.42684	-1.65027	1	0.99961	0.453	0.230
53	propiolactone	-1.9	-1.78819	-2.11616	1	0.99917	0.112	0.216
41	butirolactone	-1.93	-0.70745	-2.09888	0.99991	0.99705	1.223	0.169
52	Propene	-1.99	-2.09855	-2.56645	1	0.9983	0.109	0.576
47	diterbutylperoxide	-2	0.20718	-2.56012	0.99999	0.9982	2.207	0.560
44	cyclobuteno	-2	-1.92434	-2.29798	1	0.99889	0.076	0.298
48	formamide	-2.05	-2.10117	-2.45655	1	0.99911	0.051	0.407
56	trasnbuteno	-2.1	0.48965	0.39605	0.9991	0.9866	2.590	2.496
50	imidazole	-2.13	-1.76256	-2.17404	1	0.9982	0.367	0.044
45	cyclopenteno	-2.14	-2.03648	-2.46237	0.99999	0.99852	0.104	0.322
43	cis-2-buteno	-2.22	-2.21656	-2.64332	0.99999	0.99854	0.003	0.423
51	methylvynilether	-2.3	-2.09855	-2.56645	1	0.9983	0.201	0.266
46	dimethylformamide	-2.4	-1.15506	-2.16253	1	0.99893	1.245	0.237
57	ethylisocianate	-2.63	-0.82095	-1.24139	0.99999	0.99726	1.809	1.389
58	acetonitrile	-2.82	-0.96236	-0.95543	1	1	1.858	1.865
59	tetrafluorethylene	-3	-2.7882	-2.7517	1	1	0.212	0.248
60	2butyne	-3.43	-0.90695	-1.53895	0.99985	0.99157	2.523	1.891
						MAD	0.140	0.264
						V ratio	0.61	0.78

	PW91	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-0.70902	-1.27065	0.99989	0.99605	0.591	0.029
49	guanine	-1.4	-0.80851	-1.53561	1	0.99984	0.591	0.136
55	transcloropropene	-1.49	-1.09076	-1.42901	1	0.99873	0.399	0.061
42	cis-bromopropeno	-1.49	-1.14975	-1.76722	--	0.99999	0.340	0.277
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	0.99993	0.99129	0.111	0.169
39	acetic-acid	-1.8	-0.80711	-1.26747	0.99997	0.99663	0.993	0.533
40	allene	-1.88	-1.36485	-1.69496	1	0.99879	0.515	0.185
53	propiolactone	-1.9	0.16781	-1.58634	0.99999	0.996	2.068	0.314
41	butirolactone	-1.93	-0.43629	-1.37168	0.99998	0.99769	1.494	0.558
52	Propene	-1.99	-0.29216	-2.02964	1	0.99953	1.698	0.040
47	diterbutylperoxide	-2	1.05132	-1.70105	0.99998	0.998	3.051	0.299
44	cyclobuteno	-2	-0.94636	-1.93972	0.99997	0.98975	1.054	0.060
48	formamide	-2.05	0.16986	-2.04025	1	0.99933	2.220	0.010
56	trasnbuteno	-2.1	-0.55436	-1.82519	0.99999	0.99796	1.546	0.275
50	imidazole	-2.13	-0.7996	-0.84012	1	0.99994	1.330	1.290
45	cyclopenteno	-2.14	-0.04724	-1.90475	1	0.99895	2.093	0.235
43	cis-2-buteno	-2.22	--	-1.74406	--	--		0.476
51	methylvynilether	-2.3	-0.29216	-2.02964	1	0.99953	2.008	0.270
46	dimethylformamide	-2.4	0.45657	-1.62603	1	0.9992	2.857	0.774
57	ethylisocianate	-2.63	-0.50738	-1.06585	1	0.99942	2.123	1.564
58	acetonitrile	-2.82	-0.8298	-0.83614	0.99999	0.99999	1.990	1.984
59	tetrafluorethylene	-3	-1.07619	-1.11629	1	0.99996	1.924	1.884
60	2butyne	-3.43	-0.727	-1.27696	0.99972	0.99231	2.703	2.153
						MAD	0.111	0.169
						V ratio	0.04	0.61

	B97D	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.06	-1.4892	0.99997	0.99771	0.240	0.189
49	guanine	-1.4	-0.97996	-1.51652	1	0.99969	0.420	0.117
55	transcloropropene	-1.49	-1.41164	-1.64809	1	0.99938	0.078	0.158
42	cis-bromopropeno	-1.49	-1.36956	-1.87405	--	0.99996	0.120	0.384
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	1	0.99912	0.111	0.169
39	acetic-acid	-1.8	-1.14818	-1.84566	1	0.99849	0.652	0.046
40	allene	-1.88	-1.63553	-1.9503	1	0.99893	0.244	0.070
53	propiolactone	-1.9	-1.31425	-2.10765	0.99999	0.99867	0.586	0.208
41	butirolactone	-1.93	-0.77887	-1.77154	0.99998	0.98768	1.151	0.158
52	Propene	-1.99	-1.8689	-2.25952	1	0.99867	0.121	0.270
47	diterbutylperoxide	-2	-0.20585	-1.84088	0.99998	0.99446	1.794	0.159
44	cyclobuteno	-2	-1.96374	-2.43979	1	0.99965	0.036	0.440
48	formamide	-2.05	-0.96724	-2.545	0.98323	0.98267	1.083	0.495
56	trasnbuteno	-2.1	-1.18339	-2.19802	0.99983	0.98717	0.917	0.098
50	imidazole	-2.13	-1.8732	-2.44126	--	0.99995	0.257	0.311
45	cyclopenteno	-2.14	-1.24164	-2.20132	0.99999	0.98936	0.898	0.061
43	cis-2-buteno	-2.22	-1.00539	-1.97761	0.99954	0.98415	1.215	0.242
51	methylvynilether	-2.3	-0.72592	-2.02487	0.99895	0.9747	1.574	0.275
46	dimethylformamide	-2.4	0.48614	1.43594	0.9601	0.92231	2.886	3.836
57	ethylisocianate	-2.63	-0.99491	-1.41169	0.99999	0.99715	1.635	1.218
58	acetonitrile	-2.82	-0.9177	-1.28671	0.99836	0.99381	1.902	1.533
59	tetrafluorethylene	-3	-1.5749	-1.66225	1	0.99982	1.425	1.338
60	2butyne	-3.43	-1.04001	-2.28527	--	0.99967	2.390	1.145
						MAD	0.151	0.214
						V ratio	0.35	0.65

	B3PW91	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.19948	-1.47367	1	0.99919	0.101	0.174
49	guanine	-1.4	-1.12884	-1.68008	1	0.99965	0.271	0.280
55	transcloropropene	-1.49	-1.32401	-1.58401	1	0.9993	0.166	0.094
42	cis-bromopropeno	-1.49	-1.46929	-1.7133	1	0.99939	0.021	0.223
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	0.99999	0.99903	0.111	0.169
39	acetic-acid	-1.8	-2.10237	-2.32636	1	0.99963	0.302	0.526
40	allene	-1.88	-1.53728	-1.87824	1	0.99881	0.343	0.002
53	propiolactone	-1.9	-1.79421	-2.18241	1	0.99878	0.106	0.282
41	butirolactone	-1.93	-0.23656	-2.22595	0.99996	0.99884	1.693	0.296
52	Propene	-1.99	-1.77651	-2.20649	1	0.99851	0.213	0.216
47	diterbutylperoxide	-2	-0.00962	-1.31903	0.95243	0.90705	1.990	0.681
44	cyclobuteno	-2	-1.95518	-2.32791	1	0.99888	0.045	0.328
48	formamide	-2.05	-2.09127	-2.48968	1	0.99883	0.041	0.440
56	trasnbuteno	-2.1	-2.01123	-2.46158	0.99999	0.99822	0.089	0.362
50	imidazole	-2.13	-1.7303	-2.15714	1	0.99794	0.400	0.027
45	cyclopenteno	-2.14	-2.06158	-2.48331	0.99999	0.99853	0.078	0.343
43	cis-2-buteno	-2.22	-2.2586	-2.68112	0.99999	0.99855	0.039	0.461
51	methylvynilether	-2.3	-2.11891	-2.58471	1	0.99827	0.181	0.285
46	dimethylformamide	-2.4	-1.16569	-1.91297	0.99999	0.99345	1.234	0.487
57	ethylisocianate	-2.63	-0.80017	-1.20091	0.99999	0.99721	1.830	1.429
58	acetonitrile	-2.82	-2.23743	-3.08849	0.99999	0.9994	0.583	0.268
59	tetrafluorethylene	-3	-1.29265	-1.32635	1	0.99997	1.707	1.674
60	2butyne	-3.43	--	-3.14925	--	--	--	0.281
			1	0.99965		MAD	0.126	0.227
						V ratio	0.65	0.70

	B3LYP	Exp (eV)	Quad Fit	Linear Fit	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.17995	-1.42863	0.120	0.129
49	guanine	-1.4	-1.15807	-1.54005	0.242	0.140
55	transcloropropene	-1.49	-1.40954	-1.744	0.080	0.254
42	cis-bromopropeno	-1.49	-1.29132	-1.53769	0.199	0.048
38	1-2-cyclohexadiene	-1.75	-2.06795	-1.9841	0.318	0.234
39	acetic-acid	-1.8	-2.02578	-2.24181	0.226	0.442
40	allene	-1.88	-1.66688	-1.66688	0.213	0.213
53	propiolactone	-1.9	-1.66648	-2.1056	0.234	0.206
41	butirolactone	-1.93	-1.72578	-1.49224	0.204	0.438
52	Propene	-1.99	-1.75167	-2.1607	0.238	0.171
47	diterbutylperoxide	-2	-1.86269	-2.38007	0.137	0.380
44	cyclobuteno	-2	-2.06026	-2.42817	0.060	0.428
48	formamide	-2.05	-1.96216	-2.39975	0.088	0.350
56	trasnbuteno	-2.1	-2.10035	-2.10035	0.000	0.000
50	imidazole	-2.13	-2.05687	-2.45191	0.073	0.322
45	cyclopenteno	-2.14	-2.13976	-2.73477	0.000	0.595
43	cis-2-buteno	-2.22	-2.10429	-2.54133	0.116	0.321
51	methylvynilether	-2.3	-1.17124	-1.83649	1.129	0.464
46	dimethylformamide	-2.4	-0.72593	-1.08366	1.674	1.316
57	ethylisocianate	-2.63	0.16797	-1.82696	2.798	0.803
58	acetonitrile	-2.82	-0.88448	-0.89465	1.936	1.925
59	tetrafluorethylene	-3	-1.86857	-1.94737	1.131	1.053
60	2butyne	-3.43	-0.9825	-1.38054	2.448	2.049
				MAD	0.145	0.199
				V ratio	0.65	0.70

	B3LYP-D	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.17108	-1.43194	1	0.99921	0.129	0.132
49	guanine	-1.4	-0.27892	-0.47553	0.99999	0.9996	1.121	0.924
55	transcloropropene	-1.49	-1.28868	-1.53398	1	0.99934	0.201	0.044
42	cis-bromopropeno	-1.49	-1.45821	-1.69038	1	0.99942	0.032	0.200
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	0.99999	0.99908	0.111	0.169
39	acetic-acid	-1.8	-2.01865	-2.25238	1	0.99958	0.219	0.452
40	allene	-1.88	-1.71	-1.66635	1	0.99961	0.170	0.214
53	propiolactone	-1.9	-1.65633	-2.10864	0.99999	0.99825	0.244	0.209
41	butirolactone	-1.93	-2.0747	-2.0747	0.99999	0.99885	0.145	0.145
52	Propene	-1.99	-1.69602	-2.24511	1	0.99956	0.294	0.255
47	diterbutylperoxide	-2	-1.84958	-1.84958	0.99993	0.99707	0.150	0.150
44	cyclobuteno	-2	-1.93122	-2.28887	1	0.99891	0.069	0.289
48	formamide	-2.05	-2.06113	-2.4198	1	0.99901	0.011	0.370
56	trasnbuteno	-2.1	-1.9603	-2.3914	0.99999	0.99823	0.140	0.291
50	imidazole	-2.13	-2.17815	-2.17815	1	0.99952	0.048	0.048
45	cyclopenteno	-2.14	-2.04758	-2.43952	0.99999	0.99865	0.092	0.300
43	cis-2-buteno	-2.22	-2.1265	-2.75069	1	0.99964	0.094	0.531
51	methylvynilether	-2.3	-2.12037	-2.79683	1	0.99961	0.180	0.497
46	dimethylformamide	-2.4	-1.05386	-2.02235	1	0.99884	1.346	0.378
57	ethylisocianate	-2.63	-0.73286	-1.08141	0.99999	0.99781	1.897	1.549
58	acetonitrile	-2.82	-0.88489	-0.89303	1	1	1.935	1.927
59	tetrafluorethylene	-3	-1.86992	-1.94932	1	0.99987	1.130	1.051
60	2butyne	-3.43	-0.98375	-1.38139	0.99994	0.99628	2.446	2.049
						MAD	0.137	0.188
						V ratio	0.74	0.57

	CAM-B3LYP	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.26959	-1.52474	1	0.99928	0.030	0.225
49	guanine	-1.4	-1.1794	-1.76552	1	0.99967	0.221	0.366
55	transcloropropene	-1.49	-1.38513	-1.62503	1	0.99939	0.105	0.135
42	cis-bromopropeno	-1.49	-1.52843	-1.75444	1	0.99946	0.038	0.264
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	0.99999	0.99907	0.111	0.169
39	acetic-acid	-1.8	-2.14993	-2.33758	1	0.99974	0.350	0.538
40	allene	-1.88	-1.50416	-1.71725	1	0.99963	0.376	0.163
53	propiolactone	-1.9	-1.9065	-2.29862	1	0.99876	0.007	0.399
41	butirolactone	-1.93	-2.14574	-2.33648	0.99986	0.99961	0.216	0.406
52	Propene	-1.99	-1.9065	-2.29862	1	0.99876	0.083	0.309
47	diterbutylperoxide	-2	-0.61395	-1.85361	1	0.96193	1.386	0.146
44	cyclobuteno	-2	-1.52843	-1.75444	1	0.99946	0.472	0.246
48	formamide	-2.05	-2.29961	-2.56236	1	0.99952	0.250	0.512
56	trasnbuteno	-2.1	0.48965	0.39605	0.9991	0.9866	2.590	2.496
50	imidazole	-2.13	-1.9628	-2.32043	1	0.99865	0.167	0.190
45	cyclopenteno	-2.14	-2.16031	-2.55805	0.99999	0.99868	0.020	0.418
43	cis-2-buteno	-2.22	-2.37328	-2.76375	0.99999	0.99875	0.153	0.544
51	methylvynilether	-2.3	-2.26004	-2.68037	1	0.99862	0.040	0.380
46	dimethylformamide	-2.4	-1.50559	-2.15881	1	0.99574	0.894	0.241
57	ethylisocianate	-2.63	-0.90397	-1.29232	0.99999	0.99741	1.726	1.338
58	acetonitrile	-2.82	-2.3887	-3.1059	1	0.99609	0.431	0.286
59	tetrafluorethylene	-3	-2.10532	-2.18652	1	0.99987	0.895	0.813
60	2butyne	-3.43	-4.32352	-2.25492	0.9959	0.10414	0.894	1.175
						MAD	0.111	0.216
						V ratio	0.56	0.48

	LC-BLYP	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.27596	-1.53552	1	0.9993	0.024	0.236
49	guanine	-1.4	-1.33308	-1.7286	1	0.99967	0.067	0.329
55	transcloropropene	-1.49	-1.39906	-1.64077	1	0.99942	0.091	0.151
42	cis-bromopropeno	-1.49	-1.49764	-1.72758	1	0.99947	0.008	0.238
38	1-2-cyclohexadiene	-1.75	-1.63909	-1.91934	0.99999	0.99904	0.111	0.169
39	acetic-acid	-1.8	-2.07601	-2.2465	1	0.9998	0.276	0.447
40	allene	-1.88	-1.49592	-1.7063	1	0.99965	0.384	0.174
53	propiolactone	-1.9	-1.98935	-2.22488	1	0.9996	0.089	0.325
41	butirolactone	-1.93	-2.27044	-2.39837	0.99999	0.9999	0.340	0.468
52	Propene	-1.99	-2.00362	-2.37567	1	0.99897	0.014	0.386
47	diterbutylperoxide	-2	-1.77301	-3.3736	0.99967	0.99945	0.227	1.374
44	cyclobuteno	-2	-2.10655	-2.44846	1	0.99911	0.107	0.448
48	formamide	-2.05	-2.33276	-2.52756	1	0.99975	0.283	0.478
56	trasnbuteno	-2.1	-2.23798	-2.64075	0.99999	0.99869	0.138	0.541
50	imidazole	-2.13	-2.13046	-2.42959	1	0.99918	0.000	0.300
45	cyclopenteno	-2.14	-2.21325	-2.61611	0.99999	0.99873	0.073	0.476
43	cis-2-buteno	-2.22	-2.32504	-2.88144	1	0.99959	0.105	0.661
51	methylvynilether	-2.3	-2.33427	-2.7317	1	0.99887	0.034	0.432
46	dimethylformamide	-2.4	-1.93926	-2.41016	1	0.99827	0.461	0.010
57	ethylisocianate	-2.63	-1.09448	-1.54327	1	0.99721	1.536	1.087
58	acetonitrile	-2.82	-1.17486	-1.17677	0.99999	0.99999	1.645	1.643
59	tetrafluorethylene	-3	-2.34285	-2.43417	1	0.99984	0.657	0.566
60	2butyne	-3.43	-1.50284	-1.9594	0.99996	0.99604	1.927	1.471
						MAD	0.095	0.200
						V ratio	0.65	0.48

	BHandHLYP	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.398	-1.657	1	0.99927	0.098	0.357
49	guanine	-1.4	-1.491	-2.053	1	0.9986	0.091	0.653
55	transcloropropene	-1.49	-1.526	-1.771	1	0.99938	0.036	0.281
42	cis-bromopropeno	-1.49	-1.649	-1.877	1	0.99947	0.159	0.387
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99904	0.111	0.169
39	acetic-acid	-1.8	-2.275	-2.493	1	0.99994	0.475	0.693
40	allene	-1.88	-1.589	-1.804	1	0.99963	0.291	0.076
53	propiolactone	-1.9	-2.148	-2.390	1	0.99957	0.248	0.490
41	butirolactone	-1.93	-2.038	-2.602	1	0.99992	0.108	0.672
52	Propene	-1.99	-2.052	-2.458	1	0.99871	0.062	0.468
47	diterbutylperoxide	-2	-1.773	-3.374	0.99967	0.99945	0.227	1.374
44	cyclobuteno	-2	-2.145	-2.634	1	0.99967	0.145	0.634
48	formamide	-2.05	-2.474	-2.756	1	0.9999	0.424	0.706
56	trasnbuteno	-2.1	-2.292	-2.713	1	0.99852	0.192	0.613
50	imidazole	-2.13	-2.075	-2.468	1	0.99842	0.055	0.338
45	cyclopenteno	-2.14	-2.326	-2.731	0.99999	0.99866	0.186	0.591
43	cis-2-buteno	-2.22	-2.445	-3.004	1	0.99957	0.225	0.784
51	methylvynilether	-2.3	-2.385	-2.823	1	0.99854	0.085	0.523
46	dimethylformamide	-2.4	-1.667	-2.483	1	0.99897	0.733	0.083
57	ethylisocianate	-2.63	-1.000	-1.402	0.99999	0.99726	1.630	1.228
58	acetonitrile	-2.82	-1.097	-1.108	0.99999	0.99999	1.723	1.712
59	tetrafluorethylene	-3	-2.216	-2.298	1	0.99986	0.784	0.702
60	2butyne	-3.43	-1.280	-1.716	0.99995	0.99589	2.150	1.714
						MAD	0.135	0.242
						V ratio	0.65	0.48

	wB97	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.424	-1.687	1	0.99929	0.124	0.387
49	guanine	-1.4	-1.243	-1.789	1	0.99958	0.157	0.389
55	transcloropropene	-1.49	-1.547	-1.791	1	0.99942	0.057	0.301
42	cis-bromopropeno	-1.49	-1.640	-1.873	1	0.99946	0.150	0.383
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99909	0.111	0.169
39	acetic-acid	-1.8	-2.299	-2.470	1	0.99979	0.499	0.670
40	allene	-1.88	-1.588	-1.799	1	0.99965	0.292	0.081
53	propiolactone	-1.9	-2.194	-2.429	1	0.9996	0.294	0.529
41	butirolactone	-1.93	-2.311	-2.538	1	0.99969	0.381	0.608
52	Propene	-1.99	-2.148	-2.517	1	0.99901	0.158	0.527
47	diterbutylperoxide	-2	-0.893	-3.441	0.99999	0.99924	1.107	1.441
44	cyclobuteno	-2	-2.243	-2.584	1	0.99912	0.243	0.584
48	formamide	-2.05	-2.545	-2.750	1	0.99973	0.495	0.700
56	trasnbuteno	-2.1	-1.385	-1.625	1	0.99939	0.715	0.475
50	imidazole	-2.13	-2.296	-2.591	1	0.9992	0.166	0.461
45	cyclopenteno	-2.14	-2.330	-2.730	0.99999	0.99876	0.190	0.590
43	cis-2-buteno	-2.22	-1.158	-2.642	0.99841	0.9782	1.062	0.422
51	methylvynilether	-2.3	-2.501	-2.901	1	0.99887	0.201	0.601
46	dimethylformamide	-2.4	-2.130	-2.599	1	0.99829	0.270	0.199
57	ethylisocianate	-2.63	-1.270	-1.783	1	0.99637	1.360	0.847
58	acetonitrile	-2.82	-2.299	-2.470	1	0.99979	0.521	0.350
59	tetrafluorethylene	-3	-2.535	-2.661	1	0.99969	0.465	0.339
60	2butyne	-3.43	-1.676	-2.192	0.99998	0.995	1.754	1.238
						MAD	0.194	0.187
						V ratio	0.43	0.17

	wB97X	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.381	-1.645	1	0.99927	0.081	0.345
49	guanine	-1.4	-1.323	-1.912	1	0.99968	0.077	0.512
55	transcloropropene	-1.49	-1.504	-1.751	1	0.9994	0.014	0.261
42	cis-bromopropeno	-1.49	-1.603	-1.838	1	0.99945	0.113	0.348
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99908	0.111	0.169
39	acetic-acid	-1.8	-2.268	-2.443	1	0.99979	0.468	0.643
40	allene	-1.88	-1.557	-1.773	1	0.99963	0.323	0.107
53	propiolactone	-1.9	-2.155	-2.393	1	0.99958	0.255	0.493
41	butirolactone	-1.93	-2.049	-2.437	1	0.99886	0.119	0.507
52	Propene	-1.99	-2.087	-2.464	1	0.99894	0.097	0.474
47	diterbutylperoxide	-2	-0.810	-3.353	0.99999	0.99922	1.190	1.353
44	cyclobuteno	-2	-2.194	-2.541	1	0.99908	0.194	0.541
48	formamide	-2.05	-2.490	-2.710	1	0.99968	0.440	0.660
56	trasnbuteno	-2.1	-2.311	-2.714	0.99999	0.99869	0.211	0.614
50	imidazole	-2.13	-2.228	-2.537	1	0.99911	0.098	0.407
45	cyclopenteno	-2.14	-2.286	-2.690	0.99999	0.99872	0.146	0.550
43	cis-2-buteno	-2.22	-0.787	-2.542	0.99732	0.9674	1.433	0.322
51	methylvynilether	-2.3	-2.437	-2.846	1	0.99879	0.137	0.546
46	dimethylformamide	-2.4	-2.011	-2.516	1	0.99793	0.389	0.116
57	ethylisocianate	-2.63	-1.218	-1.690	0.99999	0.99686	1.412	0.940
58	acetonitrile	-2.82	-1.311	-1.255	1	0.99986	1.509	1.565
59	tetrafluorethylene	-3	-2.509	-2.624	1	0.99974	0.491	0.376
60	2butyne	-3.43	-1.622	-2.144	0.99997	0.99507	1.808	1.286
						MAD	0.127	0.163
						V ratio	0.61	0.17

	wB97XD	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.350	-1.621	1	0.99923	0.050	0.321
49	guanine	-1.4	-1.323	-1.912	0.99999	0.99867	0.077	0.512
55	transcloropropene	-1.49	-1.378	-1.771	1	0.99936	0.112	0.281
42	cis-bromopropeno	-1.49	-1.586	-1.826	1	0.99942	0.096	0.336
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99906	0.111	0.169
39	acetic-acid	-1.8	-2.255	-2.439	1	0.99976	0.455	0.639
40	allene	-1.88	-1.549	-1.769	1	0.99962	0.331	0.111
53	propiolactone	-1.9	-2.114	-2.370	1	0.99952	0.214	0.470
41	butirolactone	-1.93	-2.012	-2.508	1	0.99969	0.082	0.578
52	Propene	-1.99	0.436	0.399	0.99815	0.99623	2.426	2.389
47	diterbutylperoxide	-2	2.899	-3.368	0.99615	0.99213	4.899	1.368
44	cyclobuteno	-2	-2.142	-2.499	1	0.99901	0.142	0.499
48	formamide	-2.05	-2.402	-2.669	1	0.99952	0.352	0.619
56	trasnbuteno	-2.1	-2.246	-2.664	0.99999	0.99856	0.146	0.564
50	imidazole	-2.13	-2.104	-2.444	1	0.99887	0.026	0.314
45	cyclopenteno	-2.14	-2.244	-2.656	0.99999	0.99865	0.104	0.516
43	cis-2-buteno	-2.22	-2.359	-2.925	1	0.99957	0.139	0.705
51	methylvynilether	-2.3	-2.362	-2.788	1	0.99865	0.062	0.488
46	dimethylformamide	-2.4	-1.776	-2.530	1	0.99948	0.624	0.130
57	ethylisocianate	-2.63	-1.124	-1.555	0.99999	0.99721	1.506	1.075
58	acetonitrile	-2.82	-1.213	-1.158	1	0.99988	1.607	1.662
59	tetrafluorethylene	-3	-2.387	-2.493	1	0.99978	0.613	0.507
60	2butyne	-3.43	-1.505	-2.034	0.99997	0.99493	1.925	1.396
						MAD	0.105	0.173
						V ratio	0.61	0.17

