Supplementary material to: Short- and long-range corrected hybrid density functionals with the D3 dispersion corrections

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TABLES

TABLE I. Root-mean-square error (in kcal/mol) of SLC-LDA-D3 for the training set as a function of ω_{SR} and ω_{LR} (in bohr^{-1}).

$\omega_{\mathrm{LR}}\backslash\omega_{\mathrm{SR}}$	0.8	1.0	1.5	2.0	2.5	3.0	3.5	4.0
0.30	19.13	16.86	28.33	34.73	38.49	41.04	42.91	44.33
0.35	19.24	10.66	19.42	25.56	29.24	31.75	33.59	34.99
0.40	21.34	10.84	12.82	18.19	21.67	24.08	25.87	27.23
0.45	23.76	13.48	**9.65**	12.98	15.91	18.09	19.74	21.03
0.50	24.80	16.31	10.64	10.63	12.33	13.97	15.33	16.44

TABLE II. Root-mean-square error (in kcal/mol) of SLC-PBE-D3 for the training set as a function of ω_{SR} and ω_{LR} (in bohr^{-1}).

$\omega_{\mathrm{LR}}\backslash\omega_{\mathrm{SR}}$	0.8	1.0	1.5	2.0	2.5	3.0	3.5	4.0
0.30	11.90	8.60	6.00	8.06	9.24	9.81	10.17	10.44
0.35	13.26	9.70	5.36	5.87	6.78	7.27	7.60	7.85
0.40	14.80	11.11	5.94	**4.90**	5.20	5.51	5.75	5.96
0.45	16.32	12.66	7.12	5.34	5.02	5.03	5.11	5.21
0.50	17.83	14.20	8.54	6.44	5.85	5.72	5.70	5.71

TABLE III: Nonhydrogen transfer barrier heights (in kcal/mol) of the NHTBH38/04 set [1].

Reaction	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
Heavy-atom transfer reactions										
$H + N_2O \rightarrow OH + N_2$										

V^f	18.14	9.97	17.86	20.68	19.23	17.47	18.16	15.31	17.59	20.18
V^r	83.22	52.46	77.26	81.91	80.58	77.75	78.82	85.59	79.02	81.91
$H + FH \rightarrow HF + H$										
V^f	42.18	27.07	40.39	44.78	43.10	40.56	41.46	37.83	40.09	43.74
V^r	42.18	27.07	40.39	44.78	43.10	40.56	41.46	37.83	40.09	43.74
$H + ClH \rightarrow HCl + H$										
V^f	18.00	9.64	18.30	23.17	20.71	18.19	19.33	17.30	17.99	22.25
V^r	18.00	9.64	18.30	23.17	20.71	18.19	19.33	17.30	17.99	22.25
$H + FCH_3 \rightarrow HF + CH_3$										
V^f	30.38	18.51	32.56	33.44	32.11	30.02	30.98	30.25	32.09	33.45
V^r	57.02	41.00	56.65	55.78	55.35	54.47	54.75	57.90	56.16	55.38
$H + F_2 \rightarrow HF + F$										
V^f	2.27	-9.86	0.32	1.99	0.89	-0.60	0.10	-1.56	0.30	2.26
V^r	106.18	80.86	102.53	103.62	104.26	103.96	104.08	108.23	103.81	104.40
$CH_3 + FCl \rightarrow CH_3F + Cl$										
V^f	7.43	-6.48	9.39	4.61	3.88	2.76	3.61	9.22	8.61	5.54
V^r	60.17	41.63	63.40	59.96	58.48	56.55	57.85	65.59	62.69	60.96
Nucleophilic substitution reactions										
$F^- + CH_3F \rightarrow FCH_3 + F^-$										
V^f	-0.34	-8.31	0.96	-2.61	-2.27	-1.37	-1.55	3.03	1.16	-1.34
V^r	-0.34	-8.31	0.96	-2.61	-2.27	-1.37	-1.55	3.03	1.16	-1.34
$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$										
V^f	13.38	7.06	14.37	13.29	13.25	12.85	13.06	16.66	14.86	13.54
V^r	13.38	7.06	14.37	13.29	13.25	12.85	13.06	16.66	14.86	13.54

$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$										
V^f	3.10	-3.80	8.42	6.22	4.72	3.70	4.38	8.56	7.82	6.48
V^r	3.10	-3.80	8.42	6.22	4.72	3.70	4.38	8.56	7.82	6.48
$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$										
V^f	13.61	7.15	17.80	17.69	16.04	14.30	15.20	18.38	17.81	17.24
V^r	13.61	7.15	17.80	17.69	16.04	14.30	15.20	18.38	17.81	17.24
$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$										
V^f	-12.54	-19.52	-9.42	-11.70	-13.14	-13.58	-13.14	-9.57	-9.94	-11.43
V^r	20.11	12.31	23.54	20.15	20.79	21.26	21.33	26.89	23.87	21.89
$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$										
V^f	2.89	-0.67	5.42	5.41	4.20	3.07	3.60	5.59	5.36	4.96
V^r	29.62	21.45	32.11	30.89	31.08	30.50	30.91	35.79	32.90	31.72
$OH^- + CH_3F \rightarrow HOCH_3 + F^-$										
V^f	-2.78	-10.59	-1.19	-4.00	-3.67	-3.31	-3.19	1.35	-1.01	-2.84
V^r	17.33	9.14	21.34	17.87	17.58	17.90	17.89	22.68	21.01	18.47
$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$										
V^f	10.96	3.88	11.88	11.62	11.54	10.57	11.06	14.69	12.39	11.75
V^r	47.20	43.21	52.43	49.19	49.36	49.20	49.43	54.19	52.50	50.19

Unimolecular and association reactions

$H + N_2 \rightarrow HN_2$										
V^f	14.69	5.19	12.14	15.46	13.99	12.32	12.96	11.36	12.33	15.20
V^r	10.72	9.08	13.10	15.08	14.32	13.40	13.74	13.10	12.72	14.42
$H + CO \rightarrow HCO$										
V^f	3.17	-1.69	2.32	5.64	4.55	3.37	3.71	1.27	2.29	5.33

V^r	22.68	24.66	26.04	27.07	26.74	26.20	26.24	24.79	25.37	26.13
$H + C_2H_4 \rightarrow CH_3CH_2$										
V^f	1.72	-0.14	2.05	4.95	4.09	3.03	3.42	0.44	1.80	4.54
V^r	41.75	40.19	47.53	48.46	47.01	45.37	46.01	46.97	47.22	47.82
$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$										
V^f	6.85	1.50	6.98	4.80	5.03	4.57	4.93	8.35	6.06	4.90
V^r	32.97	29.76	39.34	36.71	35.37	33.85	34.64	37.18	39.06	37.03
$HCN \rightarrow HNC$										
V^f	48.16	45.60	46.67	45.86	46.28	46.42	46.19	46.35	46.24	45.26
V^r	33.11	30.50	33.20	32.79	33.13	33.27	33.07	33.59	32.57	32.36
MSE		-8.52	1.39	1.32	0.55	-0.45	0.04	1.99	1.29	1.38
MAE		8.62	2.47	2.32	1.75	1.51	1.53	3.32	2.38	2.13
rms		10.61	3.07	2.82	2.08	2.00	1.89	3.77	2.86	2.55

TABLE IV: Hydrogen transfer barrier heights (in kcal/mol) of the HTBH38/04 set [1].

Reaction	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
$H + HCl \rightarrow H_2 + Cl$										
V^f	5.70	0.56	5.85	6.55	5.24	4.08	4.71	2.61	5.54	6.44
V^r	8.70	-1.95	5.78	6.58	5.30	4.58	4.98	8.27	5.98	6.34
$OH + H_2 \rightarrow H + H_2O$										
V^f	5.10	-6.36	2.74	3.24	2.54	2.22	2.48	4.45	3.27	3.11
V^r	21.20	13.69	21.14	20.38	19.50	18.77	19.13	17.23	20.34	20.44
$CH_3 + H_2 \rightarrow H + CH_4$										

V^f	12.10	3.82	9.98	10.25	9.58	9.06	9.36	11.35	9.69	9.80
V^r	15.30	9.32	14.87	16.29	15.05	13.54	14.22	11.74	14.56	16.10
$OH + CH_4 \rightarrow CH_3 + H_2O$										
V^f	6.70	-5.65	4.88	4.46	3.89	3.04	3.43	6.24	5.09	4.27
V^r	19.60	8.91	18.39	15.56	15.37	15.11	15.22	18.62	17.30	15.30
$H + H_2 \rightarrow H_2 + H$										
V^f	9.60	3.64	7.89	12.37	10.73	9.21	9.77	5.84	7.84	11.67
V^r	9.60	3.64	7.89	12.37	10.73	9.21	9.77	5.84	7.84	11.67
$OH + NH_3 \rightarrow H_2O + NH_2$										
V^f	3.20	-11.94	2.93	2.80	1.60	-0.02	0.85	4.90	3.32	2.71
V^r	12.70	-0.71	13.00	12.06	10.96	9.69	10.38	14.55	12.67	11.89
$HCl + CH_3 \rightarrow Cl + CH_4$										
V^f	1.70	-5.94	1.28	-0.58	-1.19	-1.86	-1.45	1.80	0.60	-0.77
V^r	7.90	-2.95	6.10	5.49	4.34	3.11	3.69	7.85	5.91	5.43
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$										
V^f	3.40	-9.03	2.42	1.76	1.16	0.17	0.56	3.47	2.40	1.49
V^r	19.90	10.76	20.06	17.27	17.18	16.57	16.82	19.97	18.64	16.90
$F + H_2 \rightarrow HF + H$										
V^f	1.80	-12.97	-2.87	-3.79	-3.89	-3.70	-3.55	-1.06	-1.71	-2.85
V^r	33.40	25.12	32.70	29.79	29.17	29.01	29.20	27.67	30.93	29.99
$O + CH_4 \rightarrow OH + CH_3$										
V^f	13.70	-0.79	9.83	10.40	9.84	9.20	9.55	12.28	10.44	10.48
V^r	8.10	-0.57	7.98	4.78	4.83	4.67	4.71	7.74	7.36	4.60
$H + PH_3 \rightarrow PH_2 + H_2$										
V^f	3.10	-1.79	2.90	5.86	4.63	3.28	3.79	0.73	2.63	5.36

V^r	23.20	17.91	23.04	25.29	24.15	23.46	23.78	25.51	23.02	24.72
$H + HO \rightarrow H_2 + O$										
V^f	10.70	3.75	10.52	10.68	9.82	8.84	9.17	6.66	10.16	10.48
V^r	13.10	-1.98	7.48	10.25	9.35	8.89	9.15	10.81	8.37	10.06
$H + H_2S \rightarrow H_2 + HS$										
V^f	3.50	-1.22	3.77	6.89	5.52	4.05	4.62	1.63	3.53	6.38
V^r	17.30	9.10	15.69	18.48	17.19	16.31	16.64	18.96	15.81	17.85
$O + HCl \rightarrow OH + Cl$										
V^f	9.80	-10.54	7.88	8.39	6.94	5.47	6.42	10.89	8.52	8.38
V^r	10.40	-7.33	10.84	8.84	7.46	5.92	6.71	12.39	10.74	8.71
$NH_2 + CH_3 \rightarrow CH_4 + NH$										
V^f	8.00	0.71	9.29	6.92	6.49	5.65	6.13	9.44	8.73	6.60
V^r	22.40	10.56	20.18	20.01	19.34	18.41	18.99	22.02	19.97	19.89
$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$										
V^f	7.50	2.89	10.88	8.76	8.41	7.26	7.83	10.81	9.98	8.26
V^r	18.30	7.51	17.63	17.44	16.72	15.69	16.23	19.27	17.19	17.18
$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$										
V^f	10.40	1.44	11.31	10.92	10.03	8.60	9.26	12.33	10.74	10.33
V^r	17.40	9.99	18.90	17.17	16.70	15.29	16.00	19.17	17.63	16.56
$NH_2 + CH_4 \rightarrow CH_3 + NH_3$										
V^f	14.50	4.39	13.70	13.43	12.56	11.28	11.95	14.98	13.37	12.96
V^r	17.80	7.71	17.15	15.26	14.69	13.65	14.21	17.71	16.23	14.80
s-trans cis-$C_5H_8 \rightarrow$ s-trans cis-C_5H_8										
V^f	38.40	31.19	40.09	42.88	41.46	39.07	39.92	44.37	39.90	41.80
V^r	38.40	31.19	40.09	42.88	41.46	39.07	39.92	44.37	39.90	41.80

MSE	-9.67	-0.77	-0.66	-1.55	2.57	-2.08	-0.27	-1.03	-0.96
MAE	9.67	1.39	2.11	2.27	2.70	2.40	1.99	1.41	2.04
rms	10.37	1.90	2.47	2.60	3.10	2.75	2.59	1.77	2.33

TABLE V: Interaction energies (in kcal/mol) of the S22 set [2, 3].

Complex	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
Hydrogen bonded complexes										
NH_3 dimer [C_{2h}]	-3.133	-2.83	-2.35	-3.66	-3.59	-3.08	-3.09	-2.82	-2.85	-3.27
H_2O dimer [C_s]	-4.989	-4.91	-4.37	-5.65	-5.59	-4.97	-5.04	-4.95	-4.69	-5.21
Formic acid dimer [C_{2h}]	-18.753	-18.08	-17.79	-20.11	-19.95	-19.28	-19.51	-19.20	-18.88	-19.83
Formamide dimer [C_{2h}]	-16.062	-14.69	-14.00	-16.77	-16.65	-16.17	-16.26	-15.73	-15.40	-16.40
Uracil dimer [C_{2h}]	-20.641	-18.45	-17.54	-20.31	-20.29	-20.43	-20.51	-20.19	-19.61	-20.56
2-pyridone$\cdots$2-aminopyridine [C_1]	-16.934	-15.27	-13.80	-16.39	-16.37	-17.06	-16.98	-16.28	-16.36	-16.93
Adenine$\cdots$thymine WC [C_1]	-16.66	-14.29	-13.04	-16.04	-15.90	-16.46	-16.43	-15.94	-15.91	-16.47
Dispersion complexes										
CH_4 dimer [D_{3d}]	-0.527	-0.08	0.13	-0.43	-0.57	-0.57	-0.61	-0.74	-0.69	-0.56
C_2H_4 dimer [D_{2d}]	-1.472	-0.31	-0.15	-1.90	-1.77	-1.79	-1.54	-1.52	-1.53	-1.46
Benzene$\cdots CH_4$ [C_3]	-1.448	-0.01	0.01	-1.58	-1.43	-1.70	-1.64	-1.38	-1.57	-1.68
Benzene dimer [C_{2h}]	-2.654	1.90	1.64	-2.27	-1.52	-3.16	-3.00	-1.99	-2.89	-3.18
Pyrazine dimer [C_s]	-4.255	0.73	0.36	-3.73	-2.91	-4.27	-4.15	-3.40	-4.13	-4.27
Uracil dimer [C_2]	-9.805	-2.69	-3.24	-8.92	-7.85	-9.79	-9.83	-9.49	-9.83	-9.96
Indole$\cdots$benzene [C_1]	-4.524	2.24	1.73	-3.68	-2.46	-5.10	-4.61	-3.13	-4.49	-4.90

Adenine$\cdots$thymine stack [C_1]	-11.73	-1.33	-2.57	-10.38	-8.49	-11.86	-11.26	-10.08	-11.32	-11.76
Mixed complexes										
Ethene$\cdots$ethine [C_{2v}]	-1.496	-1.16	-0.87	-1.62	-1.66	-1.63	-1.65	-1.59	-1.61	-1.63
Benzene$\cdots$$H_2O$ [C_s]	-3.275	-2.03	-2.13	-3.56	-3.39	-3.50	-3.58	-3.52	-3.73	-3.71
Benzene$\cdots$$NH_3$ [C_s]	-2.312	-0.91	-0.95	-2.44	-2.30	-2.53	-2.56	-2.42	-2.60	-2.63
Benzene$\cdots$HCN [C_s]	-4.541	-2.81	-3.30	-4.90	-4.61	-4.79	-4.65	-4.41	-4.80	-4.88
Benzene dimer [C_{2v}]	-2.717	-0.10	-0.21	-2.37	-2.11	-2.89	-2.82	-2.37	-2.75	-2.94
Indole$\cdots$benzene T-shape [C_1]	-5.627	-2.02	-2.27	-4.87	-4.46	-5.64	-5.52	-5.14	-5.77	-5.75
Phenol dimer [C_1]	-7.097	-3.86	-3.84	-6.93	-6.48	-6.99	-7.00	-6.83	-6.73	-7.14
MSE		2.71	2.82	0.10	0.47	-0.14	-0.07	0.34	0.11	-0.20
MAE		2.71	2.82	0.53	0.79	0.19	0.18	0.45	0.30	0.23
rms		3.73	3.58	0.63	1.11	0.25	0.25	0.61	0.39	0.33

TABLE VI: The 23 core ionization energies (in eV) of 14 molecules taken from Ref. [4]. Bold type denotes the atom at which the $1s$ electron is ionized. The relativistic corrections are not considered.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
$\mathbf{C}_2H_2$	290.82	269.16	275.23	275.90	279.36	280.14	279.93	292.73	287.04	287.76
$\mathbf{C}H_4$	290.91	268.37	274.41	275.13	278.54	279.29	279.09	291.82	286.15	286.91
$\mathbf{C}H_3OH$	292.42	269.96	276.09	276.81	280.22	280.96	280.76	293.53	287.83	288.59
$CH_3\mathbf{C}N$	292.45	270.03	276.22	276.85	280.32	281.09	280.88	293.79	288.04	288.74
$\mathbf{C}H_3CN$	292.98	270.39	276.50	277.19	280.61	281,37	281.16	293.93	288.24	288.99

H**C**N	293.40	270.38	276.51	277.15	280.63	281.42	281.19	294.09	288.32	289.04
H_2**C**O	294.47	271.57	277.78	278.47	281.91	282.67	282.46	295.34	289.55	290.31
CO	296.21	272.02	278.23	278.88	282.39	283.17	282.95	295.99	290.13	290.87
CO_2	297.69	273.66	280.33	280.95	284.44	285.21	284.99	298.14	292.14	292.87
NH_3	405.56	379.92	385.83	386.69	391.09	392.19	391.86	409.67	403.09	403.97
CH_3C**N**	405.64	380.34	386.40	387.17	391.64	392.76	392.42	410.37	403.74	404.57
HC**N**	406.78	381.10	387.12	387.89	392.37	393.50	393.15	411.13	404.47	405.31
NNO	408.71	382.89	389.27	390.02	394.50	395.63	395.28	413.43	406.61	407.45
N$_2$	409.98	383.12	389.27	390.02	394.52	395.67	395.31	413.38	406.63	407.46
N**N**O	412.59	386.30	393.02	393.76	398.20	399.26	398.94	417.13	410.30	411.12
CH_3**O**H	539.11	510.22	516.05	516.94	522.38	523.87	523.37	546.62	539.34	540.28
H_2C**O**	539.48	510.77	516.56	517.41	522.89	524.39	523.89	547.21	539.90	540.80
H_2**O**	539.90	510.28	516.15	517.07	522.50	523.97	523.48	546.76	539.43	540.40
C**O**$_2$	541.28	512.36	518.34	519.16	524.64	526.13	525.64	549.05	541.66	542.55
NN**O**	541.42	512.97	518.72	519.56	525.06	526.61	526.08	549.40	542.04	542.95
C**O**	542.55	513.06	518.98	519.76	525.26	526.76	526.26	549.66	542.33	543.17
H**F**	694.23	659.88	665.77	666.71	673.16	675.00	674.35	703.26	695.36	696.38
F$_2$	696.69	662.88	668.98	669.87	676.34	678.19	677.54	706.57	698.58	699.58
MSE		-26.25	-20.15	-19.39	-14.88	-13.74	-14.10	4.25	-2.36	-1.53
MAE		26.25	20.15	19.39	14.88	13.74	14.10	4.27	2.77	2.53
rms		26.48	20.47	19.70	15.10	13.91	14.29	5.27	3.36	2.91

TABLE VII: The 23 core ionization energies (in eV) of 14 molecules taken from Ref. [4]. Bold type denotes the atom at which the 1s electron is ionized. The relativistic corrections (0.12 eV for C, 0.24 eV for N, 0.45 eV for O, and 0.75 eV for F) [5] are subtracted from the reference values.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
$\mathbf{C}_2H_2$	290.70	269.16	275.23	275.90	279.36	280.14	279.93	292.73	287.04	287.76
$\mathbf{C}H_4$	290.79	268.37	274.41	275.13	278.54	279.29	279.09	291.82	286.15	286.91
$\mathbf{C}H_3OH$	292.30	269.96	276.09	276.81	280.22	280.96	280.76	293.53	287.83	288.59
$CH_3\mathbf{C}N$	292.33	270.03	276.22	276.85	280.32	281.09	280.88	293.79	288.04	288.74
$\mathbf{C}H_3CN$	292.86	270.39	276.50	277.19	280.61	281,37	281.16	293.93	288.24	288.99
H$\mathbf{C}$N	293.28	270.38	276.51	277.15	280.63	281.42	281.19	294.09	288.32	289.04
$H_2\mathbf{C}O$	294.35	271.57	277.78	278.47	281.91	282.67	282.46	295.34	289.55	290.31
$\mathbf{C}O$	296.09	272.02	278.23	278.88	282.39	283.17	282.95	295.99	290.13	290.87
$\mathbf{C}O_2$	297.57	273.66	280.33	280.95	284.44	285.21	284.99	298.14	292.14	292.87
$\mathbf{N}H_3$	405.32	379.92	385.83	386.69	391.09	392.19	391.86	409.67	403.09	403.97
$CH_3C\mathbf{N}$	405.40	380.34	386.40	387.17	391.64	392.76	392.42	410.37	403.74	404.57
HC$\mathbf{N}$	406.54	381.10	387.12	387.89	392.37	393.50	393.15	411.13	404.47	405.31
$\mathbf{N}NO$	408.47	382.89	389.27	390.02	394.50	395.63	395.28	413.43	406.61	407.45
$\mathbf{N}_2$	409.74	383.12	389.27	390.02	394.52	395.67	395.31	413.38	406.63	407.46
N$\mathbf{N}$O	412.35	386.30	393.02	393.76	398.20	399.26	398.94	417.13	410.30	411.12
$CH_3\mathbf{O}H$	538.66	510.22	516.05	516.94	522.38	523.87	523.37	546.62	539.34	540.28
$H_2C\mathbf{O}$	539.03	510.77	516.56	517.41	522.89	524.39	523.89	547.21	539.90	540.80
$H_2\mathbf{O}$	539.45	510.28	516.15	517.07	522.50	523.97	523.48	546.76	539.43	540.40
$C\mathbf{O}_2$	540.83	512.36	518.34	519.16	524.64	526.13	525.64	549.05	541.66	542.55

NN**O**	540.97	512.97	518.72	519.56	525.06	526.61	526.08	549.40	542.04	542.95
C**O**	542.10	513.06	518.98	519.76	525.26	526.76	526.26	549.66	542.33	543.17
H**F**	693.48	659.88	665.77	666.71	673.16	675.00	674.35	703.26	695.36	696.38
$\mathbf{F}_2$	695.94	662.88	668.98	669.87	676.34	678.19	677.54	706.57	698.58	699.58
MSE		-25.95	-19.86	-19.10	-14.59	-13.45	-13.81	4.54	-2.07	-1.24
MAE		25.95	19.86	19.10	14.59	13.45	13.81	4.55	2.78	2.60
rms		26.16	20.15	19.38	14.78	13.60	13.97	5.62	3.30	2.93

TABLE VIII: The 38 core excitation energies (in eV) of 13 molecules taken from Ref. [6]. The relativistic corrections are not considered.

