Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary material to: Assessment of density functional methods with correct asymptotic behavior

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TABLE I: Reference values (in eV) for the IP131[a] EA131[b] FG131[b] and AE113 databases. For the CCSD(T) calculations, the correlation energies in the basis-set limit are extrapolated from calculations using the aug-cc-pVTZ and aug-cc-pVQZ basis sets. The reference atomization energies for AE113 are calculated without the zero-point energy correction. All the databases contain the 18 atoms and 113 molecules collected in IP131.

	IP131	EA131	FG131	AE113
Molecule	Experimental Vertical Ionization Potential	CCSD(T) Vertical Electron Affinity	CCSD(T) Fundamental Gap	CCSD(T) Atomization Energy
H (Hydrogen atom)	13.60	0.75	12.86	
He (Helium atom)	24.59	-2.63	27.23	
Li (Lithium atom)	5.39	0.62	4.22	
Be (Beryllium atom)	9.32	-0.36	9.66	
B (Boron atom)	8.30	0.25	7.99	
C (Carbon atom)	11.26	1.25	9.97	
N (Nitrogen atom)	14.53	-0.22	14.74	
O (Oxygen atom)	13.62	1.45	12.14	
F (Fluorine atom)	17.42	3.44	13.98	
Ne (Neon atom)	21.57	-5.31	26.92	
Na (Sodium atom)	5.14	0.54	4.14	
Mg (Magnesium atom)	7.65	-0.23	7.76	
Al (Aluminum atom)	5.99	0.45	5.53	
Si (Silicon atom)	8.15	1.42	6.73	
P (Phosphorus atom)	10.49	0.74	9.78	
S (Sulfur atom)	10.36	2.10	8.23	
Cl (Chlorine atom)	12.97	3.69	9.30	
Ar (Argon atom)	15.76	-2.81	18.65	
CH_3 (Methyl radical)	9.84	-0.07	9.86	13.32
CH_4 (Methane)	13.60	-0.62	15.06	18.19
NH (Imidogen) ($3\Sigma^-$)	13.49	0.33	13.17	3.60
NH_2 (Amino radical)	12.00	0.74	11.34	7.91
NH_3 (Ammonia)	10.82	-0.56	11.54	12.91
OH (Hydroxyl radical)	13.02	1.84	11.27	4.65
H_2O (Water)	12.62	-0.56	13.35	10.11
HF (Hydrogen fluoride)	16.12	-0.63	16.91	6.16
SiH_3 (Silyl)	8.74	0.93	7.95	9.88
SiH_4 (Silane)	12.30	-1.11	14.03	14.07
PH_3 (Phosphine)	10.59	-1.21	11.83	10.46
H_2S (Hydrogen sulfide)	10.50	-0.49	11.00	7.94
HCl (Hydrogen chloride)	12.77	-0.52	13.36	4.65
C_2H_2 (Acetylene)	11.49	-1.90	13.43	17.49
C_2H_4 (Ethylene)	10.68	-1.87	12.57	24.38

C_2H_6 (Ethane)	11.99	-0.63	13.41	30.84
HCN (Hydrogen cyanide)	13.61	-0.48	14.31	13.51
CO (Carbon monoxide)	14.01	-1.51	15.57	11.22
HCO (Formy l radical)	9.31	0.02	9.56	12.01
H_2CO (Formaldehyde)	10.89	-0.55	11.56	16.20
CH_3OH (Methyl alcohol)	10.96	-0.55	11.67	22.22
N_2 (Nitrogen diatomic)	15.58	-2.24	17.88	9.85
N_2H_4 (Hydrazine)	8.98	-0.45	10.30	18.82
NO (Nitric oxide)	9.26	-0.42	10.11	6.57
O_2 (Oxygen diatomic) ($3\Sigma_g$)	12.30	-0.08	12.52	5.20
H_2O_2 (Hydrogen peroxide)	11.70	-0.92	12.65	11.62
F_2 (Fluorine diatomic)	15.70	0.42	15.53	1.67
CO_2 (Carbon dioxide)	13.78	-0.65	14.58	16.85
P_2 (Phosphorus diatomic)	10.62	0.48	10.19	4.99
S_2 (Sulfur diatomic) ($3\Sigma_g$)	9.55	1.53	7.96	4.41
Cl_2 (Chlorine diatomic)	11.49	0.75	10.93	2.53
NaCl (Sodium Chloride)	9.80	0.65	8.64	4.32
SiO (Silicon monoxide)	11.61	0.03	11.60	8.25
CS (Carbon monosulfide)	11.34	-0.09	11.58	7.37
ClO (Monochlorine monoxide)	11.01	2.19	8.86	2.74
ClF (Chlorine monofluoride)	12.77	0.44	12.43	2.68
Si_2H_6 (Disilane)	10.53	-0.69	11.33	23.19
CH_3Cl (Methyl chloride)	11.29	-0.51	12.01	17.08
CH_3SH (Methanethiol)	9.44	-0.50	10.01	20.50
SO_2 (Sulfur dioxide)	12.50	0.81	11.74	10.97
BF_3 (Borane, trifluoro-)	15.96	-1.04	17.22	20.40
BCl_3 (Borane, trichloro-)	11.64	-0.17	12.07	14.02
$AlCl_3$ (Aluminum trichloride)	12.01	0.06	12.14	13.57
CF_4 (Carbon tetrafluoride)	16.20	-1.33	17.85	20.80
CCl_4 (Carbon tetrachloride)	11.69	-0.46	11.97	13.59
OCS (Carbonyl sulfide)	11.19	-0.74	12.13	14.45
CS_2 (Carbon disulfide)	10.09	0.01	10.19	12.00
CF_2O (Carbonic difluoride)	13.60	-2.37	16.08	18.22
SiF_4 (Silicon tetrafluoride)	16.40	-0.81	16.95	24.92
N_2O (Nitrous oxide)	12.89	-2.01	15.01	11.66
NF_3 (Nitrogen trifluoride)	13.60	-2.06	15.76	8.94
PF_3 (Phosphorus trifluoride)	12.20	-1.23	13.00	15.64
O_3 (Ozone)	12.73	1.93	11.06	6.26
F_2O (Difluorine monoxide)	13.26	-0.31	13.82	4.04
ClF_3 (Chlorine trifluoride)	13.05	1.20	11.79	5.43
C_2F_4 (Tetrafluoroethylene)	10.69	-1.65	12.45	25.54
CF_3CN (Acetonitrile, trifluoro-)	14.30	-0.96[b]	15.40[b]	27.77
CH_3CCH (Propyne)	10.37	-1.13	11.70	30.44