	PBE0	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.230	-1.504	1	0.99918	0.070	0.204
49	guanine	-1.4	-1.223	-1.772	1	0.99955	0.177	0.372
55	transcloropropene	-1.49	-1.360	-1.620	1	0.99931	0.130	0.130
42	cis-bromopropeno	-1.49	-1.502	-1.746	1	0.99939	0.012	0.256
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99902	0.111	0.169
39	acetic-acid	-1.8	-2.159	-2.389	1	0.99961	0.359	0.589
40	allene	-1.88	-1.598	-1.935	1	0.99884	0.282	0.055
53	propiolactone	-1.9	-1.859	-2.246	1	0.99878	0.041	0.346
41	butirolactone	-1.93	0.437	-1.925	0.99992	0.98919	2.367	0.005
52	Propene	-1.99	-1.819	-2.247	1	0.99853	0.171	0.257
47	diterbutylperoxide	-2	1.835	-1.698	0.99858	0.98928	3.835	0.302
44	cyclobuteno	-2	-2.006	-2.374	1	0.99891	0.006	0.374
48	formamide	-2.05	-2.185	-2.562	1	0.99896	0.135	0.512
56	trasnbuteno	-2.1	-2.048	-2.496	0.99999	0.99824	0.052	0.396
50	imidazole	-2.13	-1.779	-2.212	1	0.99787	0.351	0.082
45	cyclopenteno	-2.14	-2.093	-2.517	0.99999	0.99852	0.047	0.377
43	cis-2-buteno	-2.22	-2.303	-2.723	0.99999	0.99856	0.083	0.503
51	methylvynilether	-2.3	-2.176	-2.638	1	0.99831	0.124	0.338
46	dimethylformamide	-2.4	-1.123	-2.100	1	0.99819	1.277	0.300
57	ethylisocianate	-2.63	-0.809	-1.196	0.99999	0.99732	1.821	1.434
58	acetonitrile	-2.82	-0.938	-0.941	0.99999	0.99999	1.882	1.879
59	tetrafluorethylene	-3	-3.084	-3.054	--	1	0.084	0.054
60	2butyne	-3.43	-1.144	-2.869	0.99997	0.99589	2.286	0.561
					MAD		0.089	0.132
					V ratio		0.61	0.26

	LC-wPBE	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.264	-1.538	1	0.99925	0.037	0.238
49	guanine	-1.4	-1.300	-1.708	1	0.99862	0.100	0.308
55	transcloropropene	-1.49	-1.395	-1.651	1	0.99938	0.095	0.161
42	cis-bromopropeno	-1.49	-1.468	-1.712	1	0.99943	0.022	0.222
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99906	0.111	0.169
39	acetic-acid	-1.8	-2.182	-2.410	1	0.99994	0.382	0.610
40	allene	-1.88	-1.432	-1.648	1	0.99965	0.448	0.232
53	propiolactone	-1.9	-2.026	-2.268	1	0.99959	0.126	0.368
41	butirolactone	-1.93	-2.021	-2.362	1	0.99921	0.091	0.432
52	Propene	-1.99	-1.977	-2.362	1	0.99895	0.013	0.372
47	diterbutylperoxide	-2	-1.421	-3.189	0.99997	0.99652	0.579	1.189
44	cyclobuteno	-2	-2.075	-2.429	1	0.99908	0.075	0.429
48	formamide	-2.05	-2.377	-2.586	1	0.99972	0.327	0.536
56	trasnbuteno	-2.1	-2.216	-2.630	0.99999	0.99869	0.116	0.530
50	imidazole	-2.13	-2.142	-2.447	1	0.99917	0.012	0.317
45	cyclopenteno	-2.14	-2.174	-2.594	0.99999	0.99868	0.034	0.454
43	cis-2-buteno	-2.22	-2.365	-2.770	0.99999	0.9988	0.145	0.550
51	methylvynilether	-2.3	-2.321	-2.737	1	0.9988	0.021	0.437
46	dimethylformamide	-2.4	-1.934	-2.439	1	0.99806	0.466	0.039
57	ethylisocianate	-2.63	-1.107	-1.586	0.99999	0.99682	1.523	1.044
58	acetonitrile	-2.82	-3.033	-3.313	1	0.99951	0.213	0.493
59	tetrafluorethylene	-3	-2.366	-2.482	1	0.99974	0.634	0.518
60	2butyne	-3.43	-2.946	-3.751	0.99997	0.99474	0.484	0.321
						MAD	0.102	0.211
						V ratio	0.65	0.39

	TPSS	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.245	-1.512	1	0.9992	0.055	0.212
49	guanine	-1.4	-1.136	-1.717	1	0.9995	0.264	0.317
55	transcloropropene	-1.49	-1.373	-1.627	1	0.99932	0.117	0.137
42	cis-bromopropeno	-1.49	-0.388	-1.398	0.98659	0.9736	1.102	0.092
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99981	0.99481	0.111	0.169
39	acetic-acid	-1.8	-0.836	-1.570	0.9994	0.99212	0.964	0.230
40	allene	-1.88	-1.560	-1.907	1	0.99872	0.320	0.027
53	propiolactone	-1.9	-1.233	-2.117	0.99975	0.99264	0.667	0.217
41	butirolactone	-1.93	0.312	-1.903	1	0.99823	2.242	0.027
52	Propene	-1.99	-1.233	-2.117	0.99975	0.99264	0.757	0.127
47	diterbutylperoxide	-2	0.779	-2.020	1	0.99753	2.779	0.020
44	cyclobuteno	-2	-1.256	-2.212	0.99956	0.9911	0.744	0.212
48	formamide	-2.05	-0.720	-1.321	1	0.99938	1.330	0.729
56	trasnbuteno	-2.1	-1.773	-1.947	0.99819	0.99841	0.327	0.153
50	imidazole	-2.13	-1.624	-2.400	--	0.99999	0.506	0.270
45	cyclopenteno	-2.14	-1.805	-2.712	1	0.99991	0.335	0.572
43	cis-2-buteno	-2.22	-1.162	-1.444	1	0.99997	1.058	0.776
51	methylvynilether	-2.3	-1.918	-2.893	--	0.99999	0.382	0.593
46	dimethylformamide	-2.4	-0.897	-2.201	1	0.99977	1.503	0.199
57	ethylisocianate	-2.63	-0.795	-1.209	0.99999	0.99718	1.835	1.421
58	acetonitrile	-2.82	-1.006	-0.990	0.99999	0.99998	1.814	1.830
59	tetrafluorethylene	-3	-1.286	-1.338	1	0.99994	1.714	1.662
60	2butyne	-3.43	0.130	-1.865	1	0.99907	3.560	1.565
						MAD	0.137	0.161
						V ratio	0.17	0.65

	TPSSh	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.284	-1.550	1	0.9992	0.016	0.250
49	guanine	-1.4	-1.186	-1.733	1	0.9995	0.214	0.333
55	transcloropropene	-1.49	-1.415	-1.667	1	0.99932	0.075	0.177
42	cis-bromopropeno	-1.49	-1.544	-1.783	0.98659	0.9736	0.054	0.293
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99981	0.99481	0.111	0.169
39	acetic-acid	-1.8	-2.122	-2.400	0.9994	0.99212	0.322	0.600
40	allene	-1.88	-1.506	-1.728	1	0.99872	0.374	0.152
53	propiolactone	-1.9	-1.845	-2.292	0.99975	0.99264	0.055	0.392
41	butirolactone	-1.93	-0.240	-2.220	1	0.99823	1.691	0.290
52	Propene	-1.99	-1.861	-2.287	0.99975	0.99264	0.129	0.297
47	diterbutylperoxide	-2	0.710	-2.295	1	0.99753	2.710	0.295
44	cyclobuteno	-2	-2.046	-2.411	0.99956	0.9911	0.046	0.411
48	formamide	-2.05	-2.214	-2.653	1	0.99938	0.164	0.603
56	trasnbuteno	-2.1	-2.099	-2.535	0.99819	0.99841	0.001	0.435
50	imidazole	-2.13	-1.763	-2.355	--	0.99999	0.367	0.225
45	cyclopenteno	-2.14	-2.047	-2.637	1	0.99991	0.093	0.497
43	cis-2-buteno	-2.22	-2.205	-2.875	1	0.99997	0.015	0.655
51	methylvynilether	-2.3	-2.138	-2.768	--	0.99999	0.162	0.468
46	dimethylformamide	-2.4	-1.107	-2.111	1	0.99977	1.293	0.289
57	ethylisocianate	-2.63	-0.807	-1.369	0.99999	0.99718	1.823	1.261
58	acetonitrile	-2.82	-1.041	-1.017	0.99999	0.99998	1.779	1.803
59	tetrafluorethylene	-3	-1.347	-1.392	1	0.99994	1.653	1.608
60	2butyne	-3.43	-0.206	-1.627	1	0.99907	3.224	1.803
						MAD	0.084	0.252
						V ratio	0.61	0.48

	M06-L	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.489	-1.750	1	0.9993	0.189	0.450
49	guanine	-1.4	-1.293	-1.649	1	0.99961	0.107	0.249
55	transcloropropene	-1.49	-1.602	-1.861	1	0.99935	0.112	0.371
42	cis-bromopropeno	-1.49	-1.678	-1.905	1	0.99949	0.188	0.415
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	1	0.99928	0.111	0.169
39	acetic-acid	-1.8	-2.535	-2.660	0.99999	0.99997	0.735	0.860
40	allene	-1.88	-1.545	-1.749	1	0.99968	0.335	0.131
53	propiolactone	-1.9	-2.168	-2.530	1	0.9999	0.268	0.630
41	butirolactone	-1.93	0.027	-2.347	0.99981	0.99507	1.957	0.417
52	Propene	-1.99	-2.058	-2.456	1	0.99877	0.068	0.466
47	diterbutylperoxide	-2	7.605	-2.766	0.99983	0.98856	9.605	0.766
44	cyclobuteno	-2	-2.128	-2.536	1	0.99868	0.128	0.536
48	formamide	-2.05	-2.264	-2.810	1	0.99961	0.214	0.760
56	trasnbuteno	-2.1	-2.313	-2.857	1	0.99958	0.213	0.757
50	imidazole	-2.13	-1.938	-2.536	1	0.99935	0.192	0.406
45	cyclopenteno	-2.14	-2.204	-2.778	1	0.99954	0.064	0.638
43	cis-2-buteno	-2.22	-2.325	-2.971	1	0.9996	0.105	0.751
51	methylvynilether	-2.3	-2.232	-3.006	1	0.99985	0.068	0.706
46	dimethylformamide	-2.4	-1.743	-2.629	1	0.99977	0.657	0.229
57	ethylisocianate	-2.63	-1.301	-1.639	0.99988	0.99784	1.329	0.991
58	acetonitrile	-2.82	-1.436	-1.374	1	0.99985	1.384	1.446
59	tetrafluorethylene	-3	-2.051	-2.226	1	0.99936	0.949	0.774
60	2butyne	-3.43	-1.934	-2.563	0.99999	0.99923	1.496	0.867
						MAD	0.145	0.195
						V ratio	0.61	0.48

	M06	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.228	-1.489	1	0.99927	0.072	0.189
49	guanine	-1.4	-1.594	-1.677	0.99972	0.99967	0.194	0.277
55	transcloropropene	-1.49	-1.348	-1.601	1	0.99934	0.142	0.111
42	cis-bromopropeno	-1.49	-1.508	-1.666	--	0.99986	0.018	0.176
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99916	0.111	0.169
39	acetic-acid	-1.8	-1.077	-2.157	0.99888	0.98865	0.723	0.357
40	allene	-1.88	-1.585	-1.889	1	0.99905	0.295	0.009
53	propiolactone	-1.9	-1.884	-2.256	1	0.9998	0.016	0.356
41	butirolactone	-1.93	-0.962	-2.155	0.99997	0.9977	0.968	0.225
52	Propene	-1.99	-1.897	-2.270	1	0.99888	0.093	0.280
47	diterbutylperoxide	-2	--	-2.965	--	--		0.965
44	cyclobuteno	-2	-1.930	-2.419	1	0.99966	0.070	0.419
48	formamide	-2.05	-2.302	-2.649	1	0.99984	0.252	0.599
56	trasnbuteno	-2.1	-2.162	-2.492	0.99998	0.99904	0.062	0.392
50	imidazole	-2.13	-1.891	-2.317	1	0.99967	0.239	0.187
45	cyclopenteno	-2.14	-1.957	-2.529	1	0.99952	0.183	0.389
43	cis-2-buteno	-2.22	-2.145	-2.769	1	0.99972	0.075	0.549
51	methylvynilether	-2.3	-1.784	-2.676	0.99998	0.9994	0.516	0.376
46	dimethylformamide	-2.4	-1.514	-2.321	1	0.99945	0.886	0.079
57	ethylisocianate	-2.63	-1.006	-1.347	0.99984	0.99752	1.624	1.283
58	acetonitrile	-2.82	-1.183	-1.158	1	0.99998	1.637	1.662
59	tetrafluorethylene	-3	-1.564	-1.647	1	0.99984	1.436	1.353
60	2butyne	-3.43	-1.204	-1.990	0.99526	0.9858	2.226	1.440
						MAD	0.130	0.170
						V ratio	0.56	0.43

	M06-L	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.214	-1.508	0.99999	0.99911	0.086	0.208
49	guanine	-1.4	-1.227	-1.678	0.99999	0.99838	0.173	0.278
55	transcloropropene	-1.49	-1.367	-1.646	1	0.99925	0.123	0.156
42	cis-bromopropeno	-1.49	-1.481	-1.744	1	0.99932	0.009	0.254
38	1-2-cyclohexadiene	-1.75	-1.639	-1.919	0.99999	0.99886	0.111	0.169
39	acetic-acid	-1.8	-2.224	-2.416	1	0.99975	0.424	0.616
40	allene	-1.88	-1.673	-1.908	1	0.99957	0.207	0.028
53	propiolactone	-1.9	-1.946	-2.209	1	0.99953	0.046	0.309
41	butirolactone	-1.93	-1.883	-2.277	1	0.99896	0.047	0.347
52	Propene	-1.99	-2.284	-2.719	1	0.99866	0.294	0.729
47	diterbutylperoxide	-2	-1.335	-3.480	0.99998	0.9972	0.665	1.480
44	cyclobuteno	-2	-2.086	-2.464	1	0.99894	0.086	0.464
48	formamide	-2.05	-2.314	-2.522	1	0.99972	0.264	0.472
56	trasnbuteno	-2.1	-2.113	-2.575	0.99999	0.99851	0.013	0.475
50	imidazole	-2.13	-2.041	-2.435	1	0.99858	0.089	0.305
45	cyclopenteno	-2.14	-2.139	-2.599	0.99999	0.99841	0.001	0.459
43	cis-2-buteno	-2.22	-2.355	-2.801	0.99999	0.99852	0.135	0.581
51	methylvynilether	-2.3	-2.284	-2.719	1	0.99866	0.016	0.419
46	dimethylformamide	-2.4	-1.367	-2.203	0.98994	0.98524	1.033	0.197
57	ethylisocianate	-2.63	-0.472	-1.105	0.99996	0.9946	2.158	1.525
58	acetonitrile	-2.82	-3.090	-3.429	1	0.99928	0.270	0.609
59	tetrafluorethylene	-3	-1.840	-1.944	1	0.99979	1.160	1.056
60	2butyne	-3.43	--	-3.898	--	--	#¡VALOR!	0.468
						MAD	0.116	0.212
						V ratio	0.74	0.39

	M06-2X	Exp (eV)	Quad Fit	Linear Fit	Corr.Coef. QF	Corr.Coef. LF	MAD - QF	MAD - LF
54	transbromopropene	-1.3	-1.316	-1.593	1	0.99919	0.016	0.293
49	guanine	-1.4	-1.358	-1.754	0.99999	0.99868	0.042	0.354
55	transcloropropene	-1.49	-1.443	-1.708	1	0.99929	0.047	0.218
42	cis-bromopropeno	-1.49	-1.586	-1.827	1	0.99941	0.096	0.337
38	1-2-cyclohexadiene	-1.75	-1.950	-2.264	0.99999	0.999	0.200	0.514
39	acetic-acid	-1.8	-2.368	-2.546	1	0.99978	0.568	0.746
40	allene	-1.88	-1.616	-1.834	1	0.99963	0.264	0.046
53	propiolactone	-1.9	-2.130	-2.374	1	0.99956	0.230	0.474
41	butirolactone	-1.93	-2.046	-2.533	1	0.99969	0.116	0.603
52	Propene	-1.99	-1.976	-2.394	1	0.99865	0.014	0.404
47	diterbutylperoxide	-2	0.689	-2.277	0.94353	0.85256	2.689	0.277
44	cyclobuteno	-2	-2.143	-2.509	1	0.99895	0.143	0.509
48	formamide	-2.05	-2.362	-2.662	1	0.99938	0.312	0.612
56	trasnbuteno	-2.1	-2.214	-2.649	0.99999	0.99843	0.114	0.549
50	imidazole	-2.13	-1.917	-2.391	1	0.99768	0.213	0.261
45	cyclopenteno	-2.14	-2.209	-2.632	0.99999	0.99857	0.069	0.492
43	cis-2-buteno	-2.22	-2.460	-2.863	0.99999	0.99872	0.240	0.643
51	methylvynilether	-2.3	-2.270	-2.746	1	0.99827	0.030	0.446
46	dimethylformamide	-2.4	-1.339	-2.391	1	0.99825	1.061	0.009
57	ethylisocianate	-2.63	-0.680	-1.291	0.99989	0.99347	1.950	1.339
58	acetonitrile	-2.82	-1.015	-0.988	1	0.99997	1.805	1.832
59	tetrafluorethylene	-3	-2.162	-2.280	1	0.99972	0.838	0.720
60	2butyne	-3.43	-2.445	-3.931	1	0.99977	0.985	0.501
						MAD	0.122	0.194
						V ratio	0.65	0.26

Table S9. Results of the calculations of the E^0_{Red} and E^0_{expRed} potentials of co
chart S-3ab with different DFT functionals.

Functional	MAD (V)[a]	Range (V)[b]	Slope[c]	(Eq. 9) y-intercept[c]	R^2
BLYP	0.13	0.59	1.010	-4.21	0.956
BPW91	0.15	0.55	1.019	-4.39	0.967
PW91	0.15	0.56	1.017	-4.44	0.966
B97D	0.14	0.57	1.027	-4.34	0.964
B3PW91	0.14	0.57	0.980	-4.29	0.954
B3LYP	0.13	0.69	0.963	-4.20	0.942
B3LYP-D	0.13	0.69	0.967	-4.21	0.942
CAM-B3LYP	0.15	0.80	0.935	-4.09	0.924
LC-BLYP	0.17	0.97	0.902	-4.00	0.897
BHandHLYP	0.18	1.01	0.900	-3.82	0.884
ω-B97	0.14	0.76	0.961	-4.12	0.928
ω-B97X	0.14	0.74	0.951	-4.11	0.929
ω-B97XD	0.13	0.69	0.955	-4.13	0.941
PBE0	0.14	0.54	0.978	-4.24	0.952
LC-ωPBE	0.17	0.77	0.958	-4.22	0.919
TPSS	0.14	0.62	1.008	-4.29	0.959
TPSSh	0.14	0.58	0.985	-4.21	0.950
M06	0.13	0.63	0.996	-4.32	0.956
M06-2X	0.12	0.74	0.940	-4.16	0.949
M06-L	0.14	0.62	1.012	-4.26	0.968
M06-HF	0.17	0.78	0.873	-4.08	0.914

[a]MAD of the calculated (by using eq. 12) *vs.* experimental E^0_{expRed}. [b] Differenc
biggest and smallest deviation of the calculated E^0_{expRed} to measure the dispers
calculated values. [c] Results of the plot of calculated absolute E^0_{Red} *vs*. experim
(Eq. 9).[d] Results of the plot of calculated relative E^0_{Red} *vs*. experimental E^0_{Red}
the extrapolations are included in the supporting information, figures S-4.1 to S

Tables S10.1-21. Detailed values of the energies employed for computing the E^0_{Red} in table 3 for each DFT method employed.

FUNCTIONAL BLYP

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	ΔG (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.967388	0.055960	-156.027483	0.047835	42.808592	1.856	-2.420	-2.56	0.140
2	-233.371051	0.090108	-233.424226	0.083949	37.232790	1.615	-2.662	-2.71	0.048
3	-191.933275	0.033483	-192.027410	0.029241	61.732382	2.677	-1.599	-1.19	0.409
4	-345.573449	0.075575	-345.665136	0.072073	59.732426	2.590	-1.686	-1.38	0.306
5	-384.880819	0.100636	-384.966360	0.096816	56.074539	2.432	-1.845	-1.55	0.295
6	-534.405693	0.096278	-534.509832	0.093050	67.374001	2.922	-1.355	-1.29	0.065
7	-306.496005	0.061034	-306.577305	0.056133	54.091920	2.346	-1.931	-1.86	0.071
8	-362.985662	0.097277	-363.090215	0.095469	66.742044	2.894	-1.382	-1.55	0.163
9	-362.983402	0.098482	-363.090560	0.094524	69.726304	3.024	-1.253	-1.43	0.177
10	-284.385225	0.046650	-284.493081	0.043920	69.393279	3.009	-1.267	-1.40	0.133
11	-245.082567	0.021354	-245.192238	0.018529	70.592060	3.061	-1.215	-1.39	0.170
12	-436.803108	0.067341	-436.924343	0.063435	78.527312	3.405	-0.871	-0.95	0.079
13	-476.107824	0.092048	-476.226331	0.088198	76.780431	3.330	-0.947	-0.97	0.023
14	-280.355523	0.034612	-280.454712	0.030796	64.636359	2.803	-1.474	-1.39	0.084
15	-319.664518	0.058277	-319.760484	0.054585	62.536140	2.712	-1.565	-1.46	0.105
16	-508.268684	0.068523	-508.374300	0.063637	69.341121	3.007	-1.270	-1.18	0.090
17	-586.886736	0.117495	-586.984530	0.111989	64.821327	2.811	-1.466	-1.42	0.046
18	-296.374953	0.022664	-296.503810	0.020390	82.285769	3.568	-0.708	-0.63	0.078
19	-374.994731	0.068906	-375.116315	0.065011	78.739337	3.415	-0.862	-0.79	0.072
21	-270.875271	0.081595	-270.983684	0.078715	69.837276	3.029	-1.248	-1.21	0.038
22	-349.461126	0.130694	-349.543857	0.131336	51.511490	2.234	-2.043	-1.49	0.553
23	-501.908868	0.154002	-502.021381	0.154040	70.579158	3.061	-1.216	-0.90	0.316
24	-173.787997	0.075501	-173.869466	0.074986	51.445678	2.231	-2.046	-1.76	0.286
25	-310.178550	0.106257	-310.278965	0.104647	64.021145	2.776	-1.500	-1.36	0.140
26	-541.203806	0.178705	-541.308523	0.177758	66.305140	2.875	-1.401	-1.10	0.301
28	-500.723975	0.135091	-500.851965	0.134586	80.632100	3.497	-0.780	-0.52	0.260
29	-365.517487	0.121530	-365.604250	0.119825	55.514447	2.407	-1.869	-1.79	0.079
30	-385.412819	0.109780	-385.511948	0.105131	65.121655	2.824	-1.453	-1.51	0.057
31	-310.178468	0.106349	-310.282463	0.100787	68.747840	2.981	-1.295	-1.38	0.085
32	-310.178041	0.105523	-310.285223	0.103481	68.538979	2.972	-1.304	-1.26	0.044
33	-370.153669	0.071901	-370.259888	0.068749	68.631298	2.976	-1.300	-1.26	0.040
34	-730.495388	0.069811	-730.605826	0.066118	71.618217	3.106	-1.171	-1.16	0.011
35	-423.544476	0.112673	-423.674516	0.111646	82.245745	3.567	-0.710	-0.47	0.240
36	-363.150792	0.077660	-363.278153	0.076334	80.751945	3.502	-0.775	-0.53	0.245
37	-363.147253	0.077279	-363.263596	0.075484	74.132486	3.215	-1.062	-0.87	0.192
38	-608.024715	0.078437	-608.138641	0.078410	71.506246	3.101	-1.176	-0.96	0.216
40	-540.635439	0.169704	-540.712171	0.165069	51.058724	2.214	-2.062	-1.96	0.102
41	-424.184695	0.124093	-424.266914	0.121534	53.198998	2.307	-1.970	-1.96	0.010
42	-460.136621	0.104142	-460.213102	0.099012	51.211430	2.221	-2.056	-2.13	0.074
43	-499.440740	0.128936	-499.516599	0.124720	50.247541	2.179	-2.098	-2.16	0.062
44	-385.840817	0.111495	-385.902820	0.105273	42.811492	1.857	-2.420	-2.42	0.000
45	-539.467639	0.153182	-539.530237	0.146979	43.173292	1.872	-2.404	-2.38	0.024
46	-615.695462	0.165345	-615.770936	0.159290	51.160225	2.219	-2.058	-1.98	0.078
47	-264.333082	0.047346	-264.401311	0.041188	46.678745	2.024	-2.252	-2.10	0.152
48	-555.528982	0.142253	-555.601092	0.135540	49.462331	2.145	-2.132	-1.97	0.164
49	-401.899758	0.100286	-401.973105	0.094780	49.481081	2.146	-2.131	-1.98	0.151
50	-248.273793	0.058689	-248.327366	0.051596	38.068790	1.651	-2.626	-2.40	0.230
52	-2255.194718	0.015122	-2255.312776	0.011586	76.301317	3.309	-0.968	-0.71	0.258
53	-601.280911	0.054230	-601.408829	0.049892	82.992104	3.599	-0.678	-0.50	0.178
54	-723.999413	0.143648	-724.117469	0.141697	75.305599	3.266	-1.011	-0.65	0.361
57	-499.414186	0.125105	-499.549916	0.124714	85.416993	3.704	-0.572	-0.51	0.062
58	-460.113264	0.101757	-460.252503	0.100484	88.172688	3.824	-0.453	-0.39	0.063
59	-420.807077	0.076237	-420.949882	0.074929	90.432739	3.922	-0.355	-0.34	0.015
60	-381.500594	0.051477	-381.646831	0.051302	91.874905	3.984	-0.292	-0.23	0.062
61	-841.117016	0.039877	-841.267511	0.038279	95.439285	4.139	-0.138	-0.10	0.038
62	-1300.731708	0.027613	-1300.886356	0.026953	97.457268	4.226	-0.050	0.06	0.110