Excitation	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
Core→Valence										
C_2H_4 C(1s) $\rightarrow \pi^*$	284.7	268.07	269.02	269.74	273.37	274.76	274.20	284.98	280.51	281.23
C_2H_2 C(1s) $\rightarrow \pi^*$	285.8	268.92	269.99	270.69	274.34	275.74	275.18	286.02	281.52	282.22
H_2CO C(1s) $\rightarrow \pi^*$	286.0	269.25	269.79	270.48	274.08	275.51	274.93	285.48	281.18	281.85
CO C(1s) $\rightarrow \pi^*$	287.4	270.40	270.79	271.37	274.93	276.35	275.78	286.38	282.18	282.78
CO_2 C(1s) $\rightarrow \pi^*$	290.8	273.74	274.49	275.08	278.62	280.01	279.44	289.97	285.73	286.33
N_2 N(1s) $\rightarrow \pi^*$	401.0	381.56	382.07	382.83	387.32	389.03	388.34	403.64	398.66	399.42
H_2CO O(1s) $\rightarrow \pi^*$	530.8	508.53	509.21	510.13	515.48	517.45	516.66	537.09	531.52	532.43
CO O(1s) $\rightarrow \pi^*$	534.2	511.37	512.23	513.14	518.59	520.59	519.79	540.48	534.72	535.64
HF F(1s) $\rightarrow \sigma^*$	687.4	659.07	660.67	661.81	668.40	670.68	669.71	696.00	689.59	690.68
SiH_4 Si(1s) $\rightarrow \sigma^*$	1842.5	1779.27	1781.21	1782.55	1794.84	1799.52	1797.60	1852.21	1843.94	1845.54
PH_3 P(1s) $\rightarrow \sigma^*$	2145.8	2075.69	2077.03	2078.32	2091.78	2096.99	2094.85	2154.80	2146.59	2148.12

H_2S S(1s) $\rightarrow \sigma^*$	2473.1	2395.39	2396.48	2397.78	2412.37	2418.02	2415.71	2481.33	2473.07	2474.61
SO_2 S(1s) $\rightarrow \pi^*$	2473.8	2396.11	2396.92	2398.22	2412.79	2418.47	2416.14	2481.35	2473.12	2474.67
HCl Cl(1s) $\rightarrow \sigma^*$	2823.9	2739.15	2740.77	2742.07	2757.51	2763.51	2761.06	2831.99	2823.59	2825.08
Cl_2 Cl(1s) $\rightarrow \sigma_u^*$	2821.3	2737.15	2738.27	2739.59	2754.88	2760.83	2758.40	2828.90	2820.64	2822.15
Core→Rydberg										
C_2H_4 C(1s) $\rightarrow$ 3s	287.1	268.59	271.54	272.41	275.96	276.93	276.54	288.25	283.25	284.08
C_2H_2 C(1s) $\rightarrow$ 3s	287.7	268.88	271.81	272.66	276.25	277.21	276.82	288.57	283.54	284.36
C_2H_2 C(1s) $\rightarrow 3p_\pi$	288.7	269.60	272.84	273.66	277.24	278.08	277.76	289.96	284.64	285.45
C_2H_2 C(1s) $\rightarrow 3p_\sigma$	288.8	269.21	272.32	273.12	276.75	277.76	277.38	289.16	284.08	284.88
H_2CO C(1s) $\rightarrow 3sa_1$	290.2	271.21	273.98	274.86	278.42	279.44	279.01	290.59	285.62	286.45
H_2CO C(1s) $\rightarrow 3pb_2$	291.3	271.87	274.91	275.77	279.46	280.46	280.07	291.96	286.72	287.58
H_2CO C(1s) $\rightarrow 3pa_1$	291.7	271.77	274.97	275.84	279.39	280.29	279.92	291.64	286.66	287.49
CO C(1s) $\rightarrow$ 3s	292.4	272.05	274.96	275.79	279.49	280.44	280.04	292.14	286.81	287.65
CO C(1s) $\rightarrow 3p_\pi$	293.3	272.58	275.78	276.58	280.24	281.08	280.75	293.14	287.65	288.48
CO C(1s) $\rightarrow 3p_\sigma$	293.5	272.53	275.74	276.55	280.24	281.12	280.79	293.14	287.66	288.49
CO_2 C(1s) $\rightarrow$ 3s	292.7	272.78	274.99	275.72	279.60	281.03	280.43	291.85	286.79	287.58
CO_2 C(1s) $\rightarrow 3p_\pi$	295.0	274.12	277.74	278.55	282.22	283.08	282.73	295.19	289.56	290.39
N_2 N(1s) $\rightarrow$ 3s	406.2	383.23	385.80	386.75	391.46	392.81	392.24	409.28	403.09	404.02
N_2 N(1s) $\rightarrow 3p_\pi$	407.1	383.82	386.66	387.59	392.28	393.54	393.03	410.37	404.00	404.93
N_2 N(1s) $\rightarrow 3p_\sigma$	407.3	383.77	386.88	387.80	392.50	393.71	393.23	410.70	404.26	405.18
H_2CO O(1s) $\rightarrow 3sa_1$	535.4	510.30	513.14	514.20	519.85	521.54	520.86	543.15	536.40	537.43
H_2CO O(1s) $\rightarrow 3pa_1$	536.3	510.95	514.00	515.06	520.70	522.26	521.65	544.32	537.36	538.38
CO O(1s) $\rightarrow$ 3s	538.9	513.06	515.39	516.39	522.13	523.86	523.14	545.37	538.63	539.60
CO O(1s) $\rightarrow 3p_\pi$	539.9	513.58	516.37	517.35	523.07	524.66	524.02	546.71	539.72	540.68

H_2S S(1s) $\rightarrow$ 4p	2476.3	2396.11	2399.32	2400.71	2415.18	2420.27	2418.20	2485.48	2476.55	2478.13
SO_2 S(1s) $\rightarrow$ 4p	2478.4	2400.56	2402.69	2404.00	2418.65	2424.29	2421.98	2487.91	2479.43	2480.98
HCl Cl(1s) $\rightarrow$ 4p$_\pi$	2827.8	2740.76	2743.73	2745.09	2760.58	2766.13	2763.87	2836.44	2827.28	2828.81
Cl_2 Cl(1s) $\rightarrow$ 4p	2828.5	2741.19	2743.97	2745.32	2760.78	2766.55	2764.20	2836.39	2827.47	2829.01
Core$\rightarrow$Valence	MSE	-42.32	-41.30	-40.31	-31.95	-28.74	-30.05	4.81	-1.46	-0.38
(15)	MAE	42.32	41.30	40.31	31.95	28.74	30.05	5.12	2.22	2.53
	rms	50.91	49.93	48.96	39.29	35.56	37.08	6.25	2.91	2.84
Core$\rightarrow$Rydberg	MSE	-32.26	-29.35	-28.38	-22.26	-20.35	-21.12	3.36	-2.93	-1.93
(23)	MAE	32.26	29.35	28.38	22.26	20.35	21.12	3.50	3.22	2.94
	rms	39.91	37.64	36.78	29.43	26.90	27.93	4.94	3.81	3.26

TABLE IX: The 38 core excitation energies (in eV) of 13 molecules taken from Ref. [6]. The relativistic corrections [(0.12 eV for C, 0.24 eV for N, 0.45 eV for O, and 0.75 eV for F) [5] and (3.4 eV for Si, 4.6 eV for P, 5.9 eV for S, and 7.9 eV for Cl) [6]] are subtracted from the reference values.

Excitation	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
Core$\rightarrow$Valence										
C_2H_4 C(1s) $\rightarrow \pi^*$	284.58	268.07	269.02	269.74	273.37	274.76	274.20	284.98	280.51	281.23
C_2H_2 C(1s) $\rightarrow \pi^*$	285.68	268.92	269.99	270.69	274.34	275.74	275.18	286.02	281.52	282.22
H_2CO C(1s) $\rightarrow \pi^*$	285.88	269.25	269.79	270.48	274.08	275.51	274.93	285.48	281.18	281.85
CO C(1s) $\rightarrow \pi^*$	287.28	270.40	270.79	271.37	274.93	276.35	275.78	286.38	282.18	282.78
CO_2 C(1s) $\rightarrow \pi^*$	290.68	273.74	274.49	275.08	278.62	280.01	279.44	289.97	285.73	286.33
N_2 N(1s) $\rightarrow \pi^*$	400.76	381.56	382.07	382.83	387.32	389.03	388.34	403.64	398.66	399.42

H_2CO O(1s) $\rightarrow \pi^*$	530.35	508.53	509.21	510.13	515.48	517.45	516.66	537.09	531.52	532.43
CO O(1s) $\rightarrow \pi^*$	533.75	511.37	512.23	513.14	518.59	520.59	519.79	540.48	534.72	535.64
HF F(1s) $\rightarrow \sigma^*$	686.65	659.07	660.67	661.81	668.40	670.68	669.71	696.00	689.59	690.68
SiH_4 Si(1s) $\rightarrow \sigma^*$	1839.1	1779.27	1781.21	1782.55	1794.84	1799.52	1797.60	1852.21	1843.94	1845.54
PH_3 P(1s) $\rightarrow \sigma^*$	2141.2	2075.69	2077.03	2078.32	2091.78	2096.99	2094.85	2154.80	2146.59	2148.12
H_2S S(1s) $\rightarrow \sigma^*$	2467.2	2395.39	2396.48	2397.78	2412.37	2418.02	2415.71	2481.33	2473.07	2474.61
SO_2 S(1s) $\rightarrow \pi^*$	2467.9	2396.11	2396.92	2398.22	2412.79	2418.47	2416.14	2481.35	2473.12	2474.67
HCl Cl(1s) $\rightarrow \sigma^*$	2816.0	2739.15	2740.77	2742.07	2757.51	2763.51	2761.06	2831.99	2823.59	2825.08
Cl_2 Cl(1s) $\rightarrow \sigma_u^*$	2813.4	2737.15	2738.27	2739.59	2754.88	2760.83	2758.40	2828.90	2820.64	2822.15
Core→Rydberg										
C_2H_4 C(1s) $\rightarrow$ 3s	286.98	268.59	271.54	272.41	275.96	276.93	276.54	288.25	283.25	284.08
C_2H_2 C(1s) $\rightarrow$ 3s	287.58	268.88	271.81	272.66	276.25	277.21	276.82	288.57	283.54	284.36
C_2H_2 C(1s) $\rightarrow 3p_\pi$	288.58	269.60	272.84	273.66	277.24	278.08	277.76	289.96	284.64	285.45
C_2H_2 C(1s) $\rightarrow 3p_\sigma$	288.68	269.21	272.32	273.12	276.75	277.76	277.38	289.16	284.08	284.88
H_2CO C(1s) $\rightarrow 3sa_1$	290.08	271.21	273.98	274.86	278.42	279.44	279.01	290.59	285.62	286.45
H_2CO C(1s) $\rightarrow 3pb_2$	291.18	271.87	274.91	275.77	279.46	280.46	280.07	291.96	286.72	287.58
H_2CO C(1s) $\rightarrow 3pa_1$	291.58	271.77	274.97	275.84	279.39	280.29	279.92	291.64	286.66	287.49
CO C(1s) $\rightarrow$ 3s	292.28	272.05	274.96	275.79	279.49	280.44	280.04	292.14	286.81	287.65
CO C(1s) $\rightarrow 3p_\pi$	293.18	272.58	275.78	276.58	280.24	281.08	280.75	293.14	287.65	288.48
CO C(1s) $\rightarrow 3p_\sigma$	293.38	272.53	275.74	276.55	280.24	281.12	280.79	293.14	287.66	288.49
CO_2 C(1s) $\rightarrow$ 3s	292.58	272.78	274.99	275.72	279.60	281.03	280.43	291.85	286.79	287.58
CO_2 C(1s) $\rightarrow 3p_\pi$	294.88	274.12	277.74	278.55	282.22	283.08	282.73	295.19	289.56	290.39
N_2 N(1s) $\rightarrow$ 3s	405.96	383.23	385.80	386.75	391.46	392.81	392.24	409.28	403.09	404.02
N_2 N(1s) $\rightarrow 3p_\pi$	406.86	383.82	386.66	387.59	392.28	393.54	393.03	410.37	404.00	404.93

N_2 N(1s) $\rightarrow 3p_\sigma$	407.06	383.77	386.88	387.80	392.50	393.71	393.23	410.70	404.26	405.18
H_2CO O(1s) $\rightarrow 3sa_1$	534.95	510.30	513.14	514.20	519.85	521.54	520.86	543.15	536.40	537.43
H_2CO O(1s) $\rightarrow 3pa_1$	535.85	510.95	514.00	515.06	520.70	522.26	521.65	544.32	537.36	538.38
CO O(1s) $\rightarrow$ 3s	538.45	513.06	515.39	516.39	522.13	523.86	523.14	545.37	538.63	539.60
CO O(1s) $\rightarrow 3p_\pi$	539.45	513.58	516.37	517.35	523.07	524.66	524.02	546.71	539.72	540.68
H_2S S(1s) $\rightarrow$ 4p	2470.4	2396.11	2399.32	2400.71	2415.18	2420.27	2418.20	2485.48	2476.55	2478.13
SO_2 S(1s) $\rightarrow$ 4p	2472.5	2400.56	2402.69	2404.00	2418.65	2424.29	2421.98	2487.91	2479.43	2480.98
HCl Cl(1s) $\rightarrow 4p_\pi$	2819.9	2740.76	2743.73	2745.09	2760.58	2766.13	2763.87	2836.44	2827.28	2828.81
Cl_2 Cl(1s) $\rightarrow$ 4p	2820.6	2741.19	2743.97	2745.32	2760.78	2766.55	2764.20	2836.39	2827.47	2829.01
Core→Valence	MSE	-39.78	-38.76	-37.77	-29.41	-26.20	-27.51	7.35	1.08	2.16
(15)	MAE	39.78	38.76	37.77	29.41	26.20	27.51	7.61	4.42	4.96
	rms	47.20	46.21	45.23	35.54	31.80	33.33	9.73	4.80	5.50
Core→Rydberg	MSE	-30.89	-27.98	-27.01	-20.89	-18.97	-19.75	4.73	-1.56	-0.56
(23)	MAE	30.89	27.98	27.01	20.89	18.97	19.75	4.83	4.23	4.12
	rms	37.32	34.99	34.11	26.74	24.21	25.24	7.43	4.67	4.69

TABLE X: Interaction energies (in kcal/mol) of the S66 set [7].

Complex	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
Hydrogen bonded complexes										
Water$\cdots$Water	-4.918	-4.87	-4.37	-5.62	-5.56	-4.93	-5.01	-4.96	-4.69	-5.17
Water$\cdots$MeOH	-5.592	-5.16	-4.70	-6.18	-6.10	-5.56	-5.64	-5.68	-5.33	-5.81
Water$\cdots$$MeNH_2$	-6.908	-7.15	-6.34	-7.58	-7.57	-7.33	-7.34	-7.08	-7.03	-7.43
Water$\cdots$Peptide	-8.103	-7.28	-6.98	-9.03	-8.82	-8.13	-8.27	-8.23	-7.90	-8.50

MeOH$\cdots$MeOH	-5.757	-5.08	-4.54	-6.04	-6.00	-5.69	-5.75	-5.78	-5.45	-5.88
MeOH$\cdots$$MeNH_2$	-7.554	-7.19	-6.29	-7.93	-7.93	-7.99	-7.92	-7.68	-7.68	-7.95
MeOH$\cdots$Peptide	-8.230	-7.18	-6.64	-8.81	-8.64	-8.39	-8.47	-8.33	-8.07	-8.64
MeOH$\cdots$Water	-5.009	-4.78	-4.22	-5.50	-5.46	-4.94	-5.03	-4.97	-4.70	-5.16
$MeNH_2\cdots$MeOH	-3.059	-2.22	-1.68	-3.16	-3.16	-3.05	-3.11	-3.19	-3.00	-3.13
$MeNH_2\cdots MeNH_2$	-4.160	-3.08	-2.51	-4.61	-4.43	-4.36	-4.16	-3.88	-3.92	-4.28
$MeNH_2\cdots$Peptide	-5.419	-3.39	-3.08	-5.86	-5.54	-5.54	-5.51	-5.21	-5.19	-5.68
$MeNH_2\cdots$Water	-7.266	-7.14	-6.45	-7.96	-7.89	-7.52	-7.52	-7.32	-7.25	-7.66
Peptide$\cdots$MeOH	-6.187	-4.53	-4.24	-6.36	-6.22	-6.14	-6.22	-6.25	-6.00	-6.35
Peptide$\cdots$$MeNH_2$	-7.454	-6.12	-5.42	-7.53	-7.46	-7.91	-7.73	-7.41	-7.49	-7.77
Peptide$\cdots$Peptide	-8.630	-6.36	-6.04	-8.72	-8.50	-8.94	-8.95	-8.83	-8.69	-9.03
Peptide$\cdots$Water	-5.124	-4.32	-3.96	-5.41	-5.36	-4.88	-5.07	-5.09	-4.85	-5.20
Uracil$\cdots$Uracil (BP)	-17.182	-15.49	-14.38	-17.19	-17.16	-17.26	-17.36	-16.98	-16.49	-17.39
Water$\cdots$Pyridine	-6.857	-6.82	-6.01	-7.34	-7.31	-7.06	-7.16	-7.02	-6.83	-7.21
MeOH$\cdots$Pyridine	-7.410	-6.92	-6.01	-7.50	-7.50	-7.57	-7.65	-7.46	-7.32	-7.65
AcOH$\cdots$AcOH	-19.093	-18.59	-18.12	-20.50	-20.34	-19.84	-20.06	-19.76	-19.39	-20.37
$AcNH_2\cdots AcNH_2$	-16.265	-15.02	-14.14	-16.94	-16.83	-16.50	-16.58	-16.04	-15.69	-16.72
AcOH$\cdots$Uracil	-19.491	-18.31	-17.58	-20.20	-20.10	-19.87	-20.03	-19.70	-19.22	-20.22
$AcNH_2\cdots$Uracil	-19.189	-17.67	-16.83	-19.56	-19.51	-19.44	-19.52	-19.12	-18.65	-19.60
MSE		0.88	1.49	-0.46	-0.37	-0.17	-0.23	-0.05	0.18	-0.34
MAE		0.90	1.49	0.46	0.38	0.21	0.23	0.15	0.23	0.34
rms		1.10	1.63	0.56	0.48	0.28	0.31	0.20	0.29	0.43
Dispersion complexes										
Benzene$\cdots$Benzene (pi-pi)	-2.822	1.22	1.11	-2.38	-1.84	-3.26	-3.25	-2.47	-3.10	-3.35

Pyridine···Pyridine (pi-pi)	-3.895	0.48	0.22	-3.43	-2.81	-4.32	-4.24	-3.51	-4.17	-4.34
Uracil···Uracil (pi-pi)	-9.829	-2.51	-3.13	-8.91	-7.79	-9.74	-9.77	-9.36	-9.78	-9.92
Benzene···Pyridine (pi-pi)	-3.439	0.81	0.61	-2.99	-2.40	-3.86	-3.81	-3.05	-3.71	-3.91
Benzene···Uracil (pi-pi)	-5.713	0.36	-0.25	-5.08	-4.06	-5.79	-5.80	-5.11	-5.87	-6.07
Pyridine···Uracil (pi-pi)	-6.819	-0.74	-1.33	-6.22	-5.23	-6.80	-6.82	-6.29	-6.86	-7.06
Benzene···Ethene	-1.432	0.76	0.89	-1.58	-1.26	-1.71	-1.80	-1.15	-1.59	-1.91
Uracil···Ethene	-3.380	-0.34	-0.44	-3.48	-3.00	-3.54	-3.59	-3.19	-3.48	-3.74
Uracil···Ethyne	-3.738	-1.03	-1.16	-4.02	-3.59	-3.72	-3.82	-3.41	-3.63	-3.94
Pyridine···Ethene	-1.872	0.45	0.59	-2.02	-1.67	-2.10	-2.16	-1.56	-1.95	-2.25
Pentane···Pentane	-3.776	0.42	0.68	-4.17	-3.48	-5.32	-4.34	-4.05	-4.34	-4.54
Pentane···Neopentane	-2.613	0.18	0.59	-2.47	-2.13	-3.38	-2.88	-2.61	-2.81	-3.08
Neopentane···Neopentane	-1.777	0.14	0.52	-2.70	-2.35	-3.58	-3.08	-2.75	-2.98	-3.31
Neopentane···Cyclopentane	-2.404	0.11	0.62	-3.02	-2.56	-4.10	-3.31	-3.05	-3.21	-3.52
Cyclopentane···Cyclopentane	-2.997	0.05	0.54	-1.69	-1.59	-2.38	-2.22	-1.98	-2.11	-2.38
Benzene···Cyclopentane	-3.575	0.30	0.24	-3.41	-2.82	-4.38	-4.00	-3.49	-3.96	-4.10
Benzene···Neopentane	-2.895	0.09	0.12	-2.77	-2.41	-3.50	-3.42	-2.97	-3.35	-3.54
Uracil···Pentane	-4.848	0.52	0.34	-4.65	-3.77	-5.63	-5.21	-4.91	-5.30	-5.37
Uracil···Cyclopentane	-4.138	0.58	0.59	-3.72	-3.01	-4.68	-4.30	-4.07	-4.34	-4.45
Uracil···Neopentane	-3.712	0.08	0.08	-3.41	-2.91	-4.22	-4.03	-3.85	-4.04	-4.14
Ethene···Pentane	-2.005	0.01	0.29	-2.32	-2.04	-2.59	-2.22	-2.08	-2.19	-2.24
Ethyne···Pentane	-1.748	-0.09	0.17	-1.94	-1.81	-2.05	-2.03	-1.87	-1.99	-2.00
Peptide···Pentane	-4.264	0.07	0.14	-4.55	-3.79	-5.13	-4.55	-4.26	-4.52	-4.73
MSE		3.72	3.73	0.12	0.67	-0.53	-0.30	0.12	-0.24	-0.44
MAE		3.72	3.73	0.42	0.74	0.59	0.38	0.32	0.33	0.50
rms		4.00	3.92	0.51	0.92	0.77	0.47	0.42	0.44	0.58

Mixed complexes										
Benzene$\cdots$Benzene (TS)	-2.876	-0.19	-0.30	-2.61	-2.31	-3.12	-3.02	-2.67	-3.00	-3.07
Pyridine$\cdots$Pyridine (TS)	-3.535	-0.75	-0.87	-3.42	-3.05	-3.72	-3.60	-3.28	-3.52	-3.62
Benzene$\cdots$Pyridine (TS)	-3.331	-0.61	-0.82	-3.13	-2.80	-3.62	-3.50	-3.15	-3.51	-3.57
Benzene$\cdots$Ethyne (CH-pi)	-2.867	-1.23	-1.41	-3.03	-2.82	-3.02	-2.91	-2.70	-2.96	-3.00
Ethyne$\cdots$Ethyne (TS)	-1.524	-1.20	-0.89	-1.71	-1.73	-1.56	-1.56	-1.48	-1.48	-1.57
Benzene$\cdots$AcOH (OH-pi)	-4.707	-2.32	-2.62	-4.57	-4.22	-4.64	-4.75	-4.60	-5.05	-4.97
Benzene$\cdots$$AcNH_2$ (NH-pi)	-4.361	-2.34	-2.29	-4.45	-4.18	-4.51	-4.56	-4.43	-4.60	-4.62
Benzene$\cdots$Water (OH-pi)	-3.277	-1.98	-2.10	-3.61	-3.40	-3.50	-3.57	-3.48	-3.73	-3.72
Benzene$\cdots$MeOH (OH-pi)	-4.188	-1.86	-1.95	-4.26	-3.89	-4.41	-4.35	-4.14	-4.54	-4.51
Benzene$\cdots$$MeNH_2$ (NH-pi)	-3.231	-0.77	-0.83	-3.28	-2.93	-3.58	-3.49	-3.18	-3.54	-3.61
Benzene$\cdots$Peptide (NH-pi)	-5.282	-1.68	-2.02	-5.05	-4.56	-5.79	-5.62	-5.23	-5.80	-5.81
Pyridine$\cdots$Pyridine (CH-N)	-4.146	-2.49	-2.18	-4.21	-4.01	-3.89	-3.85	-3.54	-3.54	-4.05
Ethyne$\cdots$Water (CH-O)	-2.850	-2.63	-2.30	-3.23	-3.24	-2.73	-2.86	-2.91	-2.73	-2.94
Ethyne$\cdots$AcOH (OH-pi)	-4.868	-4.10	-3.78	-5.65	-5.41	-4.98	-5.10	-4.79	-4.91	-5.28
Pentane$\cdots$AcOH	-2.912	0.07	0.30	-2.99	-2.59	-3.37	-3.21	-3.21	-3.29	-3.30
Pentane$\cdots$$AcNH_2$	-3.534	-0.26	-0.01	-3.81	-3.28	-4.14	-3.87	-3.68	-3.85	-3.99
Benzene$\cdots$AcOH	-3.801	-0.53	-0.84	-3.82	-3.32	-4.12	-4.05	-3.64	-4.07	-4.26
Peptide$\cdots$Ethene	-2.999	-0.95	-0.74	-3.27	-3.00	-3.14	-3.14	-3.05	-3.06	-3.17
Pyridine$\cdots$Ethyne	-3.991	-3.64	-3.04	-4.20	-4.24	-4.15	-4.20	-4.04	-3.94	-4.19
$MeNH_2\cdots$Pyridine	-3.968	-1.73	-1.44	-4.11	-3.78	-4.08	-3.99	-3.65	-3.78	-4.09
MSE		2.05	2.11	-0.11	0.17	-0.19	-0.15	0.07	-0.13	-0.25
MAE		2.05	2.11	0.20	0.33	0.24	0.18	0.16	0.23	0.26
rms		2.28	2.27	0.26	0.38	0.28	0.21	0.21	0.29	0.30