CH_2CCH_2 (Allene)	10.20	-0.56	10.83	30.40
C_3H_4 (Cyclopropene)	9.86	-1.82	11.87	29.45
C_3H_6 (Cyclopropane)	10.54	-0.65	11.64	36.91
C_3H_8 (Propane)	11.51	-0.60[b]	12.72[b]	43.58
CH_3CCCH_3 (2-Butyne)	9.79	-0.68[b]	10.46[b]	43.32
C_4H_6 (Cyclobutene)	9.43	-1.41[b]	11.14[b]	43.28
$CH_3CH(CH_3)CH_3$ (Isobutane)	11.13	-0.56[b]	12.28[b]	56.37
C_6H_6 (Benzene)	9.25	-0.71[b]	10.16[b]	59.14
CH_2F_2 (Methane, difluoro-)	13.27	-0.58	14.15	18.99
CHF_3 (Methane, trifluoro-)	15.50	-0.60	15.44	19.92
CH_2Cl_2 (Methylene chloride)	11.40	-0.49	12.18	16.05
$CHCl_3$ (Chloroform)	11.50	-0.83	12.38	14.87
CH_3NO_2 (Methane, nitro-)	11.29	-0.37	11.95	26.01
CH_3SiH_3 (Methyl silane)	11.60	-0.53	12.35	27.23
HCOOH (Formic acid)	11.50	-0.57	11.98	21.49
CH_3CONH_2 (Acetamide)	10.00	-0.31	10.05	37.48
C_2H_5N (Aziridine)	9.85	-0.56[b]	10.44[b]	31.11
C_2N_2 (Cyanogen)	13.51	-0.19	13.90	21.60
CH_3NHCH_3 (Dimethylamine)	8.95	-0.56[b]	9.65[b]	37.66
CH_2CO (Ketene)	9.64	-0.51	10.32	23.03
C_2H_4O (Ethylene oxide)	10.57	-0.86	11.68	28.18
$C_2H_2O_2$ (Ethanedial)	10.60	0.69	10.04	27.39
CH_3CH_2OH (Ethanol)	10.64	-0.53	11.38	35.06
CH_3OCH_3 (Dimethyl ether)	10.10	-0.58	10.79	34.56
C_2H_4S (Thiirane)	9.05	-0.78	9.93	27.06
CH_3SOCH_3 (Dimethyl sulfoxide)	9.10	-0.40[b]	9.54[b]	36.89
CH_2CHF (Ethene, fluoro-)	10.63	-0.88	11.55	24.81
CH_3CH_2Cl (Ethyl chloride)	11.06	-0.51	11.74	29.96
CH_2CHCl (Ethene, chloro-)	10.20	-1.12	11.35	23.51
CH_3COCl (Acetyl Chloride)	11.03	-0.85	11.97	28.90
$CH_2ClCH_2CH_3$ (Propane, 1-chloro-)	10.88	-0.49[b]	11.63[b]	42.65
$N(CH_3)_3$ (Trimethylamine)	8.54	-0.54[b]	9.10[b]	50.20
C_4H_4O (Furan)	8.90	-0.74[b]	9.82[b]	42.99
C_4H_5N (Pyrrole)	8.23	-0.51[b]	8.89[b]	46.34
NO_2 (Nitrogen dioxide)	11.23	1.44	9.79	9.80
SF_6 (Sulfur Hexafluoride)	15.70	-1.05[b]	16.98[b]	20.77
$CFCl_3$ (Trichloromonofluoromethane)	11.76	-0.68	12.61	15.22
CF_3Cl (Methane, chlorotrifluoro-)	13.08	-1.06	14.27	18.85
CF_3Br (Bromotrifluoromethane)	12.08	-0.81[b]	12.97[b]	18.35
HCCF (Fluoroacetylene)	11.50	-0.55	12.04	17.19
HCCCN (Cyanoacetylene)	11.75	-0.36	12.20	25.93
C_4N_2 (2-Butynedinitrile)	11.84	0.68	11.52	34.15
C_2N_2 (Cyanogen)	13.51	-0.19	13.90	21.60