FUNCTIONAL BPW91

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	ΔG (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.018685	0.056310	-156.085399	0.049291	46.267869	2.006	-2.472	-2.56	0.088
2	-233.455140	0.090729	-233.514989	0.084758	41.302953	1.791	-2.688	-2.71	0.022
3	-191.967413	0.033750	-192.067249	0.029577	65.266390	2.830	-1.649	-1.19	0.459
4	-345.651371	0.076118	-345.749360	0.072627	63.679347	2.761	-1.717	-1.38	0.337
5	-384.977299	0.101279	-385.069058	0.097613	59.880086	2.597	-1.882	-1.55	0.332
6	-534.482634	0.097148	-534.591911	0.094043	70.520454	3.058	-1.421	-1.29	0.131
7	-306.548500	0.061529	-306.635255	0.057039	57.256978	2.483	-1.996	-1.86	0.136
9	-363.063724	0.099304	-363.170907	0.095287	69.779345	3.026	-1.453	-1.43	0.023
10	-284.430357	0.047418	-284.537783	0.044580	69.191758	3.001	-1.478	-1.40	0.078
11	-245.109869	0.021843	-245.219079	0.019034	70.293007	3.048	-1.431	-1.39	0.046
12	-436.879014	0.068055	-437.003005	0.064327	80.145212	3.476	-1.003	-0.95	0.053
13	-476.201994	0.092897	-476.323257	0.089250	78.382208	3.399	-1.080	-0.97	0.110
14	-280.404283	0.035103	-280.508263	0.031356	67.599518	2.931	-1.547	-1.39	0.157
15	-319.731561	0.058871	-319.832422	0.055279	65.545503	2.842	-1.636	-1.46	0.176
16	-508.341969	0.069224	-508.453295	0.064698	72.698147	3.153	-1.326	-1.18	0.146
17	-586.996773	0.118545	-587.100191	0.113328	68.169235	2.956	-1.523	-1.42	0.103
18	-296.416475	0.023058	-296.549451	0.020949	84.767247	3.676	-0.803	-0.63	0.173
19	-375.072845	0.068594	-375.198698	0.067470	79.678977	3.455	-1.024	-0.79	0.234
21	-270.959630	0.082137	-271.074002	0.078502	74.050648	3.211	-1.268	-1.21	0.058
23	-502.060274	0.155035	-502.180004	0.154985	75.163004	3.259	-1.219	-0.90	0.319
24	-173.850640	0.076271	-173.935408	0.075633	53.593399	2.324	-2.155	-1.76	0.395
25	-310.281488	0.106866	-310.387841	0.105438	67.633549	2.933	-1.546	-1.36	0.186
26	-541.374801	0.179747	-541.486574	0.178904	70.667573	3.065	-1.414	-1.10	0.314
28	-500.872767	0.136035	-501.008559	0.135701	85.420151	3.704	-0.775	-0.52	0.255
29	-365.630682	0.122227	-365.721722	0.120429	58.257148	2.526	-1.953	-1.79	0.163
30	-385.514680	0.110400	-385.618979	0.106124	68.131772	2.955	-1.524	-1.51	0.014
31	-310.281168	0.107026	-310.391263	0.102123	72.162614	3.129	-1.350	-1.38	0.030
32	-310.280753	0.106155	-310.393931	0.104352	72.151620	3.129	-1.350	-1.26	0.090
33	-370.229778	0.072528	-370.341334	0.069443	71.938397	3.120	-1.359	-1.26	0.099
34	-730.592369	0.070446	-730.708522	0.067317	74.850716	3.246	-1.233	-1.16	0.073
35	-423.652865	0.113390	-423.788806	0.112410	85.919413	3.726	-0.753	-0.47	0.283
36	-363.237764	0.078249	-363.371422	0.076956	84.682663	3.672	-0.807	-0.53	0.277
37	-363.234385	0.077873	-363.356756	0.076150	77.869755	3.377	-1.102	-0.87	0.232
38	-608.102223	0.079242	-608.221931	0.079337	75.058206	3.255	-1.224	-0.96	0.264
40	-540.798192	0.170466	-540.882776	0.166699	55.440616	2.404	-2.075	-1.96	0.115
41	-424.299539	0.124480	-424.387979	0.120675	57.884454	2.510	-1.969	-1.96	0.009
42	-460.233085	0.104805	-460.315553	0.100104	54.699161	2.372	-2.107	-2.13	0.023
43	-499.554917	0.129963	-499.636784	0.125805	53.981758	2.341	-2.138	-2.16	0.022
44	-385.956462	0.112215	-386.026072	0.106164	47.477813	2.059	-2.420		
45	-539.626970	0.154088	-539.697463	0.148183	47.940109	2.079	-2.400	-2.38	0.020
46	-615.874613	0.166451	-615.958343	0.160504	56.273269	2.440	-2.039	-1.98	0.059
47	-264.389551	0.047789	-264.463423	0.041752	50.143558	2.174	-2.304	-2.10	0.204
48	-555.680286	0.143217	-555.759886	0.136583	54.112482	2.347	-2.132	-1.97	0.164
49	-402.007165	0.101005	-402.087902	0.095632	54.034547	2.343	-2.136	-1.98	0.156
50	-248.337959	0.059169	-248.397523	0.052172	41.767683	1.811	-2.668	-2.40	0.272
52	-2255.325493	0.016023	-2255.450166	0.013013	80.122068	3.475	-1.004	-0.71	0.294
53	-601.363543	0.054615	-601.499161	0.050501	87.682640	3.802	-0.677	-0.50	0.177
54	-724.164132	0.145869	-724.290653	0.142902	81.255106	3.524	-0.955	-0.65	0.305
57	-499.528995	0.125472	-499.671574	0.125425	89.499282	3.881	-0.598	-0.51	0.088
58	-460.209076	0.102260	-460.355080	0.101004	92.406614	4.007	-0.472	-0.39	0.082
59	-420.884376	0.076772	-421.033903	0.075471	94.646064	4.104	-0.375	-0.34	0.035
60	-381.559345	0.051897	-381.712302	0.051788	96.050506	4.165	-0.314	-0.23	0.084
61	-841.189080	0.040411	-841.346069	0.038918	99.448790	4.313	-0.166	-0.10	0.066
62	-1300.817037	0.028326	-1300.977989	0.027764	101.351376	4.395	-0.084	0.06	0.144

FUNCTIONAL PW91

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	ΔG (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.968464	0.057079	-156.036811	0.049365	47.729091	2.070	-2.454	-2.56	0.106
2	-233.385709	0.090769	-233.447573	0.084683	42.639084	1.849	-2.674	-2.71	0.036
3	-191.916109	0.033793	-192.017671	0.029603	66.360772	2.878	-1.646	-1.19	0.456
4	-345.561967	0.076192	-345.661813	0.072616	64.898082	2.814	-1.709	-1.38	0.329
5	-384.876872	0.101493	-384.970585	0.097693	61.190253	2.654	-1.870	-1.55	0.320
6	-534.362784	0.097303	-534.474583	0.094305	72.036225	3.124	-1.399	-1.29	0.109
7	-306.473797	0.061692	-306.562416	0.057196	58.430158	2.534	-1.989	-1.86	0.129
9	-362.974820	0.099301	-363.084387	0.095226	71.311273	3.092	-1.431	-1.43	0.001
10	-284.364643	0.047447	-284.474328	0.044616	70.604697	3.062	-1.462	-1.40	0.062
11	-245.055569	0.021890	-245.166958	0.019106	71.644376	3.107	-1.416	-1.39	0.031
12	-436.777486	0.068202	-436.903546	0.064544	81.399236	3.530	-0.993	-0.95	0.043
13	-476.089012	0.093026	-476.212293	0.089437	79.612201	3.452	-1.071	-0.97	0.101
14	-280.335511	0.035174	-280.441204	0.031402	68.690357	2.979	-1.545	-1.39	0.155
15	-319.651327	0.058889	-319.753989	0.055318	66.662214	2.891	-1.633	-1.46	0.173
16	-508.227630	0.069294	-508.340979	0.064774	73.963752	3.207	-1.316	-1.18	0.136
17	-586.860046	0.118941	-586.965451	0.113133	69.787736	3.026	-1.497	-1.42	0.077
18	-296.347127	0.023156	-296.481786	0.020997	85.854241	3.723	-0.800	-0.63	0.170
19	-374.980518	0.068786	-375.108233	0.067632	80.866767	3.507	-1.017	-0.79	0.227
21	-270.881503	0.082248	-270.997965	0.078872	75.199498	3.261	-1.262	-1.21	0.052
23	-501.923379	0.154921	-502.045176	0.155161	76.278193	3.308	-1.216	-0.90	0.316
24	-173.798064	0.076357	-173.885063	0.075789	54.948704	2.383	-2.140	-1.76	0.380
25	-310.191952	0.106845	-310.300486	0.105550	68.918407	2.989	-1.535	-1.36	0.175
26	-541.227280	0.179944	-541.341318	0.179145	72.060920	3.125	-1.398	-1.10	0.298
28	-500.738827	0.136092	-500.876604	0.135822	86.625662	3.757	-0.767	-0.52	0.247
29	-365.531153	0.122619	-365.624252	0.120804	59.558999	2.583	-1.941	-1.79	0.151
30	-385.413269	0.110320	-385.519377	0.106075	69.247725	3.003	-1.520	-1.51	0.010
31	-310.191575	0.107097	-310.303655	0.102221	73.390655	3.183	-1.341	-1.38	0.039
32	-310.191179	0.106241	-310.306517	0.104451	73.499138	3.187	-1.336	-1.26	0.076
33	-370.138495	0.072643	-370.252045	0.069458	73.252346	3.177	-1.347	-1.26	0.087
34	-730.493311	0.070558	-730.611408	0.067422	76.074883	3.299	-1.224	-1.16	0.064
35	-423.541838	0.113492	-423.679930	0.112382	87.350671	3.788	-0.735	-0.47	0.265
36	-363.139375	0.078369	-363.275078	0.077012	86.006092	3.730	-0.794	-0.53	0.264
37	-363.135928	0.077917	-363.260474	0.076249	79.200385	3.435	-1.089	-0.87	0.219
38	-607.974031	0.079325	-608.096047	0.079492	76.461266	3.316	-1.208	-0.96	0.248
40	-540.650698	0.170185	-540.737170	0.166852	56.353646	2.444	-2.080	-1.96	0.120
41	-424.187647	0.124074	-424.278001	0.120620	58.865336	2.553	-1.971	-1.96	0.011
42	-460.120442	0.104827	-460.204816	0.100249	55.818149	2.421	-2.103	-2.13	0.027
43	-499.430709	0.130034	-499.514527	0.125845	55.225390	2.395	-2.128	-2.16	0.032
44	-385.851090	0.112261	-385.922360	0.106237	48.502563	2.103	-2.420		
45	-539.484032	0.154479	-539.556138	0.148447	49.032635	2.126	-2.397	-2.38	0.017
46	-615.714724	0.166682	-615.800016	0.160672	57.292877	2.485	-2.039	-1.98	0.059
47	-264.321341	0.047856	-264.396957	0.041783	51.260497	2.223	-2.300	-2.10	0.200
48	-555.536889	0.143400	-555.618223	0.136728	55.225028	2.395	-2.128	-1.97	0.160
49	-401.901429	0.101060	-401.983838	0.095682	55.086694	2.389	-2.134	-1.98	0.154
50	-248.270161	0.059228	-248.331466	0.052222	42.865737	1.859	-2.664	-2.40	0.268
52	-2255.135652	0.016140	-2255.261975	0.013215	81.104082	3.517	-1.006	-0.71	0.296
53	-601.215143	0.052556	-601.352745	0.050493	87.640815	3.801	-0.723	-0.50	0.223
54	-723.981816	0.146321	-724.110041	0.143191	82.426727	3.574	-0.949	-0.65	0.299
57	-499.405353	0.126290	-499.549993	0.125279	91.397401	3.963	-0.560	-0.51	0.050
58	-460.096111	0.102415	-460.244153	0.100966	93.807500	4.068	-0.455	-0.39	0.065
59	-420.782604	0.076848	-420.934145	0.075458	95.965531	4.162	-0.362	-0.34	0.022
60	-381.468792	0.051979	-381.623746	0.051854	97.313570	4.220	-0.303	-0.23	0.073
61	-841.077733	0.040520	-841.236673	0.039014	100.681771	4.366	-0.157	-0.10	0.057
62	-1300.684877	0.028487	-1300.847785	0.027911	102.587669	4.449	-0.075	0.06	0.135

FUNCTIONAL B97D

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.983993	0.059450	-156.050492	0.051571	46.672763	2.024	-2.423	-2.56	0.137
2	-233.405368	0.094246	-233.464961	0.088138	41.228119	1.788	-2.659	-2.71	0.051
3	-191.912887	0.035630	-192.013509	0.031361	65.820326	2.854	-1.592	-1.19	0.402
4	-345.556291	0.079420	-345.654439	0.075786	63.869114	2.770	-1.677	-1.38	0.297
5	-384.877105	0.105530	-384.968575	0.101557	59.891344	2.597	-1.850	-1.55	0.300
6	-534.326426	0.101759	-534.436285	0.098222	71.156751	3.086	-1.361	-1.29	0.071
7	-306.463296	0.064711	-306.550659	0.060142	57.688462	2.502	-1.945	-1.86	0.085
9	-362.960675	0.103349	-363.073565	0.099278	73.393520	3.183	-1.264	-1.43	0.166
10	-284.338464	0.049592	-284.451460	0.046890	72.601534	3.148	-1.298	-1.40	0.102
11	-245.023626	0.023735	-245.138377	0.020721	73.898393	3.205	-1.242	-1.39	0.143
12	-436.738314	0.071435	-436.866761	0.067717	82.934354	3.596	-0.850	-0.95	0.100
13	-476.055372	0.097011	-476.181335	0.093328	81.354473	3.528	-0.919	-0.97	0.051
14	-280.313335	0.037538	-280.418871	0.033740	68.608191	2.975	-1.472	-1.39	0.082
15	-319.634918	0.062008	-319.737624	0.058379	66.726251	2.894	-1.553	-1.46	0.093
16	-508.181042	0.073156	-508.291294	0.068380	72.181024	3.130	-1.317	-1.18	0.137
17	-586.824385	0.123782	-586.926932	0.119353	67.128272	2.911	-1.536	-1.42	0.116
18	-296.312409	0.025546	-296.447925	0.023237	86.486466	3.750	-0.696	-0.63	0.066
19	-374.957001	0.073400	-375.086287	0.069154	83.792556	3.634	-0.813	-0.79	0.023
21	-270.894543	0.085300	-271.007966	0.081737	73.409758	3.183	-1.263	-1.21	0.053
23	-501.934975	0.160502	-502.053509	0.160752	74.224547	3.219	-1.228	-0.90	0.328
24	-173.816576	0.079280	-173.901887	0.078850	53.803309	2.333	-2.114	-1.76	0.354
25	-310.210420	0.110716	-310.315634	0.109538	66.761980	2.895	-1.552	-1.36	0.192
26	-541.244108	0.186165	-541.354195	0.185542	69.471713	3.013	-1.434	-1.10	0.334
28	-500.742599	0.140945	-500.879064	0.140928	85.643633	3.714	-0.733	-0.52	0.213
29	-365.542029	0.126568	-365.632832	0.125073	57.917714	2.512	-1.935	-1.79	0.145
30	-385.417292	0.114250	-385.521379	0.110774	67.497077	2.927	-1.520	-1.51	0.010
31	-310.210152	0.110887	-310.319240	0.105400	71.897304	3.118	-1.329	-1.38	0.051
32	-310.209875	0.109992	-310.322350	0.108146	71.737128	3.111	-1.336	-1.26	0.076
33	-370.132578	0.075620	-370.242969	0.072617	71.155442	3.086	-1.361	-1.26	0.101
34	-730.471216	0.073503	-730.586614	0.070500	74.297863	3.222	-1.225	-1.16	0.065
35	-423.542860	0.117612	-423.677126	0.116659	84.850992	3.680	-0.767	-0.47	0.297
36	-363.135870	0.081480	-363.268508	0.080296	83.974908	3.642	-0.805	-0.53	0.275
37	-363.132929	0.081079	-363.253742	0.079557	76.766558	3.329	-1.118	-0.87	0.248
38	-607.938397	0.082967	-608.056793	0.083332	74.065598	3.212	-1.235	-0.96	0.275
40	-540.663393	0.179346	-540.746404	0.172124	56.621909	2.455	-1.991	-1.96	0.031
41	-424.193467	0.128828	-424.281613	0.125462	57.424391	2.490	-1.957	-1.96	0.003
42	-460.107503	0.109054	-460.189503	0.104530	54.294656	2.354	-2.092	-2.13	0.038
43	-499.423782	0.135019	-499.505237	0.130837	53.738057	2.330	-2.116	-2.16	0.044
44	-385.859135	0.116411	-385.927457	0.110252	46.737432	2.027	-2.420		
45	-539.488958	0.160093	-539.557339	0.153860	46.820702	2.030	-2.416	-2.38	0.036
46	-615.713464	0.172715	-615.796049	0.166517	55.712135	2.416	-2.031	-1.98	0.051
47	-264.311926	0.050286	-264.386223	0.044210	50.434438	2.187	-2.260	-2.10	0.160
48	-555.531169	0.148753	-555.609083	0.141915	53.182728	2.306	-2.140	-1.97	0.172
49	-401.898652	0.105033	-401.978460	0.099600	53.489271	2.320	-2.127	-1.98	0.147
50	-248.270914	0.061829	-248.330979	0.054967	41.997295	1.821	-2.626	-2.40	0.230
52	-2254.971880	0.018517	-2255.097993	0.015743	80.877865	3.507	-0.939	-0.71	0.229
53	-601.160871	0.056814	-601.296753	0.053701	87.220170	3.782	-0.664	-0.50	0.164
54	-723.951526	0.152582	-724.079347	0.149098	82.394572	3.573	-0.874	-0.65	0.224
57	-499.394603	0.131118	-499.539383	0.130195	91.429360	3.965	-0.482	-0.51	0.028
58	-460.080633	0.106712	-460.228631	0.105040	93.919067	4.073	-0.374	-0.39	0.016
59	-420.761512	0.080451	-420.912951	0.078843	96.038250	4.165	-0.282	-0.34	0.058
60	-381.442176	0.054674	-381.596882	0.054555	97.154188	4.213	-0.234	-0.23	0.004
61	-841.015386	0.043114	-841.174499	0.041598	100.796135	4.371	-0.076	-0.10	0.024
62	-1300.586937	0.031034	-1300.750454	0.030464	102.965906	4.465	0.018	0.06	0.042

FUNCTIONAL B3PW91

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.983993	0.059450	-156.050492	0.051571	46.672763	2.024	-2.423	-2.56	0.137
2	-233.405368	0.094246	-233.464961	0.088138	41.228119	1.788	-2.659	-2.71	0.051
3	-191.912887	0.035630	-192.013509	0.031361	65.820326	2.854	-1.592	-1.19	0.402
4	-345.556291	0.079420	-345.654439	0.075786	63.869114	2.770	-1.677	-1.38	0.297
5	-384.877105	0.105530	-384.968575	0.101557	59.891344	2.597	-1.850	-1.55	0.300
6	-534.326426	0.101759	-534.436285	0.098222	71.156751	3.086	-1.361	-1.29	0.071
7	-306.463296	0.064711	-306.550659	0.060142	57.688462	2.502	-1.945	-1.86	0.085
9	-362.960675	0.103349	-363.073565	0.099278	73.393520	3.183	-1.264	-1.43	0.166
10	-284.338464	0.049592	-284.451460	0.046890	72.601534	3.148	-1.298	-1.40	0.102
11	-245.023626	0.023735	-245.138377	0.020721	73.898393	3.205	-1.242	-1.39	0.143
12	-436.738314	0.071435	-436.866761	0.067717	82.934354	3.596	-0.850	-0.95	0.100
13	-476.055372	0.097011	-476.181335	0.093328	81.354473	3.528	-0.919	-0.97	0.051
14	-280.313335	0.037538	-280.418871	0.033740	68.608191	2.975	-1.472	-1.39	0.082
15	-319.634918	0.062008	-319.737624	0.058379	66.726251	2.894	-1.553	-1.46	0.093
16	-508.181042	0.073156	-508.291294	0.068380	72.181024	3.130	-1.317	-1.18	0.137
17	-586.824385	0.123782	-586.926932	0.119353	67.128272	2.911	-1.536	-1.42	0.116
18	-296.312409	0.025546	-296.447925	0.023237	86.486466	3.750	-0.696	-0.63	0.066
19	-374.957001	0.073400	-375.086287	0.069154	83.792556	3.634	-0.813	-0.79	0.023
21	-270.894543	0.085300	-271.007966	0.081737	73.409758	3.183	-1.263	-1.21	0.053
23	-501.934975	0.160502	-502.053509	0.160752	74.224547	3.219	-1.228	-0.90	0.328
24	-173.816576	0.079280	-173.901887	0.078850	53.803309	2.333	-2.114	-1.76	0.354
25	-310.210420	0.110716	-310.315634	0.109538	66.761980	2.895	-1.552	-1.36	0.192
26	-541.244108	0.186165	-541.354195	0.185542	69.471713	3.013	-1.434	-1.10	0.334
28	-500.742599	0.140945	-500.879064	0.140928	85.643633	3.714	-0.733	-0.52	0.213
29	-365.542029	0.126568	-365.632832	0.125073	57.917714	2.512	-1.935	-1.79	0.145
30	-385.417292	0.114250	-385.521379	0.110774	67.497077	2.927	-1.520	-1.51	0.010
31	-310.210152	0.110887	-310.319240	0.105400	71.897304	3.118	-1.329	-1.38	0.051
32	-310.209875	0.109992	-310.322350	0.108146	71.737128	3.111	-1.336	-1.26	0.076
33	-370.132578	0.075620	-370.242969	0.072617	71.155442	3.086	-1.361	-1.26	0.101
34	-730.471216	0.073503	-730.586614	0.070500	74.297863	3.222	-1.225	-1.16	0.065
35	-423.542860	0.117612	-423.677126	0.116659	84.850992	3.680	-0.767	-0.47	0.297
36	-363.135870	0.081480	-363.268508	0.080296	83.974908	3.642	-0.805	-0.53	0.275
37	-363.132929	0.081079	-363.253742	0.079557	76.766558	3.329	-1.118	-0.87	0.248
38	-607.938397	0.082967	-608.056793	0.083332	74.065598	3.212	-1.235	-0.96	0.275
40	-540.663393	0.179346	-540.746404	0.172124	56.621909	2.455	-1.991	-1.96	0.031
41	-424.193467	0.128828	-424.281613	0.125462	57.424391	2.490	-1.957	-1.96	0.003
42	-460.107503	0.109054	-460.189503	0.104530	54.294656	2.354	-2.092	-2.13	0.038
43	-499.423782	0.135019	-499.505237	0.130837	53.738057	2.330	-2.116	-2.16	0.044
44	-385.859135	0.116411	-385.927457	0.110252	46.737432	2.027	-2.420		
45	-539.488958	0.160093	-539.557339	0.153860	46.820702	2.030	-2.416	-2.38	0.036
46	-615.713464	0.172715	-615.796049	0.166517	55.712135	2.416	-2.031	-1.98	0.051
47	-264.311926	0.050286	-264.386223	0.044210	50.434438	2.187	-2.260	-2.10	0.160
48	-555.531169	0.148753	-555.609083	0.141915	53.182728	2.306	-2.140	-1.97	0.172
49	-401.898652	0.105033	-401.978460	0.099600	53.489271	2.320	-2.127	-1.98	0.147
50	-248.270914	0.061829	-248.330979	0.054967	41.997295	1.821	-2.626	-2.40	0.230
52	-2254.971880	0.018517	-2255.097993	0.015743	80.877865	3.507	-0.939	-0.71	0.229
53	-601.160871	0.056814	-601.296753	0.053701	87.220170	3.782	-0.664	-0.50	0.164
54	-723.951526	0.152582	-724.079347	0.149098	82.394572	3.573	-0.874	-0.65	0.224
57	-499.394603	0.131118	-499.539383	0.130195	91.429360	3.965	-0.482	-0.51	0.028
58	-460.080633	0.106712	-460.228631	0.105040	93.919067	4.073	-0.374	-0.39	0.016
59	-420.761512	0.080451	-420.912951	0.078843	96.038250	4.165	-0.282	-0.34	0.058
60	-381.442176	0.054674	-381.596882	0.054555	97.154188	4.213	-0.234	-0.23	0.004
61	-841.015386	0.043114	-841.174499	0.041598	100.796135	4.371	-0.076	-0.10	0.024
62	-1300.586937	0.031034	-1300.750454	0.030464	102.965906	4.465	0.018	0.06	0.042

FUNCTIONAL B3LYP

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.051841	0.058500	-156.115899	0.050823	45.014156	1.952	-2.410	-2.56	0.150
2	-233.498177	0.093959	-233.555203	0.087738	39.688449	1.721	-2.641	-2.71	0.069
3	-191.995870	0.035524	-192.094759	0.031195	64.770208	2.809	-1.553	-1.19	0.363
4	-345.699924	0.079167	-345.795914	0.075491	62.541705	2.712	-1.650	-1.38	0.270
5	-385.034855	0.105265	-385.124204	0.101213	58.609587	2.542	-1.821	-1.55	0.271
6	-534.545982	0.101399	-534.654606	0.097898	70.359431	3.051	-1.311	-1.29	0.021
7	-306.590756	0.064356	-306.676548	0.059639	56.794864	2.463	-1.899	-1.86	0.039
8	-363.104426	0.102082	-363.217727	0.099940	72.441447	3.141	-1.221	-1.55	0.324
9	-363.101496	0.102977	-363.217271	0.098869	75.227478	3.262	-1.100	-1.43	0.330
10	-284.449601	0.049111	-284.565846	0.046604	74.518077	3.231	-1.131	-1.40	0.269
11	-245.120107	0.023389	-245.238121	0.020414	75.921316	3.292	-1.070	-1.39	0.315
12	-436.913796	0.071073	-437.043294	0.067188	83.699073	3.630	-0.733	-0.95	0.217
13	-476.245157	0.096560	-476.372166	0.092725	82.106033	3.561	-0.802	-0.97	0.168
14	-280.429303	0.037250	-280.533824	0.033419	67.992174	2.948	-1.414	-1.39	0.024
15	-319.765215	0.061719	-319.866811	0.057995	66.089175	2.866	-1.496	-1.46	0.036
16	-508.389079	0.072758	-508.497621	0.067705	71.281744	3.091	-1.271	-1.18	0.091
17	-587.060928	0.123543	-587.161894	0.118648	66.428898	2.881	-1.481	-1.42	0.061
18	-296.434560	0.025271	-296.569620	0.022897	86.240781	3.740	-0.622	-0.63	0.008
19	-375.107797	0.073321	-375.236487	0.069126	83.386889	3.616	-0.746	-0.79	0.044
21	-271.005757	0.085053	-271.117730	0.082187	72.062297	3.125	-1.237	-1.21	0.027
22	-349.645962	0.136045	-349.732066	0.136858	53.520640	2.321	-2.041	-1.49	0.551
23	-502.139469	0.159900	-502.255534	0.160275	72.596373	3.148	-1.214	-0.90	0.314
24	-173.885703	0.078912	-173.971449	0.078495	54.067773	2.345	-2.017	-1.76	0.257
25	-310.335728	0.110402	-310.439477	0.109116	65.910376	2.858	-1.504	-1.36	0.144
26	-541.461880	0.185717	-541.569574	0.184943	68.064631	2.952	-1.411	-1.10	0.311
28	-500.942375	0.140398	-501.075886	0.140279	83.854481	3.636	-0.726	-0.52	0.206
29	-365.688671	0.126473	-365.779275	0.124917	57.831206	2.508	-1.854	-1.79	0.064
30	-385.573644	0.114089	-385.676849	0.110168	67.222326	2.915	-1.447	-1.51	0.063
31	-310.335622	0.110565	-310.443128	0.107723	69.244406	3.003	-1.359	-1.38	0.021
32	-310.335333	0.109734	-310.446313	0.107717	70.906410	3.075	-1.287	-1.26	0.027
33	-370.281386	0.075309	-370.390808	0.072242	70.587781	3.061	-1.301	-1.26	0.041
34	-730.634870	0.073172	-730.748984	0.069912	73.652776	3.194	-1.168	-1.16	0.008
35	-423.716295	0.117330	-423.849205	0.116126	84.157805	3.650	-0.713	-0.47	0.243
36	-363.290041	0.081212	-363.420997	0.079968	82.956921	3.597	-0.765	-0.53	0.235
37	-363.286965	0.080780	-363.406296	0.079193	75.877118	3.290	-1.072	-0.87	0.202
38	-608.177028	0.082494	-608.294115	0.082778	73.294847	3.178	-1.184	-0.96	0.224
40	-540.884725	0.175427	-540.964326	0.171757	52.253456	2.266	-2.096	-1.96	0.136
41	-424.365463	0.128690	-424.451441	0.124998	56.268856	2.440	-1.922	-1.96	0.038
42	-460.295482	0.108741	-460.375528	0.103971	53.222880	2.308	-2.054	-2.13	0.076
43	-499.626520	0.134514	-499.706015	0.130254	52.557056	2.279	-2.083	-2.16	0.077
44	-386.015746	0.116043	-386.080819	0.109745	44.785992	1.942			
45	-539.706336	0.159630	-539.771182	0.153314	44.654715	1.936	-2.426	-2.38	0.046
46	-615.959413	0.172130	-616.038224	0.165834	53.405512	2.316	-2.046	-1.98	0.066
47	-264.421304	0.050045	-264.493872	0.043874	49.409313	2.143	-2.220	-2.10	0.120
48	-555.755511	0.148269	-555.830329	0.141425	51.243899	2.222	-2.140	-1.97	0.172
49	-402.062417	0.104673	-402.139180	0.099136	51.644288	2.240	-2.123	-1.98	0.143
50	-248.373589	0.061572	-248.431665	0.054648	40.788013	1.769	-2.593	-2.40	0.197
52	-2255.361118	0.017957	-2255.484762	0.015034	79.421825	3.444	-0.918	-0.71	0.208
53	-601.428551	0.057755	-601.561061	0.053377	85.898409	3.725	-0.637	-0.50	0.137
54	-724.254721	0.151709	-724.378669	0.148364	79.877727	3.464	-0.898	-0.65	0.248
57	-499.596975	0.131016	-499.739188	0.129525	90.175258	3.910	-0.452	-0.51	0.058
58	-460.269243	0.106531	-460.414758	0.104825	92.382038	4.006	-0.356	-0.39	0.034
59	-420.935966	0.080204	-421.084957	0.078597	94.501651	4.098	-0.264	-0.34	0.076
60	-381.602492	0.054481	-381.754789	0.054305	95.678032	4.149	-0.213	-0.23	0.017
61	-841.227643	0.042821	-841.384485	0.041247	99.407138	4.311	-0.051	-0.10	0.049
62	-1300.851166	0.030586	-1301.012512	0.029944	101.649122	4.408	0.046	0.06	0.014