MSE	2.22	2.46	-0.15	0.16	-0.30	-0.23	0.04	-0.06	-0.35
MAE	2.23	2.46	0.37	0.49	0.35	0.26	0.21	0.27	0.37
rms	2.75	2.80	0.47	0.65	0.51	0.35	0.30	0.35	0.46

TABLE XI: Atomization energies (in eV) of the AE113 database [8, 9]. The atomization energies are calculated without the zero-point energy correction.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
CH_3	13.32	13.44	13.38	13.27	13.30	13.31	13.30	13.65	13.33	13.24
CH_4	18.19	18.21	18.11	18.11	18.14	18.16	18.15	18.58	18.06	18.10
NH	3.60	3.84	3.70	3.66	3.65	3.65	3.65	3.73	3.69	3.65
NH_2	7.91	8.18	5.95	7.94	7.94	7.95	7.94	8.11	7.93	7.93
NH_3	12.91	13.10	12.83	12.86	12.88	12.90	12.89	13.16	12.78	12.87
OH	4.65	4.78	4.65	4.60	4.63	4.65	4.64	4.73	4.60	4.60
H_2O	10.11	10.18	9.97	9.92	9.97	10.02	10.00	10.20	9.85	9.94
HF	6.16	6.18	6.06	6.04	6.04	6.07	6.06	6.16	5.93	6.01
SiH_3	9.88	9.62	9.77	9.86	9.89	9.88	9.88	10.24	9.71	9.84
SiH_4	14.07	13.58	13.78	14.07	14.07	14.04	14.05	14.53	13.72	14.04
PH_3	10.46	10.40	10.25	10.48	10.57	10.62	10.61	10.84	10.22	10.50
SH_2	7.93	7.90	7.72	7.86	7.92	7.96	7.96	8.05	7.69	7.88
HCl	4.65	4.64	4.52	4.58	4.60	4.63	4.63	4.67	4.50	4.59
HCCH	17.49	18.00	17.45	17.35	17.39	17.40	17.39	17.47	17.38	17.31
CH_2CH_2	24.38	24.80	24.35	24.28	24.33	24.35	24.34	24.63	24.28	24.26
CH_3CH_3	30.84	31.09	30.88	30.82	30.84	30.85	30.85	31.40	30.80	30.81

HCN	13.51	14.17	13.51	13.47	13.46	13.45	13.45	13.42	13.46	13.47
CO	11.22	11.70	11.26	11.19	11.17	11.17	11.17	11.13	11.15	11.22
HCO	12.01	12.78	12.20	12.05	12.06	12.09	12.07	12.06	12.07	12.05
CH_2O	16.20	16.78	16.26	16.17	16.19	16.22	16.21	16.31	16.12	16.17
CH_3OH	22.22	22.57	22.23	22.13	22.17	22.21	22.19	22.55	22.08	22.15
N_2	9.85	10.56	9.91	9.95	9.86	9.79	9.82	9.71	9.88	9.98
NH_2NH_2	18.82	19.49	18.90	18.91	18.90	18.90	18.90	19.15	18.81	18.95
NO	6.57	7.23	6.74	6.52	6.48	6.45	6.46	6.89	6.59	6.53
O_2	5.20	6.24	5.60	5.51	5.44	5.42	5.43	5.31	5.46	5.53
HOOH	11.62	12.19	11.51	11.42	11.46	11.52	11.50	11.56	11.32	11.46
F_2	1.67	2.25	1.60	1.61	1.54	1.52	1.53	1.36	1.42	1.56
CO_2	16.85	18.13	17.20	16.95	16.97	17.03	17.00	16.76	16.96	16.98
P_2	4.99	5.30	4.39	4.71	4.93	5.07	5.01	4.47	4.36	4.74
S_2	4.41	4.97	4.26	4.38	4.48	4.57	4.54	4.08	4.23	4.42
Cl_2	2.53	2.82	2.36	2.41	2.47	2.54	2.51	2.22	2.34	2.45
NaCl	4.32	4.13	4.18	4.46	4.46	4.35	4.36	4.25	4.14	4.39
SiO	8.25	8.48	8.02	8.12	8.14	8.13	8.13	8.03	7.89	8.13
CS	7.37	7.79	7.01	7.17	7.22	7.28	7.26	6.89	6.99	7.18
ClO	2.74	3.53	2.85	2.81	2.85	2.90	2.88	2.63	2.77	2.84
ClF	2.68	3.12	2.67	2.67	2.67	2.68	2.68	2.52	2.55	2.66
SiH_3SiH_3	23.19	22.49	22.82	23.30	23.27	23.19	23.23	23.76	22.72	23.25
CH_3Cl	17.08	17.35	17.05	17.07	17.09	17.10	17.10	17.23	16.98	17.06
CH_3SH	20.50	20.72	20.39	20.47	20.52	20.54	20.54	20.73	20.32	20.48
SO_2	10.97	12.09	11.03	10.92	10.99	11.07	11.04	10.68	10.81	11.00
BF_3	20.40	20.93	20.65	20.37	20.35	20.30	20.31	20.39	20.22	20.29

BCl_3	14.02	14.67	14.17	14.18	14.19	14.18	14.18	13.67	14.07	14.16
$AlCl_3$	13.57	13.35	13.35	13.52	13.49	13.42	13.46	13.06	13.23	13.51
CF_4	20.80	21.94	21.35	21.00	20.91	20.82	20.88	20.83	20.83	20.97
CCl_4	13.59	14.57	13.59	13.70	13.67	13.62	13.65	12.83	13.49	13.70
OCS	14.45	15.64	14.53	14.47	14.53	14.63	14.59	14.14	14.37	14.50
CS_2	12.00	13.09	11.70	11.83	11.96	12.12	12.05	11.35	11.62	11.85
CF_2O	18.21	19.53	18.71	18.42	18.38	18.36	18.38	18.21	18.33	18.41
SiF_4	24.92	24.58	24.54	24.59	24.44	24.24	24.33	24.35	23.94	24.45
N_2O	11.66	13.51	11.97	11.89	11.82	11.82	11.83	11.38	11.80	11.90
NF_3	8.94	10.67	9.47	9.40	9.22	9.11	9.17	8.90	9.10	9.35
PF_3	15.64	15.99	15.62	15.59	15.59	15.52	15.56	15.52	15.21	15.58
O_3	6.26	8.04	6.10	6.00	5.95	6.01	5.98	5.40	5.82	5.99
F_2O	4.04	5.35	4.15	4.11	4.02	3.98	4.00	3.71	3.87	4.07
ClF_3	5.43	7.12	5.70	5.60	5.54	5.54	5.54	5.09	5.32	5.54
CF_2CF_2	25.54	27.50	26.37	25.91	25.84	25.78	25.81	25.56	25.80	25.83
CF_3CN	27.77	29.67	28.40	28.06	27.94	27.83	27.89	27.61	27.96	28.02
CH_3CCH	30.43	31.26	30.57	30.39	30.43	30.42	30.42	30.65	30.46	30.36
CH_2CCH_2	30.40	31.42	30.56	30.39	30.45	30.48	30.46	30.63	30.46	30.36
$cylC_3H_4$	29.45	30.45	29.83	29.65	29.59	29.52	29.57	29.72	29.71	29.60
$cylC_3H_6$	36.91	37.68	37.33	37.15	37.09	37.02	37.06	37.50	37.22	37.12
$CH_3CH_2CH_3$	43.58	44.02	43.72	43.61	43.62	43.63	43.62	44.31	43.63	43.60
CH_3CCCH_3	43.32	44.48	43.60	43.37	43.39	43.37	43.37	43.73	43.47	43.33
$cylC_4H_6$	43.28	44.43	43.73	43.43	43.40	43.39	43.40	43.67	43.61	43.42
isobutane	56.37	56.98	56.57	56.44	56.42	56.42	56.41	57.25	56.49	56.42
benzene	59.14	61.17	59.69	59.19	59.26	59.29	59.28	59.26	59.53	59.19

CH_2F_2	18.99	19.62	19.22	19.08	19.04	19.01	19.03	19.18	18.93	19.03
CF_3H	19.92	20.84	20.31	20.07	20.01	19.94	19.98	20.02	19.90	20.03
CH_2Cl_2	16.05	16.55	16.05	16.09	16.11	16.11	16.11	15.93	15.97	16.09
CCl_3H	14.87	15.61	14.87	14.95	14.94	14.91	14.94	14.44	14.78	14.95
CH_3NO_2	26.01	27.91	26.45	26.29	26.24	26.22	26.24	26.14	26.19	26.31
CH_3SiH_3	27.22	26.95	27.05	27.26	27.26	27.22	27.24	27.82	26.97	27.23
HCOOH	21.49	22.50	21.71	21.49	21.54	21.58	21.56	21.61	21.47	21.53
CH_3CONH_2	37.48	38.87	37.89	37.70	37.69	37.69	37.70	37.96	37.69	37.72
$cylNHC_2H_4$	31.11	32.10	31.53	31.39	31.32	31.26	31.30	31.57	31.41	31.39
NCCN	21.59	23.39	21.85	21.68	21.64	21.62	21.62	21.23	21.73	21.67
CH_3NHCH_3	37.66	38.33	37.83	37.75	37.75	37.76	37.75	38.31	37.72	37.76
CH_2CO	23.03	24.26	23.35	23.13	23.17	23.22	23.20	23.17	23.18	23.14
$cylOC_2H_4$	28.18	29.11	28.55	28.33	28.30	28.28	28.30	28.53	28.37	28.35
OCHCHO	27.39	28.84	27.69	27.47	27.48	27.49	27.49	27.40	27.44	27.48
CH_3CH_2OH	35.06	35.62	35.17	35.02	35.05	35.07	35.06	35.57	35.00	35.04
CH_3OCH_3	34.55	35.15	34.67	34.54	34.58	34.59	34.59	35.11	34.50	34.56
$cylSC_2H_4$	27.06	27.78	27.20	27.18	27.16	27.14	27.17	27.15	27.10	27.18
CH_3SOCH_3	36.89	37.82	36.98	36.92	36.96	36.99	36.99	37.19	36.81	36.95
CH_2CHF	24.81	25.62	25.00	24.84	24.85	24.85	24.85	25.01	24.80	24.80
CH_3CH_2Cl	29.96	30.42	30.03	30.00	30.02	30.01	30.02	30.28	29.96	30.00
CH_2CHCl	23.51	24.22	23.55	23.49	23.53	23.54	23.54	23.53	23.46	23.48
CH_3CClO	28.90	30.11	29.13	29.00	29.02	29.04	29.04	28.96	28.96	29.01
prplCl	42.65	43.35	42.81	42.75	42.74	42.73	42.74	43.14	42.72	42.74
NC_3H_9	50.20	51.08	50.45	50.35	50.33	50.32	50.32	51.03	50.34	50.36
$cylOC_4H_4$	42.99	44.80	43.60	43.07	43.12	43.14	43.15	43.15	43.37	43.11

cylNHC$_4$H$_4$	46.34	48.23	47.02	46.54	46.56	46.58	46.58	46.62	46.85	46.56
NO_2	9.80	11.75	7.41	10.14	10.07	10.08	10.09	9.66	10.07	10.15
SF_6	20.77	21.99	21.20	20.79	20.66	20.46	20.59	20.33	20.42	20.76
$CFCl_3$	15.22	16.35	15.41	15.42	15.37	15.30	15.34	14.71	15.20	15.40
$CClF_3$	18.85	20.06	19.32	19.10	19.01	18.92	18.98	18.74	18.90	19.07
$CBrF_3$	18.34	19.60	18.81	18.55	18.46	18.37	18.43	18.16	18.36	18.51
HCCF	17.19	18.19	17.45	17.23	17.24	17.24	17.24	17.17	17.24	17.18
HCCCN	25.93	27.58	26.11	25.88	25.90	25.90	25.89	25.61	25.98	25.84
NCCCCN	34.15	36.94	34.64	34.26	34.27	34.27	34.24	33.66	34.46	34.22
C_2N_2	21.59	23.39	21.85	21.68	21.64	21.62	21.62	21.23	21.73	21.67
C_3O_2	28.58	31.24	29.25	28.77	28.88	29.03	28.94	28.40	28.93	28.78
FCN	13.19	14.37	13.45	13.31	13.27	13.25	13.26	13.04	13.26	13.29
HCCCCH	30.05	31.55	30.19	29.89	29.97	30.00	29.96	29.81	30.04	29.83
H_2CS	14.07	14.45	13.85	13.92	14.00	14.06	14.04	13.92	13.78	13.92
$HCONH_2$	24.56	25.70	24.86	24.70	24.73	24.75	24.74	24.84	24.67	24.72
CH_2CHCHO	35.76	37.06	35.97	35.76	35.81	35.83	35.82	35.91	35.79	35.75
CH_2CCl_2	22.48	23.46	22.60	22.55	22.57	22.55	22.57	22.26	22.49	22.54
$CHFCF_2$	25.31	26.91	25.91	25.57	25.52	25.48	25.50	25.38	25.47	25.50
CH_2CF_2	25.38	26.57	25.80	25.54	25.52	25.50	25.52	25.55	25.48	25.49
CH_3F	18.31	18.64	18.39	18.32	18.32	18.32	18.32	18.60	18.22	18.29
CF_2Cl_2	16.97	18.17	17.33	17.23	17.15	17.06	17.11	16.67	17.01	17.20
SiF_2	12.93	12.95	12.70	12.86	12.79	12.67	12.72	12.68	12.40	12.78
MSE		0.83	0.10	0.05	0.05	0.04	0.05	0.04	-0.03	0.04
MAE		0.88	0.27	0.11	0.10	0.10	0.10	0.28	0.17	0.11

rms	1.06	0.41	0.15	0.13	0.14	0.13	0.34	0.23	0.14

TABLE XII: Vertical ionization potentials (in eV) of the IP131 database [8], calculated using $\mathrm{IP}(1) = E_{\mathrm{total}}(N-1) - E_{\mathrm{total}}(N)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	13.60	13.60	13.77	13.64	13.65	13.68	13.67	13.90	13.76	13.66
He	24.59	24.47	24.63	24.67	24.65	24.71	24.69	25.19	24.55	24.62
Li	5.39	5.57	3.74	5.31	5.29	5.36	5.36	5.82	5.58	5.39
Be	9.32	9.00	9.03	8.91	8.86	8.83	8.85	9.55	9.05	8.96
B	8.30	8.67	8.76	8.39	8.51	8.55	8.52	9.04	8.74	8.39
C	11.26	11.54	11.68	11.30	11.40	11.44	11.41	11.99	11.64	11.32
N	14.53	14.74	14.89	14.53	14.59	14.63	14.60	15.21	14.82	14.53
O	13.62	14.07	14.12	13.83	13.83	13.82	13.81	14.31	14.03	13.79
F	17.42	17.68	17.78	17.51	17.52	17.54	17.52	18.02	17.58	17.44
Ne	21.57	21.70	21.82	21.61	21.58	21.62	21.58	22.05	21.52	21.45
Na	5.14	5.35	5.20	4.87	4.87	4.95	4.94	5.58	5.22	4.95
Mg	7.65	7.62	7.47	7.65	7.60	7.48	7.48	8.03	7.50	7.56
Al	5.99	6.07	6.20	5.89	5.95	6.00	5.98	6.37	6.17	5.91
Si	8.15	8.20	8.32	8.03	8.07	8.11	8.10	8.51	8.29	8.05
P	10.49	10.49	10.62	10.39	10.39	10.41	10.42	10.83	10.59	10.41
S	10.36	10.43	10.52	10.41	10.46	10.49	10.48	10.96	10.49	10.44
Cl	12.97	12.98	13.07	12.96	13.01	13.03	13.02	13.53	13.03	13.00
Ar	15.76	15.72	15.83	15.75	15.76	15.79	15.78	16.29	15.78	15.78
CH_3	9.84	10.02	10.11	9.72	9.76	9.77	9.76	10.33	10.08	9.73

CH_4	13.60	13.96	14.23	14.19	14.19	14.16	14.18	14.70	14.23	14.21
NH	13.49	13.80	13.92	13.56	13.60	13.63	13.61	14.20	13.86	13.57
NH_2	12.00	12.18	10.17	12.14	12.10	12.08	12.10	12.64	12.16	12.18
NH_3	10.82	10.97	10.97	10.95	10.93	10.93	10.93	11.45	10.95	10.98
OH	13.02	13.30	13.34	13.17	13.18	13.17	13.16	13.70	13.26	13.16
H_2O	12.62	12.81	12.83	12.75	12.73	12.73	12.73	13.25	12.75	12.75
HF	16.12	16.34	16.40	16.27	16.23	16.24	16.23	16.74	16.23	16.21
SiH_3	8.74	8.95	9.11	8.77	8.84	8.88	8.86	9.35	9.09	8.79
SiH_4	12.30	12.14	12.82	12.74	12.68	12.58	12.63	13.27	12.77	12.76
PH_3	10.59	10.48	10.52	10.48	10.53	10.56	10.55	10.98	10.53	10.53
SH_2	10.50	10.41	10.46	10.39	10.43	10.46	10.45	10.87	10.43	10.42
HCl	12.77	12.73	12.79	12.72	12.75	12.77	12.77	13.23	12.76	12.75
HCCH	11.49	11.41	11.36	11.21	11.25	11.28	11.27	11.74	11.33	11.24
CH_2CH_2	10.68	10.62	10.50	10.39	10.42	10.44	10.43	10.88	10.48	10.41
CH_3CH_3	11.99	11.91	12.60	12.56	12.49	12.38	12.43	13.10	12.59	12.57
HCN	13.61	13.75	13.70	13.53	13.56	13.59	13.58	14.09	13.66	13.55
CO	14.01	13.86	14.17	14.19	14.16	14.12	14.15	14.84	14.18	14.26
HCO	9.31	9.77	10.14	9.92	9.96	9.97	9.96	10.56	10.12	9.94
CH_2O	10.89	10.75	10.94	10.85	10.86	10.85	10.85	11.36	10.89	10.86
CH_3OH	10.96	10.69	11.04	10.96	10.93	10.90	10.91	11.48	10.99	10.96
N_2	15.58	15.40	16.06	15.92	15.94	15.90	15.91	16.71	16.06	15.98
NH_2NH_2	8.98	9.40	9.80	9.74	9.71	9.67	9.69	10.31	9.79	9.77
NO	9.26	9.91	10.29	10.04	10.12	10.15	10.13	10.76	10.25	10.06
O_2	12.30	12.58	13.07	12.89	12.97	13.00	12.98	13.66	13.03	12.92
HOOH	11.70	11.30	11.83	11.73	11.73	11.71	11.72	12.39	11.79	11.76

F_2	15.70	15.39	16.03	15.90	15.97	15.99	15.97	16.71	15.97	15.93
CO_2	13.78	13.67	14.00	13.87	13.85	13.83	13.84	14.44	13.93	13.88
P_2	10.62	10.52	10.43	10.30	10.38	10.45	10.42	10.70	10.39	10.32
S_2	9.55	9.47	9.97	9.81	9.75	9.69	9.73	10.29	9.94	9.83
Cl_2	11.49	11.21	11.76	11.67	11.62	11.54	11.58	12.22	11.72	11.69
NaCl	9.80	9.35	9.28	9.23	9.27	9.29	9.28	9.72	9.25	9.24
SiO	11.61	11.31	11.67	11.54	11.57	11.54	11.56	12.14	11.64	11.58
CS	11.34	11.29	12.96	11.54	11.50	11.49	11.51	12.07	11.52	11.59
ClO	11.01	10.77	11.23	11.08	11.09	11.06	11.07	11.69	11.18	11.09
ClF	12.77	12.43	12.85	12.74	12.76	12.76	12.76	13.37	12.81	12.78
SiH_3SiH_3	10.53	10.29	10.59	10.48	10.49	10.48	10.50	10.97	10.57	10.51
CH_3Cl	11.29	11.10	11.43	11.34	11.34	11.32	11.33	11.86	11.39	11.37
CH_3SH	9.44	9.26	9.43	9.35	9.37	9.38	9.38	9.84	9.40	9.38
SO_2	12.50	12.14	13.61	12.58	12.59	12.55	12.56	13.26	12.68	12.63
BF_3	15.96	14.47	15.77	15.63	15.59	15.46	15.52	16.57	15.75	15.70
BCl_3	11.64	10.81	12.04	11.95	11.79	11.55	11.68	12.54	12.01	11.97
$AlCl_3$	12.01	10.89	12.29	12.20	12.03	11.76	11.90	12.79	12.27	12.22
CF_4	16.20	14.56	16.05	15.88	15.86	15.73	15.79	16.93	16.02	15.97
CCl_4	11.69	10.55	11.95	11.87	11.68	11.40	11.54	12.48	11.92	11.88
OCS	11.19	11.25	11.34	11.23	11.27	11.32	11.30	11.74	11.30	11.27
CS_2	10.09	10.04	10.10	10.00	10.03	10.08	10.07	10.46	10.06	10.03
CF_2O	13.60	13.17	13.63	13.49	13.50	13.48	13.49	14.11	13.55	13.50
SiF_4	16.40	14.47	16.16	15.99	15.91	15.71	15.81	17.01	16.13	16.08
N_2O	12.89	12.91	12.95	12.81	12.84	12.87	12.85	13.35	12.88	12.82
NF_3	13.60	12.95	13.58	13.49	13.51	13.49	13.49	14.21	13.53	13.51

PF_3	12.20	11.29	11.63	11.59	11.64	11.64	11.64	12.28	11.64	11.66
O_3	12.73	12.64	13.38	13.29	13.29	13.23	13.25	13.59	13.35	13.32
F_2O	13.26	12.73	13.52	13.40	13.45	13.44	13.44	14.19	13.48	13.43
ClF_3	13.05	12.00	13.02	12.92	12.92	12.84	12.87	13.72	13.00	12.97
CF_2CF_2	10.69	10.10	10.55	10.41	10.48	10.48	10.47	11.13	10.52	10.44
CF_3CN	14.30	13.49	14.09	13.92	13.94	13.92	13.93	14.55	14.05	13.94
CH_3CCH	10.37	10.21	10.36	10.23	10.25	10.24	10.25	10.75	10.34	10.25
CH_2CCH_2	10.20	10.08	10.15	10.04	10.06	10.07	10.07	10.55	10.13	10.07
$cylC_3H_4$	9.86	9.71	9.86	9.73	9.73	9.72	9.73	10.23	9.84	9.74
$cylC_3H_6$	10.54	10.74	10.96	10.84	10.83	10.81	10.82	11.36	10.94	10.86
$CH_3CH_2CH_3$	11.51	11.10	11.94	11.91	11.83	11.68	11.75	12.46	11.94	11.93
CH_3CCCH_3	9.79	9.30	9.56	9.44	9.45	9.42	9.43	9.95	9.54	9.46
$cylC_4H_6$	9.43	9.41	9.50	9.37	9.38	9.39	9.39	9.86	9.48	9.39
isobutane	11.13	10.74	11.52	11.51	11.44	11.30	11.36	11.99	11.48	11.51
benzene	9.25	9.27	9.39	9.26	9.27	9.26	9.27	9.74	9.37	9.28
CH_2F_2	13.27	12.43	13.23	13.16	13.16	13.10	13.12	13.90	13.22	13.20
CF_3H	15.50	13.54	14.48	14.41	14.40	14.32	14.35	15.20	14.46	14.45
CH_2Cl_2	11.40	10.70	11.74	11.63	11.52	11.33	11.43	12.21	11.68	11.65
CCl_3H	11.50	10.53	11.70	11.61	11.46	11.23	11.35	12.20	11.66	11.62
CH_3NO_2	11.29	11.01	11.58	11.73	11.68	11.58	11.63	12.40	11.79	11.76
CH_3SiH_3	11.60	11.26	11.77	11.65	11.65	11.62	11.64	12.18	11.75	11.68
HCOOH	11.50	11.11	11.34	11.24	11.23	11.21	11.22	11.77	11.27	11.24
CH_3CONH_2	10.00	9.66	10.54	9.87	9.85	9.81	9.82	10.37	9.89	9.87
$cylNHC_2H_4$	9.85	9.62	9.84	9.76	9.75	9.72	9.73	10.27	9.82	9.79
NCCN	13.51	13.14	13.58	13.40	13.38	13.32	13.35	14.00	13.54	13.43