FUNCTIONAL B3LYP-D

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.057494	0.059393	-156.121289	0.050901	45.360518	1.967	-2.396	-2.56	0.164
2	-233.509477	0.093911	-233.566721	0.087739	39.793805	1.726	-2.638	-2.71	0.072
3	-191.999638	0.035558	-192.098316	0.031158	64.682164	2.805	-1.558	-1.19	0.368
4	-345.710784	0.079132	-345.806816	0.075464	62.562607	2.713	-1.650	-1.38	0.270
5	-385.050364	0.105516	-385.139780	0.101914	58.369253	2.531	-1.832	-1.55	0.282
6	-534.562737	0.102420	-534.671958	0.098799	70.809523	3.071	-1.293	-1.29	0.003
7	-306.598435	0.064789	-306.684141	0.060086	56.732482	2.460	-1.903	-1.86	0.043
9	-363.116485	0.103399	-363.232090	0.099296	75.117377	3.257	-1.106	-1.43	0.324
10	-284.456017	0.049694	-284.572284	0.046667	74.858364	3.246	-1.117	-1.40	0.283
11	-245.122949	0.023681	-245.240956	0.020526	76.030299	3.297	-1.066	-1.39	0.319
12	-436.924509	0.071045	-437.054121	0.067174	83.762021	3.632	-0.731	-0.95	0.219
13	-476.260208	0.095804	-476.387257	0.091987	82.119541	3.561	-0.802	-0.97	0.168
14	-280.433140	0.037189	-280.537811	0.033367	68.080330	2.952	-1.411	-1.39	0.021
15	-319.772362	0.062267	-319.874116	0.058521	66.201712	2.871	-1.493	-1.46	0.033
16	-508.399107	0.072997	-508.507830	0.067987	71.368378	3.095	-1.268	-1.18	0.088
17	-587.079849	0.124283	-587.180842	0.119651	66.280970	2.874	-1.489	-1.42	0.069
18	-296.437450	0.025219	-296.572623	0.022851	86.308491	3.743	-0.621	-0.63	0.009
19	-375.117198	0.074550	-375.246043	0.071683	82.650718	3.584	-0.779	-0.79	0.011
21	-271.016426	0.085084	-271.128317	0.082131	72.065151	3.125	-1.238	-1.21	0.028
23	-502.164200	0.160172	-502.279677	0.160291	72.388443	3.139	-1.224	-0.90	0.324
24	-173.895370	0.079300	-173.981392	0.078739	54.331935	2.356	-2.007	-1.76	0.247
25	-310.350570	0.110927	-310.454285	0.109276	66.117544	2.867	-1.496	-1.36	0.136
26	-541.494130	0.186007	-541.601786	0.185228	68.044188	2.951	-1.413	-1.10	0.313
28	-500.963487	0.140311	-501.097068	0.140294	83.834364	3.635	-0.728	-0.52	0.208
29	-365.708546	0.126641	-365.799025	0.125063	57.767168	2.505	-1.858	-1.79	0.068
30	-385.590104	0.113719	-385.692672	0.110998	66.069631	2.865	-1.498	-1.51	0.012
31	-310.350536	0.109890	-310.457808	0.107047	69.097974	2.996	-1.367	-1.38	0.013
32	-310.350345	0.110408	-310.461274	0.108302	70.930216	3.076	-1.287	-1.26	0.027
33	-370.292521	0.075339	-370.401828	0.072176	70.576377	3.061	-1.303	-1.26	0.043
34	-730.646700	0.073205	-730.760720	0.069872	73.640158	3.193	-1.170	-1.16	0.010
35	-423.735124	0.117403	-423.868007	0.116884	83.711145	3.630	-0.733	-0.47	0.263
36	-363.302750	0.081247	-363.433625	0.079930	82.951423	3.597	-0.766	-0.53	0.236
37	-363.299689	0.080759	-363.418963	0.079187	75.832086	3.288	-1.075	-0.87	0.205
38	-608.193430	0.082690	-608.310480	0.080202	75.010951	3.253	-1.111	-0.96	0.151
40	-540.911084	0.178499	-540.990691	0.171938	54.071350	2.345	-2.019	-1.96	0.059
41	-424.385271	0.130169	-424.471161	0.126655	56.101540	2.433	-1.931	-1.96	0.029
42	-460.310526	0.109023	-460.390682	0.104266	53.284072	2.311	-2.053	-2.13	0.077
43	-499.644953	0.135112	-499.724555	0.130715	52.710034	2.286	-2.078	-2.16	0.082
44	-386.031989	0.115962	-386.097171	0.109729	44.814084	1.943	-2.420		
45	-539.732742	0.159621	-539.797670	0.153303	44.707457	1.939	-2.425	-2.38	0.045
46	-615.989852	0.172179	-616.068690	0.165837	53.450923	2.318	-2.045	-1.98	0.065
47	-264.426131	0.049983	-264.498933	0.043821	49.550906	2.149	-2.215	-2.10	0.115
48	-555.779325	0.148279	-555.854259	0.141446	51.309595	2.225	-2.138	-1.97	0.170
49	-402.077192	0.104602	-402.154038	0.099097	51.675911	2.241	-2.122	-1.98	0.142
50	-248.379667	0.061507	-248.437993	0.054627	40.916892	1.774	-2.589	-2.40	0.193
52	-2255.377780	0.017995	-2255.501465	0.014963	79.516221	3.448	-0.915	-0.71	0.205
53	-601.444742	0.057700	-601.577315	0.053293	85.956557	3.728	-0.636	-0.50	0.136
54	-724.287081	0.151716	-724.410937	0.148357	79.828724	3.462	-0.902	-0.65	0.252
57	-499.620310	0.132294	-499.762568	0.129877	90.784670	3.937	-0.426	-0.51	0.084
58	-460.286655	0.106884	-460.432053	0.105053	92.387738	4.006	-0.357	-0.39	0.033
59	-420.948910	0.080397	-421.097706	0.078806	94.369254	4.092	-0.271	-0.34	0.069
60	-381.611012	0.054416	-381.763053	0.054244	95.514896	4.142	-0.221	-0.23	0.009
61	-841.237191	0.042766	-841.393826	0.041184	99.282475	4.305	-0.058	-0.10	0.042
62	-1300.861744	0.030583	-1301.022925	0.029878	101.584922	4.405	0.042	0.06	0.018

FUNCTIONAL CAM-B3LYP

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.947718	0.059339	-156.010309	0.052114	43.810279	1.900	-2.402	-2.56	0.158
2	-233.352681	0.095547	-233.407916	0.089274	38.597370	1.674	-2.628	-2.71	0.082
3	-191.897989	0.036250	-191.996508	0.031941	64.525490	2.798	-1.503	-1.19	0.313
4	-345.514920	0.080582	-345.610169	0.077014	62.008900	2.689	-1.612	-1.38	0.232
5	-384.825836	0.107064	-384.913895	0.103018	57.796940	2.506	-1.795	-1.55	0.245
6	-534.320563	0.103431	-534.427523	0.100221	69.132453	2.998	-1.303	-1.29	0.013
7	-306.450014	0.065726	-306.535052	0.061040	56.302956	2.442	-1.860	-1.86	0.000
9	-362.931270	0.104023	-363.049747	0.100570	76.512304	3.318	-0.983	-1.43	0.447
10	-284.329718	0.049441	-284.448250	0.047577	75.549570	3.276	-1.025	-1.40	0.375
11	-245.025094	0.024216	-245.145391	0.021161	77.404008	3.357	-0.945	-1.39	0.440
12	-436.709004	0.072574	-436.840565	0.068715	84.977328	3.685	-0.616	-0.95	0.334
13	-476.015125	0.098386	-476.144477	0.094531	83.588135	3.625	-0.677	-0.97	0.293
14	-280.294133	0.038358	-280.399452	0.034604	68.444369	2.968	-1.333	-1.39	0.057
15	-319.605198	0.063175	-319.707777	0.059449	66.707785	2.893	-1.409	-1.46	0.051
16	-508.169334	0.074478	-508.275883	0.069782	69.807045	3.027	-1.274	-1.18	0.094
17	-586.791500	0.125870	-586.890755	0.121535	65.003266	2.819	-1.483	-1.42	0.063
18	-296.301196	0.026372	-296.437747	0.024058	87.139123	3.779	-0.523	-0.63	0.107
19	-374.924406	0.075093	-375.055232	0.071262	84.498427	3.664	-0.637	-0.79	0.153
21	-270.838701	0.086330	-270.948922	0.083585	70.887207	3.074	-1.227	-1.21	0.017
23	-501.837151	0.162267	-501.950373	0.162872	70.668418	3.065	-1.237	-0.90	0.337
24	-173.781335	0.079993	-173.866560	0.079955	53.503472	2.320	-1.981	-1.76	0.221
25	-310.143545	0.111967	-310.245162	0.110973	64.389202	2.792	-1.509	-1.36	0.149
26	-541.135733	0.188272	-541.239989	0.187898	65.656171	2.847	-1.454	-1.10	0.354
28	-500.646677	0.142523	-500.779466	0.142859	83.115477	3.604	-0.697	-0.52	0.177
29	-365.474920	0.128207	-365.564280	0.126855	56.922568	2.468	-1.833	-1.79	0.043
30	-385.362126	0.115446	-385.463833	0.112265	65.818192	2.854	-1.447	-1.51	0.063
31	-310.143449	0.112139	-310.249108	0.109424	68.005248	2.949	-1.352	-1.38	0.028
32	-310.143254	0.111259	-310.252675	0.109439	69.804849	3.027	-1.274	-1.26	0.014
33	-370.098036	0.076573	-370.205577	0.073688	69.293346	3.005	-1.296	-1.26	0.036
34	-730.471398	0.074501	-730.583801	0.071519	72.405219	3.140	-1.162	-1.16	0.002
35	-423.482814	0.118896	-423.612652	0.117931	82.079914	3.559	-0.742	-0.47	0.272
36	-363.082289	0.082522	-363.210883	0.081415	81.388864	3.529	-0.772	-0.53	0.242
37	-363.079664	0.082089	-363.196607	0.080735	74.232406	3.219	-1.082	-0.87	0.212
38	-607.937926	0.083957	-608.052999	0.084623	71.791666	3.113	-1.188	-0.96	0.228
40	-540.558675	0.181670	-540.634791	0.175048	51.918780	2.251	-2.050	-1.96	0.090
41	-424.131313	0.130248	-424.216027	0.127035	55.174914	2.393	-1.909	-1.96	0.051
42	-460.067808	0.110546	-460.146369	0.106014	52.141729	2.261	-2.040	-2.13	0.090
43	-499.373958	0.136546	-499.452011	0.132487	51.525553	2.234	-2.067	-2.16	0.093
44	-385.784539	0.117922	-385.847311	0.111556	43.384596	1.881	-2.420		
45	-539.388103	0.162608	-539.449961	0.156034	42.941255	1.862	-2.439	-2.38	0.059
46	-615.599866	0.175188	-615.676270	0.168699	52.016144	2.256	-2.046	-1.98	0.066
47	-264.284366	0.051137	-264.357173	0.045067	49.495662	2.146	-2.155	-2.10	0.055
48	-555.440185	0.150905	-555.512474	0.143988	49.702399	2.155	-2.146	-1.97	0.178
49	-401.834056	0.106514	-401.909205	0.100980	50.629248	2.196	-2.106	-1.98	0.126
50	-248.233345	0.062734	-248.291438	0.056038	40.655447	1.763	-2.538	-2.40	0.142
52	-2255.152540	0.019510	-2255.275377	0.016812	78.774518	3.416	-0.885	-0.71	0.175
53	-601.124047	0.059492	-601.254528	0.054848	84.792309	3.677	-0.624	-0.50	0.124
54	-723.854263	0.155216	-723.978086	0.151580	79.981301	3.468	-0.833	-0.65	0.183
57	-499.343297	0.133078	-499.485391	0.132049	89.810905	3.895	-0.407	-0.51	0.103
58	-460.040230	0.108520	-460.185459	0.106625	92.321654	4.004	-0.298	-0.39	0.092
59	-420.731718	0.081802	-420.880265	0.080098	94.283500	4.089	-0.213	-0.34	0.127
60	-381.423094	0.055694	-381.574769	0.055578	95.250047	4.131	-0.171	-0.23	0.059
61	-841.051595	0.044125	-841.207934	0.042596	99.063103	4.296	-0.005	-0.10	0.095
62	-1300.678553	0.032040	-1300.839614	0.031446	101.439967	4.399	0.098	0.06	0.038

FUNCTIONAL LC-BLYP

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.5384824	0.061605	-155.60045	0.053763	43.8043382	1.89958	-2.386	-2.56	0.174
2	-232.7545161	0.097638	-232.80855	0.091365	37.8444466	1.64113	-2.645	-2.71	0.065
3	-191.4798626	0.037188	-191.57956	0.032961	65.211632	2.82791	-1.458	-1.19	0.268
4	-344.7119939	0.082417	-344.80885	0.07886	63.0095843	2.73242	-1.553	-1.38	0.173
5	-383.9236715	0.109387	-384.01268	0.105241	58.4521935	2.53479	-1.751	-1.55	0.201
6	-533.2784578	0.105784	-533.38521	0.102574	69.0027948	2.99232	-1.293	-1.29	0.003
7	-305.8233318	0.06751	-305.90909	0.062715	56.8242626	2.46419	-1.822	-1.86	0.038
9	-362.1904031	0.10487	-362.31349	0.102705	78.5962164	3.40834	-0.877	-1.43	0.553
10	-283.7906448	0.050911	-283.91331	0.048983	78.1854653	3.39052	-0.895	-1.40	0.505
11	-244.5864881	0.025223	-244.71096	0.022107	80.0607427	3.47184	-0.814	-1.39	0.571
12	-435.7881328	0.074482	-435.92465	0.070768	87.9976001	3.81603	-0.470	-0.95	0.480
13	-474.9938094	0.10074	-475.12822	0.09696	86.7152554	3.76042	-0.525	-0.97	0.445
14	-279.6837349	0.03966	-279.79211	0.036065	70.261719	3.04691	-1.239	-1.39	0.151
15	-318.8947655	0.064968	-319.00054	0.061294	68.6773774	2.9782	-1.308	-1.46	0.152
16	-507.1433475	0.076713	-507.25064	0.072279	70.1103739	3.04035	-1.245	-1.18	0.065
17	-585.565572	0.127881	-585.66556	0.124897	64.6174669	2.80215	-1.484	-1.42	0.064
18	-295.6844368	0.027598	-295.82531	0.025471	89.7330867	3.89129	-0.394	-0.63	0.236
19	-374.107067	0.077093	-374.24288	0.073363	87.5675117	3.79738	-0.488	-0.79	0.302
21	-270.1441956	0.087919	-270.2538	0.085152	70.5141514	3.05786	-1.228	-1.21	0.018
23	-500.5596651	0.165073	-500.67135	0.166235	69.3514074	3.00743	-1.278	-0.90	0.378
24	-173.363606	0.081589	-173.44831	0.081947	52.9300396	2.29532	-1.990	-1.76	0.230
25	-309.3484049	0.114133	-309.44907	0.113503	63.5612978	2.75634	-1.529	-1.36	0.169
26	-539.7589401	0.191778	-539.86119	0.191774	64.1638946	2.78248	-1.503	-1.10	0.403
28	-499.3802027	0.145131	-499.51366	0.146176	83.0891789	3.60317	-0.683	-0.52	0.163
29	-364.5764248	0.130806	-364.66474	0.130264	55.7600933	2.41804	-1.868	-1.79	0.078
30	-384.4576424	0.117331	-384.55844	0.114958	64.7421982	2.80755	-1.478	-1.51	0.032
31	-309.3484802	0.114145	-309.45321	0.111664	67.2753108	2.9174	-1.368	-1.38	0.012
32	-309.3483581	0.113218	-309.45742	0.111795	69.3320801	3.00659	-1.279	-1.26	0.019
33	-369.2860195	0.078155	-369.39267	0.07555	68.5562167	2.97295	-1.313	-1.26	0.053
34	-729.514331	0.076156	-729.62606	0.073817	71.5759626	3.1039	-1.182	-1.16	0.022
35	-422.4820139	0.120893	-422.61101	0.120198	81.3826594	3.52917	-0.757	-0.47	0.287
36	-362.1917649	0.084214	-362.31987	0.083415	80.8861711	3.50764	-0.778	-0.53	0.248
37	-362.1893571	0.083776	-362.30508	0.082839	73.2027815	3.17445	-1.111	-0.87	0.241
38	-606.7907396	0.085861	-606.90501	0.084218	72.7367287	3.15424	-1.132	-0.96	0.172
40	-539.181977	0.185059	-539.25707	0.17841	51.2967228	2.22449	-2.061	-1.96	0.101
41	-423.1286965	0.132259	-423.21433	0.12978	55.2930528	2.39779	-1.888	-1.96	0.072
42	-459.0564775	0.113113	-459.13597	0.108804	52.5882731	2.2805	-2.005	-2.13	0.125
43	-498.2620562	0.139362	-498.34112	0.135391	52.1074676	2.25965	-2.026	-2.16	0.134
44	-384.8036936	0.120253	-384.86586	0.11386	43.0244417	1.86576	-2.420		
45	-538.0234397	0.166027	-538.08465	0.159452	42.5359774	1.84458	-2.441	-2.38	0.061
46	-614.0481074	0.179063	-614.12383	0.172356	51.7239912	2.24302	-2.043	-1.98	0.063
47	-263.6800065	0.052451	-263.75534	0.046562	50.9686134	2.21026	-2.075	-2.10	0.025
48	-554.0711418	0.154216	-554.14344	0.147193	49.7724357	2.15839	-2.127	-1.97	0.159
49	-400.8488129	0.108815	-400.92462	0.103408	50.9632294	2.21003	-2.076	-1.98	0.096
50	-247.6329377	0.064171	-247.69299	0.057808	41.6749428	1.80724	-2.479	-2.40	0.083
52	-2253.115603	0.021516	-2253.2402	0.019141	79.658308	3.45439	-0.831	-0.71	0.121
53	-599.7438992	0.059564	-599.87533	0.056755	84.2387233	3.65302	-0.633	-0.50	0.133
54	-722.0966109	0.159512	-722.22194	0.155932	80.893619	3.50796	-0.778	-0.65	0.128
57	-498.2331328	0.13575	-498.37525	0.135379	89.4110441	3.87732	-0.408	-0.51	0.102
58	-459.0291382	0.111125	-459.17503	0.109005	92.8814663	4.02782	-0.258	-0.39	0.132
59	-419.8206196	0.083836	-419.96968	0.082106	94.6205058	4.10323	-0.183	-0.34	0.157
60	-380.6120562	0.057284	-380.76407	0.057188	95.4474315	4.13909	-0.147	-0.23	0.083
61	-839.9777259	0.045823	-840.13449	0.044294	99.3318547	4.30754	0.022	-0.10	0.122
62	-1299.34195	0.034029	-1299.5036	0.033377	101.855811	4.41699	0.131	0.06	0.071

FUNCTIONAL BHandHLYP

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	D_G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.942382	0.062620	-155.998326	0.054019	40.502700	1.756	-2.360	-2.56	0.200
2	-233.342910	0.098714	-233.391828	0.092290	34.727104	1.506	-2.610	-2.71	0.100
3	-191.878467	0.038011	-191.970743	0.033462	60.758127	2.635	-1.481	-1.19	0.291
4	-345.490466	0.083519	-345.579381	0.079723	58.177279	2.523	-1.593	-1.38	0.213
5	-384.798950	0.110710	-384.880469	0.106249	53.953304	2.340	-1.776	-1.55	0.226
6	-534.245217	0.107437	-534.345990	0.103822	65.504875	2.841	-1.275	-1.29	0.015
7	-306.411723	0.068556	-306.490406	0.063498	52.548171	2.279	-1.837	-1.86	0.023
9	-362.873551	0.108351	-362.989800	0.104181	75.563595	3.277	-0.839	-1.43	0.591
10	-284.275469	0.054338	-284.392048	0.049505	76.186650	3.304	-0.812	-1.40	0.588
11	-244.972902	0.025818	-245.091255	0.022521	76.336469	3.310	-0.806	-1.39	0.579
12	-436.650391	0.075373	-436.779605	0.071273	83.656105	3.628	-0.488	-0.95	0.462
13	-475.954353	0.101853	-476.081367	0.097760	82.270984	3.568	-0.548	-0.97	0.422
14	-280.258761	0.040288	-280.358659	0.036416	65.116780	2.824	-1.292	-1.39	0.098
15	-319.567554	0.065828	-319.664852	0.061996	63.459760	2.752	-1.364	-1.46	0.096
16	-508.097954	0.077704	-508.197596	0.071558	66.383040	2.879	-1.237	-1.18	0.057
17	-586.715401	0.129900	-586.807638	0.126041	60.300843	2.615	-1.501	-1.42	0.081
18	-296.255543	0.028080	-296.387579	0.025648	84.380341	3.659	-0.457	-0.63	0.173
19	-374.873907	0.077922	-375.000688	0.074239	81.867387	3.550	-0.566	-0.79	0.224
21	-270.832540	0.089091	-270.932928	0.086379	64.696361	2.806	-1.310	-1.21	0.100
23	-501.822919	0.166823	-501.926863	0.167791	64.618416	2.802	-1.314	-0.90	0.414
24	-173.765379	0.082914	-173.843202	0.082762	48.930413	2.122	-1.994	-1.76	0.234
25	-310.134855	0.115391	-310.226808	0.114476	58.275819	2.527	-1.589	-1.36	0.229
26	-541.118267	0.193828	-541.213300	0.193580	59.789938	2.593	-1.523	-1.10	0.423
28	-500.632537	0.146650	-500.756355	0.147141	77.388882	3.356	-0.760	-0.52	0.240
29	-365.452191	0.132342	-365.533808	0.130968	52.077062	2.258	-1.858	-1.79	0.068
30	-385.336409	0.119031	-385.428734	0.116055	59.802078	2.593	-1.523	-1.51	0.013
31	-310.134936	0.115591	-310.230714	0.112875	61.805783	2.680	-1.436	-1.38	0.056
32	-310.134826	0.114661	-310.234575	0.112895	63.701108	2.762	-1.354	-1.26	0.094
33	-370.074073	0.079202	-370.171377	0.076358	62.843738	2.725	-1.391	-1.26	0.131
34	-730.449070	0.077040	-730.551630	0.073941	66.302368	2.875	-1.241	-1.16	0.081
35	-423.457290	0.122693	-423.577840	0.121531	76.375234	3.312	-0.804	-0.47	0.334
36	-363.065793	0.085283	-363.185164	0.084321	75.509933	3.274	-0.842	-0.53	0.312
37	-363.063194	0.084869	-363.169994	0.083561	67.838584	2.942	-1.174	-0.87	0.304
38	-607.879720	0.087141	-607.984664	0.085010	67.190590	2.914	-1.202	-0.96	0.242
40	-540.540623	0.187105	-540.610536	0.179514	48.634752	2.109	-2.007	-1.96	0.047
41	-424.102196	0.134399	-424.180412	0.130814	51.330992	2.226	-1.890	-1.96	0.070
42	-460.024578	0.114463	-460.096535	0.109696	48.144748	2.088	-2.028	-2.13	0.102
43	-499.328776	0.141192	-499.400223	0.136566	47.736958	2.070	-2.046	-2.16	0.114
44	-385.772279	0.121595	-385.828012	0.115001	39.110673	1.696	-2.420		
45	-539.370872	0.167410	-539.425712	0.160549	38.717895	1.679	-2.437	-2.38	0.057
46	-615.581054	0.180306	-615.650628	0.173572	47.883651	2.076	-2.040	-1.98	0.060
47	-264.259585	0.053260	-264.325832	0.047015	45.489488	1.973	-2.143	-2.10	0.043
48	-555.414113	0.155530	-555.479859	0.148482	45.678350	1.981	-2.135	-1.97	0.167
49	-401.812876	0.109989	-401.881194	0.104272	46.458025	2.015	-2.101	-1.98	0.121
50	-248.216876	0.065058	-248.268738	0.058276	36.799726	1.596	-2.520	-2.40	0.124
52	-2255.056966	0.021040	-2255.175052	0.018306	75.816001	3.288	-0.828	-0.71	0.118
53	-601.073106	0.060285	-601.199140	0.057247	80.993824	3.512	-0.604	-0.50	0.104
54	-723.815326	0.160358	-723.932955	0.156341	76.333936	3.310	-0.806	-0.65	0.156
57	-499.297477	0.137369	-499.432259	0.136534	85.100643	3.690	-0.426	-0.51	0.084
58	-459.996305	0.112297	-460.135198	0.110196	88.474907	3.837	-0.279	-0.39	0.111
59	-420.690029	0.084945	-420.832300	0.083037	90.473556	3.923	-0.193	-0.34	0.147
60	-381.383642	0.058089	-381.529103	0.057849	91.429191	3.965	-0.151	-0.23	0.079
61	-840.995729	0.046316	-841.146095	0.044623	95.418073	4.138	0.022	-0.10	0.122
62	-1300.606236	0.034059	-1300.761590	0.033299	97.962978	4.248	0.132	0.06	0.072