CH_3NHCH_3	8.95	8.77	9.02	8.97	8.95	8.91	8.93	9.46	9.00	8.99
CH_2CO	9.64	9.71	9.80	9.70	9.74	9.75	9.74	10.25	9.78	9.73
$cylOC_2H_4$	10.57	10.47	10.74	10.64	10.63	10.60	10.61	11.14	10.69	10.65
OCHCHO	10.60	9.99	10.84	10.76	10.73	10.60	10.66	11.43	10.82	10.79
CH_3CH_2OH	10.64	10.19	10.72	10.65	10.62	10.56	10.58	11.18	10.67	10.65
CH_3OCH_3	10.10	9.73	10.10	10.02	10.00	9.96	9.97	10.52	10.05	10.03
$cylSC_2H_4$	9.05	8.93	9.07	8.98	9.00	9.01	9.02	9.46	9.04	9.01
CH_3SOCH_3	9.10	8.81	9.06	8.98	8.97	8.94	8.95	9.49	9.03	9.00
CH_2CHF	10.63	10.37	10.46	10.33	10.37	10.39	10.38	10.89	10.43	10.36
CH_3CH_2Cl	11.06	10.66	11.15	11.08	11.07	11.02	11.05	11.59	11.12	11.09
CH_2CHCl	10.20	9.83	10.12	10.00	9.98	9.94	9.97	10.52	10.09	10.02
CH_3CClO	11.03	10.75	11.98	11.09	11.06	11.01	11.03	11.59	11.12	11.09
prplCl	10.88	10.36	11.02	10.95	10.92	10.84	10.88	11.46	10.99	10.96
NC_3H_9	8.54	8.25	8.46	8.43	8.40	8.36	8.38	8.89	8.44	8.43
$cylOC_4H_4$	8.90	8.90	9.00	8.86	8.87	8.87	8.87	9.37	8.97	8.87
$cylNHC_4H_4$	8.23	8.27	8.31	8.19	8.21	8.21	8.21	8.68	8.29	8.21
NO_2	11.23	11.18	9.01	11.70	11.74	11.71	11.71	12.51	11.88	11.74
SF_6	15.70	13.73	15.52	15.44	15.40	15.22	15.31	16.48	15.57	15.53
$CFCl_3$	11.76	10.84	12.07	11.98	11.83	11.59	11.71	12.59	12.04	12.00
$CClF_3$	13.08	12.56	13.11	13.02	13.04	13.02	13.03	13.61	13.07	13.05
$CBrF_3$	12.08	11.70	12.06	11.90	11.95	11.95	11.97	12.57	12.04	11.99
HCCF	11.50	11.17	11.30	11.16	11.20	11.22	11.21	11.75	11.28	11.19
HCCCN	11.75	11.37	11.68	11.52	11.51	11.48	11.50	12.08	11.65	11.55
NCCCCN	11.84	11.51	12.07	11.91	11.87	11.80	11.83	12.50	12.04	11.93
C_2N_2	13.51	13.14	13.58	13.40	13.38	13.32	13.35	14.00	13.54	13.43

C_3O_2	10.80	10.76	10.85	10.72	10.77	10.81	10.79	11.30	10.81	10.75
FCN	13.65	13.31	13.49	13.33	13.37	13.39	13.38	13.96	13.46	13.36
HCCCCH	10.30	9.93	10.19	10.04	10.04	10.01	10.02	10.59	10.17	10.07
H_2CS	9.38	9.26	9.36	9.26	9.30	9.32	9.32	9.75	9.32	9.29
$HCONH_2$	10.40	10.23	10.91	10.30	10.29	10.27	10.28	10.80	10.31	10.30
CH_2CHCHO	10.10	9.81	10.13	10.04	10.02	9.98	10.00	10.54	10.08	10.04
CH_2CCl_2	10.00	9.56	10.00	9.88	9.85	9.78	9.82	10.41	9.97	9.90
$CHFCF_2$	10.62	10.01	10.33	10.20	10.26	10.27	10.26	10.85	10.30	10.23
CH_2CF_2	10.70	10.38	10.58	10.45	10.50	10.51	10.51	11.06	10.55	10.48
CH_3F	13.04	12.72	13.25	13.17	13.16	13.12	13.14	13.78	13.21	13.18
CF_2Cl_2	12.24	11.51	12.46	12.38	12.28	12.13	12.21	12.96	12.42	12.39
SiF_2	11.08	10.83	11.00	11.10	11.10	11.07	11.09	11.64	11.03	11.14
MSE		-0.26	0.10	0.00	0.00	-0.03	-0.02	0.57	0.09	0.02
MAE		0.36	0.28	0.19	0.18	0.19	0.18	0.58	0.20	0.18
rms		0.52	0.46	0.26	0.26	0.27	0.26	0.64	0.28	0.26

TABLE XIII: Vertical ionization potentials (in eV) of the IP131 database [8], calculated using $\mathrm{IP}(2) = -\epsilon_{\mathrm{HOMO}}(N)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	13.60	7.59	12.21	11.91	11.62	11.05	11.38	12.68	12.21	11.98
He	24.59	15.76	21.19	21.13	20.90	20.26	20.62	22.41	21.30	21.28
Li	5.39	3.22	3.78	5.32	5.31	5.21	5.30	5.83	5.61	5.38
Be	9.32	5.61	8.92	8.76	8.63	8.29	8.49	9.33	8.94	8.81
B	8.30	4.17	8.21	7.91	7.73	7.24	7.51	8.66	8.20	7.92

C	11.26	6.10	10.69	10.36	10.14	9.57	9.88	11.30	10.68	10.41
N	14.53	8.31	13.27	12.94	12.72	12.14	12.46	14.12	13.30	13.03
O	13.62	7.60	12.60	12.38	12.12	11.49	11.83	13.39	12.63	12.43
F	17.42	10.32	15.58	15.43	15.23	14.63	14.96	16.76	15.67	15.57
Ne	21.57	13.38	18.83	18.73	18.63	18.08	18.39	20.47	19.06	19.02
Na	5.14	3.03	5.24	4.82	4.91	4.87	4.92	5.58	5.26	4.87
Mg	7.65	4.70	7.50	7.35	7.31	7.08	7.22	7.92	7.52	7.37
Al	5.99	3.09	6.20	5.88	5.77	5.47	5.66	6.39	6.18	5.90
Si	8.15	4.61	8.23	7.93	7.72	7.30	7.55	8.49	8.20	7.95
P	10.49	6.30	10.33	10.08	9.78	9.26	9.57	10.69	10.31	10.10
S	10.36	6.15	10.31	10.08	9.83	9.31	9.60	10.83	10.29	10.11
Cl	12.97	8.14	12.60	12.45	12.15	11.56	11.88	13.24	12.59	12.48
Ar	15.76	10.30	15.00	14.89	14.56	13.92	14.28	15.77	15.01	14.95
CH_3	9.84	5.42	9.80	9.41	9.15	8.59	8.90	10.27	9.79	9.44
CH_4	13.60	9.45	14.00	13.91	13.60	12.99	13.32	14.69	14.01	13.95
NH	13.49	7.92	12.81	12.49	12.24	11.65	11.97	13.59	12.82	12.56
NH_2	12.00	7.22	9.88	11.65	11.36	10.75	11.09	12.52	11.81	11.72
NH_3	10.82	6.18	10.72	10.64	10.33	9.73	10.06	11.48	10.74	10.70
OH	13.02	7.38	12.30	12.16	11.89	11.27	11.61	13.21	12.34	12.24
H_2O	12.62	7.24	12.11	12.02	11.73	11.11	11.45	13.06	12.15	12.11
HF	16.12	9.65	14.82	14.73	14.50	13.89	14.23	16.06	14.92	14.90
SiH_3	8.74	5.37	9.13	8.78	8.59	8.16	8.41	9.46	9.12	8.81
SiH_4	12.30	8.52	12.76	12.66	12.37	11.82	12.13	13.34	12.76	12.69
PH_3	10.59	6.72	10.61	10.49	10.26	9.77	10.04	11.14	10.62	10.54
SH_2	10.50	6.31	10.42	10.30	10.01	9.46	9.77	10.95	10.40	10.33

HCl	12.77	8.05	12.46	12.37	12.05	11.44	11.78	13.10	12.45	12.40
HCCH	11.49	7.20	11.35	11.21	10.92	10.36	10.67	11.88	11.34	11.23
CH_2CH_2	10.68	6.74	10.70	10.55	10.28	9.75	10.05	11.18	10.68	10.57
CH_3CH_3	11.99	8.17	12.51	12.43	12.15	11.59	11.90	13.17	12.52	12.46
HCN	13.61	9.02	13.41	13.25	12.94	12.35	12.68	14.02	13.40	13.28
CO	14.01	9.04	13.84	13.75	13.44	12.81	13.16	14.69	13.87	13.83
HCO	9.31	5.16	9.61	9.40	9.17	8.63	8.93	10.32	9.64	9.46
CH_2O	10.89	6.26	10.68	10.58	10.36	9.82	10.13	11.51	10.71	10.66
CH_3OH	10.96	6.26	10.84	10.75	10.49	9.92	10.24	11.68	10.87	10.83
N_2	15.58	10.28	15.30	15.17	14.91	14.29	14.63	16.29	15.34	15.27
NH_2NH_2	8.98	5.30	9.74	9.66	9.38	8.80	9.12	10.49	9.76	9.72
NO	9.26	4.52	9.38	9.15	8.93	8.35	8.67	10.26	9.40	9.23
O_2	12.30	6.84	11.94	11.79	11.59	11.01	11.33	13.08	12.02	11.92
HOOH	11.70	6.46	11.34	11.24	10.98	10.38	10.71	12.32	11.38	11.34
F_2	15.70	9.48	14.74	14.64	14.47	13.90	14.22	16.09	14.87	14.83
CO_2	13.78	9.09	13.54	13.41	13.18	12.65	12.95	14.38	13.56	13.49
P_2	10.62	7.15	10.64	10.49	10.30	9.90	10.14	10.96	10.61	10.49
S_2	9.55	5.83	9.88	9.70	9.41	8.88	9.19	10.33	9.85	9.72
Cl_2	11.49	7.33	11.60	11.50	11.20	10.63	10.95	12.21	11.58	11.52
NaCl	9.80	5.30	9.34	9.25	8.96	8.41	8.71	9.94	9.34	9.27
SiO	11.61	7.48	11.59	11.44	11.25	10.77	11.05	12.25	11.60	11.51
CS	11.34	7.40	11.88	11.78	11.50	10.92	11.25	12.58	11.88	11.84
ClO	11.01	6.30	10.87	10.73	10.48	9.91	10.23	11.64	10.88	10.79
ClF	12.77	7.86	12.43	12.33	12.04	11.45	11.78	13.20	12.44	12.38
SiH_3SiH_3	10.53	7.19	10.94	10.82	10.59	10.13	10.39	11.41	10.93	10.84

CH_3Cl	11.29	7.12	11.39	11.31	11.00	10.43	10.75	12.01	11.39	11.33
CH_3SH	9.44	5.57	9.60	9.49	9.21	8.68	8.98	10.13	9.59	9.51
SO_2	12.50	8.08	12.48	12.35	12.13	11.61	11.90	13.29	12.50	12.43
BF_3	15.96	10.07	15.15	15.01	14.84	14.28	14.59	16.38	15.25	15.19
BCl_3	11.64	7.72	12.00	11.90	11.59	11.02	11.34	12.61	11.98	11.92
$AlCl_3$	12.01	8.02	12.27	12.17	11.86	11.30	11.61	12.87	12.26	12.19
CF_4	16.20	10.42	15.55	15.43	15.26	14.69	15.01	16.81	15.65	15.61
CCl_4	11.69	7.69	11.99	11.90	11.59	11.01	11.33	12.61	11.97	11.92
OCS	11.19	7.50	11.35	11.22	10.99	10.53	10.80	11.89	11.33	11.26
CS_2	10.09	6.82	10.31	10.18	9.97	9.57	9.80	10.75	10.28	10.21
CF_2O	13.60	8.52	13.33	13.20	12.97	12.39	12.71	14.31	13.36	13.30
SiF_4	16.40	10.69	15.73	15.61	15.42	14.85	15.17	16.92	15.82	15.77
N_2O	12.89	8.40	12.58	12.44	12.23	11.74	12.02	13.33	12.58	12.50
NF_3	13.60	8.45	13.21	13.13	12.90	12.33	12.64	14.20	13.23	13.21
PF_3	12.20	7.36	11.54	11.44	11.21	10.69	10.98	12.29	11.57	11.52
O_3	12.73	8.02	12.88	12.78	12.55	11.97	12.29	13.75	12.93	12.88
F_2O	13.26	7.72	12.91	12.81	12.62	12.03	12.35	14.12	12.99	12.95
ClF_3	13.05	8.00	12.78	12.68	12.44	11.87	12.19	13.74	12.81	12.77
CF_2CF_2	10.69	6.31	10.57	10.42	10.22	9.71	9.99	11.31	10.55	10.47
CF_3CN	14.30	9.57	14.06	13.90	13.60	13.00	13.33	14.72	14.04	13.93
CH_3CCH	10.37	6.49	10.55	10.42	10.14	9.60	9.90	11.07	10.53	10.44
CH_2CCH_2	10.20	6.56	10.51	10.38	10.12	9.60	9.89	11.03	10.50	10.40
$cylC_3H_4$	9.86	6.11	10.01	9.88	9.62	9.11	9.40	10.51	10.00	9.90
$cylC_3H_6$	10.54	7.07	11.24	11.11	10.83	10.28	10.59	11.82	11.23	11.14
$CH_3CH_2CH_3$	11.51	7.75	12.00	11.93	11.66	11.11	11.41	12.64	12.00	11.96

CH_3CCCH_3	9.79	5.93	9.89	9.78	9.51	8.99	9.28	10.41	9.88	9.79
$cylC_4H_6$	9.43	6.04	9.87	9.74	9.49	8.99	9.27	10.35	9.86	9.76
isobutane	11.13	7.58	11.74	11.68	11.42	10.87	11.17	12.38	11.74	11.70
benzene	9.25	6.33	9.83	9.69	9.49	9.06	9.30	10.25	9.81	9.71
CH_2F_2	13.27	8.15	12.85	12.76	12.54	11.98	12.29	13.79	12.89	12.85
CF_3H	15.50	9.35	14.09	14.01	13.79	13.22	13.53	15.08	14.13	14.10
CH_2Cl_2	11.40	7.38	11.67	11.58	11.29	10.72	11.03	12.29	11.65	11.60
CCl_3H	11.50	7.42	11.69	11.60	11.29	10.71	11.03	12.30	11.67	11.61
CH_3NO_2	11.29	6.92	11.64	11.53	11.30	10.73	11.05	12.59	11.68	11.63
CH_3SiH_3	11.60	7.92	12.06	11.94	11.66	11.13	11.43	12.63	12.05	11.97
HCOOH	11.50	6.73	11.26	11.16	10.92	10.35	10.67	12.14	11.29	11.24
CH_3CONH_2	10.00	5.79	10.23	10.15	9.91	9.35	9.66	11.08	10.27	10.23
$cylNHC_2H_4$	9.85	5.78	10.04	9.94	9.67	9.12	9.43	10.71	10.05	9.99
NCCN	13.51	9.39	13.51	13.34	13.07	12.54	12.83	14.11	13.49	13.37
CH_3NHCH_3	8.95	5.06	9.27	9.19	8.93	8.39	8.69	9.96	9.28	9.24
CH_2CO	9.64	5.91	9.86	9.72	9.50	9.01	9.29	10.45	9.85	9.76
$cylOC_2H_4$	10.57	6.27	10.79	10.70	10.46	9.90	10.22	11.65	10.84	10.78
OCHCHO	10.60	6.39	10.70	10.62	10.41	9.88	10.18	11.53	10.73	10.68
CH_3CH_2OH	10.64	6.15	10.70	10.62	10.37	9.79	10.11	11.53	10.73	10.69
CH_3OCH_3	10.10	5.83	10.21	10.14	9.90	9.36	9.66	11.02	10.24	10.21
$cylSC_2H_4$	9.05	5.37	9.38	9.26	8.98	8.46	8.75	9.90	9.36	9.28
CH_3SOCH_3	9.10	5.38	9.38	9.29	9.07	8.58	8.85	10.07	9.40	9.35
CH_2CHF	10.63	6.52	10.57	10.43	10.18	9.66	9.95	11.14	10.56	10.46
CH_3CH_2Cl	11.06	6.97	11.24	11.16	10.86	10.28	10.60	11.86	11.23	11.18
CH_2CHCl	10.20	6.42	10.30	10.18	9.92	9.41	9.70	10.82	10.28	10.19

CH_3CClO	11.03	7.13	11.36	11.27	11.04	10.52	10.81	12.12	11.38	11.32
prplCl	10.88	6.94	11.20	11.12	10.82	10.25	10.57	11.82	11.19	11.14
NC_3H_9	8.54	4.85	8.89	8.83	8.59	8.07	8.35	9.56	8.90	8.87
$cylOC_4H_4$	8.90	5.67	9.34	9.20	8.97	8.51	8.77	9.80	9.32	9.21
$cylNHC_4H_4$	8.23	5.13	8.71	8.58	8.36	7.92	8.17	9.15	8.69	8.59
NO_2	11.23	6.50	8.49	11.16	10.94	10.37	10.69	12.31	11.39	11.26
SF_6	15.70	10.14	15.24	15.12	14.96	14.41	14.72	16.50	15.34	15.29
$CFCl_3$	11.76	7.75	12.07	11.97	11.66	11.08	11.40	12.69	12.04	11.99
$CClF_3$	13.08	8.56	13.08	12.97	12.66	12.06	12.40	13.78	13.07	13.01
$CBrF_3$	12.08	7.82	12.08	11.88	11.64	11.12	11.42	12.73	12.08	11.95
HCCF	11.50	7.01	11.23	11.09	10.82	10.28	10.58	11.84	11.22	11.12
HCCCN	11.75	7.87	11.77	11.62	11.36	10.87	11.14	12.32	11.76	11.64
NCCCCN	11.84	8.44	12.24	12.08	11.83	11.36	11.62	12.79	12.22	12.10
C_2N_2	13.51	9.39	13.51	13.34	13.07	12.54	12.83	14.11	13.49	13.37
C_3O_2	10.80	7.27	10.95	10.81	10.63	10.22	10.46	11.56	10.94	10.86
FCN	13.65	8.73	13.17	13.02	12.74	12.17	12.49	13.88	13.17	13.06
HCCCCH	10.30	6.64	10.39	10.24	10.00	9.52	9.79	10.89	10.37	10.26
H_2CS	9.38	5.53	9.52	9.40	9.14	8.62	8.91	10.05	9.51	9.43
$HCONH_2$	10.40	6.02	10.47	10.39	10.15	9.59	9.90	11.34	10.51	10.47
CH_2CHCHO	10.10	6.00	10.46	10.37	10.14	9.59	9.90	11.30	10.50	10.45
CH_2CCl_2	10.00	6.44	10.30	10.17	9.92	9.42	9.70	10.81	10.27	10.18
$CHFCF_2$	10.62	6.22	10.38	10.24	10.02	9.52	9.80	11.06	10.37	10.28
CH_2CF_2	10.70	6.57	10.68	10.54	10.30	9.78	10.07	11.30	10.67	10.58
CH_3F	13.04	8.09	12.79	12.70	12.48	11.91	12.23	13.73	12.85	12.81
CF_2Cl_2	12.24	8.08	12.44	12.35	12.04	11.45	11.78	13.09	12.42	12.37

SiF_2	11.08	7.14	11.00	10.88	10.70	10.24	10.50	11.65	11.03	10.96
MSE		-4.40	-0.15	-0.24	-0.48	-1.01	-0.71	0.61	-0.09	-0.18
MAE		4.40	0.42	0.40	0.51	1.01	0.72	0.70	0.36	0.37
rms		4.50	0.68	0.63	0.75	1.18	0.93	0.77	0.56	0.59

TABLE XIV: Vertical electron affinities (in eV) of the EA131 database [8, 9], calculated using EA(1) = $E_{\text{total}}(N) - E_{\text{total}}(N+1)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	0.75	0.65	0.63	0.65	0.73	0.79	0.75	1.31	0.63	0.64
He	-2.63	-3.81	-3.92	-4.18	-4.12	-4.02	-4.05	-3.75	-3.92	-4.13
Li	0.62	0.52	-0.33	0.40	0.48	0.51	0.47	0.78	0.48	0.40
Be	-0.36	-0.16	-0.27	-0.55	-0.45	-0.35	-0.40	-0.08	-0.28	-0.53
B	0.25	0.54	0.41	0.09	0.22	0.32	0.27	0.63	0.40	0.11
C	1.25	1.55	1.45	1.11	1.23	1.31	1.27	1.72	1.43	1.14
N	-0.22	0.17	-0.02	-0.10	-0.10	-0.11	-0.12	0.31	-0.05	-0.13
O	1.45	1.66	1.54	1.47	1.46	1.44	1.44	1.90	1.46	1.43
F	3.44	3.54	3.48	3.44	3.38	3.35	3.35	3.81	3.30	3.35
Ne	-5.31	-6.61	-6.84	-7.21	-7.09	-6.99	-7.03	-6.41	-6.81	-7.15
Na	0.54	0.55	0.46	0.52	0.57	0.52	0.49	0.75	0.46	0.46
Mg	-0.23	-0.15	-0.21	-0.49	-0.43	-0.33	-0.37	-0.10	-0.22	-0.46
Al	0.45	0.50	0.46	0.14	0.23	0.32	0.28	0.58	0.44	0.17
Si	1.42	1.46	1.44	1.14	1.21	1.29	1.26	1.60	1.42	1.16
P	0.74	0.85	0.75	0.71	0.82	0.87	0.83	1.17	0.73	0.70

S	2.10	2.14	2.06	2.03	2.12	2.16	2.13	2.49	2.04	2.04
Cl	3.69	3.65	3.60	3.60	3.66	3.68	3.66	4.05	3.58	3.60
Ar	-2.81	-2.98	-3.29	-3.58	-3.43	-3.31	-3.37	-2.90	-3.27	-3.56
CH_3	-0.07	-0.04	-0.30	-0.23	-0.17	-0.14	-0.16	0.15	-0.31	-0.23
CH_4	-0.62	-0.72	-0.92	-1.12	-1.07	-0.98	-1.02	-0.71	-0.92	-1.09
NH	0.33	0.46	0.28	0.27	0.29	0.29	0.28	0.70	0.26	0.26
NH_2	0.74	0.75	2.57	0.59	0.61	0.62	0.61	1.01	0.53	0.59
NH_3	-0.56	-0.69	-0.89	-1.10	-1.05	-0.96	-1.00	-0.65	-0.89	-1.07
OH	1.83	1.85	1.70	1.71	1.69	1.68	1.67	2.11	1.62	1.68
H_2O	-0.56	-0.72	-0.87	-1.09	-1.04	-0.95	-0.98	-0.61	-0.87	-1.06
HF	-0.63	-0.77	-0.87	-1.10	-1.05	-0.96	-0.99	-0.61	-0.87	-1.06
SiH_3	0.93	0.91	0.76	0.81	0.88	0.91	0.89	1.17	0.75	0.81
SiH_4	-1.11	-0.78	-1.08	-1.28	-1.22	-1.13	-1.17	-0.84	-1.07	-1.25
PH_3	-1.21	-0.64	-0.89	-1.12	-1.04	-0.94	-0.99	-0.64	-0.88	-1.08
SH_2	-0.49	-0.59	-0.81	-1.04	-0.96	-0.87	-0.91	-0.57	-0.81	-1.01
HCl	-0.52	-0.62	-0.77	-0.99	-0.92	-0.82	-0.87	-0.52	-0.77	-0.97
HCCH	-1.90	-0.69	-0.96	-1.13	-1.09	-1.00	-1.04	-0.77	-0.96	-1.10
CH_2CH_2	-1.86	-0.82	-1.83	-1.29	-1.25	-1.15	-1.19	-0.89	-1.09	-1.26
CH_3CH_3	-0.62	-0.68	-0.96	-1.14	-1.10	-1.02	-1.05	-0.74	-0.96	-1.11
HCN	-0.48	-0.69	-1.86	-0.90	-0.85	-0.78	-0.81	-0.50	-0.71	-0.87
CO	-1.50	-1.30	-1.52	-1.75	-1.66	-1.56	-1.61	-1.22	-1.54	-1.74
HCO	0.02	-0.02	-0.07	-0.07	-0.01	0.01	-0.01	0.43	-0.09	-0.06
CH_2O	-0.55	-0.56	-0.88	-1.09	-1.03	-0.97	-1.00	-0.54	-0.91	-1.08
CH_3OH	-0.55	-0.59	-0.83	-1.01	-0.97	-0.89	-0.92	-0.61	-0.83	-0.98
N_2	-2.24	-2.05	-2.07	-2.25	-2.20	-2.16	-2.18	-1.70	-2.11	-2.26