FUNCTIONAL ω–B97

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.000728	0.060547	-156.061059	0.052487	42.916372	1.861	-2.419	-2.56	0.141
2	-233.441155	0.096219	-233.494443	0.090053	37.307641	1.618	-2.663	-2.71	0.047
3	-191.947953	0.036390	-192.044174	0.032173	63.025644	2.733	-1.547	-1.19	0.357
4	-345.619034	0.080630	-345.713026	0.077228	61.115203	2.650	-1.630	-1.38	0.250
5	-384.948298	0.107565	-385.035141	0.103606	56.979009	2.471	-1.810	-1.55	0.260
6	-534.451462	0.105232	-534.555424	0.101101	67.829183	2.941	-1.339	-1.29	0.049
7	-306.527366	0.066198	-306.610058	0.061837	54.626334	2.369	-1.912	-1.86	0.052
9	-363.037345	0.105564	-363.152297	0.101745	74.530065	3.232	-1.049	-1.43	0.381
10	-284.401179	0.052692	-284.515912	0.048376	74.704225	3.240	-1.041	-1.40	0.359
11	-245.079212	0.024566	-245.195536	0.021703	74.790700	3.243	-1.037	-1.39	0.348
12	-436.827558	0.072917	-436.956451	0.069216	83.203957	3.608	-0.672	-0.95	0.278
13	-476.150942	0.099053	-476.277902	0.095252	82.053552	3.558	-0.722	-0.97	0.248
14	-280.371943	0.038580	-280.476795	0.035032	68.021890	2.950	-1.331	-1.39	0.059
15	-319.700239	0.063445	-319.802742	0.059779	66.621638	2.889	-1.391	-1.46	0.069
16	-508.299318	0.074705	-508.403289	0.069997	68.196946	2.957	-1.323	-1.18	0.143
17	-586.956591	0.125754	-587.053687	0.122416	63.023470	2.733	-1.548	-1.42	0.128
18	-296.379521	0.026517	-296.515443	0.024477	86.572386	3.754	-0.526	-0.63	0.104
19	-375.036804	0.075922	-375.167983	0.072972	84.167201	3.650	-0.631	-0.79	0.159
21	-270.932698	0.086405	-271.041565	0.083276	70.278645	3.048	-1.233	-1.21	0.023
23	-502.014156	0.162335	-502.125301	0.163165	69.223876	3.002	-1.279	-0.90	0.379
24	-173.839730	0.080820	-173.927301	0.080761	54.988963	2.385	-1.896	-1.76	0.136
25	-310.255329	0.112387	-310.355574	0.111435	63.501934	2.754	-1.527	-1.36	0.167
26	-541.332390	0.189296	-541.434578	0.188626	64.544387	2.799	-1.482	-1.10	0.382
28	-500.821811	0.142383	-500.954335	0.143065	82.732262	3.588	-0.693	-0.52	0.173
29	-365.599517	0.128773	-365.689866	0.128045	57.151509	2.478	-1.802	-1.79	0.012
30	-385.482724	0.115481	-385.582914	0.112672	64.632786	2.803	-1.478	-1.51	0.032
31	-310.254935	0.112447	-310.359301	0.108368	68.049887	2.951	-1.330	-1.38	0.050
32	-310.254787	0.110419	-310.363180	0.110736	67.818271	2.941	-1.340	-1.26	0.080
33	-370.198350	0.076579	-370.304276	0.073986	68.096810	2.953	-1.328	-1.26	0.068
34	-730.551087	0.074706	-730.661975	0.072236	71.133274	3.085	-1.196	-1.16	0.036
35	-423.619480	0.118456	-423.746881	0.117733	80.398919	3.487	-0.794	-0.47	0.324
36	-363.200550	0.082579	-363.327360	0.081695	80.128863	3.475	-0.806	-0.53	0.276
37	-363.198205	0.081943	-363.313159	0.080777	72.866303	3.160	-1.121	-0.87	0.251
38	-608.069687	0.083962	-608.183064	0.084525	70.791635	3.070	-1.211	-0.96	0.251
40	-540.748529	0.182084	-540.823248	0.174159	51.859942	2.249	-2.032	-1.96	0.072
41	-424.271147	0.130919	-424.354872	0.128042	54.343836	2.357	-1.924	-1.96	0.036
42	-460.199427	0.110574	-460.276783	0.105983	51.422315	2.230	-2.051	-2.13	0.079
43	-499.522513	0.136589	-499.599468	0.132815	50.658020	2.197	-2.084	-2.16	0.076
44	-385.918248	0.118134	-385.980254	0.111768	42.903848	1.861	-2.420		
45	-539.577324	0.163000	-539.638658	0.156458	42.592901	1.847	-2.433	-2.38	0.053
46	-615.814866	0.175395	-615.890663	0.168900	51.638892	2.239	-2.041	-1.98	0.061
47	-264.362019	0.051279	-264.434822	0.045464	49.333597	2.139	-2.141	-2.10	0.041
48	-555.627632	0.151052	-555.699136	0.144126	49.215602	2.134	-2.146	-1.97	0.178
49	-401.966230	0.106675	-402.041197	0.101340	50.390315	2.185	-2.095	-1.98	0.115
50	-248.311514	0.062912	-248.369896	0.056560	40.621346	1.762	-2.519	-2.40	0.123
52	-2255.228253	0.020324	-2255.350250	0.017756	78.166035	3.390	-0.891	-0.71	0.181
53	-601.301936	0.059257	-601.430737	0.054640	83.721461	3.631	-0.650	-0.50	0.150
54	-724.092144	0.154527	-724.216113	0.151256	79.844029	3.462	-0.818	-0.65	0.168
57	-499.499351	0.134595	-499.638463	0.133349	88.076053	3.819	-0.461	-0.51	0.049
58	-460.177130	0.109036	-460.319842	0.107414	90.571154	3.928	-0.353	-0.39	0.037
59	-420.850938	0.081750	-420.996533	0.080169	92.354501	4.005	-0.276	-0.34	0.064
60	-381.524646	0.055855	-381.673022	0.055859	93.105291	4.038	-0.243	-0.23	0.013
61	-841.139214	0.044426	-841.292243	0.042963	96.945124	4.204	-0.076	-0.10	0.024
62	-1300.752124	0.032539	-1300.909969	0.032042	99.361036	4.309	0.028	0.06	0.032

FUNCTIONAL ω–B97X

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.992745	0.060528	-156.053614	0.052390	43.302162	1.878	-2.404	-2.56	0.156
2	-233.425463	0.096069	-233.479298	0.089769	37.735228	1.636	-2.645	-2.71	0.065
3	-191.933567	0.036366	-192.030080	0.032116	63.229466	2.742	-1.540	-1.19	0.350
4	-345.594365	0.080681	-345.688159	0.077243	61.013528	2.646	-1.636	-1.38	0.256
5	-384.920262	0.107405	-385.006920	0.103258	56.981018	2.471	-1.810	-1.55	0.260
6	-534.403486	0.103912	-534.508134	0.100752	67.650641	2.934	-1.348	-1.29	0.058
7	-306.502063	0.066136	-306.585031	0.061618	54.898785	2.381	-1.901	-1.86	0.041
9	-363.002842	0.105444	-363.117580	0.101204	74.659929	3.238	-1.044	-1.43	0.386
10	-284.372762	0.052537	-284.487364	0.048205	74.631938	3.236	-1.045	-1.40	0.355
11	-245.053907	0.024464	-245.170109	0.021597	74.717015	3.240	-1.041	-1.39	0.344
12	-436.790045	0.072982	-436.918670	0.069236	83.063567	3.602	-0.679	-0.95	0.271
13	-476.110396	0.099019	-476.237012	0.095165	81.871197	3.550	-0.731	-0.97	0.239
14	-280.347481	0.038584	-280.451830	0.034925	67.776345	2.939	-1.342	-1.39	0.048
15	-319.672744	0.063046	-319.774660	0.059292	66.308801	2.875	-1.406	-1.46	0.054
16	-508.252593	0.074670	-508.356905	0.069964	68.409752	2.967	-1.315	-1.18	0.135
17	-586.903630	0.126290	-587.000966	0.122240	63.620789	2.759	-1.523	-1.42	0.103
18	-296.351031	0.026520	-296.486308	0.024343	86.253786	3.740	-0.541	-0.63	0.089
19	-375.002451	0.075588	-375.132701	0.072384	83.743624	3.632	-0.650	-0.79	0.140
21	-270.916086	0.086522	-271.025948	0.083902	70.583104	3.061	-1.221	-1.21	0.011
23	-501.982027	0.162476	-502.094272	0.163190	69.986686	3.035	-1.246	-0.90	0.346
24	-173.827546	0.080580	-173.914817	0.080467	54.833973	2.378	-1.904	-1.76	0.144
25	-310.235693	0.112183	-310.336800	0.111186	64.071318	2.778	-1.503	-1.36	0.143
26	-541.296741	0.189292	-541.399874	0.188548	65.183408	2.827	-1.455	-1.10	0.355
28	-500.788898	0.142566	-500.921951	0.143067	83.177309	3.607	-0.674	-0.52	0.154
29	-365.574650	0.128827	-365.665250	0.127940	57.408490	2.490	-1.792	-1.79	0.002
30	-385.455341	0.115437	-385.556593	0.112368	65.462431	2.839	-1.443	-1.51	0.067
31	-310.235246	0.112507	-310.340661	0.107359	69.379584	3.009	-1.273	-1.38	0.107
32	-310.235079	0.112454	-310.344340	0.110591	69.731368	3.024	-1.258	-1.26	0.002
33	-370.172744	0.076747	-370.279700	0.074019	68.827604	2.985	-1.297	-1.26	0.037
34	-730.532327	0.074762	-730.644336	0.072043	71.992981	3.122	-1.159	-1.16	0.001
35	-423.588158	0.118353	-423.716501	0.119169	80.024086	3.470	-0.811	-0.47	0.341
36	-363.174275	0.082692	-363.302030	0.081666	80.810678	3.504	-0.777	-0.53	0.247
37	-363.171878	0.082035	-363.288091	0.080753	73.728981	3.197	-1.084	-0.87	0.214
38	-608.022773	0.084080	-608.137218	0.084541	71.525899	3.102	-1.180	-0.96	0.220
40	-540.714748	0.182106	-540.789533	0.174765	51.535065	2.235	-2.047	-1.96	0.087
41	-424.240066	0.132383	-424.323541	0.127500	55.445377	2.404	-1.877	-1.96	0.083
42	-460.163799	0.110566	-460.240906	0.106170	51.143948	2.218	-2.064	-2.13	0.066
43	-499.483880	0.139001	-499.560562	0.132578	52.149373	2.261	-2.020	-2.16	0.140
44	-385.894217	0.118177	-385.956234	0.111789	42.925280	1.861	-2.420		
45	-539.542214	0.162971	-539.603389	0.156435	42.489610	1.843	-2.439	-2.38	0.059
46	-615.773859	0.175556	-615.849708	0.169052	51.677501	2.241	-2.040	-1.98	0.060
47	-264.341577	0.051313	-264.413683	0.045372	48.975257	2.124	-2.158	-2.10	0.058
48	-555.589260	0.151168	-555.660660	0.144250	49.144959	2.131	-2.150	-1.97	0.182
49	-401.938799	0.106710	-402.013462	0.101278	50.260178	2.180	-2.102	-1.98	0.122
50	-248.294801	0.062951	-248.352504	0.056433	40.299489	1.748	-2.534	-2.40	0.138
52	-2255.185592	0.020104	-2255.307632	0.017415	78.268451	3.394	-0.887	-0.71	0.177
53	-601.249655	0.059154	-601.378916	0.054714	83.898467	3.638	-0.643	-0.50	0.143
54	-724.037674	0.154912	-724.161806	0.151395	80.100815	3.474	-0.808	-0.65	0.158
57	-499.456900	0.133741	-499.597721	0.129645	90.936843	3.943	-0.338	-0.51	0.172
58	-460.138762	0.108966	-460.282478	0.107169	91.311120	3.960	-0.322	-0.39	0.068
59	-420.815732	0.081660	-420.962450	0.079858	93.197748	4.042	-0.240	-0.34	0.100
60	-381.492570	0.055909	-381.642220	0.055876	93.927435	4.073	-0.208	-0.23	0.022
61	-841.104987	0.044391	-841.259298	0.042896	97.769468	4.240	-0.042	-0.10	0.058
62	-1300.715653	0.032443	-1300.874794	0.031894	100.207257	4.346	0.064	0.06	0.004

FUNCTIONAL ω–B97XD

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.986084	0.060238	-156.047764	0.052005	43.871062	1.902	-2.402	-2.56	0.158
2	-233.412682	0.095508	-233.467351	0.089145	38.298071	1.661	-2.644	-2.71	0.066
3	-191.921308	0.036107	-192.017898	0.031859	63.276675	2.744	-1.561	-1.19	0.371
4	-345.569924	0.080257	-345.663671	0.076764	61.019160	2.646	-1.659	-1.38	0.279
5	-384.894043	0.106851	-384.980776	0.102475	57.171751	2.479	-1.825	-1.55	0.275
6	-534.363854	0.103462	-534.469025	0.099597	68.421553	2.967	-1.338	-1.29	0.048
7	-306.480780	0.065500	-306.563925	0.061125	54.919313	2.382	-1.923	-1.86	0.063
9	-362.979685	0.105163	-363.093061	0.101015	73.747712	3.198	-1.107	-1.43	0.323
10	-284.351938	0.052129	-284.465415	0.047831	73.904941	3.205	-1.100	-1.40	0.300
11	-245.034763	0.024080	-245.149948	0.021343	73.997430	3.209	-1.096	-1.39	0.289
12	-436.755322	0.072573	-436.883139	0.068795	82.577125	3.581	-0.724	-0.95	0.226
13	-476.074500	0.098454	-476.200158	0.094502	81.331190	3.527	-0.778	-0.97	0.192
14	-280.323301	0.038206	-280.427014	0.034474	67.422585	2.924	-1.381	-1.39	0.009
15	-319.646774	0.063939	-319.747898	0.060338	65.716436	2.850	-1.455	-1.46	0.005
16	-508.208821	0.074183	-508.313785	0.069057	69.082587	2.996	-1.309	-1.18	0.129
17	-586.857297	0.125613	-586.955009	0.121191	64.090202	2.779	-1.525	-1.42	0.105
18	-296.323308	0.026104	-296.457810	0.023862	85.808091	3.721	-0.584	-0.63	0.046
19	-374.971393	0.074685	-375.100365	0.071195	83.121114	3.605	-0.700	-0.79	0.090
21	-270.899057	0.086218	-271.010419	0.082028	72.509950	3.144	-1.160	-1.21	0.050
23	-501.948947	0.162119	-502.062840	0.162416	71.282400	3.091	-1.213	-0.90	0.313
24	-173.821088	0.080252	-173.907696	0.079795	54.633855	2.369	-1.935	-1.76	0.175
25	-310.217434	0.111634	-310.320033	0.110491	65.098860	2.823	-1.482	-1.36	0.122
26	-541.263099	0.188665	-541.367926	0.187425	66.558335	2.886	-1.418	-1.10	0.318
28	-500.754140	0.141986	-500.888327	0.142301	84.006351	3.643	-0.662	-0.52	0.142
29	-365.553159	0.128097	-365.643884	0.126845	57.716190	2.503	-1.802	-1.79	0.012
30	-385.430659	0.115164	-385.533287	0.113717	65.308066	2.832	-1.473	-1.51	0.037
31	-310.216946	0.112104	-310.323913	0.107231	70.180841	3.043	-1.261	-1.38	0.119
32	-310.216764	0.111967	-310.327335	0.110030	70.599546	3.062	-1.243	-1.26	0.017
33	-370.147916	0.076516	-370.256305	0.073667	69.803053	3.027	-1.278	-1.26	0.018
34	-730.513075	0.074410	-730.626596	0.071547	73.031910	3.167	-1.138	-1.16	0.022
35	-423.559115	0.117574	-423.689212	0.118665	80.952729	3.511	-0.794	-0.47	0.324
36	-363.145976	0.082368	-363.275351	0.081250	81.885821	3.551	-0.754	-0.53	0.224
37	-363.143483	0.081623	-363.261563	0.080224	74.974150	3.251	-1.053	-0.87	0.183
38	-607.979786	0.083699	-608.095769	0.083979	72.604623	3.149	-1.156	-0.96	0.196
40	-540.679449	0.181437	-540.755355	0.173281	52.749835	2.288	-2.017	-1.96	0.057
41	-424.212612	0.131423	-424.296056	0.126187	55.647366	2.413	-1.891	-1.96	0.069
42	-460.130467	0.109939	-460.207692	0.105485	51.254258	2.223	-2.082	-2.13	0.048
43	-499.449019	0.137915	-499.525738	0.133601	50.848771	2.205	-2.100	-2.16	0.060
44	-385.868950	0.117959	-385.931547	0.111299	43.459845	1.885	-2.420		
45	-539.505205	0.161725	-539.567173	0.155496	42.794222	1.856	-2.449	-2.38	0.069
46	-615.730985	0.174761	-615.807505	0.168386	52.017010	2.256	-2.049	-1.98	0.069
47	-264.320831	0.050953	-264.392264	0.044922	48.609520	2.108	-2.197	-2.10	0.097
48	-555.548863	0.150475	-555.620919	0.143504	49.590668	2.151	-2.154	-1.97	0.186
49	-401.910165	0.106172	-401.985128	0.100695	50.477175	2.189	-2.116	-1.98	0.136
50	-248.277540	0.062590	-248.334700	0.055945	40.037992	1.736	-2.568	-2.40	0.172
52	-2255.138425	0.019404	-2255.260653	0.016518	78.510004	3.405	-0.900	-0.71	0.190
53	-601.190188	0.058869	-601.320411	0.054268	84.603504	3.669	-0.636	-0.50	0.136
54	-723.979144	0.153894	-724.103557	0.150315	80.316093	3.483	-0.822	-0.65	0.172
57	-499.421743	0.133573	-499.563186	0.132295	89.558994	3.884	-0.421	-0.51	0.089
58	-460.104659	0.108215	-460.249103	0.106360	91.803940	3.981	-0.324	-0.39	0.066
59	-420.783062	0.080870	-420.930634	0.078510	94.083758	4.080	-0.225	-0.34	0.115
60	-381.461303	0.055524	-381.612000	0.055505	94.575744	4.101	-0.203	-0.23	0.027
61	-841.071577	0.043920	-841.226841	0.042410	98.377498	4.266	-0.038	-0.10	0.062
62	-1300.679946	0.031856	-1300.839992	0.031314	100.769989	4.370	0.065	0.06	0.005

FUNCTIONAL PBE0

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.842830	0.059017	-155.907813	0.051046	45.779231	1.985	-2.416	-2.56	0.144
2	-233.203155	0.094853	-233.261446	0.088709	40.433537	1.753	-2.647	-2.71	0.063
3	-191.761403	0.035954	-191.860402	0.031659	64.818334	2.811	-1.590	-1.19	0.400
4	-345.285049	0.079998	-345.381581	0.076429	62.814075	2.724	-1.677	-1.38	0.297
5	-384.571050	0.106287	-384.660858	0.102301	58.856819	2.552	-1.848	-1.55	0.298
6	-533.938232	0.102701	-534.046498	0.099494	69.950144	3.033	-1.367	-1.29	0.077
7	-306.230990	0.065414	-306.316717	0.060718	56.741424	2.461	-1.940	-1.86	0.080
9	-362.682729	0.102287	-362.794064	0.100020	71.286745	3.091	-1.309	-1.43	0.121
10	-284.131236	0.050105	-284.242443	0.047383	71.491286	3.100	-1.301	-1.40	0.099
11	-244.851601	0.024125	-244.964512	0.021089	72.757760	3.155	-1.246	-1.39	0.139
12	-436.417113	0.072092	-436.543937	0.068446	81.871048	3.550	-0.850	-0.95	0.100
13	-475.698901	0.097779	-475.823274	0.094156	80.318330	3.483	-0.918	-0.97	0.052
14	-280.103294	0.038008	-280.207213	0.034202	67.598922	2.931	-1.469	-1.39	0.079
15	-319.389617	0.062591	-319.490842	0.058988	65.780098	2.853	-1.548	-1.46	0.088
16	-507.815055	0.073915	-507.923262	0.069137	70.899015	3.075	-1.326	-1.18	0.146
17	-586.388235	0.126763	-586.488706	0.120411	67.032688	2.907	-1.494	-1.42	0.074
18	-296.097823	0.026023	-296.231636	0.023693	85.430635	3.705	-0.696	-0.63	0.066
19	-374.671766	0.074165	-374.799671	0.069717	83.052537	3.602	-0.799	-0.79	0.009
21	-270.666637	0.085845	-270.777822	0.082523	71.854435	3.116	-1.285	-1.21	0.075
23	-501.522643	0.161393	-501.639098	0.161810	72.814988	3.158	-1.243	-0.90	0.343
24	-173.662778	0.079754	-173.746274	0.079513	52.545674	2.279	-2.122	-1.76	0.362
25	-309.947287	0.111412	-310.050303	0.110279	65.354488	2.834	-1.567	-1.36	0.207
26	-540.797235	0.187212	-540.905281	0.186797	68.060221	2.951	-1.449	-1.10	0.349
28	-500.339088	0.141768	-500.474006	0.141909	84.574144	3.668	-0.733	-0.52	0.213
29	-365.239428	0.127573	-365.328103	0.125948	56.664540	2.457	-1.944	-1.79	0.154
30	-385.108147	0.114792	-385.209791	0.111626	65.769039	2.852	-1.549	-1.51	0.039
31	-309.946989	0.111534	-310.053794	0.106251	70.336231	3.050	-1.351	-1.38	0.029
32	-309.946762	0.110660	-310.057100	0.108845	70.377092	3.052	-1.349	-1.26	0.089
33	-369.852961	0.076167	-369.960838	0.073189	69.563025	3.017	-1.384	-1.26	0.124
34	-730.136682	0.074059	-730.249753	0.071145	72.781605	3.156	-1.245	-1.16	0.085
35	-423.204870	0.118286	-423.336605	0.117387	83.228854	3.609	-0.792	-0.47	0.322
36	-362.844330	0.082046	-362.974652	0.080893	82.501898	3.578	-0.823	-0.53	0.293
37	-362.841495	0.081621	-362.959944	0.080193	75.223875	3.262	-1.139	-0.87	0.269
38	-607.521768	0.083642	-607.637873	0.084164	72.529487	3.145	-1.256	-0.96	0.296
40	-540.218146	0.180442	-540.299572	0.173947	55.171193	2.393	-2.008	-1.96	0.048
41	-423.852172	0.131768	-423.938648	0.126307	57.691009	2.502	-1.899	-1.96	0.061
42	-459.755589	0.109874	-459.835813	0.105434	53.127407	2.304	-2.097	-2.13	0.033
43	-499.036563	0.135943	-499.116283	0.131748	52.657149	2.283	-2.117	-2.16	0.043
44	-385.543156	0.117117	-385.609804	0.110975	45.676806	1.981	-2.420		
45	-539.053534	0.161212	-539.120107	0.154908	45.730744	1.983	-2.418	-2.38	0.038
46	-615.222633	0.173814	-615.303612	0.167595	54.717727	2.373	-2.028	-1.98	0.048
47	-264.106659	0.050739	-264.179368	0.044664	49.437673	2.144	-2.257	-2.10	0.157
48	-555.090975	0.149767	-555.167146	0.142879	52.120385	2.260	-2.141	-1.97	0.173
49	-401.577948	0.105740	-401.656121	0.100318	52.456920	2.275	-2.126	-1.98	0.146
50	-248.070112	0.062304	-248.128769	0.055484	41.087462	1.782	-2.619	-2.40	0.223
52	-2254.223587	0.019105	-2254.348272	0.016426	79.922445	3.466	-0.935	-0.71	0.225
53	-600.710663	0.058582	-600.844978	0.054175	87.049683	3.775	-0.626	-0.50	0.126
54	-723.389265	0.153919	-723.515952	0.150287	81.775914	3.546	-0.855	-0.65	0.205
57	-499.007509	0.131957	-499.151033	0.131298	90.476128	3.924	-0.477	-0.51	0.033
58	-459.728275	0.107525	-459.874939	0.105726	93.162051	4.040	-0.361	-0.39	0.029
59	-420.444160	0.081106	-420.594224	0.079430	95.218514	4.129	-0.272	-0.34	0.068
60	-381.159841	0.055191	-381.313146	0.055062	96.280927	4.175	-0.226	-0.23	0.004
61	-840.626575	0.043662	-840.784309	0.042136	99.937635	4.334	-0.067	-0.10	0.033
62	-1300.091651	0.031678	-1300.253845	0.031080	102.153439	4.430	0.029	0.06	0.031

FUNCTIONAL LC-ωPBE

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	ΔG (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.924014	0.060975	-155.990380	0.052528	46.945457	2.036	-2.398	-2.56	0.162
2	-233.326396	0.096777	-233.385216	0.090486	40.857518	1.772	-2.662	-2.71	0.048
3	-191.853646	0.036706	-191.955855	0.032512	66.769035	2.895	-1.539	-1.19	0.349
4	-345.436987	0.081452	-345.536568	0.077883	64.727453	2.807	-1.627	-1.38	0.247
5	-384.748646	0.108113	-384.840837	0.104248	60.276284	2.614	-1.820	-1.55	0.270
6	-534.195561	0.104729	-534.303789	0.101601	69.876910	3.030	-1.404	-1.29	0.114
7	-306.382687	0.066681	-306.471022	0.062083	58.316391	2.529	-1.905	-1.86	0.045
9	-362.873964	0.104484	-362.992068	0.101909	75.727169	3.284	-1.150	-1.43	0.280
10	-284.272714	0.050932	-284.390569	0.048474	75.497296	3.274	-1.160	-1.40	0.240
11	-244.968192	0.024846	-245.087750	0.021799	76.935469	3.336	-1.098	-1.39	0.287
12	-436.603383	0.073486	-436.736429	0.069685	85.873188	3.724	-0.710	-0.95	0.240
13	-475.909617	0.099637	-476.040725	0.095813	84.670515	3.672	-0.763	-0.97	0.207
14	-280.222661	0.039040	-280.332338	0.035411	71.100340	3.083	-1.351	-1.39	0.039
15	-319.533864	0.064158	-319.641019	0.060519	69.523962	3.015	-1.419	-1.46	0.041
16	-508.039677	0.075616	-508.148954	0.071230	71.324700	3.093	-1.341	-1.18	0.161
17	-586.662207	0.126732	-586.764338	0.123416	66.168551	2.869	-1.565	-1.42	0.145
18	-296.220448	0.026964	-296.361148	0.024870	89.604669	3.886	-0.549	-0.63	0.081
19	-374.843717	0.076205	-374.979260	0.072757	87.218079	3.782	-0.652	-0.79	0.138
21	-270.791569	0.087012	-270.902430	0.084282	71.279444	3.091	-1.343	-1.21	0.133
23	-501.741521	0.163570	-501.855361	0.164471	70.870367	3.073	-1.361	-0.90	0.461
24	-173.769553	0.080907	-173.855218	0.081151	53.602988	2.325	-2.110	-1.76	0.350
25	-310.096707	0.113165	-310.199001	0.112363	64.693658	2.805	-1.629	-1.36	0.269
26	-541.041872	0.189895	-541.146518	0.189676	65.803800	2.854	-1.581	-1.10	0.481
28	-500.547752	0.143740	-500.683723	0.144675	84.736359	3.675	-0.760	-0.52	0.240
29	-365.416451	0.129505	-365.506276	0.128945	56.717608	2.460	-1.975	-1.79	0.185
30	-385.290627	0.116360	-385.392823	0.113930	65.654043	2.847	-1.587	-1.51	0.077
31	-310.096597	0.113144	-310.203081	0.108672	69.626088	3.019	-1.415	-1.38	0.035
32	-310.096460	0.112150	-310.206725	0.110808	70.034536	3.037	-1.397	-1.26	0.137
33	-370.015110	0.077232	-370.122920	0.074669	69.260172	3.003	-1.431	-1.26	0.171
34	-730.281713	0.075298	-730.394722	0.073018	72.345090	3.137	-1.297	-1.16	0.137
35	-423.400293	0.119848	-423.529737	0.119450	81.476781	3.533	-0.901	-0.47	0.431
36	-363.000161	0.083220	-363.129134	0.082423	81.431959	3.531	-0.903	-0.53	0.373
37	-362.997996	0.082837	-363.114921	0.081824	74.007237	3.209	-1.225	-0.87	0.355
38	-607.782683	0.084822	-607.897945	0.085767	71.734720	3.111	-1.323	-0.96	0.363
40	-540.453616	0.183210	-540.533870	0.176513	54.562214	2.366	-2.068	-1.96	0.108
41	-424.054370	0.131362	-424.143473	0.128872	57.475097	2.492	-1.942	-1.96	0.018
42	-459.966932	0.111768	-460.049443	0.107476	54.469855	2.362	-2.072	-2.13	0.058
43	-499.272831	0.137822	-499.354902	0.134086	53.845067	2.335	-2.099	-2.16	0.061
44	-385.708276	0.119445	-385.775551	0.112699	46.448823	2.014	-2.420		
45	-539.278466	0.164223	-539.345360	0.157596	46.134683	2.001	-2.434	-2.38	0.054
46	-615.470218	0.176813	-615.551697	0.170417	55.142202	2.391	-2.043	-1.98	0.063
47	-264.222495	0.051785	-264.300725	0.045947	52.753386	2.288	-2.147	-2.10	0.047
48	-555.320294	0.152475	-555.397110	0.145155	52.796187	2.290	-2.145	-1.97	0.177
49	-401.747377	0.107646	-401.827701	0.102221	53.808121	2.333	-2.101	-1.98	0.121
50	-248.181011	0.063487	-248.244436	0.057025	43.854449	1.902	-2.533	-2.40	0.137
52	-2254.472739	0.020860	-2254.599920	0.018202	81.475304	3.533	-0.901	-0.71	0.191
53	-600.942981	0.057718	-601.077421	0.055677	85.642856	3.714	-0.720	-0.50	0.220
54	-723.673421	0.157026	-723.803276	0.153309	83.817421	3.635	-0.800	-0.65	0.150
57	-499.246145	0.134140	-499.390850	0.134024	90.876152	3.941	-0.493	-0.51	0.017
58	-459.941784	0.109706	-460.090020	0.107843	94.188653	4.085	-0.350	-0.39	0.040
59	-420.632961	0.082758	-420.784227	0.081069	95.980846	4.162	-0.272	-0.34	0.068
60	-381.324019	0.056379	-381.478111	0.056306	96.739510	4.195	-0.239	-0.23	0.009
61	-840.810168	0.044947	-840.968911	0.043457	100.547645	4.360	-0.074	-0.10	0.026
62	-1300.294824	0.033104	-1300.458291	0.032527	102.938798	4.464	0.030	0.06	0.030

FUNCTIONAL TPSS

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.073293	0.057474	-156.136257	0.046257	46.549661	2.019	-2.356	-2.56	0.204
2	-233.533776	0.092249	-233.590555	0.085996	39.553253	1.715	-2.659	-2.71	0.051
3	-192.020289	0.034639	-192.117475	0.030214	63.761552	2.765	-1.609	-1.19	0.419
4	-345.752440	0.077397	-345.847554	0.073637	62.044289	2.691	-1.684	-1.38	0.304
5	-385.092543	0.103043	-385.181695	0.099108	58.412427	2.533	-1.841	-1.55	0.291
6	-534.617829	0.098768	-534.725540	0.095764	69.474750	3.013	-1.362	-1.29	0.072
7	-306.630775	0.063075	-306.715105	0.058185	55.986661	2.428	-1.947	-1.86	0.087
9	-363.156852	0.100812	-363.264596	0.096682	70.202439	3.044	-1.330	-1.43	0.100
10	-284.494315	0.048165	-284.602553	0.045373	69.672527	3.021	-1.353	-1.40	0.047
11	-245.159307	0.022447	-245.269286	0.019558	70.825439	3.071	-1.303	-1.39	0.082
12	-436.988664	0.069098	-437.111651	0.065269	79.578248	3.451	-0.924	-0.95	0.026
13	-476.325462	0.094297	-476.445895	0.090526	77.939165	3.380	-0.995	-0.97	0.025
14	-280.477836	0.035870	-280.579985	0.032009	66.522493	2.885	-1.490	-1.39	0.100
15	-319.818773	0.060002	-319.918044	0.056244	64.651561	2.804	-1.571	-1.46	0.111
16	-508.468805	0.070377	-508.577591	0.065834	71.115208	3.084	-1.291	-1.18	0.111
17	-587.151172	0.120731	-587.252390	0.115319	66.911458	2.902	-1.473	-1.42	0.053
18	-296.488514	0.023666	-296.620272	0.021435	84.079361	3.646	-0.728	-0.63	0.098
19	-375.172067	0.070745	-375.297254	0.067002	80.904808	3.508	-0.866	-0.79	0.076
21	-271.050230	0.083393	-271.159816	0.080443	70.617338	3.062	-1.312	-1.21	0.102
23	-502.225019	0.156836	-502.340449	0.157018	72.319131	3.136	-1.238	-0.90	0.338
24	-173.909678	0.077561	-173.993514	0.076904	53.020321	2.299	-2.075	-1.76	0.315
25	-310.385962	0.108446	-310.487883	0.106903	64.924500	2.815	-1.559	-1.36	0.199
26	-541.554227	0.182196	-541.661940	0.181431	68.071120	2.952	-1.423	-1.10	0.323
28	-501.033343	0.137845	-501.164944	0.137442	82.833663	3.592	-0.782	-0.52	0.262
29	-365.749089	0.124255	-365.838171	0.122156	57.217195	2.481	-1.893	-1.79	0.103
30	-385.634384	0.111846	-385.734218	0.107258	65.525488	2.842	-1.533	-1.51	0.023
31	-310.385579	0.108622	-310.491090	0.105674	68.058573	2.951	-1.423	-1.38	0.043
32	-310.385281	0.107861	-310.493844	0.105608	69.537749	3.016	-1.359	-1.26	0.099
33	-370.333147	0.073620	-370.440129	0.070454	69.119055	2.997	-1.377	-1.26	0.117
34	-730.687520	0.071538	-730.799267	0.067636	72.570856	3.147	-1.227	-1.16	0.067
35	-423.781739	0.115143	-423.913537	0.114037	83.398337	3.617	-0.758	-0.47	0.288
36	-363.350282	0.079413	-363.479416	0.078049	81.889003	3.551	-0.823	-0.53	0.293
37	-363.347037	0.079025	-363.464418	0.077153	74.832516	3.245	-1.129	-0.87	0.259
38	-608.246943	0.080299	-608.362020	0.080326	72.195439	3.131	-1.244	-0.96	0.284
40	-540.975401	0.172916	-541.056011	0.168343	53.453227	2.318	-2.056	-1.96	0.096
41	-424.428637	0.126144	-424.514641	0.122324	56.365158	2.444	-1.930	-1.96	0.030
42	-460.363789	0.106370	-460.443427	0.101733	52.882955	2.293	-2.081	-2.13	0.049
43	-499.699889	0.132109	-499.778967	0.127747	52.359387	2.271	-2.104	-2.16	0.056
44	-386.081176	0.113810	-386.146678	0.107489	45.069217	1.954	-2.420		
45	-539.800039	0.156458	-539.866270	0.150112	45.542676	1.975	-2.399	-2.38	0.019
46	-616.069142	0.168560	-616.148848	0.162358	53.907492	2.338	-2.037	-1.98	0.057
47	-264.464536	0.048697	-264.535690	0.042483	48.549200	2.105	-2.269	-2.10	0.169
48	-555.852293	0.145141	-555.928084	0.138301	51.851638	2.249	-2.126	-1.97	0.158
49	-402.130914	0.102453	-402.207886	0.096860	51.810477	2.247	-2.128	-1.98	0.148
50	-248.413908	0.060244	-248.470485	0.053089	39.992779	1.734	-2.640	-2.40	0.244
52	-2255.464487	0.016327	-2255.587348	0.013220	79.046016	3.428	-0.947	-0.71	0.237
53	-601.528143	0.055223	-601.660792	0.051069	85.844870	3.723	-0.652	-0.50	0.152
54	-724.381637	0.147863	-724.504937	0.144628	79.401664	3.443	-0.931	-0.65	0.281
57	-499.670182	0.127575	-499.811118	0.127314	88.602440	3.842	-0.532	-0.51	0.022
58	-460.335869	0.104159	-460.479971	0.102542	91.439632	3.965	-0.409	-0.39	0.019
59	-420.997059	0.078141	-421.144501	0.076595	93.491363	4.054	-0.320	-0.34	0.020
60	-381.658004	0.052865	-381.808655	0.052649	94.670464	4.105	-0.269	-0.23	0.039
61	-841.292110	0.041206	-841.447241	0.039615	98.344446	4.265	-0.110	-0.10	0.010
62	-1300.924401	0.028985	-1301.083926	0.028305	100.530293	4.360	-0.015	0.06	0.075

FUNCTIONAL TPSSh

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	D_G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.056512	0.059310	-156.119076	0.049348	45.510836	1.974	-2.378	-2.56	0.182
2	-233.510952	0.093820	-233.567290	0.087550	39.287065	1.704	-2.648	-2.71	0.062
3	-191.996948	0.035472	-192.094096	0.031024	63.752728	2.765	-1.587	-1.19	0.397
4	-345.712841	0.078886	-345.807612	0.075109	61.839901	2.682	-1.670	-1.38	0.290
5	-385.050106	0.104952	-385.138668	0.100936	58.093411	2.519	-1.832	-1.55	0.282
6	-534.552855	0.100985	-534.660148	0.097694	69.392051	3.009	-1.342	-1.29	0.052
7	-306.594453	0.064515	-306.678620	0.059579	55.912703	2.425	-1.927	-1.86	0.067
9	-363.112324	0.102686	-363.221860	0.098554	71.327261	3.093	-1.258	-1.43	0.172
10	-284.455954	0.049165	-284.565876	0.046456	70.676664	3.065	-1.286	-1.40	0.114
11	-245.124054	0.023318	-245.235712	0.020351	71.928321	3.119	-1.232	-1.39	0.153
12	-436.931430	0.070676	-437.055858	0.066871	80.467269	3.489	-0.862	-0.95	0.088
13	-476.265040	0.096196	-476.387042	0.092434	78.917822	3.422	-0.929	-0.97	0.041
14	-280.441057	0.037003	-280.543399	0.033134	66.648071	2.890	-1.461	-1.39	0.071
15	-319.778924	0.061444	-319.878511	0.057710	64.834820	2.812	-1.540	-1.46	0.080
16	-508.403863	0.072230	-508.511526	0.067557	70.491946	3.057	-1.294	-1.18	0.114
17	-587.080036	0.123032	-587.180219	0.118126	65.943733	2.860	-1.492	-1.42	0.072
18	-296.447002	0.024841	-296.579330	0.022534	84.484470	3.664	-0.688	-0.63	0.058
19	-375.124252	0.072791	-375.250385	0.066606	83.031128	3.601	-0.751	-0.79	0.039
21	-271.021927	0.084807	-271.130499	0.081902	69.952405	3.033	-1.318	-1.21	0.108
23	-502.171621	0.159412	-502.285936	0.159656	71.580981	3.104	-1.247	-0.90	0.347
24	-173.892412	0.078854	-173.975603	0.078351	52.518382	2.277	-2.074	-1.76	0.314
25	-310.354464	0.110172	-310.455236	0.108764	64.118736	2.781	-1.571	-1.36	0.211
26	-541.497850	0.184973	-541.604170	0.184436	67.053272	2.908	-1.443	-1.10	0.343
28	-500.979565	0.140067	-501.111049	0.139848	82.644675	3.584	-0.767	-0.52	0.247
29	-365.709911	0.126386	-365.798111	0.124280	56.667738	2.457	-1.894	-1.79	0.104
30	-385.592294	0.113577	-385.691454	0.109537	64.758942	2.808	-1.543	-1.51	0.033
31	-310.354104	0.110352	-310.458564	0.107445	67.373203	2.922	-1.430	-1.38	0.050
32	-310.353863	0.109548	-310.461497	0.107407	68.884735	2.987	-1.364	-1.26	0.104
33	-370.293522	0.075017	-370.399333	0.071931	68.333814	2.963	-1.388	-1.26	0.128
34	-730.652559	0.072928	-730.763326	0.069235	71.824890	3.115	-1.237	-1.16	0.077
35	-423.735048	0.117031	-423.865341	0.116015	82.397635	3.573	-0.778	-0.47	0.308
36	-363.308000	0.080880	-363.436030	0.079595	81.146397	3.519	-0.832	-0.53	0.302
37	-363.305000	0.080479	-363.421053	0.078738	73.916940	3.205	-1.146	-0.87	0.276
38	-608.183153	0.082003	-608.296972	0.082203	71.297286	3.092	-1.259	-0.96	0.299
40	-540.917609	0.175509	-540.997137	0.171760	52.257428	2.266	-2.085	-1.96	0.125
41	-424.383032	0.127806	-424.468483	0.122276	57.091334	2.476	-1.875	-1.96	0.085
42	-460.311275	0.108341	-460.390230	0.103712	52.450155	2.275	-2.077	-2.13	0.053
43	-499.644340	0.134390	-499.722760	0.130047	51.933988	2.252	-2.099	-2.16	0.061
44	-386.040073	0.115721	-386.104701	0.109378	44.535110	1.931	-2.420		
45	-539.742578	0.159146	-539.807527	0.152712	44.793546	1.942	-2.409	-2.38	0.029
46	-616.003115	0.171431	-616.082022	0.165138	53.463754	2.318	-2.033	-1.98	0.053
47	-264.432640	0.049843	-264.503585	0.043636	48.413987	2.099	-2.252	-2.10	0.152
48	-555.790958	0.147680	-555.865621	0.140776	51.183953	2.220	-2.132	-1.97	0.164
49	-402.085886	0.104300	-402.162138	0.098707	51.358685	2.227	-2.124	-1.98	0.144
50	-248.385592	0.061445	-248.442055	0.054396	39.854776	1.728	-2.623	-2.40	0.227
52	-2255.385646	0.017586	-2255.508595	0.014610	79.018776	3.427	-0.925	-0.71	0.215
53	-601.448200	0.056818	-601.580459	0.052629	85.622219	3.713	-0.638	-0.50	0.138
54	-724.295657	0.150959	-724.419236	0.147507	79.713054	3.457	-0.895	-0.65	0.245
57	-499.613464	0.130166	-499.754910	0.129568	89.133491	3.865	-0.486	-0.51	0.024
58	-460.282418	0.106185	-460.426949	0.104386	91.823045	3.982	-0.369	-0.39	0.021
59	-420.946643	0.079844	-421.094489	0.078144	93.841917	4.069	-0.282	-0.34	0.058
60	-381.610663	0.054155	-381.761669	0.053924	94.902537	4.115	-0.236	-0.23	0.006
61	-841.237935	0.042480	-841.393535	0.040880	98.644458	4.278	-0.074	-0.10	0.026
62	-1300.863457	0.030289	-1301.023606	0.028941	101.340739	4.395	0.043	0.06	0.017

FUNCTIONAL M06

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.907695	0.058773	-155.972198	0.050825	45.463634	1.972	-2.453	-2.56	0.107
2	-233.296627	0.093481	-233.355325	0.087284	40.722293	1.766	-2.659	-2.71	0.051
3	-191.858129	0.035246	-191.955282	0.030872	63.708740	2.763	-1.662	-1.19	0.472
4	-345.440713	0.078838	-345.536201	0.075198	62.203921	2.697	-1.727	-1.38	0.347
5	-384.743124	0.104085	-384.832228	0.101085	57.795950	2.506	-1.919	-1.55	0.369
6	-534.225684	0.102460	-534.332991	0.099240	69.357211	3.008	-1.417	-1.29	0.127
7	-306.390483	0.064803	-306.475156	0.060049	56.116289	2.433	-1.991	-1.86	0.131
9	-362.857500	0.102262	-362.970069	0.098876	72.762822	3.155	-1.270	-1.43	0.160
10	-284.274269	0.049356	-284.386234	0.046918	71.788868	3.113	-1.312	-1.40	0.088
11	-244.978204	0.023035	-245.092055	0.020218	73.210705	3.175	-1.250	-1.39	0.135
12	-436.619609	0.070993	-436.747912	0.067175	82.907153	3.595	-0.830	-0.95	0.120
13	-475.917849	0.096175	-476.043665	0.092431	81.300078	3.526	-0.899	-0.97	0.071
14	-280.229684	0.036946	-280.335216	0.033148	68.606013	2.975	-1.450	-1.39	0.060
15	-319.532749	0.062321	-319.635607	0.058701	66.816292	2.897	-1.527	-1.46	0.067
16	-508.068880	0.072339	-508.177432	0.067321	71.266183	3.090	-1.334	-1.18	0.154
17	-586.675898	0.123591	-586.776722	0.119396	65.900536	2.858	-1.567	-1.42	0.147
18	-296.233212	0.024967	-296.370214	0.022787	87.338047	3.787	-0.637	-0.63	0.007
19	-374.840260	0.074784	-374.971681	0.072691	83.780952	3.633	-0.792	-0.79	0.002
21	-270.773062	0.084211	-270.887548	0.081546	73.513235	3.188	-1.237	-1.21	0.027
23	-501.721107	0.159344	-501.839245	0.159499	74.035274	3.211	-1.214	-0.90	0.314
24	-173.736788	0.077969	-173.829439	0.077998	58.121291	2.520	-1.904	-1.76	0.144
25	-310.070509	0.108582	-310.176706	0.108117	66.931447	2.902	-1.522	-1.36	0.162
26	-541.013182	0.184613	-541.122994	0.183844	69.390795	3.009	-1.416	-1.10	0.316
28	-500.532829	0.139415	-500.668480	0.139694	84.947446	3.684	-0.741	-0.52	0.221
29	-365.389277	0.125213	-365.484882	0.124375	60.519164	2.624	-1.800	-1.79	0.010
30	-385.277658	0.112202	-385.383209	0.110719	67.164768	2.913	-1.512	-1.51	0.002
31	-310.069864	0.109557	-310.179801	0.106904	70.650894	3.064	-1.361	-1.38	0.019
32	-310.069592	0.109346	-310.183520	0.107528	72.631991	3.150	-1.275	-1.26	0.015
33	-370.021900	0.074713	-370.133422	0.071832	71.789262	3.113	-1.312	-1.26	0.052
34	-730.373856	0.072426	-730.490276	0.068532	75.497750	3.274	-1.151	-1.16	0.009
35	-423.392261	0.116693	-423.526474	0.116040	84.629377	3.670	-0.755	-0.47	0.285
36	-363.000197	0.080477	-363.133257	0.079353	84.201366	3.651	-0.773	-0.53	0.243
37	-362.997172	0.080015	-363.118770	0.078844	77.038632	3.341	-1.084	-0.87	0.214
38	-607.831545	0.082924	-607.951094	0.083447	74.690075	3.239	-1.186	-0.96	0.226
40	-540.432656	0.178030	-540.514275	0.171305	55.436486	2.404	-2.021	-1.96	0.061
41	-424.040632	0.130138	-424.126465	0.125760	56.608489	2.455	-1.970	-1.96	0.010
42	-459.973950	0.108396	-460.054129	0.104259	52.908782	2.294	-2.131	-2.13	0.001
43	-499.270707	0.133741	-499.350322	0.130143	52.216623	2.264	-2.161	-2.16	0.001
44	-385.694256	0.115135	-385.761915	0.109117	46.232998	2.005	-2.420		
45	-539.265033	0.158709	-539.332338	0.152360	46.218551	2.004	-2.421	-2.38	0.041
46	-615.462409	0.171332	-615.543798	0.165053	55.012863	2.386	-2.039	-1.98	0.059
47	-264.223107	0.049458	-264.297166	0.043546	50.182791	2.176	-2.249	-2.10	0.149
48	-555.315099	0.147524	-555.391939	0.140704	52.497512	2.277	-2.148	-1.97	0.180
49	-401.741721	0.103915	-401.820953	0.098493	53.121429	2.304	-2.121	-1.98	0.141
50	-248.173859	0.060975	-248.233317	0.054211	41.555119	1.802	-2.623	-2.40	0.227
52	-2254.942920	0.018860	-2255.067130	0.015995	79.740738	3.458	-0.967	-0.71	0.257
53	-601.001853	0.057709	-601.135281	0.052819	86.795684	3.764	-0.661	-0.50	0.161
54	-723.701802	0.152322	-723.828067	0.148550	81.599425	3.539	-0.886	-0.65	0.236
57	-499.246197	0.132134	-499.387595	0.129495	90.384508	3.920	-0.505	-0.51	0.005
58	-459.949987	0.105746	-460.094530	0.103605	92.045274	3.992	-0.433	-0.39	0.043
59	-420.649149	0.080586	-420.796810	0.078703	93.840255	4.069	-0.356	-0.34	0.016
60	-381.348019	0.054378	-381.498705	0.054140	94.706579	4.107	-0.318	-0.23	0.088
61	-840.945800	0.043002	-841.101021	0.041382	98.419353	4.268	-0.157	-0.10	0.057
62	-1300.542149	0.030992	-1300.701900	0.030370	100.635482	4.364	-0.061	0.06	0.121