NH_2NH_2	-0.45	-0.55	-0.77	-0.98	-0.93	-0.84	-0.88	-0.53	-0.77	-0.95
NO	-0.42	-0.26	-0.13	-0.29	-0.25	-0.23	-0.24	0.30	-0.17	-0.29
O_2	-0.08	-0.20	0.00	-0.10	-0.07	-0.08	-0.09	0.46	-0.07	-0.12
HOOH	-0.92	-0.76	-1.33	-1.23	-1.19	-1.09	-1.13	-0.76	-1.02	-1.20
F_2	0.42	0.48	0.72	0.63	0.63	0.62	0.61	1.26	0.66	0.62
CO_2	-0.65	-0.87	-1.14	-1.33	-1.28	-1.19	-1.23	-0.82	-1.14	-1.31
P_2	0.48	0.57	0.81	0.64	0.65	0.63	0.63	1.08	0.78	0.64
S_2	1.53	1.35	1.58	1.48	1.51	1.49	1.49	1.98	1.54	1.49
Cl_2	0.75	0.87	0.86	0.72	0.76	0.77	0.76	1.24	0.84	0.73
NaCl	0.65	0.79	0.76	0.56	0.57	0.64	0.62	1.01	0.76	0.60
SiO	0.03	0.10	0.17	-0.07	-0.01	0.04	0.01	0.42	0.14	-0.06
CS	-0.09	0.07	0.26	0.06	0.10	0.09	0.08	0.58	0.23	0.06
ClO	2.19	1.93	2.14	2.09	2.08	2.05	2.06	2.59	2.09	2.08
ClF	0.44	0.55	0.57	0.45	0.47	0.47	0.47	0.98	0.55	0.45
SiH_3SiH_3	-0.69	-0.72	-1.20	-1.21	-1.16	-1.06	-1.11	-0.77	-1.01	-1.18
CH_3Cl	-0.51	-0.55	-0.78	-0.96	-0.91	-0.82	-0.86	-0.55	-0.78	-0.93
CH_3SH	-0.50	-0.54	-0.82	-1.01	-0.96	-0.87	-0.91	-0.59	-0.82	-0.99
SO_2	0.81	0.73	1.12	0.96	0.97	0.94	0.95	1.54	1.08	0.97
BF_3	-1.04	-0.82	-1.12	-1.35	-1.31	-1.23	-1.25	-0.81	-1.12	-1.31
BCl_3	-0.17	-0.10	-1.01	-0.16	-0.11	-0.13	-0.14	0.36	0.06	-0.18
$AlCl_3$	0.06	0.24	-0.14	-0.35	-0.23	-0.14	-0.20	0.18	-0.13	-0.35
CF_4	-1.33	-1.40	-1.82	-2.03	-2.01	-1.92	-1.95	-1.50	-1.81	-1.99
CCl_4	-0.46	0.22	-0.43	-0.48	-0.38	-0.25	-0.33	-0.08	-0.43	-0.45
OCS	-0.74	-0.88	-1.23	-1.28	-1.24	-1.21	-1.25	-0.94	-1.11	-1.28
CS_2	0.01	0.00	0.37	0.16	0.17	0.12	0.14	0.69	0.34	0.17

CF_2O	-2.37	-1.01	-1.36	-1.56	-1.52	-2.11	-1.47	-1.03	-1.35	-1.53
SiF_4	-0.81	-0.71	-1.16	-1.37	-1.32	-1.24	-1.27	-0.79	-1.15	-1.33
N_2O	-2.01	-1.46	-1.78	-2.16	-2.12	-2.12	-2.13	-1.46	-1.77	-1.97
NF_3	-2.06	-2.24	-2.73	-2.92	-2.84	-2.78	-2.84	-2.39	-2.74	-2.93
PF_3	-1.23	-1.07	-1.44	-1.66	-1.60	-1.48	-1.53	-1.20	-1.46	-1.63
O_3	1.93	1.88	2.64	2.52	2.53	2.46	2.48	3.28	2.62	2.54
F_2O	-0.31	-0.28	-0.14	-0.23	-0.21	-0.21	-0.22	0.37	-0.20	-0.24
ClF_3	1.20	1.02	1.32	1.21	1.22	1.19	1.20	1.83	1.29	1.23
CF_2CF_2	-1.65	-1.07	-1.49	-1.72	-1.68	-1.59	-1.62	-1.16	-1.49	-1.69
CF_3CN	-0.96	-0.98	-1.39	-1.60	-1.55	-1.51	-1.54	-1.11	-1.39	-1.55
CH_3CCH	-1.13	-0.56	-0.84	-0.99	-0.97	-0.89	-0.92	-0.63	-0.84	-0.97
CH_2CCH_2	-0.56	-0.67	-1.49	-1.16	-1.13	-1.04	-1.08	-0.78	-1.00	-1.13
$cylC_3H_4$	-1.82	-0.75	-1.82	-1.19	-1.16	-1.07	-1.11	-0.83	-1.02	-1.17
$cylC_3H_6$	-0.65	-0.77	-1.09	-1.27	-1.24	-1.15	-1.19	-0.88	-1.09	-1.24
$CH_3CH_2CH_3$	-0.60	-0.63	-0.96	-1.15	-1.11	-1.02	-1.06	-0.73	-0.96	-1.11
CH_3CCCH_3	-0.67	-0.52	-0.90	-1.06	-1.03	-0.95	-0.98	-0.67	-0.90	-1.03
$cylC_4H_6$	-1.41	-0.69	-1.00	-1.20	-1.17	-1.08	-1.11	-0.81	-1.02	-1.17
isobutane	-0.56	-0.56	-0.92	-1.10	-1.07	-0.98	-1.02	-0.70	-0.92	-1.07
benzene	-0.71	-0.52	-1.37	-1.12	-1.08	-0.99	-1.03	-0.72	-0.94	-1.09
CH_2F_2	-0.58	-0.68	-0.88	-1.07	-1.03	-0.94	-0.98	-0.67	-0.88	-1.04
CF_3H	-0.60	-0.82	-0.90	-1.11	-1.06	-0.99	-1.02	-0.69	-0.91	-1.08
CH_2Cl_2	-0.49	-0.48	-0.77	-0.96	-0.89	-0.80	-0.85	-0.54	-0.77	-0.94
CCl_3H	-0.83	-0.32	-0.77	-0.96	-0.87	-0.75	-0.82	-0.53	-0.77	-0.95
CH_3NO_2	-0.37	-0.06	-0.10	-0.24	-0.23	-0.24	-0.24	0.35	-0.14	-0.25
CH_3SiH_3	-0.53	-0.59	-0.87	-1.05	-1.01	-0.92	-0.96	-0.66	-0.87	-1.03

HCOOH	-0.57	-0.70	-1.88	-1.13	-1.08	-0.99	-1.03	-0.69	-0.92	-1.11
CH_3CONH_2	-0.31	-0.33	-0.57	-0.77	-0.72	-0.63	-0.67	-0.34	-0.57	-0.74
cylNHC_2H_4	-0.56	-0.63	-0.87	-1.06	-1.02	-0.93	-0.97	-0.67	-0.87	-1.03
NCCN	-0.19	0.14	0.24	0.06	0.11	0.12	0.11	0.59	0.21	0.07
CH_3NHCH_3	-0.56	-0.57	-0.87	-1.04	-1.01	-0.93	-0.96	-0.66	-0.87	-1.01
CH_2CO	-0.51	-0.72	-1.22	-1.08	-1.31	-1.17	-1.25	-0.68	-0.90	-1.05
cylOC_2H_4	-0.86	-0.69	-0.95	-1.13	-1.09	-1.01	-1.04	-0.75	-0.96	-1.10
OCHCHO	0.69	1.04	1.01	0.84	0.90	0.94	0.91	1.36	0.98	0.84
CH_3CH_2OH	-0.53	-0.55	-0.82	-1.00	-0.96	-0.88	-0.91	-0.60	-0.82	-0.97
CH_3OCH_3	-0.58	-0.60	-0.90	-1.09	-1.05	-0.96	-1.00	-0.69	-0.90	-1.06
cylSC_2H_4	-0.78	-0.66	-0.94	-1.12	-1.08	-1.00	-1.03	-0.74	-0.94	-1.10
CH_3SOCH_3	-0.40	-0.43	-0.67	-0.87	-0.82	-0.74	-0.78	-0.45	-0.67	-0.84
CH_2CHF	-0.88	-0.76	-1.92	-1.16	-1.12	-1.03	-1.07	-0.77	-0.97	-1.13
CH_3CH_2Cl	-0.51	-0.56	-0.82	-1.00	-0.96	-0.87	-0.91	-0.60	-0.82	-0.98
CH_2CHCl	-1.11	-0.68	-0.90	-1.09	-1.04	-0.96	-1.00	-0.70	-0.90	-1.06
CH_3CClO	-0.85	-0.36	-0.71	-0.89	-0.84	-0.76	-0.79	-0.48	-0.71	-0.86
prplCl	-0.48	-0.47	-0.79	-0.98	-0.93	-0.84	-0.88	-0.57	-0.79	-0.95
NC_3H_9	-0.54	-0.52	-0.88	-1.06	-1.02	-0.94	-0.98	-0.66	-0.88	-1.03
cylOC_4H_4	-0.74	-0.60	-1.88	-1.12	-1.08	-0.99	-1.02	-0.73	-0.93	-1.09
cylNHC_4H_4	-0.51	-0.46	-0.71	-0.91	-0.86	-0.77	-0.81	-0.50	-0.71	-0.88
NO_2	1.44	1.13	4.32	1.41	1.43	1.38	1.39	2.03	1.40	1.41
SF_6	-1.05	-0.50	-1.05	-1.15	-1.10	-1.02	-1.06	-0.55	-1.03	-1.07
$CFCl_3$	-0.68	-0.16	-0.68	-0.78	-0.68	-0.57	-0.64	-0.33	-0.69	-0.76
$CClF_3$	-1.06	-1.07	-1.49	-1.73	-1.63	-1.50	-1.56	-1.20	-1.48	-1.68
$CBrF_3$	-0.81	-0.76	-1.02	-1.26	-1.16	-1.06	-1.11	-0.67	-1.03	-1.23

HCCF	-0.55	-0.61	-0.81	-0.98	-0.94	-0.87	-0.90	-0.62	-0.81	-0.96
HCCCN	-0.36	-0.12	-0.36	-0.54	-0.49	-0.46	-0.48	-0.03	-0.38	-0.53
NCCCCN	0.68	1.08	1.15	0.97	1.01	1.03	1.02	1.47	1.12	0.98
C_2N_2	-0.19	0.14	0.24	0.06	0.11	0.12	0.11	0.59	0.21	0.07
C_3O_2	-0.74	-0.68	-0.38	-0.58	-0.56	-0.59	-0.58	0.00	-0.42	-0.57
FCN	-0.66	-0.59	-0.87	-1.07	-1.01	-0.91	-0.95	-0.53	-0.86	-1.04
HCCCCH	-0.64	-0.46	-0.99	-0.93	-1.12	-0.85	-1.09	-0.63	-0.80	-0.90
H_2CS	0.28	0.39	-0.88	0.41	0.42	0.40	0.40	0.90	0.56	0.40
$HCONH_2$	-0.35	-0.47	-0.63	-0.84	-0.78	-0.69	-0.73	-0.40	-0.63	-0.81
CH_2CHCHO	-0.46	0.02	0.03	-0.14	-0.11	-0.09	-0.11	0.34	0.00	-0.15
CH_2CCl_2	-1.07	-0.64	-0.92	-1.11	-1.06	-1.07	-1.02	-0.72	-0.92	-1.09
$CHFCF_2$	-0.54	-0.73	-0.92	-1.12	-1.08	-1.00	-1.03	-0.70	-0.92	-1.09
CH_2CF_2	-1.03	-0.73	-0.97	-1.15	-1.12	-1.03	-1.07	-0.76	-0.97	-1.12
CH_3F	-0.58	-0.66	-0.87	-1.04	-1.01	-0.92	-0.96	-0.66	-0.87	-1.01
CF_2Cl_2	-0.90	-0.65	-1.21	-1.36	-1.26	-1.12	-1.20	-0.85	-1.21	-1.34
SiF_2	0.10	0.18	0.26	0.02	0.08	0.12	0.10	0.51	0.23	0.02
MSE		0.10	-0.11	-0.24	-0.19	-0.14	-0.16	0.23	-0.08	-0.22
MAE		0.21	0.36	0.34	0.31	0.26	0.29	0.33	0.27	0.32
rms		0.34	0.54	0.44	0.41	0.36	0.39	0.45	0.35	0.42

TABLE XV: Vertical electron affinities (in eV) of the EA131 database [8, 9], calculated using $\mathrm{EA}(2) = -\epsilon_{\mathrm{HOMO}}(N+1)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	0.75	-1.97	1.34	1.37	1.21	0.85	1.05	1.77	1.35	1.35

He	-2.63	-6.06	-3.84	-4.10	-4.15	-4.26	-4.15	-3.74	-3.84	-4.05
Li	0.62	-0.88	0.17	0.69	0.73	0.70	0.71	0.97	0.79	0.68
Be	-0.36	-1.89	-0.06	-0.44	-0.34	-0.40	-0.37	0.11	-0.07	-0.43
B	0.25	-2.14	0.81	0.45	0.42	0.15	0.30	1.09	0.80	0.47
C	1.25	-2.06	1.64	1.28	1.16	0.74	0.98	2.09	1.64	1.32
N	-0.22	-3.49	0.26	0.11	-0.12	-0.62	-0.35	0.71	0.27	0.09
O	1.45	-2.91	1.48	1.43	1.16	0.55	0.88	2.22	1.50	1.45
F	3.44	-1.96	2.85	2.87	2.59	1.94	2.29	3.92	2.91	2.96
Ne	-5.31	-9.77	-6.70	-7.28	-7.29	-7.53	-7.35	-6.48	-6.67	-7.17
Na	0.54	-0.85	0.75	0.67	0.71	0.67	0.68	0.94	0.76	0.64
Mg	-0.23	-1.38	-0.03	-0.42	-0.35	-0.31	-0.31	0.02	-0.05	-0.38
Al	0.45	-1.58	0.82	0.48	0.47	0.31	0.41	0.95	0.80	0.50
Si	1.42	-1.26	1.78	1.46	1.35	1.07	1.24	2.00	1.76	1.48
P	0.74	-1.90	1.23	1.01	0.92	0.63	0.79	1.60	1.21	1.01
S	2.10	-1.20	2.43	2.34	2.15	1.71	1.95	2.91	2.42	2.33
Cl	3.69	-0.31	3.74	3.73	3.46	2.92	3.21	4.34	3.73	3.72
Ar	-2.81	-5.19	-3.06	-3.59	-3.46	-3.48	-3.43	-2.86	-3.03	-3.51
CH_3	-0.07	-2.78	0.38	0.36	0.20	-0.17	0.03	0.83	0.38	0.35
CH_4	-0.62	-1.97	-0.83	-1.05	-0.99	-0.92	-0.95	-0.67	-0.83	-1.03
NH	0.33	-3.16	0.67	0.60	0.37	-0.14	0.13	1.24	0.68	0.60
NH_2	0.74	-2.84	1.04	1.03	0.78	0.27	0.55	1.66	1.04	1.03
NH_3	-0.56	-2.18	-0.78	-1.02	-0.97	-0.90	-0.92	-0.61	-0.78	-1.00
OH	1.83	-2.56	1.83	1.84	1.56	0.96	1.28	2.65	1.85	1.88
H_2O	-0.56	-2.44	-0.76	-1.02	-0.97	-0.94	-0.94	-0.57	-0.76	-1.00
HF	-0.63	-2.65	-0.76	-1.04	-1.00	-1.00	-0.98	-0.56	-0.77	-1.01

SiH_3	0.93	-1.61	1.27	1.18	1.09	0.81	0.96	1.63	1.26	1.19
SiH_4	-1.11	-2.02	-0.97	-1.20	-1.13	-1.05	-1.09	-0.80	-0.96	-1.17
PH_3	-1.21	-1.95	-0.77	-1.05	-0.97	-0.88	-0.92	-0.60	-0.76	-1.01
SH_2	-0.49	-2.05	-0.69	-0.95	-0.88	-0.82	-0.84	-0.51	-0.68	-0.93
HCl	-0.52	-2.37	-0.63	-0.91	-0.85	-0.85	-0.83	-0.43	-0.63	-0.88
HCCH	-1.90	-1.81	-0.88	-1.10	-1.04	-0.96	-0.99	-0.73	-0.88	-1.08
CH_2CH_2	-1.86	-2.05	-1.59	-1.22	-1.17	-1.09	-1.12	-0.85	-1.00	-1.20
CH_3CH_3	-0.62	-1.89	-0.87	-1.09	-1.03	-0.95	-0.99	-0.70	-0.87	-1.07
HCN	-0.48	-2.32	-1.75	-0.81	-0.77	-0.79	-0.76	-0.39	-0.57	-0.78
CO	-1.50	-3.73	-1.45	-1.77	-1.79	-1.93	-1.83	-1.11	-1.46	-1.75
HCO	0.02	-2.94	0.24	0.22	0.06	-0.33	-0.12	0.84	0.24	0.23
CH_2O	-0.55	-2.45	-0.76	-1.02	-1.12	-1.40	-1.25	-0.31	-0.77	-0.99
CH_3OH	-0.55	-1.89	-0.73	-0.94	-0.90	-0.84	-0.86	-0.56	-0.73	-0.93
N_2	-2.24	-5.45	-2.13	-2.35	-2.50	-2.88	-2.67	-1.61	-2.16	-2.33
NH_2NH_2	-0.45	-2.11	-0.64	-0.89	-0.84	-0.81	-0.81	-0.46	-0.64	-0.87
NO	-0.42	-4.30	-0.24	-0.40	-0.61	-1.12	-0.84	0.49	-0.23	-0.37
O_2	-0.08	-4.58	-0.18	-0.26	-0.50	-1.08	-0.77	0.65	-0.17	-0.22
HOOH	-0.92	-2.40	-1.25	-1.17	-1.11	-1.06	-1.07	-0.72	-0.92	-1.15
F_2	0.42	-4.43	0.05	0.01	-0.17	-0.73	-0.43	1.27	0.20	0.18
CO_2	-0.65	-2.60	-1.03	-1.28	-1.22	-1.19	-1.19	-0.77	-1.02	-1.26
P_2	0.48	-2.13	1.05	0.89	0.72	0.35	0.55	1.37	1.03	0.87
S_2	1.53	-1.67	1.83	1.72	1.54	1.12	1.35	2.31	1.81	1.72
Cl_2	0.75	-2.20	0.99	0.86	0.68	0.28	0.49	1.50	0.99	0.87
NaCl	0.65	-0.83	0.87	0.62	0.65	0.65	0.67	1.10	0.88	0.65
SiO	0.03	-2.35	0.33	0.07	-0.01	-0.25	-0.11	0.60	0.31	0.07

CS	-0.09	-3.00	0.46	0.26	0.11	-0.32	-0.09	0.90	0.44	0.25
ClO	2.19	-1.97	2.23	2.18	1.95	1.41	1.71	3.00	2.24	2.22
ClF	0.44	-2.95	0.53	0.41	0.22	-0.23	0.02	1.16	0.56	0.45
SiH_3SiH_3	-0.69	-1.95	-1.10	-1.14	-1.07	-1.00	-1.03	-0.73	-0.91	-1.12
CH_3Cl	-0.51	-1.96	-0.65	-0.87	-0.81	-0.76	-0.78	-0.47	-0.65	-0.85
CH_3SH	-0.50	-1.90	-0.70	-0.93	-0.86	-0.80	-0.83	-0.53	-0.70	-0.91
SO_2	0.81	-2.78	1.17	1.01	0.80	0.29	0.57	1.76	1.16	1.03
BF_3	-1.04	-2.44	-1.01	-1.31	-1.24	-1.18	-1.20	-0.78	-1.01	-1.28
BCl_3	-0.17	-2.98	-0.90	0.23	0.10	-0.31	-0.10	0.90	0.48	0.22
$AlCl_3$	0.06	-1.61	0.13	-0.13	-0.07	-0.12	-0.09	0.41	0.15	-0.15
CF_4	-1.33	-2.98	-1.72	-1.96	-1.90	-1.83	-1.86	-1.47	-1.71	-1.94
CCl_4	-0.46	-2.11	-0.09	-0.14	-0.19	-0.35	-0.26	0.33	-0.08	-0.12
OCS	-0.74	-2.47	-1.10	-1.13	-1.27	-1.37	-1.42	-0.89	-0.94	-1.13
CS_2	0.01	-2.59	0.66	0.45	0.30	-0.10	0.12	1.08	0.64	0.45
CF_2O	-2.37	-2.74	-1.24	-1.51	-1.44	-2.41	-1.41	-0.98	-1.23	-1.48
SiF_4	-0.81	-2.48	-1.05	-1.36	-1.27	-1.23	-1.24	-0.75	-1.04	-1.33
N_2O	-2.01	-3.27	-1.62	-2.18	-2.34	-2.74	-2.52	-1.40	-1.61	-1.87
NF_3	-2.06	-4.45	-2.61	-2.82	-2.81	-3.05	-2.97	-2.30	-2.62	-2.86
PF_3	-1.23	-2.59	-1.31	-1.60	-1.54	-1.49	-1.50	-1.13	-1.34	-1.58
O_3	1.93	-2.29	2.49	2.39	2.16	1.55	1.88	3.47	2.54	2.47
F_2O	-0.31	-4.52	-0.41	-0.44	-0.63	-1.16	-0.87	0.62	-0.33	-0.33
ClF_3	1.20	-2.61	1.35	1.25	1.02	0.51	0.79	2.14	1.38	1.31
CF_2CF_2	-1.65	-2.65	-1.38	-1.67	-1.60	-1.54	-1.56	-1.12	-1.38	-1.65
CF_3CN	-0.96	-2.69	-1.28	-1.45	-1.60	-1.90	-1.74	-1.06	-1.28	-1.49
CH_3CCH	-1.13	-1.66	-0.74	-0.94	-0.89	-0.82	-0.85	-0.57	-0.74	-0.92

CH_2CCH_2	-0.56	-1.82	-1.39	-1.10	-1.06	-0.98	-1.01	-0.75	-0.91	-1.08
$cylC_3H_4$	-1.82	-1.88	-1.54	-1.12	-1.07	-1.00	-1.03	-0.77	-0.92	-1.10
$cylC_3H_6$	-0.65	-1.97	-1.00	-1.22	-1.17	-1.09	-1.12	-0.84	-1.00	-1.20
$CH_3CH_2CH_3$	-0.60	-1.77	-0.87	-1.10	-1.04	-0.96	-1.00	-0.70	-0.87	-1.08
CH_3CCCH_3	-0.67	-1.61	-0.82	-1.01	-0.97	-0.89	-0.93	-0.64	-0.82	-0.99
$cylC_4H_6$	-1.41	-1.81	-0.88	-1.14	-1.08	-1.01	-1.04	-0.77	-0.92	-1.12
isobutane	-0.56	-1.69	-0.83	-1.04	-0.99	-0.91	-0.95	-0.66	-0.83	-1.02
benzene	-0.71	-1.60	-1.00	-1.08	-1.03	-0.94	-0.98	-0.68	-0.87	-1.06
CH_2F_2	-0.58	-2.09	-0.78	-1.00	-0.95	-0.91	-0.92	-0.61	-0.78	-0.98
CF_3H	-0.60	-2.43	-0.78	-1.02	-0.99	-1.01	-0.98	-0.60	-0.79	-1.00
CH_2Cl_2	-0.49	-2.07	-0.61	-0.84	-0.78	-0.74	-0.75	-0.43	-0.61	-0.82
CCl_3H	-0.83	-2.25	-0.57	-0.82	-0.75	-0.74	-0.74	-0.37	-0.57	-0.80
CH_3NO_2	-0.37	-2.09	0.13	-0.01	-0.21	-0.66	-0.43	0.84	0.12	0.02
CH_3SiH_3	-0.53	-1.88	-0.76	-0.97	-0.91	-0.84	-0.87	-0.60	-0.76	-0.96
HCOOH	-0.57	-2.06	-1.70	-1.02	-0.98	-1.00	-0.96	-0.57	-0.76	-0.99
CH_3CONH_2	-0.31	-1.66	-0.42	-0.66	-0.60	-0.55	-0.57	-0.24	-0.42	-0.64
$cylNHC_2H_4$	-0.56	-1.90	-0.74	-0.97	-0.92	-0.87	-0.88	-0.58	-0.75	-0.95
NCCN	-0.19	-3.15	0.36	0.17	0.01	-0.39	-0.17	0.84	0.34	0.18
CH_3NHCH_3	-0.56	-1.71	-0.78	-0.98	-0.93	-0.86	-0.89	-0.61	-0.78	-0.96
CH_2CO	-0.51	-2.45	-1.07	-1.00	-1.33	-1.29	-1.31	-0.61	-0.79	-0.98
$cylOC_2H_4$	-0.86	-1.94	-0.86	-1.06	-1.01	-0.95	-0.97	-0.69	-0.86	-1.04
OCHCHO	0.69	-2.24	1.22	1.05	0.90	0.50	0.72	1.73	1.21	1.06
CH_3CH_2OH	-0.53	-1.82	-0.70	-0.92	-0.87	-0.81	-0.83	-0.53	-0.70	-0.90
CH_3OCH_3	-0.58	-1.77	-0.81	-1.02	-0.97	-0.90	-0.93	-0.64	-0.81	-1.00
$cylSC_2H_4$	-0.78	-1.93	-0.82	-1.03	-0.98	-0.91	-0.94	-0.66	-0.82	-1.02

CH_3SOCH_3	-0.40	-1.67	-0.53	-0.77	-0.71	-0.68	-0.68	-0.35	-0.53	-0.75
CH_2CHF	-0.88	-2.03	-1.70	-1.08	-1.03	-0.99	-1.00	-0.70	-0.86	-1.06
CH_3CH_2Cl	-0.51	-1.86	-0.69	-0.91	-0.86	-0.80	-0.82	-0.52	-0.69	-0.89
CH_2CHCl	-1.11	-1.91	-0.77	-1.00	-0.94	-0.90	-0.91	-0.61	-0.77	-0.98
CH_3CClO	-0.85	-1.99	-0.57	-0.79	-0.73	-0.68	-0.70	-0.39	-0.57	-0.77
prplCl	-0.48	-1.73	-0.67	-0.88	-0.83	-0.76	-0.79	-0.50	-0.67	-0.87
NC_3H_9	-0.54	-1.64	-0.80	-1.00	-0.95	-0.88	-0.91	-0.63	-0.79	-0.98
$cylOC_4H_4$	-0.74	-1.68	-1.58	-1.03	-0.98	-0.91	-0.94	-0.66	-0.81	-1.01
$cylNHC_4H_4$	-0.51	-1.70	-0.53	-0.78	-0.72	-0.69	-0.69	-0.36	-0.53	-0.76
NO_2	1.44	-2.44	1.52	1.51	1.31	0.77	1.05	2.34	1.53	1.53
SF_6	-1.05	-2.85	-0.94	-1.03	-1.10	-1.29	-1.18	-0.30	-0.90	-0.94
$CFCl_3$	-0.68	-2.43	-0.39	-0.50	-0.55	-0.73	-0.63	0.05	-0.39	-0.47
$CClF_3$	-1.06	-2.76	-1.31	-1.60	-1.54	-1.56	-1.53	-1.07	-1.30	-1.56
$CBrF_3$	-0.81	-2.73	-0.82	-1.11	-1.13	-1.27	-1.18	-0.42	-0.83	-1.07
HCCF	-0.55	-1.91	-0.70	-0.90	-0.86	-0.82	-0.83	-0.55	-0.70	-0.88
HCCCN	-0.36	-1.90	-0.16	-0.36	-0.49	-0.80	-0.62	0.25	-0.17	-0.35
NCCCCN	0.68	-1.75	1.40	1.20	1.06	0.72	0.91	1.82	1.38	1.22
C_2N_2	-0.19	-3.15	0.36	0.17	0.01	-0.39	-0.17	0.84	0.34	0.18
C_3O_2	-0.74	-3.04	-0.28	-0.48	-0.67	-1.11	-0.86	0.26	-0.30	-0.46
FCN	-0.66	-2.50	-0.71	-0.99	-0.93	-0.93	-0.91	-0.43	-0.71	-0.97
HCCCCH	-0.64	-1.62	-0.73	-0.88	-1.04	-0.80	-1.14	-0.59	-0.73	-0.86
H_2CS	0.28	-2.64	-0.73	0.65	0.47	0.04	0.27	1.26	0.83	0.64
$HCONH_2$	-0.35	-1.94	-0.48	-0.72	-0.67	-0.65	-0.65	-0.29	-0.48	-0.70
CH_2CHCHO	-0.46	-2.88	0.33	0.15	-0.01	-0.38	-0.17	0.77	0.32	0.15
CH_2CCl_2	-1.07	-1.96	-0.77	-0.99	-0.93	-1.16	-0.90	-0.61	-0.77	-0.97

$CHFCF_2$	-0.54	-2.22	-0.79	-1.03	-0.99	-0.98	-0.97	-0.60	-0.79	-1.00
CH_2CF_2	-1.03	-2.08	-0.86	-1.07	-1.02	-0.97	-0.98	-0.68	-0.86	-1.05
CH_3F	-0.58	-1.99	-0.77	-0.98	-0.93	-0.87	-0.89	-0.61	-0.77	-0.96
CF_2Cl_2	-0.90	-2.64	-1.01	-1.19	-1.21	-1.29	-1.25	-0.59	-1.00	-1.16
SiF_2	0.10	-2.36	0.46	0.19	0.09	-0.19	-0.03	0.73	0.44	0.18
MSE		-2.03	0.00	-0.13	-0.17	-0.32	-0.23	0.40	0.08	-0.10
MAE		2.03	0.34	0.34	0.32	0.39	0.33	0.47	0.30	0.33
rms		2.30	0.43	0.43	0.41	0.51	0.44	0.62	0.38	0.41

TABLE XVI: Vertical electron affinities (in eV) of the EA131 database [8, 9], calculated using $\mathrm{EA}(3) = -\epsilon_{\mathrm{LUMO}}(N)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	0.75	-0.51	-0.53	-0.52	-0.53	-0.53	-0.53	-0.50	-0.53	-0.52
He	-2.63	-2.29	-4.17	-4.55	-4.64	-4.30	-4.37	-3.79	-4.17	-4.36
Li	0.62	1.34	1.28	-0.28	-0.27	0.35	-0.24	1.47	-0.23	-0.27
Be	-0.36	2.02	-0.49	-0.67	-0.54	-0.29	-0.43	-0.22	-0.50	-0.63
B	0.25	3.62	0.13	-0.15	0.12	0.57	0.32	0.38	0.11	-0.13
C	1.25	5.59	1.41	1.00	1.38	1.98	1.65	1.58	1.36	1.03
N	-0.22	4.15	-0.15	-0.15	0.06	0.51	0.22	0.26	-0.20	-0.20
O	1.45	6.50	1.76	1.70	1.94	2.48	2.16	1.93	1.60	1.63
F	3.44	9.33	4.27	4.13	4.32	4.90	4.56	4.09	3.91	3.94
Ne	-5.31	-3.59	-6.98	-7.25	-7.18	-6.84	-7.00	-6.31	-6.95	-7.16
Na	0.54	1.45	0.04	-0.29	-0.29	-0.24	-0.27	1.28	0.03	-0.29
Mg	-0.23	1.34	-0.41	-0.59	-0.54	-0.38	-0.45	-0.20	-0.42	-0.54

Al	0.45	2.76	0.12	-0.08	0.07	0.36	0.20	0.33	0.10	-0.06
Si	1.42	4.37	1.12	0.87	1.11	1.55	1.31	1.30	1.10	0.90
P	0.74	3.73	0.35	0.55	0.84	1.21	0.97	1.04	0.32	0.54
S	2.10	5.64	1.76	2.01	2.34	2.79	2.51	2.28	1.72	2.00
Cl	3.69	7.75	3.51	3.65	4.03	4.58	4.26	3.93	3.47	3.66
Ar	-2.81	-0.84	-3.49	-3.74	-3.61	-3.41	-3.51	-2.90	-3.47	-3.65
CH_3	-0.07	2.95	-0.74	-0.55	-0.29	0.04	-0.19	-0.11	-0.75	-0.58
CH_4	-0.62	0.31	-1.07	-1.26	-1.36	-1.16	-1.20	-0.79	-1.07	-1.17
NH	0.33	4.32	0.03	0.12	0.38	0.83	0.55	0.49	-0.02	0.09
NH_2	0.74	4.54	2.17	0.36	0.64	1.11	0.82	0.67	0.16	0.34
NH_3	-0.56	0.66	-1.05	-1.28	-1.35	-1.12	-1.17	-0.71	-1.05	-1.17
OH	1.83	6.46	1.70	1.72	1.98	2.53	2.20	1.91	1.55	1.67
H_2O	-0.56	0.85	-1.04	-1.28	-1.35	-1.10	-1.16	-0.68	-1.04	-1.17
HF	-0.63	0.87	-1.03	-1.27	-1.36	-1.11	-1.17	-0.69	-1.04	-1.16
SiH_3	0.93	3.54	0.34	1.11	1.18	1.31	1.15	1.01	0.34	0.97
SiH_4	-1.11	0.37	-1.23	-1.45	-1.48	-1.28	-1.33	-0.89	-1.22	-1.35
PH_3	-1.21	0.61	-1.04	-1.27	-1.28	-1.09	-1.14	-0.70	-1.04	-1.17
SH_2	-0.49	0.79	-0.99	-1.22	-1.23	-1.03	-1.08	-0.65	-0.99	-1.12
HCl	-0.52	1.08	-0.98	-1.19	-1.20	-0.99	-1.06	-0.65	-0.98	-1.10
HCCH	-1.90	0.40	-1.10	-1.27	-1.38	-1.21	-1.23	-0.87	-1.10	-1.19
CH_2CH_2	-1.86	1.12	-1.25	-1.46	-1.55	-1.35	-1.38	-0.95	-1.25	-1.36
CH_3CH_3	-0.62	0.38	-1.09	-1.29	-1.38	-1.18	-1.22	-0.80	-1.09	-1.20
HCN	-0.48	1.11	-0.96	-1.14	-1.26	-1.08	-1.10	-0.71	-0.96	-1.05
CO	-1.50	2.01	-1.57	-1.77	-1.54	-1.08	-1.34	-1.28	-1.61	-1.75
HCO	0.02	3.46	-0.22	-0.14	0.12	0.57	0.31	0.26	-0.25	-0.15

CH_2O	-0.55	2.68	-0.98	-1.16	-0.92	-0.46	-0.72	-0.71	-1.03	-1.15
CH_3OH	-0.55	0.61	-0.99	-1.18	-1.28	-1.08	-1.12	-0.70	-0.99	-1.09
N_2	-2.24	1.96	-1.92	-2.10	-1.81	-1.29	-1.58	-1.70	-1.98	-2.11
NH_2NH_2	-0.45	0.91	-0.96	-1.20	-1.25	-1.01	-1.07	-0.61	-0.96	-1.09
NO	-0.42	4.25	0.14	-0.03	0.29	0.87	0.54	0.29	0.04	-0.07
O_2	-0.08	4.53	0.35	0.24	0.56	1.13	0.79	0.47	0.21	0.17
HOOH	-0.92	1.68	-1.18	-1.42	-1.50	-1.25	-1.31	-0.83	-1.18	-1.31
F_2	0.42	5.87	1.56	1.37	1.59	2.15	1.82	1.41	1.30	1.19
CO_2	-0.65	0.86	-1.29	-1.50	-1.55	-1.30	-1.37	-0.88	-1.29	-1.40
P_2	0.48	3.43	0.58	0.42	0.62	0.95	0.75	0.83	0.55	0.43
S_2	1.53	4.53	1.36	1.29	1.54	1.94	1.70	1.73	1.32	1.31
Cl_2	0.75	4.27	0.77	0.63	0.89	1.34	1.08	1.03	0.73	0.65
NaCl	0.65	2.26	0.58	0.38	0.28	0.45	0.42	0.87	0.58	0.47
SiO	0.03	2.86	-0.03	-0.20	-0.01	0.33	0.14	0.27	-0.06	-0.18
CS	-0.09	3.42	0.07	-0.12	0.12	0.55	0.30	0.29	0.03	-0.11
ClO	2.19	5.98	2.11	2.04	2.28	2.79	2.49	2.29	1.99	2.00
ClF	0.44	4.46	0.66	0.53	0.79	1.27	0.99	0.87	0.59	0.51
SiH_3SiH_3	-0.69	0.61	-1.16	-1.38	-1.38	-1.19	-1.25	-0.82	-1.16	-1.29
CH_3Cl	-0.51	0.87	-0.96	-1.15	-1.22	-1.02	-1.07	-0.66	-0.96	-1.06
CH_3SH	-0.50	0.83	-0.99	-1.19	-1.24	-1.03	-1.09	-0.68	-0.99	-1.10
SO_2	0.81	4.42	1.10	0.95	1.20	1.66	1.40	1.37	1.03	0.95
BF_3	-1.04	0.75	-1.25	-1.49	-1.56	-1.32	-1.37	-0.86	-1.25	-1.37
BCl_3	-0.17	2.74	-0.41	-0.67	-0.43	-0.03	-0.27	-0.20	-0.45	-0.68
$AlCl_3$	0.06	2.23	-0.43	-0.51	-0.39	-0.18	-0.32	-0.01	-0.42	-0.50
CF_4	-1.33	0.04	-1.96	-2.23	-2.31	-2.04	-2.10	-1.54	-1.95	-2.09

CCl_4	-0.46	2.76	-0.73	-0.79	-0.56	-0.14	-0.38	-0.42	-0.73	-0.76
OCS	-0.74	1.94	-1.25	-1.45	-1.21	-0.81	-1.05	-0.98	-1.29	-1.44
CS_2	0.01	2.85	0.06	-0.13	0.05	0.37	0.18	0.31	0.02	-0.12
CF_2O	-2.37	1.79	-1.50	-1.73	-1.79	-1.37	-1.60	-1.09	-1.50	-1.62
SiF_4	-0.81	1.15	-1.27	-1.49	-1.49	-1.24	-1.32	-0.83	-1.26	-1.38
N_2O	-2.01	1.57	-1.91	-2.10	-1.84	-1.37	-1.64	-1.52	-1.96	-2.08
NF_3	-2.06	1.03	-2.82	-3.05	-2.85	-2.36	-2.64	-2.45	-2.86	-3.02
PF_3	-1.23	0.88	-1.62	-1.82	-1.82	-1.54	-1.65	-1.30	-1.62	-1.73
O_3	1.93	6.24	2.89	2.74	3.00	3.48	3.20	3.18	2.80	2.71
F_2O	-0.31	4.32	0.19	0.02	0.28	0.82	0.50	0.21	0.01	-0.10
ClF_3	1.20	4.88	1.30	1.18	1.43	1.91	1.63	1.56	1.21	1.16
CF_2CF_2	-1.65	0.50	-1.63	-1.87	-1.91	-1.67	-1.74	-1.20	-1.63	-1.76
CF_3CN	-0.96	1.96	-1.55	-1.73	-1.48	-1.03	-1.29	-1.15	-1.55	-1.68
CH_3CCH	-1.13	0.45	-0.98	-1.16	-1.25	-1.07	-1.10	-0.71	-0.98	-1.07
CH_2CCH_2	-0.56	0.85	-1.14	-1.33	-1.42	-1.22	-1.26	-0.84	-1.14	-1.24
$cylC_3H_4$	-1.82	1.10	-1.18	-1.38	-1.49	-1.30	-1.33	-0.92	-1.18	-1.28
$cylC_3H_6$	-0.65	0.27	-1.24	-1.45	-1.54	-1.33	-1.37	-0.94	-1.23	-1.35
$CH_3CH_2CH_3$	-0.60	0.42	-1.08	-1.29	-1.36	-1.17	-1.21	-0.79	-1.08	-1.19
CH_3CCCH_3	-0.67	0.48	-1.02	-1.20	-1.29	-1.09	-1.13	-0.72	-1.02	-1.12
$cylC_4H_6$	-1.41	0.66	-1.15	-1.36	-1.45	-1.25	-1.29	-0.86	-1.15	-1.27
isobutane	-0.56	0.51	-1.05	-1.25	-1.32	-1.13	-1.17	-0.75	-1.05	-1.16
benzene	-0.71	1.23	-1.06	-1.26	-1.34	-1.15	-1.19	-0.77	-1.06	-1.17
CH_2F_2	-0.58	0.34	-1.07	-1.27	-1.38	-1.18	-1.22	-0.80	-1.08	-1.18
CF_3H	-0.60	0.30	-1.14	-1.34	-1.45	-1.26	-1.29	-0.86	-1.15	-1.25
CH_2Cl_2	-0.49	1.46	-0.99	-1.17	-1.20	-0.98	-1.06	-0.68	-0.99	-1.09

CCl_3H	-0.83	2.07	-1.04	-1.17	-1.08	-0.75	-0.94	-0.71	-1.04	-1.12
CH_3NO_2	-0.37	3.18	-0.28	-0.44	-0.20	0.26	-0.01	-0.06	-0.36	-0.47
CH_3SiH_3	-0.53	0.64	-1.04	-1.24	-1.30	-1.10	-1.15	-0.74	-1.04	-1.15
HCOOH	-0.57	1.51	-1.17	-1.39	-1.47	-1.25	-1.30	-0.86	-1.17	-1.29
CH_3CONH_2	-0.31	0.91	-0.78	-0.98	-1.05	-0.85	-0.90	-0.47	-0.78	-0.89
$cylNHC_2H_4$	-0.56	0.50	-1.07	-1.27	-1.36	-1.16	-1.20	-0.78	-1.07	-1.18
NCCN	-0.19	3.54	0.16	0.00	0.26	0.69	0.44	0.39	0.12	0.00
CH_3NHCH_3	-0.56	0.51	-1.02	-1.21	-1.29	-1.10	-1.14	-0.73	-1.01	-1.12
CH_2CO	-0.51	2.14	-1.10	-1.29	-1.33	-0.87	-1.13	-0.78	-1.09	-1.20
$cylOC_2H_4$	-0.86	0.32	-1.13	-1.33	-1.43	-1.23	-1.26	-0.84	-1.13	-1.24
OCHCHO	0.69	4.44	0.84	0.69	0.96	1.43	1.15	1.05	0.78	0.67
CH_3CH_2OH	-0.53	0.62	-0.99	-1.19	-1.28	-1.08	-1.12	-0.70	-0.99	-1.10
CH_3OCH_3	-0.58	0.45	-1.06	-1.26	-1.34	-1.14	-1.18	-0.76	-1.06	-1.17
$cylSC_2H_4$	-0.78	0.97	-1.13	-1.34	-1.41	-1.21	-1.25	-0.84	-1.13	-1.24
CH_3SOCH_3	-0.40	0.67	-0.88	-1.08	-1.16	-0.97	-1.00	-0.57	-0.88	-0.99
CH_2CHF	-0.88	1.02	-1.17	-1.38	-1.48	-1.28	-1.31	-0.89	-1.17	-1.28
CH_3CH_2Cl	-0.51	0.67	-1.01	-1.20	-1.28	-1.08	-1.12	-0.71	-1.01	-1.11
CH_2CHCl	-1.11	1.45	-1.10	-1.30	-1.39	-1.20	-1.23	-0.82	-1.10	-1.21
CH_3CClO	-0.85	2.34	-0.91	-1.10	-1.09	-0.64	-0.90	-0.59	-0.91	-1.01
prplCl	-0.48	0.81	-0.97	-1.17	-1.23	-1.03	-1.08	-0.67	-0.97	-1.08
NC_3H_9	-0.54	0.55	-1.02	-1.22	-1.28	-1.09	-1.13	-0.72	-1.02	-1.13
$cylOC_4H_4$	-0.74	0.87	-1.10	-1.29	-1.39	-1.20	-1.23	-0.82	-1.10	-1.20
$cylNHC_4H_4$	-0.51	0.57	-0.95	-1.15	-1.24	-1.04	-1.08	-0.67	-0.95	-1.05
NO_2	1.44	5.08	2.84	1.45	1.71	2.18	1.90	1.87	1.41	1.43
SF_6	-1.05	2.43	-1.14	-1.31	-1.13	-0.69	-0.93	-0.74	-1.14	-1.22

$CFCl_3$	-0.68	2.49	-0.95	-1.06	-0.82	-0.40	-0.65	-0.64	-0.96	-1.02
$CClF_3$	-1.06	1.32	-1.71	-1.97	-1.88	-1.52	-1.70	-1.31	-1.70	-1.85
$CBrF_3$	-0.81	1.92	-1.25	-1.46	-1.25	-0.86	-1.08	-0.88	-1.27	-1.41
HCCF	-0.55	0.67	-1.00	-1.16	-1.26	-1.09	-1.12	-0.75	-1.00	-1.09
HCCCN	-0.36	2.67	-0.54	-0.69	-0.46	-0.07	-0.30	-0.28	-0.57	-0.68
NCCCCN	0.68	3.97	0.92	0.76	0.99	1.37	1.15	1.16	0.88	0.77
C_2N_2	-0.19	3.54	0.16	0.00	0.26	0.69	0.44	0.39	0.12	0.00
C_3O_2	-0.74	2.55	-0.49	-0.68	-0.44	-0.05	-0.28	-0.24	-0.54	-0.68
FCN	-0.66	1.51	-1.03	-1.23	-1.23	-0.95	-1.06	-0.62	-1.03	-1.14
HCCCCH	-0.64	1.84	-0.95	-1.10	-1.18	-0.82	-1.03	-0.72	-0.95	-1.03
H_2CS	0.28	3.62	0.35	0.19	0.41	0.81	0.57	0.60	0.32	0.20
$HCONH_2$	-0.35	0.77	-0.87	-1.08	-1.17	-0.95	-1.00	-0.55	-0.87	-0.98
CH_2CHCHO	-0.46	3.07	-0.26	-0.40	-0.18	0.23	-0.01	-0.03	-0.30	-0.41
CH_2CCl_2	-1.07	1.70	-1.16	-1.35	-1.33	-0.99	-1.19	-0.85	-1.15	-1.26
$CHFCF_2$	-0.54	0.77	-1.15	-1.35	-1.45	-1.25	-1.29	-0.85	-1.15	-1.26
CH_2CF_2	-1.03	0.75	-1.18	-1.38	-1.47	-1.27	-1.31	-0.87	-1.18	-1.28
CH_3F	-0.58	0.35	-1.04	-1.23	-1.34	-1.14	-1.18	-0.76	-1.04	-1.14
CF_2Cl_2	-0.90	1.97	-1.40	-1.57	-1.35	-0.93	-1.17	-1.05	-1.40	-1.51
SiF_2	0.10	3.01	0.02	-0.13	0.07	0.43	0.22	0.33	-0.01	-0.13
MSE		2.43	-0.19	-0.38	-0.31	0.01	-0.15	0.10	-0.25	-0.34
MAE		2.45	0.42	0.49	0.52	0.54	0.49	0.30	0.39	0.44
rms		2.72	0.51	0.59	0.62	0.63	0.57	0.40	0.47	0.53

TABLE XVII: Fundamental gaps (in eV) of the FG131 database [8, 9], calculated using $E_g(1) = E_{\text{total}}(N-1) + E_{\text{total}}(N+1) - 2E_{\text{total}}(N)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	12.86	12.95	13.15	13.00	12.92	12.90	12.91	12.60	13.14	13.02
He	27.23	28.27	28.55	28.85	28.78	28.73	28.74	28.94	28.47	28.75
Li	4.22	5.06	4.07	4.91	4.81	4.85	4.88	5.05	5.10	4.99
Be	9.66	9.16	9.30	9.46	9.31	9.18	9.24	9.63	9.33	9.50
B	7.99	8.13	8.35	8.30	8.29	8.23	8.25	8.41	8.34	8.29
C	9.97	9.99	10.23	10.19	10.17	10.13	10.14	10.27	10.21	10.18
N	14.74	14.57	14.91	14.63	14.69	14.74	14.72	14.90	14.86	14.67
O	12.14	12.41	12.58	12.36	12.37	12.38	12.37	12.40	12.57	12.36
F	13.98	14.14	14.30	14.07	14.15	14.19	14.17	14.21	14.28	14.09
Ne	26.91	28.32	28.65	28.82	28.68	28.60	28.61	28.45	28.33	28.60
Na	4.14	4.80	4.75	4.35	4.30	4.44	4.45	4.83	4.76	4.49
Mg	7.76	7.76	7.68	8.14	8.03	7.81	7.85	8.14	7.72	8.03
Al	5.53	5.57	5.74	5.75	5.72	5.67	5.70	5.79	5.73	5.74
Si	6.73	6.74	6.89	6.89	6.86	6.82	6.84	6.92	6.87	6.89
P	9.78	9.64	9.87	9.69	9.58	9.54	9.58	9.66	9.86	9.71
S	8.23	8.28	8.46	8.38	8.34	8.33	8.35	8.46	8.45	8.40
Cl	9.30	9.33	9.47	9.36	9.35	9.35	9.37	9.47	9.46	9.40
Ar	18.65	18.70	19.11	19.33	19.19	19.09	19.15	19.18	19.05	19.34
CH_3	9.86	10.05	10.40	9.94	9.92	9.90	9.92	10.18	10.39	9.96
CH_4	15.06	14.68	15.16	15.31	15.26	15.15	15.20	15.42	15.15	15.30
NH	13.17	13.33	13.64	13.29	13.31	13.34	13.33	13.50	13.60	13.31