FUNCTIONAL M06-2X

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.963043	0.060034	-156.024434	0.052026	43.548473	1.888	-2.472	-2.56	0.088
2	-233.380855	0.095089	-233.436686	0.088636	39.083619	1.695	-2.665	-2.71	0.045
3	-191.902516	0.036121	-191.998207	0.031877	62.709919	2.719	-1.641	-1.19	0.451
4	-345.546980	0.080080	-345.641714	0.076853	61.471348	2.666	-1.695	-1.38	0.315
5	-384.862416	0.106207	-384.950550	0.102873	57.397064	2.489	-1.871	-1.55	0.321
6	-534.327412	0.103216	-534.435004	0.101128	68.825386	2.985	-1.376	-1.29	0.086
7	-306.454823	0.065192	-306.538253	0.060361	55.385033	2.402	-1.958	-1.86	0.098
9	-362.929217	0.104157	-363.044117	0.100708	74.264955	3.221	-1.140	-1.43	0.290
10	-284.320058	0.050000	-284.434800	0.048162	73.155160	3.172	-1.188	-1.40	0.212
11	-245.011404	0.023858	-245.127751	0.021098	74.740668	3.241	-1.119	-1.39	0.266
12	-436.729853	0.072421	-436.859636	0.068619	83.825666	3.635	-0.725	-0.95	0.225
13	-476.039822	0.098085	-476.167507	0.094301	82.497620	3.578	-0.783	-0.97	0.187
14	-280.314096	0.038200	-280.417276	0.034424	67.115802	2.910	-1.450	-1.39	0.060
15	-319.628483	0.061402	-319.729537	0.057680	65.747924	2.851	-1.509	-1.46	0.049
16	-508.190453	0.074477	-508.296023	0.069761	69.205882	3.001	-1.359	-1.18	0.179
17	-586.820447	0.125272	-586.919332	0.122187	63.986683	2.775	-1.585	-1.42	0.165
18	-296.317676	0.026173	-296.450857	0.023929	84.980395	3.685	-0.675	-0.63	0.045
19	-374.947366	0.076781	-375.076018	0.074271	82.304869	3.569	-0.791	-0.79	0.001
21	-270.871740	0.085831	-270.989539	0.083347	75.478364	3.273	-1.087	-1.21	0.123
23	-501.910291	0.161706	-502.031938	0.161720	76.326145	3.310	-1.050	-0.90	0.150
24	-173.785614	0.080244	-173.876234	0.080046	56.989002	2.471	-1.889	-1.76	0.129
25	-310.181215	0.111822	-310.291049	0.110732	69.605319	3.018	-1.342	-1.36	0.018
26	-541.215817	0.187654	-541.329524	0.187782	71.271990	3.091	-1.270	-1.10	0.170
28	-500.724189	0.142062	-500.866534	0.142229	89.218104	3.869	-0.491	-0.52	0.029
29	-365.516202	0.128040	-365.610881	0.126451	60.408944	2.620	-1.741	-1.79	0.049
30	-385.395720	0.114795	-385.504703	0.112552	69.795009	3.027	-1.334	-1.51	0.176
31	-310.180408	0.111488	-310.293920	0.108864	72.876263	3.160	-1.200	-1.38	0.180
32	-310.180368	0.111153	-310.297591	0.109540	74.570683	3.234	-1.126	-1.26	0.134
33	-370.120429	0.076314	-370.234946	0.073498	73.627045	3.193	-1.167	-1.26	0.093
34	-730.478882	0.074065	-730.598770	0.071748	76.684457	3.325	-1.035	-1.16	0.125
35	-423.521260	0.118724	-423.658259	0.118157	86.323776	3.743	-0.617	-0.47	0.147
36	-363.128073	0.081989	-363.264137	0.080971	86.019985	3.730	-0.630	-0.53	0.100
37	-363.125429	0.082193	-363.250224	0.080798	79.185369	3.434	-0.926	-0.87	0.056
38	-607.946593	0.084770	-608.069619	0.083144	78.220601	3.392	-0.968	-0.96	0.008
40	-540.641018	0.180397	-540.720576	0.173351	54.344757	2.357	-2.004	-1.96	0.044
41	-424.171827	0.131092	-424.256649	0.128829	54.646555	2.370	-1.990	-1.96	0.030
42	-460.100383	0.109829	-460.179608	0.105882	52.191418	2.263	-2.097	-2.13	0.033
43	-499.409671	0.136408	-499.488553	0.132530	51.932473	2.252	-2.108	-2.16	0.052
44	-385.843840	0.116878	-385.909229	0.110967	44.741730	1.940	-2.420		
45	-539.475947	0.160839	-539.541233	0.154618	44.871476	1.946	-2.414	-2.38	0.034
46	-615.704201	0.173770	-615.784023	0.168082	53.658041	2.327	-2.033	-1.98	0.053
47	-264.308242	0.050809	-264.379197	0.044582	48.432222	2.100	-2.260	-2.10	0.160
48	-555.523766	0.149704	-555.598361	0.142701	51.202920	2.220	-2.140	-1.97	0.172
49	-401.889151	0.105529	-401.965970	0.100313	51.477661	2.232	-2.128	-1.98	0.148
50	-248.260820	0.062402	-248.318652	0.055808	40.427657	1.753	-2.607	-2.40	0.211
52	-2255.111801	0.018219	-2255.236034	0.016102	79.285473	3.438	-0.922	-0.71	0.212
53	-601.205902	0.056708	-601.337339	0.053813	84.294109	3.655	-0.705	-0.50	0.205
54	-723.969009	0.153373	-724.095757	0.150069	81.608944	3.539	-0.821	-0.65	0.171
57	-499.378154	0.133003	-499.520573	0.131283	90.448371	3.922	-0.438	-0.51	0.072
58	-460.068993	0.108505	-460.214958	0.106529	92.834424	4.026	-0.334	-0.39	0.056
59	-420.755871	0.081458	-420.904935	0.079371	94.848318	4.113	-0.247	-0.34	0.093
60	-381.442665	0.055464	-381.594642	0.055334	95.448338	4.139	-0.221	-0.23	0.009
61	-841.046440	0.043616	-841.203207	0.042362	99.160019	4.300	-0.060	-0.10	0.040
62	-1300.648706	0.031752	-1300.810225	0.031183	101.711591	4.411	0.051	0.06	0.009

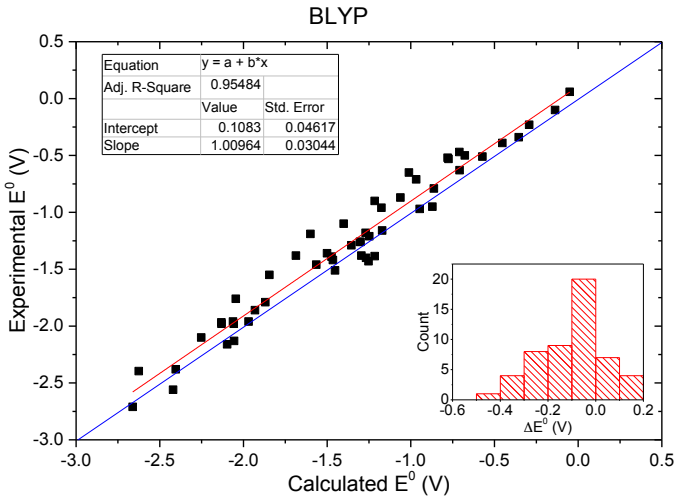
FUNCTIONAL M06-L

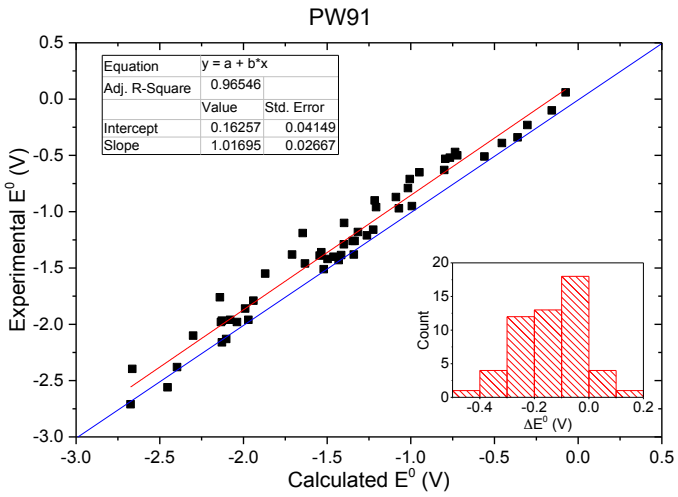
Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-156.014502	0.059190	-156.077215	0.049975	45.135083	1.957	-2.398	-2.56	0.162
2	-233.452011	0.094359	-233.507337	0.088371	38.474713	1.668	-2.687	-2.71	0.023
3	-191.959005	0.035345	-192.054110	0.030997	62.407564	2.706	-1.649	-1.19	0.459
4	-345.642419	0.078857	-345.735237	0.075362	60.437223	2.621	-1.735	-1.38	0.355
5	-384.972189	0.105827	-385.058071	0.101659	56.507317	2.450	-1.905	-1.55	0.355
6	-534.467810	0.101990	-534.572390	0.099204	67.373046	2.922	-1.434	-1.29	0.144
7	-306.538566	0.062774	-306.620279	0.059338	53.432150	2.317	-2.039	-1.86	0.179
9	-363.044758	0.104069	-363.147646	0.098394	68.124436	2.954	-1.401	-1.43	0.029
10	-284.409203	0.049999	-284.511177	0.046890	65.941008	2.860	-1.496	-1.40	0.096
11	-245.085741	0.022622	-245.190061	0.020166	67.003085	2.906	-1.450	-1.39	0.065
12	-436.853103	0.070706	-436.973585	0.067527	77.598542	3.365	-0.991	-0.95	0.041
13	-476.178446	0.096493	-476.295943	0.093334	75.712823	3.283	-1.072	-0.97	0.102
14	-280.385121	0.036925	-280.486496	0.033202	65.950055	2.860	-1.496	-1.39	0.106
15	-319.715291	0.062532	-319.813333	0.058999	63.738700	2.764	-1.592	-1.46	0.132
16	-508.318118	0.072340	-508.424564	0.067437	69.872827	3.030	-1.326	-1.18	0.146
17	-586.979510	0.123186	-587.076752	0.117743	64.435730	2.794	-1.561	-1.42	0.141
18	-296.390999	0.024563	-296.523370	0.022627	84.278588	3.655	-0.701	-0.63	0.071
19	-375.052950	0.074631	-375.177888	0.073104	79.357769	3.441	-0.914	-0.79	0.124
21	-270.954507	0.084738	-271.065769	0.082142	71.446497	3.098	-1.257	-1.21	0.047
23	-502.055030	0.160180	-502.170739	0.160507	72.403139	3.140	-1.216	-0.90	0.316
24	-173.843321	0.078677	-173.930070	0.078978	54.246846	2.352	-2.003	-1.76	0.243
25	-310.279668	0.111003	-310.381644	0.109621	64.858123	2.813	-1.543	-1.36	0.183
26	-541.374782	0.186604	-541.481652	0.186097	67.380339	2.922	-1.434	-1.10	0.334
28	-500.864616	0.140676	-500.996702	0.140342	83.094492	3.603	-0.752	-0.52	0.232
29	-365.622621	0.126752	-365.714099	0.125300	58.314455	2.529	-1.827	-1.79	0.037
30	-385.506560	0.113208	-385.605844	0.110191	64.195336	2.784	-1.572	-1.51	0.062
31	-310.278290	0.110466	-310.384797	0.107850	68.475643	2.969	-1.386	-1.38	0.006
32	-310.278064	0.110297	-310.388153	0.108217	70.386921	3.052	-1.303	-1.26	0.043
33	-370.217953	0.075043	-370.325550	0.072196	69.304362	3.005	-1.350	-1.26	0.090
34	-730.565389	0.072996	-730.678209	0.070186	72.558970	3.147	-1.209	-1.16	0.049
35	-423.647404	0.117429	-423.779218	0.116998	82.984746	3.599	-0.757	-0.47	0.287
36	-363.231217	0.080929	-363.361697	0.079904	82.520575	3.579	-0.777	-0.53	0.247
37	-363.228021	0.080650	-363.346985	0.079086	75.632882	3.280	-1.076	-0.87	0.206
38	-608.081536	0.083028	-608.197944	0.080863	74.405085	3.227	-1.129	-0.96	0.169
40	-540.792427	0.178871	-540.872695	0.172025	54.664689	2.371	-1.985	-1.96	0.025
41	-424.296659	0.131117	-424.378931	0.127338	53.997683	2.342	-2.014	-1.96	0.054
42	-460.222927	0.108257	-460.299580	0.103673	50.976492	2.211	-2.145	-2.13	0.015
43	-499.546753	0.134860	-499.622637	0.130278	50.493284	2.190	-2.166	-2.16	0.006
44	-385.950336	0.115829	-386.015458	0.109817	44.637588	1.936	-2.420		
45	-539.621293	0.160100	-539.686613	0.153506	45.126642	1.957	-2.399	-2.38	0.019
46	-615.867489	0.172034	-615.946936	0.165904	53.699880	2.329	-2.027	-1.98	0.047
47	-264.376476	0.049754	-264.446062	0.043740	47.439484	2.057	-2.298	-2.10	0.198
48	-555.670347	0.148035	-555.744923	0.141276	51.038323	2.213	-2.142	-1.97	0.174
49	-401.996901	0.104501	-402.073424	0.099129	51.389943	2.229	-2.127	-1.98	0.147
50	-248.328682	0.061427	-248.383593	0.054522	38.790236	1.682	-2.674	-2.40	0.278
52	-2255.238673	0.019018	-2255.359578	0.016368	77.531517	3.362	-0.994	-0.71	0.284
53	-601.354773	0.055846	-601.486756	0.053341	84.392865	3.660	-0.696	-0.50	0.196
54	-724.158525	0.152220	-724.281698	0.148531	79.606811	3.452	-0.904	-0.65	0.254
57	-499.524646	0.131295	-499.662987	0.131161	86.894263	3.768	-0.588	-0.51	0.078
58	-460.200688	0.106977	-460.342282	0.105314	89.895647	3.898	-0.457	-0.39	0.067
59	-420.872734	0.080606	-421.017944	0.078973	92.145360	3.996	-0.360	-0.34	0.020
60	-381.544382	0.054537	-381.693099	0.054321	93.456877	4.053	-0.303	-0.23	0.073
61	-841.153427	0.043204	-841.306397	0.041676	96.948985	4.204	-0.152	-0.10	0.052
62	-1300.760676	0.031318	-1300.917815	0.030507	99.114582	4.298	-0.058	0.06	0.118

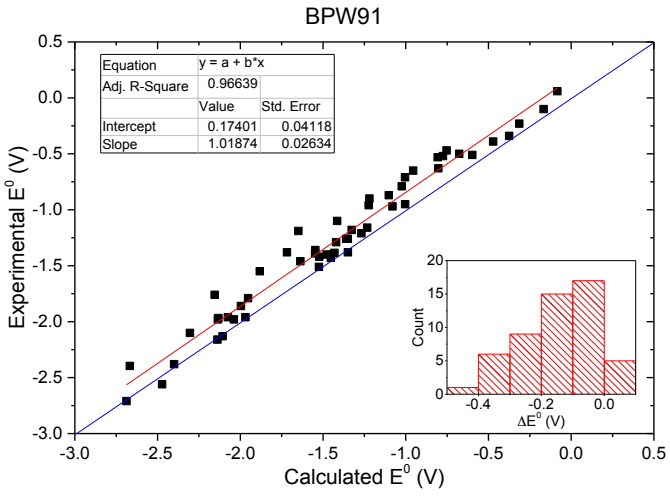
FUNCTIONAL M06-HF

Molecule	EE Neutral	Th.Correc.	EE Anion	Th.Correc.	^{D}G (Ha)	Eabs(V)	E0Calc(V)	E0exp(V)	MAD(V)
1	-155.994544	0.060738	-156.056373	0.053811	43.145522	1.871	-2.577	-2.56	0.017
2	-233.430179	0.095144	-233.488764	0.088867	40.701289	1.765	-2.683	-2.71	0.027
3	-191.928208	0.036829	-192.025989	0.032915	63.814449	2.767	-1.681	-1.19	0.491
4	-345.606755	0.081498	-345.705374	0.077362	64.479492	2.796	-1.652	-1.38	0.272
5	-384.927186	0.108023	-385.020486	0.102823	61.809385	2.680	-1.768	-1.55	0.218
6	-534.387632	0.105209	-534.500281	0.102916	72.127297	3.128	-1.320	-1.29	0.030
7	-306.493582	0.067104	-306.580700	0.062589	57.500999	2.494	-1.954	-1.86	0.094
9	-362.964105	0.105704	-363.089280	0.101197	81.376938	3.529	-0.919	-1.43	0.511
10	-284.339040	0.052915	-284.465312	0.048967	81.714582	3.544	-0.904	-1.40	0.496
11	-245.024664	0.025527	-245.151918	0.021871	82.147193	3.562	-0.886	-1.39	0.499
12	-436.783998	0.073351	-436.923718	0.069061	90.367844	3.919	-0.529	-0.95	0.421
13	-476.100041	0.099161	-476.238276	0.092684	90.808279	3.938	-0.510	-0.97	0.460
14	-280.363260	0.039094	-280.467848	0.035402	67.946575	2.947	-1.501	-1.39	0.111
15	-319.682314	0.064533	-319.785611	0.060807	67.157621	2.912	-1.536	-1.46	0.076
16	-508.259829	0.077277	-508.368452	0.073097	70.785504	3.070	-1.378	-1.18	0.198
17	-586.899893	0.126238	-587.003603	0.124389	66.238906	2.872	-1.576	-1.42	0.156
18	-296.365226	0.027335	-296.498088	0.024914	84.891559	3.681	-0.767	-0.63	0.137
19	-375.003965	0.076264	-375.133995	0.070673	85.103356	3.691	-0.757	-0.79	0.033
21	-270.926330	0.086693	-271.051092	0.084934	79.393130	3.443	-1.005	-1.21	0.205
23	-502.015039	0.161816	-502.144103	0.161957	80.900685	3.508	-0.940	-0.90	0.040
24	-173.818435	0.081855	-173.910882	0.080846	58.644583	2.543	-1.905	-1.76	0.145
25	-310.240897	0.113018	-310.359612	0.110968	75.781567	3.286	-1.162	-1.36	0.198
26	-541.327243	0.186176	-541.450281	0.187557	76.340980	3.311	-1.137	-1.10	0.037
28	-500.830626	0.142848	-500.983733	0.143356	95.756933	4.153	-0.295	-0.52	0.225
29	-365.591786	0.127986	-365.689227	0.128091	61.079215	2.649	-1.799	-1.79	0.009
30	-385.464401	0.116198	-385.582853	0.112818	76.450396	3.315	-1.133	-1.51	0.377
31	-310.241228	0.112393	-310.362488	0.109554	77.873018	3.377	-1.071	-1.38	0.309
32	-310.241230	0.112901	-310.365795	0.111466	79.065922	3.429	-1.019	-1.26	0.241
33	-370.179869	0.077264	-370.302348	0.075107	78.209843	3.392	-1.056	-1.26	0.204
34	-730.551062	0.074881	-730.678262	0.073273	80.827899	3.505	-0.943	-1.16	0.217
35	-423.590294	0.119662	-423.734529	0.118959	90.949717	3.944	-0.504	-0.47	0.034
36	-363.196798	0.082942	-363.339704	0.081610	90.511023	3.925	-0.523	-0.53	0.007
37	-363.194204	0.083257	-363.325628	0.081922	83.307402	3.613	-0.835	-0.87	0.035
38	-608.023824	0.085803	-608.154128	0.084751	82.426556	3.574	-0.874	-0.96	0.086
40	-540.758043	0.182467	-540.839364	0.176413	54.828982	2.378	-2.070	-1.96	0.110
41	-424.242858	0.132573	-424.333291	0.130098	58.300400	2.528	-1.920	-1.96	0.040
42	-460.173185	0.112564	-460.257886	0.108692	55.580445	2.410	-2.038	-2.13	0.092
43	-499.488090	0.138381	-499.572638	0.134702	55.363250	2.401	-2.047	-2.16	0.113
44	-385.928126	0.118329	-385.995848	0.111525	46.765714	2.028	-2.420		
45	-539.594708	0.163373	-539.662819	0.153335	49.039377	2.127	-2.321	-2.38	0.059
46	-615.839995	0.174892	-615.922352	0.168373	55.770324	2.418	-2.030	-1.98	0.050
47	-264.359398	0.051706	-264.432562	0.045373	49.884747	2.163	-2.285	-2.10	0.185
48	-555.642134	0.150854	-555.719638	0.143585	53.195847	2.307	-2.141	-1.97	0.173
49	-401.973229	0.106131	-402.052446	0.101114	52.857740	2.292	-2.156	-1.98	0.176
50	-248.311333	0.063167	-248.372827	0.056562	42.732991	1.853	-2.595	-2.40	0.199
52	-2255.256412	0.019230	-2255.385913	0.016015	83.280390	3.611	-0.837	-0.71	0.127
53	-601.309225	0.058086	-601.444588	0.054228	87.362171	3.788	-0.660	-0.50	0.160
54	-724.111882	0.153721	-724.244268	0.150605	85.028817	3.687	-0.761	-0.65	0.111
57	-499.447110	0.133242	-499.596673	0.132832	94.109040	4.081	-0.367	-0.51	0.143
58	-460.131603	0.109535	-460.283677	0.106041	97.620432	4.233	-0.215	-0.39	0.175
59	-420.812139	0.080860	-420.966852	0.080515	97.300671	4.219	-0.229	-0.34	0.111
60	-381.492772	0.055996	-381.649956	0.055728	98.802619	4.285	-0.163	-0.23	0.067
61	-841.113083	0.043661	-841.275184	0.042370	102.530025	4.446	-0.002	-0.10	0.098
62	-1300.731938	0.030694	-1300.898993	0.030911	104.692522	4.540	0.092	0.06	0.032

Figures S4.1 to S4.21. Plots of the correlation between the predicted and experimental E^0_{expRed} values for the different functionals. The blue line represent the ideal fit







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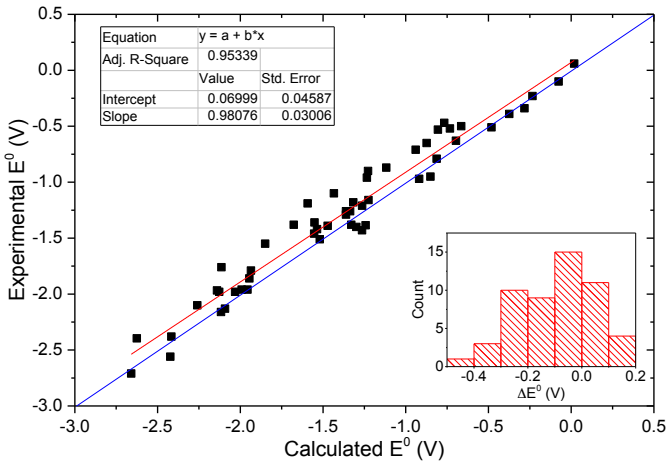

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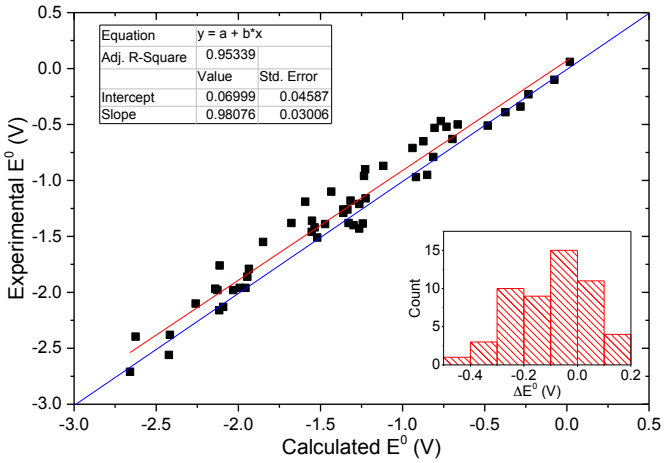

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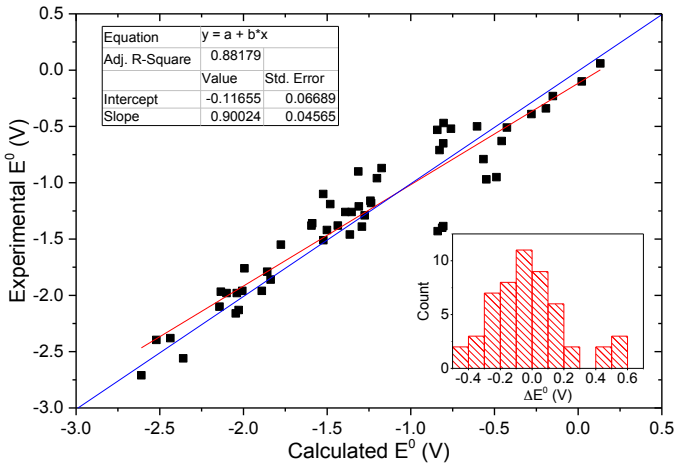
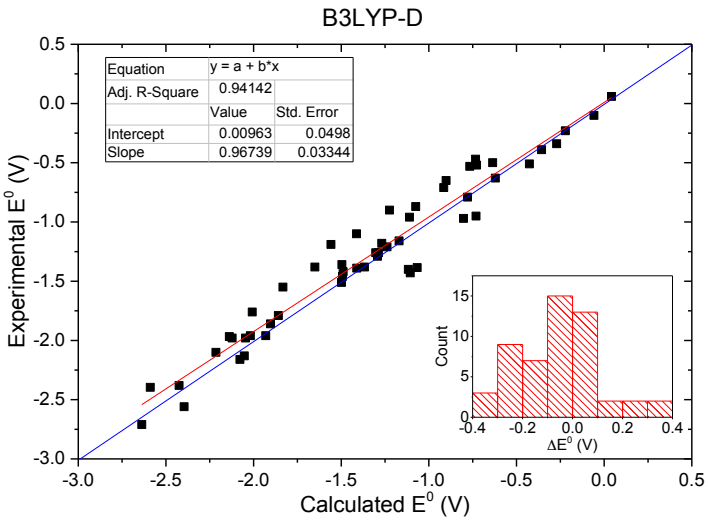
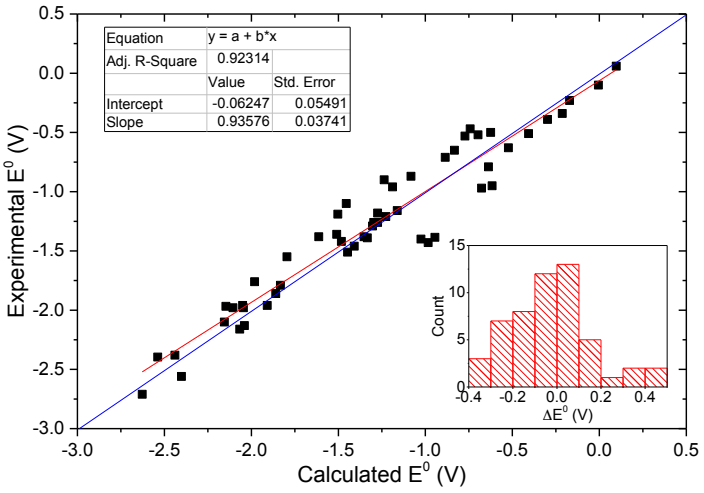
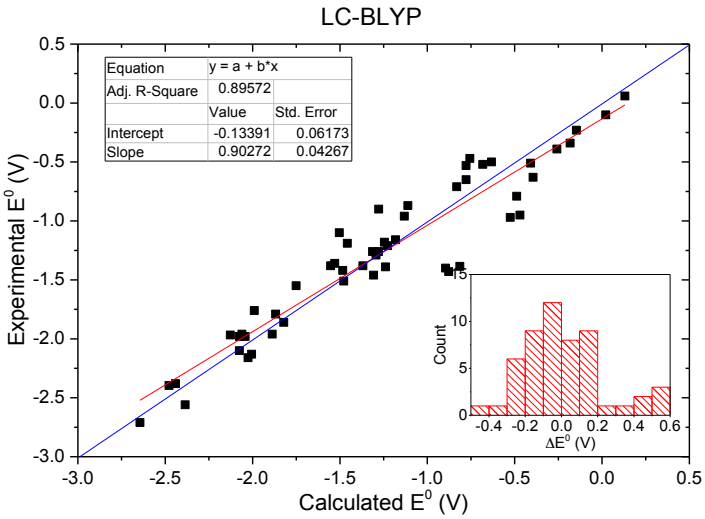
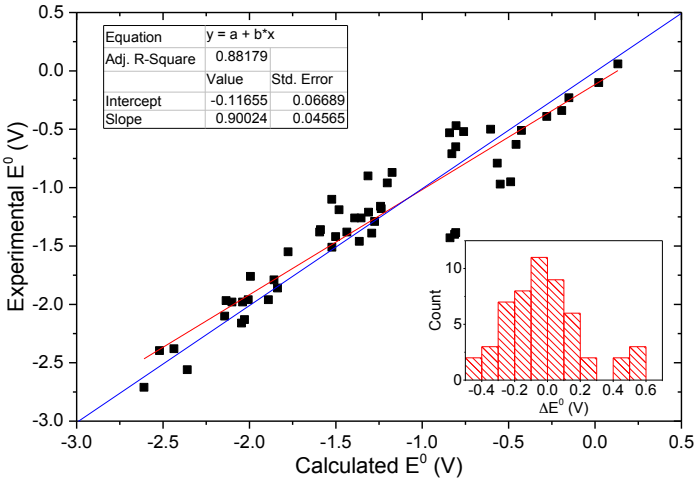



B3LYP-D
Equation y = a + b*x
Adj. R-Square 0.94142
Value Std. Error
Intercept 0.00963 0.0498
Slope 0.96739 0.03344
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)