NH_2	11.34	11.43	7.60	11.55	11.48	11.47	11.49	11.64	11.63	11.59
NH_3	11.54	11.66	11.87	12.05	11.98	11.88	11.93	12.10	11.84	12.05
OH	11.27	11.45	11.65	11.47	11.49	11.50	11.49	11.58	11.64	11.48
H_2O	13.35	13.52	13.71	13.85	13.77	13.68	13.71	13.87	13.63	13.81
HF	16.91	17.12	17.26	17.36	17.28	17.20	17.22	17.35	17.10	17.27
SiH_3	7.95	8.04	8.35	7.96	7.97	7.96	7.97	8.19	8.34	7.98
SiH_4	14.03	12.92	13.90	14.02	13.90	13.71	13.80	14.10	13.84	14.01
PH_3	11.82	11.12	11.41	11.60	11.57	11.50	11.54	11.63	11.41	11.62
SH_2	11.00	11.00	11.27	11.43	11.39	11.32	11.36	11.44	11.24	11.43
HCl	13.36	13.34	13.56	13.71	13.67	13.60	13.63	13.75	13.53	13.71
HCCH	13.43	12.10	12.31	12.35	12.35	12.28	12.31	12.51	12.29	12.34
CH_2CH_2	12.57	11.44	12.33	11.67	11.67	11.60	11.63	11.77	11.58	11.67
CH_3CH_3	13.41	12.59	13.55	13.70	13.60	13.40	13.49	13.83	13.55	13.69
HCN	14.31	14.44	15.57	14.43	14.42	14.36	14.38	14.59	14.37	14.42
CO	15.57	15.16	15.69	15.95	15.82	15.68	15.75	16.06	15.72	16.01
HCO	9.56	9.80	10.21	9.98	9.98	9.96	9.98	10.13	10.21	10.01
CH_2O	11.56	11.31	11.83	11.94	11.88	11.82	11.85	11.91	11.80	11.94
CH_3OH	11.67	11.27	11.87	11.96	11.90	11.78	11.83	12.09	11.81	11.94
N_2	17.88	17.45	18.13	18.17	18.13	18.06	18.10	18.41	18.16	18.24
NH_2NH_2	10.29	9.95	10.57	10.72	10.65	10.51	10.57	10.83	10.56	10.73
NO	10.11	10.17	10.41	10.32	10.37	10.38	10.37	10.45	10.42	10.35
O_2	12.52	12.78	13.07	12.99	13.04	13.08	13.06	13.21	13.10	13.04
HOOH	12.65	12.07	13.17	12.96	12.92	12.79	12.84	13.15	12.81	12.96
F_2	15.53	14.91	15.31	15.27	15.34	15.37	15.36	15.45	15.31	15.31
CO_2	14.58	14.54	15.14	15.20	15.13	15.02	15.06	15.27	15.06	15.18

P_2	10.19	9.96	9.62	9.66	9.73	9.82	9.79	9.62	9.61	9.69
S_2	7.96	8.12	8.40	8.33	8.24	8.20	8.23	8.31	8.39	8.34
Cl_2	10.93	10.34	10.90	10.95	10.86	10.78	10.83	10.98	10.88	10.95
NaCl	8.64	8.56	8.52	8.67	8.69	8.65	8.66	8.71	8.49	8.65
SiO	11.60	11.22	11.51	11.61	11.58	11.51	11.55	11.72	11.50	11.64
CS	11.58	11.22	12.70	11.48	11.40	11.40	11.43	11.49	11.29	11.54
ClO	8.85	8.84	9.09	8.99	9.01	9.01	9.01	9.10	9.09	9.02
ClF	12.43	11.87	12.28	12.30	12.29	12.29	12.30	12.39	12.26	12.32
SiH_3SiH_3	11.33	11.00	11.80	11.69	11.65	11.55	11.61	11.74	11.59	11.69
CH_3Cl	12.01	11.65	12.20	12.30	12.25	12.14	12.19	12.41	12.17	12.30
CH_3SH	10.01	9.80	10.26	10.36	10.33	10.25	10.29	10.43	10.22	10.37
SO_2	11.74	11.40	12.49	11.62	11.62	11.61	11.61	11.73	11.60	11.66
BF_3	17.22	15.29	16.89	16.98	16.90	16.69	16.78	17.39	16.87	17.00
BCl_3	12.07	10.90	13.05	12.11	11.90	11.68	11.81	12.18	11.95	12.15
$AlCl_3$	12.13	10.64	12.43	12.55	12.26	11.89	12.10	12.62	12.39	12.57
CF_4	17.85	15.96	17.86	17.91	17.87	17.66	17.74	18.43	17.82	17.96
CCl_4	11.97	10.34	12.38	12.35	12.06	11.65	11.87	12.56	12.35	12.33
OCS	12.13	12.13	12.57	12.51	12.52	12.52	12.55	12.68	12.41	12.54
CS_2	10.19	10.04	9.73	9.83	9.86	9.96	9.92	9.77	9.73	9.86
CF_2O	16.08	14.19	14.99	15.06	15.02	15.60	14.95	15.14	14.90	15.03
SiF_4	16.95	15.18	17.32	17.36	17.23	16.94	17.08	17.81	17.28	17.41
N_2O	15.01	14.37	14.73	14.97	14.96	14.99	14.98	14.81	14.66	14.79
NF_3	15.76	15.19	16.31	16.41	16.36	16.27	16.33	16.59	16.27	16.44
PF_3	13.00	12.36	13.07	13.25	13.23	13.11	13.17	13.48	13.10	13.29
O_3	11.06	10.76	10.74	10.77	10.77	10.77	10.77	10.32	10.73	10.79

F_2O	13.82	13.01	13.66	13.62	13.66	13.66	13.66	13.81	13.67	13.67
ClF_3	11.79	10.98	11.71	11.72	11.70	11.64	11.68	11.89	11.71	11.74
CF_2CF_2	12.45	11.17	12.05	12.13	12.16	12.07	12.10	12.29	12.01	12.13
CF_3CN	15.39	14.47	15.49	15.52	15.49	15.43	15.47	15.66	15.45	15.50
CH_3CCH	11.69	10.77	11.20	11.22	11.22	11.13	11.17	11.38	11.17	11.22
CH_2CCH_2	10.83	10.76	11.65	11.20	11.20	11.11	11.15	11.33	11.13	11.20
$cylC_3H_4$	11.87	10.46	11.68	10.92	10.89	10.79	10.84	11.07	10.86	10.91
$cylC_3H_6$	11.64	11.51	12.05	12.11	12.07	11.96	12.01	12.23	12.03	12.10
$CH_3CH_2CH_3$	12.72	11.73	12.90	13.06	12.93	12.70	12.81	13.19	12.90	13.04
CH_3CCCH_3	10.46	9.82	10.46	10.50	10.48	10.37	10.42	10.62	10.44	10.49
$cylC_4H_6$	11.14	10.10	10.50	10.57	10.55	10.46	10.50	10.67	10.49	10.56
isobutane	12.28	11.30	12.44	12.61	12.50	12.28	12.38	12.68	12.40	12.59
benzene	10.16	9.79	10.76	10.38	10.36	10.26	10.30	10.46	10.31	10.37
CH_2F_2	14.15	13.11	14.11	14.23	14.19	14.04	14.10	14.57	14.11	14.24
CF_3H	15.44	14.36	15.38	15.51	15.46	15.31	15.37	15.89	15.37	15.52
CH_2Cl_2	12.18	11.19	12.51	12.59	12.41	12.13	12.27	12.75	12.45	12.59
CCl_3H	12.38	10.85	12.46	12.57	12.33	11.98	12.16	12.72	12.43	12.57
CH_3NO_2	11.94	11.07	11.67	11.97	11.91	11.82	11.87	12.05	11.94	12.00
CH_3SiH_3	12.35	11.85	12.64	12.71	12.66	12.54	12.60	12.84	12.62	12.71
HCOOH	11.98	11.81	13.22	12.37	12.31	12.21	12.24	12.46	12.19	12.35
CH_3CONH_2	10.05	9.99	11.12	10.64	10.57	10.44	10.49	10.71	10.46	10.61
$cylNHC_2H_4$	10.44	10.26	10.71	10.82	10.76	10.65	10.70	10.94	10.69	10.82
NCCN	13.90	13.00	13.33	13.34	13.27	13.20	13.23	13.41	13.33	13.36
CH_3NHCH_3	9.65	9.34	9.88	10.01	9.96	9.84	9.89	10.11	9.86	10.00
CH_2CO	10.32	10.43	11.02	10.78	11.05	10.92	10.99	10.93	10.68	10.79

cylOC_2H_4	11.68	11.15	11.69	11.77	11.72	11.61	11.66	11.89	11.64	11.75
OCHCHO	10.04	8.95	9.82	9.92	9.83	9.67	9.75	10.07	9.84	9.94
CH_3CH_2OH	11.38	10.74	11.53	11.65	11.58	11.44	11.50	11.78	11.49	11.63
CH_3OCH_3	10.79	10.33	11.00	11.11	11.05	10.92	10.97	11.21	10.95	11.08
cylSC_2H_4	9.93	9.59	10.01	10.11	10.09	10.01	10.05	10.19	9.98	10.11
CH_3SOCH_3	9.54	9.25	9.73	9.85	9.80	9.69	9.73	9.94	9.70	9.84
CH_2CHF	11.55	11.13	12.38	11.49	11.49	11.42	11.45	11.66	11.40	11.49
CH_3CH_2Cl	11.74	11.23	11.97	12.08	12.03	11.89	11.96	12.19	11.94	12.07
CH_2CHCl	11.35	10.51	11.02	11.09	11.03	10.90	10.96	11.22	10.99	11.08
CH_3CClO	11.97	11.11	12.69	11.98	11.90	11.76	11.83	12.07	11.83	11.95
prplCl	11.63	10.83	11.81	11.92	11.85	11.68	11.76	12.03	11.78	11.91
NC_3H_9	9.10	8.77	9.34	9.48	9.43	9.31	9.36	9.55	9.32	9.46
cylOC_4H_4	9.82	9.51	10.87	9.97	9.95	9.85	9.89	10.10	9.90	9.96
cylNHC_4H_4	8.89	8.73	9.02	9.10	9.07	8.98	9.02	9.18	9.00	9.09
NO_2	9.79	10.05	4.69	10.28	10.31	10.32	10.32	10.48	10.48	10.33
SF_6	16.98	14.22	16.57	16.59	16.50	16.24	16.37	17.03	16.60	16.59
$CFCl_3$	12.61	11.00	12.75	12.76	12.51	12.16	12.35	12.91	12.72	12.75
$CClF_3$	14.27	13.64	14.59	14.75	14.67	14.52	14.59	14.81	14.55	14.73
$CBrF_3$	12.97	12.45	13.07	13.16	13.11	13.02	13.08	13.24	13.07	13.22
HCCF	12.04	11.78	12.11	12.14	12.15	12.09	12.11	12.37	12.09	12.14
HCCCN	12.20	11.48	12.03	12.06	12.01	11.93	11.97	12.12	12.03	12.07
NCCCCN	11.52	10.42	10.92	10.94	10.86	10.77	10.82	11.02	10.92	10.95
C_2N_2	13.90	13.00	13.33	13.34	13.27	13.20	13.23	13.41	13.33	13.36
C_3O_2	11.64	11.44	11.23	11.30	11.33	11.40	11.37	11.29	11.23	11.32
FCN	14.33	13.91	14.36	14.39	14.38	14.30	14.33	14.49	14.32	14.40

HCCCCH	11.00	10.38	11.18	10.97	11.16	10.86	11.12	11.22	10.97	10.97
H_2CS	9.18	8.87	10.23	8.85	8.88	8.93	8.92	8.85	8.76	8.88
$HCONH_2$	10.81	10.70	11.54	11.13	11.07	10.97	11.01	11.20	10.94	11.11
CH_2CHCHO	10.70	9.79	10.10	10.18	10.13	10.07	10.10	10.20	10.08	10.19
CH_2CCl_2	11.17	10.20	10.92	10.99	10.91	10.86	10.84	11.13	10.89	10.98
$CHFCF_2$	11.11	10.75	11.25	11.32	11.34	11.27	11.29	11.56	11.23	11.32
CH_2CF_2	11.81	11.11	11.55	11.61	11.62	11.54	11.57	11.82	11.52	11.61
CH_3F	14.09	13.38	14.12	14.22	14.17	14.04	14.09	14.44	14.08	14.20
CF_2Cl_2	13.33	12.16	13.67	13.74	13.54	13.25	13.41	13.81	13.64	13.73
SiF_2	11.04	10.66	10.74	11.07	11.02	10.96	10.99	11.13	10.79	11.11
MSE		-0.46	0.10	0.13	0.08	-0.01	0.03	0.23	0.05	0.13
MAE		0.57	0.44	0.32	0.29	0.27	0.28	0.39	0.30	0.32
rms		0.76	0.74	0.42	0.40	0.38	0.39	0.47	0.39	0.41

TABLE XVIII: Fundamental gaps (in eV) of the FG131 database [8, 9], calculated using $E_g(2) = \epsilon_{\mathrm{HOMO}}(N+1) - \epsilon_{\mathrm{HOMO}}(N)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	12.86	9.56	10.86	10.54	10.41	10.21	10.34	10.92	10.87	10.63
He	27.23	21.82	25.03	25.22	25.05	24.53	24.77	26.15	25.15	25.34
Li	4.22	4.10	3.61	4.63	4.57	4.51	4.59	4.86	4.82	4.69
Be	9.66	7.50	8.98	9.21	8.97	8.69	8.86	9.22	9.01	9.23
B	7.99	6.31	7.41	7.46	7.32	7.09	7.21	7.57	7.40	7.44
C	9.97	8.16	9.05	9.08	8.98	8.83	8.90	9.22	9.04	9.08

N	14.74	11.81	13.01	12.83	12.84	12.76	12.82	13.41	13.03	12.94
O	12.14	10.51	11.11	10.95	10.96	10.94	10.95	11.17	11.13	10.98
F	13.98	12.28	12.73	12.55	12.64	12.68	12.67	12.84	12.76	12.61
Ne	26.91	23.15	25.53	26.01	25.92	25.61	25.74	26.96	25.73	26.19
Na	4.14	3.88	4.49	4.14	4.20	4.20	4.24	4.63	4.50	4.22
Mg	7.76	6.08	7.53	7.77	7.66	7.39	7.53	7.90	7.57	7.75
Al	5.53	4.67	5.39	5.40	5.30	5.16	5.24	5.44	5.38	5.39
Si	6.73	5.87	6.45	6.47	6.37	6.24	6.32	6.50	6.44	6.47
P	9.78	8.20	9.10	9.07	8.86	8.63	8.77	9.09	9.09	9.08
S	8.23	7.35	7.88	7.74	7.67	7.59	7.66	7.92	7.87	7.79
Cl	9.30	8.45	8.86	8.72	8.69	8.64	8.68	8.90	8.85	8.76
Ar	18.65	15.49	18.06	18.48	18.01	17.40	17.71	18.63	18.04	18.47
CH_3	9.86	8.21	9.42	9.05	8.96	8.76	8.87	9.43	9.41	9.09
CH_4	15.06	11.42	14.83	14.96	14.59	13.91	14.27	15.36	14.84	14.97
NH	13.17	11.09	12.13	11.89	11.87	11.79	11.84	12.35	12.15	11.96
NH_2	11.34	10.05	8.83	10.63	10.57	10.48	10.54	10.86	10.77	10.69
NH_3	11.54	8.36	11.51	11.66	11.29	10.63	10.99	12.09	11.53	11.70
OH	11.27	9.94	10.47	10.32	10.33	10.30	10.32	10.56	10.49	10.36
H_2O	13.35	9.69	12.87	13.04	12.70	12.05	12.39	13.63	12.91	13.11
HF	16.91	12.30	15.58	15.77	15.50	14.89	15.21	16.62	15.69	15.91
SiH_3	7.95	6.98	7.87	7.60	7.50	7.35	7.44	7.83	7.86	7.63
SiH_4	14.03	10.54	13.73	13.86	13.51	12.87	13.22	14.14	13.72	13.86
PH_3	11.82	8.68	11.38	11.54	11.22	10.65	10.96	11.73	11.38	11.55
SH_2	11.00	8.36	11.11	11.25	10.89	10.29	10.62	11.45	11.09	11.26
HCl	13.36	10.43	13.09	13.28	12.90	12.30	12.61	13.53	13.08	13.28

HCCH	13.43	9.01	12.23	12.31	11.96	11.32	11.67	12.61	12.21	12.31
CH_2CH_2	12.57	8.79	12.29	11.77	11.45	10.84	11.17	12.03	11.69	11.77
CH_3CH_3	13.41	10.07	13.38	13.52	13.18	12.54	12.88	13.87	13.38	13.53
HCN	14.31	11.34	15.16	14.07	13.72	13.14	13.44	14.41	13.97	14.06
CO	15.57	12.77	15.29	15.52	15.23	14.74	14.99	15.80	15.33	15.57
HCO	9.56	8.09	9.38	9.17	9.11	8.97	9.05	9.48	9.39	9.23
CH_2O	11.56	8.71	11.44	11.60	11.48	11.23	11.37	11.82	11.48	11.65
CH_3OH	11.67	8.15	11.57	11.70	11.39	10.76	11.10	12.25	11.61	11.75
N_2	17.88	15.72	17.44	17.51	17.41	17.18	17.30	17.90	17.50	17.60
NH_2NH_2	10.29	7.41	10.37	10.55	10.21	9.61	9.93	10.94	10.40	10.59
NO	10.11	8.82	9.61	9.55	9.54	9.48	9.52	9.78	9.63	9.59
O_2	12.52	11.42	12.12	12.05	12.09	12.09	12.10	12.44	12.19	12.15
HOOH	12.65	8.85	12.59	12.41	12.09	11.44	11.79	13.03	12.30	12.49
F_2	15.53	13.92	14.70	14.63	14.65	14.63	14.65	14.82	14.67	14.65
CO_2	14.58	11.69	14.57	14.69	14.40	13.84	14.14	15.15	14.58	14.75
P_2	10.19	9.28	9.59	9.60	9.58	9.55	9.58	9.59	9.58	9.63
S_2	7.96	7.50	8.05	7.98	7.87	7.76	7.84	8.02	8.05	8.00
Cl_2	10.93	9.53	10.61	10.64	10.52	10.36	10.46	10.71	10.58	10.65
NaCl	8.64	6.13	8.46	8.63	8.31	7.75	8.04	8.85	8.46	8.62
SiO	11.60	9.83	11.26	11.37	11.26	11.02	11.16	11.64	11.29	11.44
CS	11.58	10.40	11.42	11.52	11.39	11.24	11.34	11.68	11.44	11.59
ClO	8.85	8.27	8.64	8.54	8.53	8.50	8.52	8.64	8.64	8.56
ClF	12.43	10.81	11.91	11.92	11.82	11.68	11.77	12.04	11.88	11.93
SiH_3SiH_3	11.33	9.14	12.04	11.96	11.66	11.13	11.43	12.14	11.83	11.96
CH_3Cl	12.01	9.07	12.05	12.18	11.82	11.19	11.53	12.49	12.04	12.18

CH_3SH	10.01	7.46	10.31	10.42	10.08	9.48	9.81	10.66	10.29	10.42
SO_2	11.74	10.86	11.31	11.34	11.34	11.31	11.33	11.53	11.34	11.40
BF_3	17.22	12.51	16.16	16.32	16.07	15.46	15.79	17.15	16.26	16.47
BCl_3	12.07	10.71	12.90	11.67	11.49	11.33	11.43	11.71	11.50	11.70
$AlCl_3$	12.13	9.63	12.14	12.29	11.93	11.42	11.70	12.46	12.11	12.34
CF_4	17.85	13.39	17.26	17.39	17.16	16.53	16.87	18.28	17.36	17.55
CCl_4	11.97	9.80	12.08	12.05	11.77	11.35	11.58	12.28	12.05	12.03
OCS	12.13	9.97	12.45	12.35	12.26	11.90	12.22	12.78	12.27	12.38
CS_2	10.19	9.41	9.65	9.74	9.67	9.66	9.69	9.67	9.65	9.76
CF_2O	16.08	11.26	14.57	14.71	14.41	14.80	14.12	15.28	14.60	14.78
SiF_4	16.95	13.17	16.78	16.97	16.69	16.08	16.41	17.67	16.86	17.10
N_2O	15.01	11.68	14.20	14.62	14.57	14.48	14.54	14.73	14.19	14.37
NF_3	15.76	12.90	15.82	15.95	15.71	15.38	15.61	16.50	15.85	16.07
PF_3	13.00	9.95	12.84	13.05	12.75	12.18	12.48	13.42	12.91	13.10
O_3	11.06	10.32	10.39	10.39	10.39	10.41	10.41	10.27	10.39	10.41
F_2O	13.82	12.24	13.32	13.25	13.25	13.18	13.22	13.50	13.32	13.28
ClF_3	11.79	10.61	11.43	11.43	11.42	11.37	11.40	11.60	11.42	11.46
CF_2CF_2	12.45	8.96	11.94	12.10	11.82	11.25	11.55	12.43	11.93	12.12
CF_3CN	15.39	12.27	15.33	15.35	15.20	14.90	15.07	15.78	15.31	15.41
CH_3CCH	11.69	8.15	11.29	11.35	11.03	10.42	10.75	11.64	11.27	11.35
CH_2CCH_2	10.83	8.39	11.90	11.48	11.17	10.58	10.90	11.77	11.41	11.49
$cylC_3H_4$	11.87	7.99	11.55	11.01	10.70	10.11	10.43	11.28	10.92	11.00
$cylC_3H_6$	11.64	9.04	12.25	12.33	12.00	11.37	11.71	12.67	12.24	12.33
$CH_3CH_2CH_3$	12.72	9.52	12.87	13.03	12.70	12.07	12.41	13.34	12.87	13.03
CH_3CCCH_3	10.46	7.54	10.71	10.79	10.48	9.88	10.21	11.05	10.70	10.78

$cylC_4H_6$	11.14	7.85	10.76	10.88	10.57	10.00	10.31	11.12	10.78	10.87
isobutane	12.28	9.27	12.57	12.72	12.40	11.78	12.12	13.04	12.57	12.72
benzene	10.16	7.93	10.83	10.78	10.51	10.00	10.28	10.94	10.68	10.77
CH_2F_2	14.15	10.24	13.63	13.76	13.49	12.88	13.20	14.40	13.68	13.83
CF_3H	15.44	11.78	14.88	15.03	14.78	14.23	14.51	15.68	14.92	15.09
CH_2Cl_2	12.18	9.45	12.28	12.42	12.07	11.45	11.78	12.72	12.27	12.43
CCl_3H	12.38	9.67	12.25	12.42	12.04	11.46	11.77	12.67	12.24	12.42
CH_3NO_2	11.94	9.01	11.51	11.54	11.51	11.39	11.47	11.75	11.56	11.61
CH_3SiH_3	12.35	9.79	12.81	12.91	12.58	11.97	12.30	13.23	12.80	12.92
HCOOH	11.98	8.79	12.96	12.17	11.89	11.36	11.63	12.70	12.04	12.23
CH_3CONH_2	10.05	7.46	10.66	10.82	10.51	9.91	10.23	11.33	10.69	10.87
$cylNHC_2H_4$	10.44	7.68	10.79	10.91	10.59	9.99	10.31	11.30	10.80	10.94
NCCN	13.90	12.54	13.16	13.18	13.06	12.93	13.00	13.27	13.16	13.19
CH_3NHCH_3	9.65	6.78	10.04	10.18	9.86	9.25	9.58	10.57	10.06	10.20
CH_2CO	10.32	8.36	10.93	10.72	10.83	10.30	10.59	11.06	10.64	10.74
$cylOC_2H_4$	11.68	8.21	11.65	11.76	11.47	10.85	11.19	12.34	11.70	11.83
OCHCHO	10.04	8.62	9.48	9.57	9.51	9.39	9.46	9.80	9.51	9.62
CH_3CH_2OH	11.38	7.97	11.40	11.54	11.23	10.61	10.94	12.06	11.43	11.59
CH_3OCH_3	10.79	7.60	11.02	11.16	10.87	10.26	10.59	11.66	11.05	11.21
$cylSC_2H_4$	9.93	7.30	10.20	10.29	9.96	9.37	9.69	10.56	10.18	10.30
CH_3SOCH_3	9.54	7.05	9.91	10.07	9.79	9.25	9.54	10.42	9.93	10.10
CH_2CHF	11.55	8.55	12.27	11.51	11.21	10.65	10.95	11.84	11.42	11.52
CH_3CH_2Cl	11.74	8.83	11.93	12.07	11.72	11.09	11.42	12.38	11.92	12.08
CH_2CHCl	11.35	8.34	11.07	11.18	10.86	10.31	10.61	11.43	11.06	11.17
CH_3CClO	11.97	9.12	11.94	12.06	11.77	11.20	11.51	12.51	11.95	12.09

prplCl	11.63	8.67	11.87	12.00	11.65	11.01	11.35	12.32	11.86	12.00
NC_3H_9	9.10	6.49	9.69	9.83	9.54	8.95	9.27	10.18	9.70	9.85
$cylOC_4H_4$	9.82	7.35	10.93	10.23	9.95	9.42	9.71	10.45	10.13	10.22
$cylNHC_4H_4$	8.89	6.83	9.24	9.36	9.08	8.61	8.86	9.51	9.22	9.35
NO_2	9.79	8.94	6.98	9.65	9.64	9.61	9.64	9.97	9.86	9.72
SF_6	16.98	12.98	16.18	16.14	16.06	15.70	15.89	16.80	16.24	16.23
$CFCl_3$	12.61	10.18	12.46	12.47	12.21	11.81	12.03	12.64	12.43	12.46
$CClF_3$	14.27	11.32	14.39	14.58	14.20	13.62	13.92	14.85	14.37	14.56
$CBrF_3$	12.97	10.55	12.91	12.99	12.77	12.40	12.60	13.15	12.91	13.02
HCCF	12.04	8.93	11.93	11.99	11.68	11.09	11.41	12.39	11.92	12.00
HCCCN	12.20	9.77	11.93	11.98	11.85	11.66	11.76	12.06	11.93	11.99
NCCCCN	11.52	10.19	10.84	10.87	10.77	10.64	10.71	10.97	10.84	10.88
C_2N_2	13.90	12.54	13.16	13.18	13.06	12.93	13.00	13.27	13.16	13.19
C_3O_2	11.64	10.30	11.23	11.29	11.30	11.33	11.32	11.29	11.23	11.31
FCN	14.33	11.23	13.89	14.01	13.67	13.09	13.39	14.31	13.87	14.03
HCCCCH	11.00	8.26	11.12	11.12	11.03	10.32	10.92	11.48	11.11	11.12
H_2CS	9.18	8.17	10.25	8.75	8.67	8.58	8.64	8.78	8.68	8.78
$HCONH_2$	10.81	7.96	10.94	11.11	10.82	10.24	10.55	11.63	10.98	11.17
CH_2CHCHO	10.70	8.89	10.13	10.23	10.15	9.96	10.07	10.53	10.18	10.29
CH_2CCl_2	11.17	8.40	11.07	11.16	10.85	10.59	10.60	11.42	11.04	11.15
$CHFCF_2$	11.11	8.44	11.16	11.26	11.01	10.50	10.76	11.67	11.16	11.28
CH_2CF_2	11.81	8.65	11.54	11.61	11.32	10.75	11.05	11.99	11.53	11.62
CH_3F	14.09	10.08	13.56	13.68	13.41	12.79	13.12	14.34	13.63	13.76
CF_2Cl_2	13.33	10.72	13.45	13.54	13.24	12.74	13.02	13.68	13.43	13.53
SiF_2	11.04	9.49	10.54	10.69	10.61	10.43	10.53	10.92	10.60	10.77

MSE	-2.48	-0.26	-0.22	-0.42	-0.80	-0.59	0.09	-0.27	-0.18
MAE	2.48	0.50	0.44	0.50	0.81	0.62	0.47	0.43	0.43
rms	2.69	0.70	0.59	0.65	0.93	0.77	0.57	0.57	0.57

TABLE XIX: Fundamental gaps (in eV) of the FG131 database [8, 9], calculated using $E_g(3) = \epsilon_{\mathrm{LUMO}}(N) - \epsilon_{\mathrm{HOMO}}(N)$.

Molecule	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
H	12.86	8.11	12.74	12.43	12.15	11.59	11.91	13.18	12.74	12.50
He	27.23	18.05	25.36	25.68	25.54	24.57	24.98	26.19	25.48	25.65
Li	4.22	1.88	2.50	5.60	5.57	4.86	5.54	4.36	5.83	5.65
Be	9.66	3.59	9.41	9.43	9.17	8.58	8.92	9.55	9.44	9.44
B	7.99	0.55	8.08	8.07	7.61	6.67	7.19	8.28	8.08	8.04
C	9.97	0.52	9.28	9.37	8.75	7.59	8.23	9.73	9.32	9.38
N	14.74	4.17	13.42	13.09	12.67	11.64	12.24	13.86	13.49	13.23
O	12.14	1.10	10.84	10.68	10.18	9.01	9.67	11.46	11.03	10.80
F	13.98	0.99	11.31	11.30	10.91	9.73	10.40	12.68	11.76	11.63
Ne	26.91	16.97	25.81	25.98	25.81	24.91	25.39	26.79	26.00	26.18
Na	4.14	1.58	5.20	5.11	5.20	5.12	5.19	4.30	5.22	5.15
Mg	7.76	3.36	7.91	7.93	7.85	7.46	7.67	8.12	7.94	7.91
Al	5.53	0.33	6.09	5.96	5.70	5.11	5.46	6.06	6.08	5.95
Si	6.73	0.24	7.11	7.06	6.61	5.76	6.24	7.19	7.10	7.05
P	9.78	2.57	9.98	9.53	8.93	8.05	8.59	9.66	9.98	9.55
S	8.23	0.51	8.55	8.07	7.48	6.52	7.09	8.55	8.57	8.12

Cl	9.30	0.39	9.08	8.79	8.12	6.98	7.63	9.31	9.12	8.82
Ar	18.65	11.14	18.49	18.64	18.16	17.33	17.79	18.67	18.47	18.60
CH_3	9.86	2.48	10.54	9.96	9.44	8.55	9.09	10.37	10.54	10.02
CH_4	15.06	9.14	15.07	15.18	14.96	14.15	14.52	15.48	15.08	15.12
NH	13.17	3.60	12.78	12.36	11.86	10.81	11.42	13.10	12.84	12.47
NH_2	11.34	2.68	7.71	11.29	10.71	9.65	10.27	11.85	11.65	11.38
NH_3	11.54	5.52	11.78	11.92	11.68	10.85	11.24	12.20	11.79	11.87
OH	11.27	0.92	10.61	10.44	9.91	8.74	9.40	11.30	10.79	10.58
H_2O	13.35	6.39	13.15	13.30	13.08	12.21	12.61	13.74	13.19	13.28
HF	16.91	8.78	15.85	16.00	15.86	15.00	15.40	16.75	15.96	16.06
SiH_3	7.95	1.83	8.79	7.68	7.41	6.85	7.26	8.45	8.78	7.84
SiH_4	14.03	8.15	13.99	14.11	13.85	13.10	13.46	14.23	13.98	14.04
PH_3	11.82	6.11	11.65	11.77	11.54	10.85	11.18	11.84	11.66	11.71
SH_2	11.00	5.52	11.41	11.52	11.24	10.49	10.86	11.60	11.39	11.45
HCl	13.36	6.97	13.44	13.56	13.25	12.43	12.84	13.75	13.43	13.49
HCCH	13.43	6.80	12.45	12.48	12.30	11.58	11.91	12.75	12.44	12.42
CH_2CH_2	12.57	5.62	11.95	12.02	11.83	11.10	11.43	12.13	11.93	11.94
CH_3CH_3	13.41	7.80	13.60	13.72	13.53	12.77	13.11	13.97	13.61	13.66
HCN	14.31	7.91	14.37	14.39	14.20	13.42	13.78	14.72	14.35	14.33
CO	15.57	7.04	15.41	15.52	14.98	13.89	14.49	15.97	15.48	15.58
HCO	9.56	1.69	9.84	9.54	9.05	8.06	8.63	10.06	9.89	9.61
CH_2O	11.56	3.58	11.66	11.74	11.28	10.28	10.85	12.22	11.74	11.81
CH_3OH	11.67	5.65	11.83	11.93	11.77	11.00	11.36	12.39	11.86	11.92
N_2	17.88	8.32	17.22	17.27	16.72	15.58	16.21	18.00	17.33	17.39
NH_2NH_2	10.29	4.39	10.70	10.86	10.63	9.81	10.19	11.09	10.72	10.81

NO	10.11	0.28	9.24	9.18	8.64	7.48	8.13	9.97	9.36	9.30
O_2	12.52	2.31	11.60	11.55	11.03	9.88	10.54	12.62	11.81	11.76
HOOH	12.65	4.78	12.52	12.66	12.48	11.63	12.02	13.14	12.56	12.65
F_2	15.53	3.62	13.19	13.27	12.88	11.75	12.40	14.68	13.57	13.65
CO_2	14.58	8.23	14.84	14.91	14.73	13.95	14.32	15.26	14.84	14.89
P_2	10.19	3.71	10.06	10.06	9.69	8.95	9.39	10.13	10.05	10.06
S_2	7.96	1.30	8.52	8.41	7.87	6.94	7.48	8.60	8.53	8.40
Cl_2	10.93	3.06	10.83	10.87	10.31	9.30	9.87	11.18	10.84	10.87
NaCl	8.64	3.04	8.76	8.87	8.68	7.96	8.29	9.08	8.75	8.80
SiO	11.60	4.62	11.62	11.64	11.25	10.43	10.91	11.97	11.66	11.69
CS	11.58	3.98	11.82	11.90	11.37	10.37	10.94	12.28	11.85	11.95
ClO	8.85	0.32	8.76	8.69	8.20	7.13	7.74	9.35	8.89	8.79
ClF	12.43	3.40	11.77	11.80	11.26	10.19	10.79	12.34	11.85	11.87
SiH_3SiH_3	11.33	6.58	12.11	12.19	11.97	11.32	11.64	12.24	12.08	12.12
CH_3Cl	12.01	6.24	12.36	12.46	12.22	11.45	11.82	12.68	12.35	12.39
CH_3SH	10.01	4.74	10.59	10.69	10.45	9.72	10.07	10.80	10.58	10.62
SO_2	11.74	3.66	11.39	11.40	10.93	9.94	10.50	11.92	11.46	11.48
BF_3	17.22	9.32	16.40	16.50	16.40	15.59	15.97	17.24	16.50	16.56
BCl_3	12.07	4.98	12.41	12.58	12.02	11.05	11.60	12.80	12.43	12.60
$AlCl_3$	12.13	5.79	12.71	12.68	12.25	11.48	11.93	12.89	12.68	12.69
CF_4	17.85	10.37	17.50	17.66	17.57	16.74	17.11	18.35	17.60	17.70
CCl_4	11.97	4.93	12.72	12.69	12.15	11.14	11.71	13.03	12.70	12.67
OCS	12.13	5.56	12.60	12.67	12.21	11.34	11.84	12.87	12.62	12.69
CS_2	10.19	3.97	10.26	10.32	9.92	9.20	9.62	10.45	10.26	10.33
CF_2O	16.08	6.74	14.83	14.93	14.76	13.76	14.32	15.39	14.86	14.92

SiF_4	16.95	9.54	17.00	17.09	16.90	16.09	16.49	17.75	17.08	17.15
N_2O	15.01	6.84	14.49	14.54	14.07	13.11	13.66	14.85	14.54	14.58
NF_3	15.76	7.42	16.03	16.18	15.75	14.69	15.28	16.65	16.10	16.23
PF_3	13.00	6.48	13.16	13.26	13.04	12.24	12.64	13.59	13.19	13.26
O_3	11.06	1.79	9.99	10.04	9.55	8.49	9.09	10.57	10.13	10.18
F_2O	13.82	3.40	12.72	12.80	12.34	11.20	11.85	13.91	12.98	13.05
ClF_3	11.79	3.12	11.48	11.50	11.01	9.96	10.56	12.19	11.59	11.61
CF_2CF_2	12.45	5.81	12.20	12.30	12.13	11.38	11.73	12.51	12.19	12.23
CF_3CN	15.39	7.61	15.61	15.63	15.08	14.04	14.63	15.87	15.59	15.61
CH_3CCH	11.69	6.04	11.53	11.57	11.39	10.67	11.01	11.78	11.52	11.51
CH_2CCH_2	10.83	5.71	11.65	11.71	11.54	10.82	11.15	11.86	11.64	11.64
$cylC_3H_4$	11.87	5.01	11.20	11.26	11.11	10.41	10.73	11.43	11.18	11.18
$cylC_3H_6$	11.64	6.80	12.48	12.56	12.37	11.61	11.96	12.76	12.47	12.48
$CH_3CH_2CH_3$	12.72	7.33	13.08	13.22	13.02	12.28	12.62	13.44	13.08	13.15
CH_3CCCH_3	10.46	5.45	10.91	10.98	10.79	10.08	10.41	11.13	10.90	10.91
$cylC_4H_6$	11.14	5.38	11.03	11.10	10.94	10.24	10.55	11.21	11.01	11.02
isobutane	12.28	7.06	12.79	12.93	12.73	12.00	12.33	13.14	12.79	12.86
benzene	10.16	5.10	10.89	10.95	10.83	10.21	10.49	11.02	10.88	10.87
CH_2F_2	14.15	7.81	13.92	14.03	13.92	13.16	13.50	14.59	13.97	14.03
CF_3H	15.44	9.05	15.23	15.34	15.24	14.48	14.82	15.94	15.28	15.35
CH_2Cl_2	12.18	5.92	12.66	12.75	12.49	11.70	12.09	12.97	12.65	12.69
CCl_3H	12.38	5.36	12.73	12.76	12.37	11.47	11.97	13.01	12.71	12.73
CH_3NO_2	11.94	3.74	11.92	11.98	11.50	10.47	11.06	12.66	12.04	12.10
CH_3SiH_3	12.35	7.27	13.10	13.18	12.96	12.23	12.58	13.38	13.09	13.12
HCOOH	11.98	5.22	12.43	12.54	12.39	11.60	11.96	13.00	12.46	12.53

CH_3CONH_2	10.05	4.88	11.02	11.14	10.96	10.20	10.56	11.55	11.05	11.12
cylNHC_2H_4	10.44	5.28	11.11	11.21	11.03	10.28	10.63	11.49	11.12	11.17
NCCN	13.90	5.85	13.35	13.34	12.81	11.85	12.40	13.72	13.38	13.38
CH_3NHCH_3	9.65	4.55	10.28	10.40	10.22	9.49	9.83	10.69	10.29	10.36
CH_2CO	10.32	3.76	10.95	11.02	10.83	9.88	10.42	11.23	10.94	10.96
cylOC_2H_4	11.68	5.95	11.92	12.03	11.89	11.13	11.48	12.49	11.96	12.02
OCHCHO	10.04	1.94	9.87	9.93	9.45	8.46	9.02	10.48	9.95	10.01
CH_3CH_2OH	11.38	5.54	11.69	11.82	11.64	10.87	11.23	12.23	11.72	11.79
CH_3OCH_3	10.79	5.38	11.27	11.40	11.24	10.50	10.84	11.78	11.30	11.37
cylSC_2H_4	9.93	4.39	10.51	10.60	10.40	9.67	10.01	10.73	10.50	10.52
CH_3SOCH_3	9.54	4.71	10.26	10.38	10.23	9.54	9.86	10.64	10.28	10.34
CH_2CHF	11.55	5.50	11.74	11.80	11.66	10.94	11.27	12.03	11.73	11.74
CH_3CH_2Cl	11.74	6.31	12.25	12.37	12.14	11.37	11.73	12.56	12.24	12.30
CH_2CHCl	11.35	4.97	11.41	11.48	11.30	10.61	10.93	11.63	11.39	11.40
CH_3CClO	11.97	4.79	12.27	12.36	12.13	11.16	11.71	12.71	12.28	12.33
prplCl	11.63	6.14	12.17	12.29	12.05	11.28	11.64	12.48	12.16	12.22
NC_3H_9	9.10	4.30	9.91	10.05	9.87	9.16	9.49	10.28	9.92	10.00
cylOC_4H_4	9.82	4.80	10.44	10.49	10.36	9.71	10.00	10.62	10.42	10.40
cylNHC_4H_4	8.89	4.57	9.66	9.72	9.60	8.96	9.25	9.82	9.64	9.64
NO_2	9.79	1.42	5.65	9.70	9.23	8.20	8.79	10.43	9.98	9.82
SF_6	16.98	7.70	16.38	16.42	16.10	15.09	15.65	17.24	16.48	16.51
$CFCl_3$	12.61	5.26	13.02	13.03	12.48	11.48	12.04	13.34	13.01	13.01
$CClF_3$	14.27	7.24	14.79	14.94	14.55	13.59	14.10	15.09	14.77	14.86
$CBrF_3$	12.97	5.91	13.33	13.35	12.89	11.98	12.50	13.60	13.36	13.36
HCCF	12.04	6.35	12.24	12.25	12.08	11.36	11.70	12.59	12.23	12.21

HCCCN	12.20	5.19	12.31	12.31	11.83	10.94	11.44	12.59	12.32	12.32
NCCCCN	11.52	4.47	11.32	11.31	10.84	9.99	10.47	11.63	11.34	11.33
C_2N_2	13.90	5.85	13.35	13.34	12.81	11.85	12.40	13.72	13.38	13.38
C_3O_2	11.64	4.71	11.44	11.49	11.07	10.27	10.73	11.79	11.48	11.53
FCN	14.33	7.21	14.20	14.25	13.97	13.12	13.54	14.50	14.20	14.20
HCCCCH	11.00	4.80	11.34	11.34	11.18	10.34	10.81	11.61	11.32	11.29
H_2CS	9.18	1.91	9.17	9.21	8.73	7.81	8.34	9.45	9.19	9.23
$HCONH_2$	10.81	5.25	11.33	11.47	11.31	10.54	10.90	11.89	11.37	11.45
CH_2CHCHO	10.70	2.94	10.72	10.78	10.32	9.36	9.91	11.33	10.80	10.86
CH_2CCl_2	11.17	4.74	11.45	11.53	11.25	10.41	10.89	11.66	11.43	11.45
$CHFCF_2$	11.11	5.45	11.53	11.59	11.48	10.77	11.09	11.92	11.52	11.54
CH_2CF_2	11.81	5.81	11.86	11.92	11.77	11.05	11.38	12.17	11.85	11.86
CH_3F	14.09	7.74	13.83	13.93	13.81	13.05	13.40	14.49	13.89	13.95
CF_2Cl_2	13.33	6.12	13.84	13.92	13.39	12.39	12.95	14.14	13.82	13.88
SiF_2	11.04	4.13	10.98	11.02	10.63	9.81	10.28	11.32	11.05	11.08
MSE		-6.94	-0.07	0.04	-0.27	-1.12	-0.67	0.40	0.05	0.05
MAE		6.94	0.53	0.49	0.57	1.15	0.77	0.54	0.45	0.45
rms		7.15	0.80	0.65	0.77	1.40	1.02	0.63	0.59	0.60

TABLE XX: The 19 valence and 23 Rydberg excitation energies (in eV) of nitrogen gas (N_2), carbon monoxide (CO), water (H_2O), ethylene (C_2H_4), and formaldehyde (CH_2O) taken from Ref. [10].

Molecule	State	Ref.	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3

N_2	$V^1\Pi_g$	9.31	9.11	9.46	9.47	9.42	9.36	9.39	9.54	9.47	9.49
	$V^1{\Sigma_u}^-$	9.97	9.68	9.31	9.34	9.28	9.28	9.29	9.02	9.25	9.28
	$V^1\Delta_u$	10.27	10.10	9.89	9.83	9.80	9.80	9.80	9.73	9.89	9.83
	$V^3{\Sigma_u}^+$	7.75	7.53	6.99	7.12	7.12	7.15	7.13	6.99	7.00	7.13
	$V^3\Pi_g$	8.04	7.40	7.74	7.97	7.88	7.80	7.84	7.98	7.75	7.99
	$V^3\Delta_u$	8.88	8.35	7.95	8.28	8.20	8.21	8.21	8.07	7.94	8.28
	$V^3{\Sigma_u}^-$	9.67	9.68	9.31	9.34	9.28	9.28	9.29	9.02	9.25	9.28
	$V^3\Pi_u$	11.19	10.40	10.91	11.14	11.04	10.98	11.02	11.26	11.01	11.26
CO	$V^1\Pi$	8.51	8.23	8.52	8.55	8.50	8.45	8.48	8.59	8.54	8.58
	$V^1\Sigma^-$	9.88	9.81	9.80	9.83	9.75	9.73	9.75	9.64	9.74	9.79
	$V^3\Pi$	6.32	5.72	5.83	6.13	6.09	6.05	6.08	6.14	5.86	6.19
	$V^3\Sigma^+$	8.51	8.06	7.95	7.94	7.93	7.95	7.95	7.99	7.91	7.96
	$V^3\Delta$	9.36	8.73	8.71	8.92	8.84	8.83	8.85	8.86	8.68	8.93
	$V^3\Sigma^-$	9.88	9.81	9.80	9.83	9.75	9.73	9.74	9.64	9.74	9.79
H_2O	R^1B_1	7.4	6.31	7.42	7.51	7.43	7.21	7.28	7.64	7.43	7.49
	R^1A_2	9.1	7.44	9.06	9.18	9.07	8.62	8.80	9.46	9.08	9.16
	R^1A_1	9.7	8.18	9.54	9.64	9.56	9.20	9.35	9.84	9.58	9.66
	R^1B_1	10.0	7.83	9.70	9.81	9.68	9.16	9.37	10.30	9.73	9.80
	R^1A_1	10.17	8.50	9.91	10.04	9.91	9.50	9.64	10.50	9.95	10.03
	R^3B_1	7.2	5.98	6.96	7.09	7.06	6.87	6.92	7.18	6.95	7.07
C_2H_4	R^1B_{3u}	7.11	6.43	7.60	7.61	7.45	7.06	7.22	7.65	7.58	7.56
	V^1B_{1u}	7.60	7.34	7.74	7.69	7.66	7.58	7.62	7.70	7.74	7.69

	R^1B_{1g}	7.80	6.90	8.16	8.21	8.08	7.62	7.82	8.25	8.16	8.17
	R^1B_{2g}	8.01	6.86	8.35	8.37	8.20	7.70	7.91	8.48	8.33	8.31
	R^1A_g	8.29	7.21	8.57	8.59	8.43	7.92	8.13	8.82	8.56	8.53
	R^1B_{3u}	8.62	7.45	9.11	9.06	8.88	8.39	8.63	9.34	9.09	9.04
	V^3B_{1u}	4.36	4.33	3.68	4.03	4.10	4.20	4.16	3.88	3.69	4.05
	R^3B_{3u}	6.98	6.34	7.45	7.48	7.35	6.96	7.12	7.55	7.43	7.44
	R^3B_{1g}	7.79	6.86	8.14	8.16	8.01	7.53	7.77	8.26	8.12	8.11
	R^3B_{2g}	7.79	6.81	8.24	8.23	8.07	7.60	7.81	8.39	8.22	8.19
	R^3A_g	8.15	7.09	8.36	8.26	8.10	7.66	7.88	8.64	8.35	8.26
CH_2O	V^1A_2	4.07	3.86	3.96	4.03	4.00	4.00	4.01	3.96	3.94	4.02
	R^1B_2	7.11	5.76	7.29	7.39	7.31	6.92	7.07	7.64	7.32	7.38
	R^1B_2	7.97	6.53	8.03	8.11	8.05	7.62	7.79	8.42	8.06	8.10
	R^1A_1	8.14	7.09	9.34	9.34	9.22	8.71	8.96	9.64	9.36	9.36
	R^1A_2	8.37	6.68	8.29	8.36	8.29	7.80	8.01	8.86	8.33	8.37
	R^1B_2	8.88	6.80	9.15	9.10	8.95	8.48	8.73	9.78	9.19	9.16
	V^3A_2	3.50	3.13	3.19	3.39	3.34	3.34	3.35	3.29	3.17	3.37
	V^3A_1	5.86	5.90	5.44	5.63	5.61	5.64	5.63	5.47	5.38	5.62
	R^3B_2	6.83	5.60	7.08	7.17	7.12	6.75	6.90	7.49	7.10	7.17
	R^3B_2	7.79	6.47	7.82	7.87	7.83	7.47	7.62	8.22	7.84	7.88
	R^3A_1	7.96	6.34	7.99	8.01	7.94	7.52	7.71	8.52	8.03	8.03
Valence	MSE		-0.30	-0.36	-0.23	-0.28	-0.29	-0.28	-0.32	-0.37	-0.23
(19)	MAE		0.31	0.39	0.27	0.30	0.30	0.29	0.37	0.40	0.27
	rms		0.38	0.47	0.34	0.37	0.37	0.37	0.46	0.48	0.35

Rydberg	MSE	-1.29	0.19	0.24	0.12	-0.30	-0.12	0.51	0.20	0.22
(23)	MAE	1.29	0.29	0.28	0.21	0.35	0.22	0.51	0.28	0.27
	rms	1.35	0.38	0.37	0.30	0.40	0.30	0.58	0.37	0.36

TABLE XXI: The lowest charge-transfer excitation energies (in eV) of $C_2H_4 \cdots C_2F_4$ dimer along the intermolecular distance R [11].

R (Å)	SAC-CI	PBE	LC-ωPBE	ωB97	ωB97X	ωB97X-D	ωB97X-D3	SLC-LDA-D3	SLC-PBE-D3	SLC-B97-D3
5	11.49	5.00	10.03	10.02	9.62	8.74	9.24	10.62	10.08	10.12
6	12.00	5.04	10.54	10.54	10.14	9.22	9.75	11.13	10.59	10.63
7	12.36	5.06	10.90	10.90	10.50	9.58	10.11	11.50	10.95	11.00
8	12.63	5.08	11.17	11.16	10.77	9.84	10.38	11.77	11.22	11.26
9	12.83	5.08	11.37	11.37	10.97	10.05	10.59	11.97	11.43	11.47
10	12.99	5.09	11.54	11.53	11.14	10.22	10.75	12.14	11.59	11.63