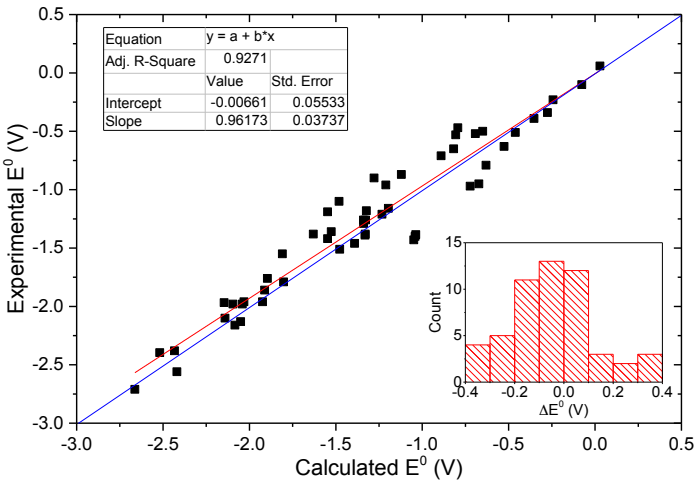

CAM-B3LYP
Equation y = a + b*x
Adj. R-Square 0.92314
Value Std. Error
Intercept -0.06247 0.05491
Slope 0.93576 0.03741
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)


LC-BLYP
Equation y = a + b*x
Adj. R-Square 0.89572
Value Std. Error
Intercept -0.13391 0.06173
Slope 0.90272 0.04267
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)

BHandHLYP



w-B97



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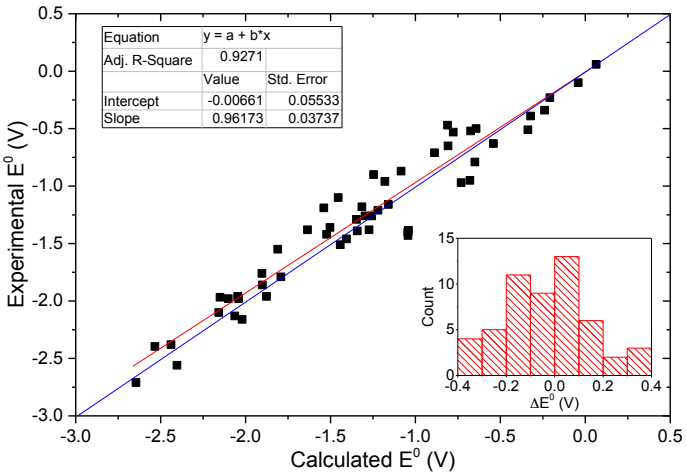
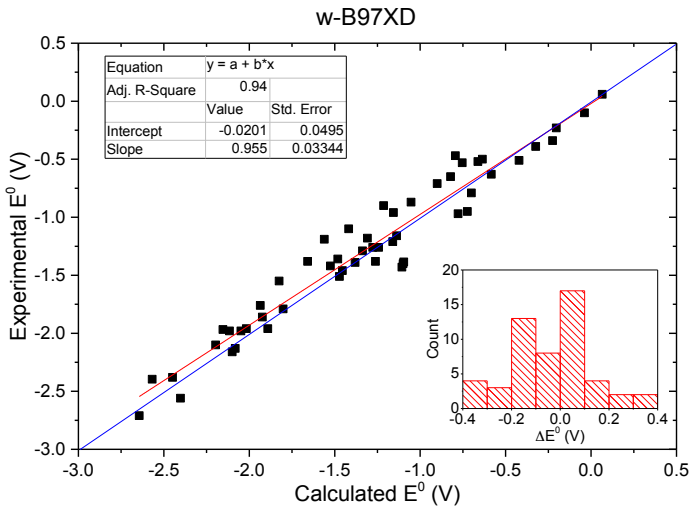
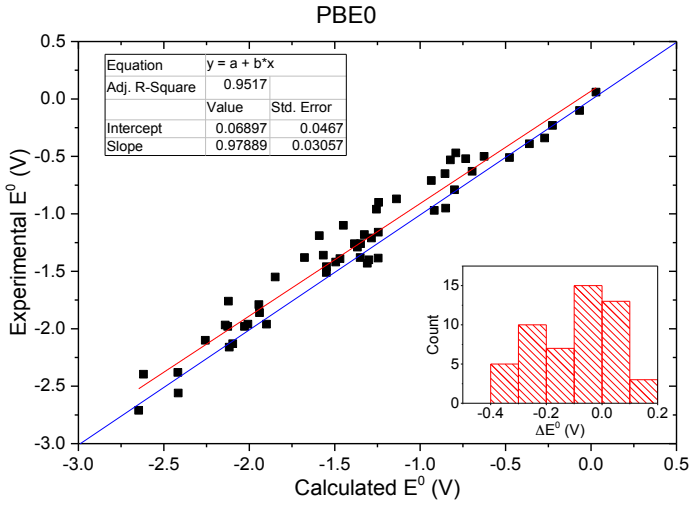
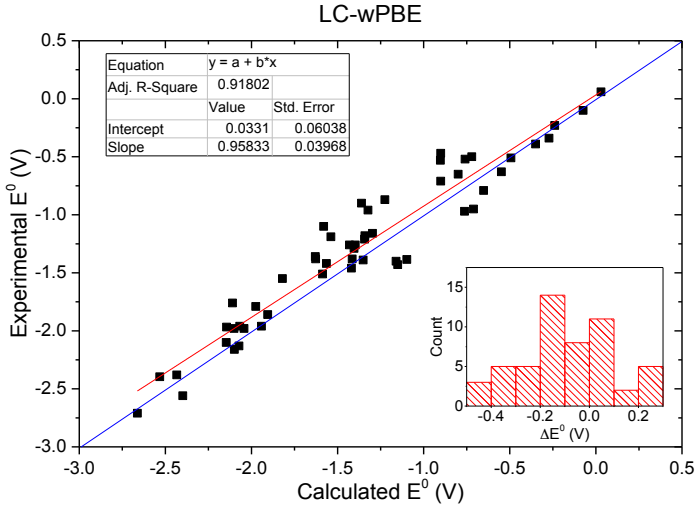
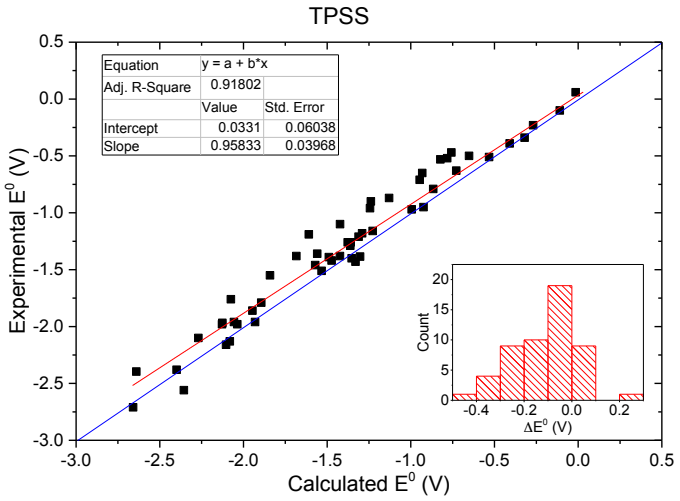
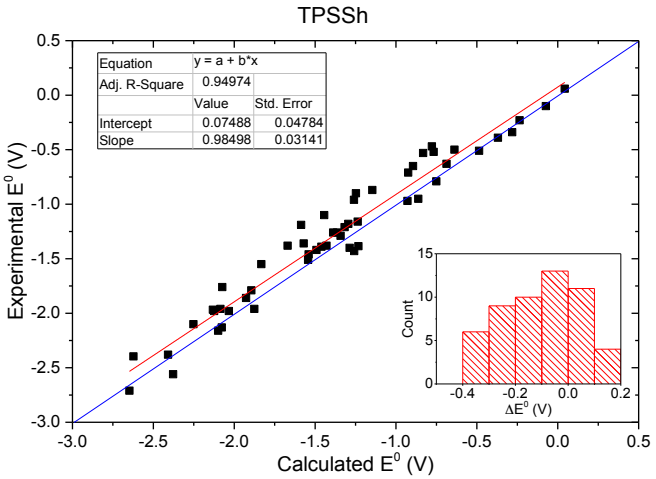


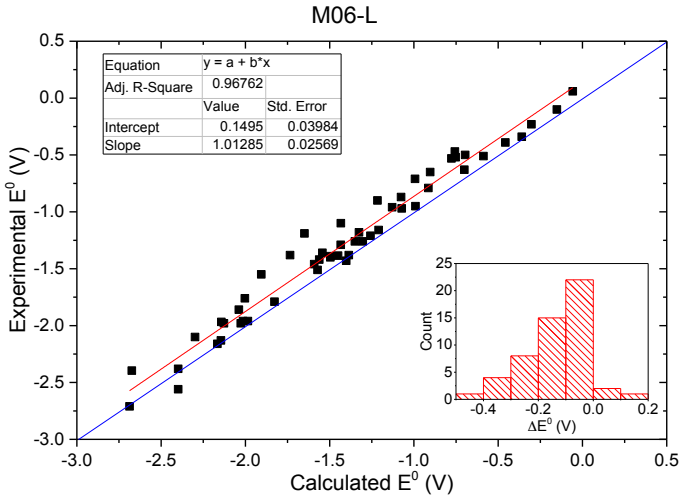

w-B97XD
Equation y = a + b*x
Adj. R-Square 0.94
Value Std. Error
Intercept -0.0201 0.0495
Slope 0.955 0.03344
Experimental E⁰ (V)
Calculated E⁰ (V)
Count
ΔE⁰ (V)

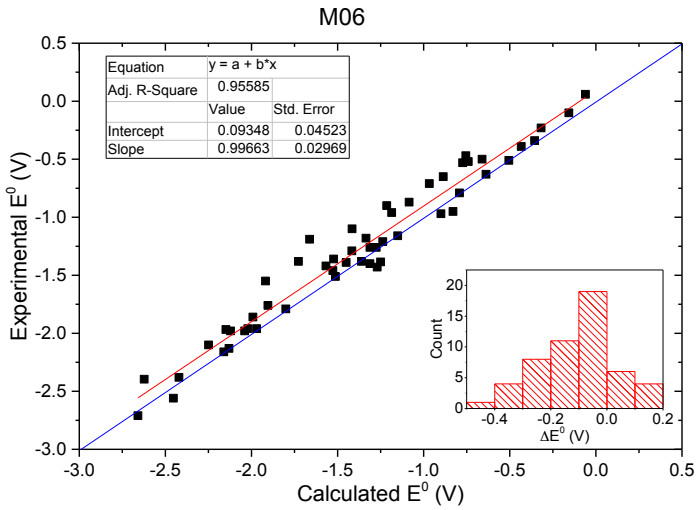

PBE0
Equation y = a + b*x
Adj. R-Square 0.9517
Value Std. Error
Intercept 0.06897 0.0467
Slope 0.97889 0.03057
Experimental E⁰ (V)
Calculated E⁰ (V)
Count
ΔE⁰ (V)

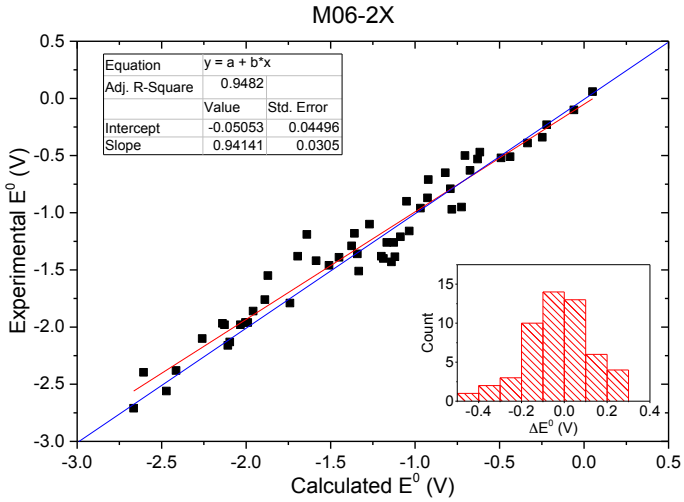

LC-wPBE
Equation y = a + b*x
Adj. R-Square 0.91802
Value Std. Error
Intercept 0.0331 0.06038
Slope 0.95833 0.03968
Experimental E⁰ (V)
Calculated E⁰ (V)
Count
ΔE⁰ (V)


TPSS
Equation y = a + b*x
Adj. R-Square 0.91802
Value Std. Error
Intercept 0.0331 0.06038
Slope 0.95833 0.03968
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)


TPSSh
Equation y = a + b*x
Adj. R-Square 0.94974
Value Std. Error
Intercept 0.07488 0.04784
Slope 0.98498 0.03141
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)


M06-L
Equation y = a + b*x
Adj. R-Square 0.96762
Value Std. Error
Intercept 0.1495 0.03984
Slope 1.01285 0.02569
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)


M06
Equation y = a + b*x
Adj. R-Square 0.95585
Value Std. Error
Intercept 0.09348 0.04523
Slope 0.99663 0.02969
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)


M06-2X
Equation y = a + b*x
Adj. R-Square 0.9482
Value Std. Error
Intercept -0.05053 0.04496
Slope 0.94141 0.0305
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)

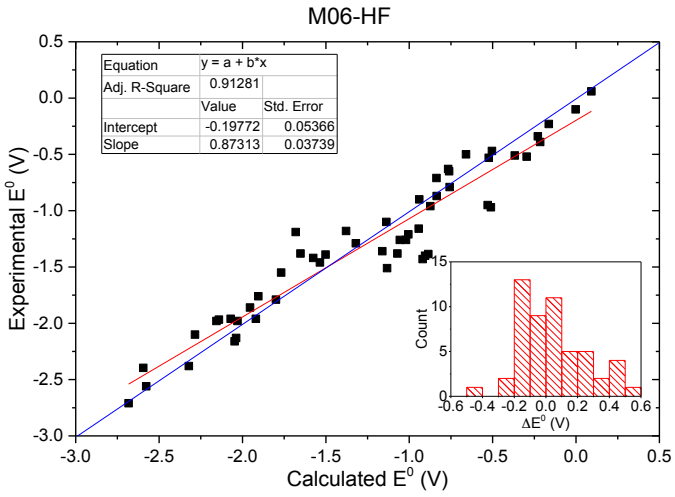
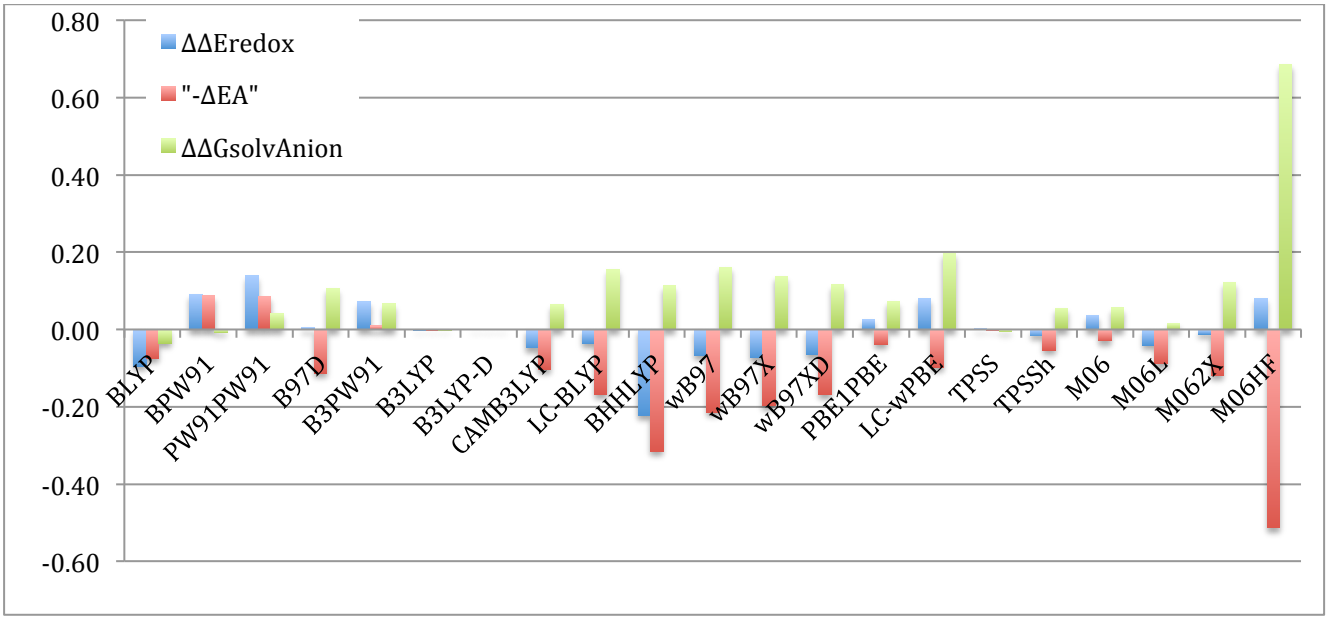

M06-HF
Equation y = a + b*x
Adj. R-Square 0.91281
Value Std. Error
Intercept -0.19772 0.05366
Slope 0.87313 0.03739
Experimental E0 (V)
Calculated E0 (V)
Count
ΔE0 (V)

Figure S5 Changes in the E^0_{Red}, (and their components *EA*s and $\Delta\Delta G_{(solv.\,A^{\bullet-}-A)}$) for compounds 40-50 with the different functionals with respect to the B3LYP-D used as reference.



Tables S11.1-3 Changes in the E^0_{Red} and their components *EA*s and $\Delta\Delta G_{(solv.\, A^{\bullet-}-A)}$ for compounds 40-50 with the different functionals with respect to the B3LYP-D used as reference.

Comp	BLYP	BPW91	PW91	B97D	B3PW91	B3LYP	B3LYP-D	CAMB3LYP	LC-BLYP	BHHLYP	wB97	wB97X	wB97XD	PBE1PBE	LC-wPBE	TPSS	TPSSh	M06	M06L	M062X	M06HF
40	-0.064	0.149	0.199	0.041	0.107	0.012	0.000	-0.077	-0.102	-0.240	-0.106	-0.105	-0.069	0.063	0.039	0.044	0.015	0.067	0.036	0.009	0.059
41	-0.093	0.071	0.123	-0.013	0.063	0.006	0.000	-0.030	-0.009	-0.201	-0.065	-0.071	-0.067	0.015	0.087	0.008	-0.006	-0.008	-0.097	-0.027	0.126
42	-0.096	0.062	0.112	-0.016	0.049	-0.002	0.000	-0.045	-0.024	-0.220	-0.074	-0.084	-0.080	-0.001	0.061	-0.013	-0.032	-0.009	-0.092	-0.034	0.110
43	-0.103	0.060	0.112	-0.018	0.050	-0.003	0.000	-0.043	-0.016	-0.216	-0.076	-0.086	-0.086	0.002	0.066	-0.013	-0.031	-0.004	-0.095	-0.026	0.122
44	-0.088	0.115	0.159	0.023	0.084	-0.002	0.000	-0.062	-0.076	-0.247	-0.082	-0.081	-0.061	0.038	0.070	0.010	-0.012	0.062	-0.008	-0.002	0.073
45	-0.065	0.145	0.190	0.049	0.091	-0.002	0.000	-0.080	-0.096	-0.264	-0.096	-0.100	-0.083	0.043	0.058	0.037	0.003	0.063	0.013	0.005	0.079
46	-0.100	0.122	0.166	0.023	0.098	-0.002	0.000	-0.062	-0.073	-0.241	-0.077	-0.075	-0.063	0.055	0.074	0.019	0.001	0.067	0.011	0.027	0.101
47	-0.126	0.025	0.073	-0.037	0.039	-0.006	0.000	-0.002	0.063	-0.175	-0.008	-0.024	-0.040	-0.005	0.140	-0.044	-0.050	0.027	-0.092	-0.049	0.012
48	-0.081	0.120	0.168	0.031	0.080	-0.003	0.000	-0.070	-0.067	-0.244	-0.091	-0.094	-0.075	0.034	0.063	0.022	-0.006	0.051	-0.013	-0.006	0.078
49	-0.096	0.102	0.147	0.014	0.079	-0.002	0.000	-0.045	-0.030	-0.226	-0.055	-0.061	-0.051	0.034	0.094	0.005	-0.014	0.063	-0.012	-0.008	0.051
50	-0.127	0.035	0.082	-0.031	0.047	-0.006	0.000	-0.010	0.036	-0.177	-0.011	-0.025	-0.037	0.007	0.130	-0.043	-0.047	0.029	-0.093	-0.021	0.077
Avg.	-0.094	0.091	0.139	0.006	0.071	-0.001	0.000	-0.048	-0.036	-0.223	-0.067	-0.073	-0.065	0.026	0.080	0.003	-0.016	0.037	-0.040	-0.012	0.081

Changes in the *EAs* of compounds 40-50 with the different functionals with respect to the B3LYP-D used as reference.

Comp	BLYP	BPW91	PW91	B97D	B3PW91	B3LYP	B3LYP-D	CAMB3LYP	LC-BLYP	BHHLYP	wB97	wB97X	wB97XD	PBE1PBE	LC-wPBE	TPSS	TPSSh	M06	M06L	M062X	M06HF
40	-0.018	-0.148	-0.231	-0.068	-0.041	-0.010	0.000	0.155	0.269	0.345	0.289	0.262	0.202	0.008	0.180	-0.046	0.018	-0.033	0.004	0.109	0.164
41	-0.007	-0.085	-0.182	-0.027	0.004	-0.002	0.000	0.114	0.190	0.327	0.253	0.232	0.196	0.057	0.134	-0.018	0.041	0.016	0.116	0.155	0.807
42	0.010	-0.075	-0.162	-0.011	0.006	0.004	0.000	0.102	0.153	0.319	0.217	0.205	0.180	0.058	0.107	0.008	0.064	0.023	0.120	0.139	0.682
43	0.669	-0.068	0.573	1.007	0.008	0.005	0.000	0.102	0.149	0.317	0.222	0.211	0.191	0.058	0.110	0.011	0.067	0.018	0.127	0.134	0.623
44	0.023	-0.092	-0.171	-0.027	-0.017	0.001	0.000	0.101	0.184	0.314	0.207	0.184	0.147	0.029	0.088	0.006	0.054	-0.028	0.073	0.100	0.551
45	-0.012	-0.136	-0.215	-0.069	-0.025	0.001	0.000	0.141	0.239	0.358	0.254	0.234	0.194	0.029	0.138	-0.032	0.034	-0.032	0.026	0.106	0.691
46	0.033	-0.105	-0.181	-0.036	-0.033	0.001	0.000	0.112	0.196	0.317	0.211	0.188	0.154	0.013	0.098	-0.008	0.036	-0.043	0.026	0.070	0.107
47	0.052	-0.021	-0.105	0.037	0.017	0.005	0.000	0.037	0.018	0.252	0.108	0.111	0.115	0.059	-0.012	0.057	0.088	0.006	0.176	0.140	0.306
48	0.002	-0.118	-0.200	-0.053	-0.020	0.003	0.000	0.133	0.226	0.344	0.256	0.233	0.186	0.032	0.136	-0.020	0.041	-0.027	0.047	0.116	0.883
49	0.021	-0.096	-0.176	-0.031	-0.019	0.001	0.000	0.094	0.161	0.317	0.197	0.178	0.145	0.030	0.081	0.002	0.051	-0.034	0.058	0.112	0.817
50	0.050	-0.019	0.114	0.521	0.019	0.005	0.000	0.052	0.066	0.252	0.136	0.132	0.129	0.056	0.027	0.061	0.094	0.457	0.197	0.127	-0.004
Avg	0.075	-0.087	-0.085	0.113	-0.009	0.001	0.000	0.104	0.168	0.315	0.214	0.197	0.167	0.039	0.099	0.002	0.053	0.029	0.088	0.119	0.512

Changes in the EAs of compounds 40-50 with the different functionals with respect to the B3LYP-D used as reference.

Comp	BLYP	BPW91	PW91	B97D	B3PW91	B3LYP	B3LYP-D	CAMB3LYP	LC-BLYP	BHHLYP	wB97	wB97X	wB97XD	PBE1PBE	LC-wPBE	TPSS	TPSSh	M06	M06L	M062X	M06HF
40	-0.106	0.003	-0.034	-0.034	0.087	0.001	0.000	0.089	0.195	0.132	0.210	0.183	0.161	0.100	0.262	-0.005	0.041	0.018	-0.003	0.160	0.396
41	-0.116	-0.041	-0.085	-0.059	0.057	0.002	0.000	0.087	0.197	0.148	0.186	0.158	0.127	0.063	0.214	-0.033	0.041	0.005	-0.009	0.118	0.969
42	-0.102	-0.038	-0.076	-0.047	0.049	0.003	0.000	0.065	0.149	0.125	0.149	0.127	0.106	0.051	0.169	-0.023	0.064	0.008	-0.003	0.107	0.852
43	0.551	-0.033	0.660	0.970	0.051	0.002	0.000	0.066	0.149	0.126	0.151	0.129	0.109	0.053	0.174	-0.020	0.067	0.006	0.002	0.106	0.800
44	-0.080	0.025	-0.013	-0.009	0.081	-0.002	0.000	0.047	0.127	0.085	0.145	0.121	0.109	0.086	0.190	0.016	0.054	0.024	0.039	0.125	0.743
45	-0.096	0.011	-0.027	-0.027	0.084	-0.001	0.000	0.072	0.169	0.118	0.183	0.157	0.135	0.096	0.233	0.002	0.034	0.018	0.004	0.148	0.923
46	-0.087	0.017	-0.017	-0.021	0.082	-0.002	0.000	0.062	0.150	0.100	0.160	0.137	0.118	0.092	0.211	0.007	0.036	0.011	0.001	0.135	0.367
47	-0.083	-0.018	-0.053	-0.017	0.046	-0.001	0.000	0.044	0.106	0.091	0.108	0.094	0.079	0.044	0.133	-0.003	0.088	0.022	0.055	0.083	0.348
48	-0.094	-0.007	-0.043	-0.035	0.066	-0.001	0.000	0.074	0.185	0.121	0.186	0.158	0.129	0.076	0.225	-0.006	0.041	0.012	-0.001	0.131	1.079
49	-0.087	-0.007	-0.042	-0.029	0.060	-0.001	0.000	0.057	0.153	0.107	0.153	0.128	0.103	0.066	0.188	-0.004	0.051	0.014	0.012	0.111	0.945
50	-0.085	0.004	0.185	0.480	0.065	-0.001	0.000	0.049	0.120	0.087	0.134	0.115	0.100	0.063	0.166	0.011	0.094	0.476	0.078	0.109	0.125
Avg	-0.035	-0.008	0.041	0.107	0.066	0.000	0.000	0.065	0.155	0.113	0.160	0.137	0.116	0.072	0.197	-0.005	0.055	0.056	0.016	0.121	0.686