C_3O_2 (Carbon suboxide)	10.80	-0.74	11.64	28.58
FCN (Cyanogen fluoride)	13.65	-0.66	14.33	13.19
C_4H_2 (Diacetylene)	10.30	-0.64	11.00	30.05
H_2CS (Thioformaldehyde)	9.38	0.28	9.18	14.07
$CHONH_2$ (Formamide)	10.40	-0.35	10.81	24.56
CH_2CHCHO (Acrolein)	10.10	-0.46[b]	10.70[b]	35.76
CH_2CCl_2 (Ethene, 1,1-dichloro-)	10.00	-1.07	11.17	22.48
C_2HF_3 (Trifluoroethylene)	10.62	-0.54	11.11	25.31
CH_2CF_2 (Ethene, 1,1-difluoro-)	10.70	-1.03	11.81	25.38
CH_3F (Methyl fluoride)	13.04	-0.58	14.09	18.31
CF_2Cl_2 (Difluorodichloromethane)	12.24	-0.90	13.33	16.97
SiF_2 (Silicon difluoride)	11.08	0.10	11.04	12.93

[a] The reference values for the IP131 database, which were published in [Y.-S. Lin, C.-W. Tsai, G.-D. Li, and J.-D. Chai, *J. Chem. Phys.*, 2012, **136**, 154109], are listed for completeness of this work.

[b] Most of the reference values for the EA131 and FG131 databases were published in the EA115 and FG115 databases [Y.-S. Lin, C.-W. Tsai, G.-D. Li, and J.-D. Chai, *J. Chem. Phys.*, 2012, **136**, 154109]. For clarity, the reference values for the additional 16 molecules are labelled with the ([b]).

TABLE II: Atomization energies (in eV) of the AE113 database. The atomization energies are calculated without the zero-point energy correction.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
CH_3	14.71	13.44	13.32	13.31	13.44	13.45	13.29	13.27	13.30	13.31	7.84	12.67	13.32
CH_4	20.04	18.21	18.08	18.14	18.24	18.26	18.15	18.11	18.14	18.16	9.69	16.58	18.19
NH	4.15	3.84	3.89	3.59	3.60	3.82	3.61	3.66	3.65	3.65	4.81	5.13	3.60
NH_2	9.02	8.18	8.23	7.86	7.92	8.16	7.86	7.94	7.94	7.95	8.73	10.25	7.91
NH_3	14.63	13.10	13.09	12.66	12.82	13.06	12.84	12.86	12.87	12.90	12.22	15.54	12.91
OH	5.40	4.78	4.77	4.55	4.67	4.71	4.63	4.60	4.63	4.65	5.86	6.58	4.65
H_2O	11.58	10.18	10.11	9.77	10.04	10.04	10.03	9.92	9.97	10.02	10.64	13.07	10.11
HF	7.05	6.18	6.14	5.92	6.17	6.07	6.07	6.04	6.04	6.07	7.53	8.63	6.16
SiH_3	10.67	9.62	9.71	10.06	9.86	9.90	9.88	9.86	9.89	9.88	-1.07	3.84	9.88
SiH_4	15.04	13.58	13.77	14.26	14.02	14.03	13.94	14.07	14.07	14.04	-0.48	6.07	14.07
PH_3	11.74	10.40	10.54	10.51	10.53	10.65	10.57	10.48	10.57	10.62	2.27	6.80	10.46
SH_2	8.95	7.90	7.84	7.89	8.02	7.91	7.90	7.86	7.92	7.96	2.86	6.40	7.93
HCl	5.24	4.64	4.55	4.65	4.67	4.58	4.61	4.58	4.60	4.63	2.58	4.40	4.65
HCCH	19.96	18.00	17.58	17.62	17.64	17.49	17.53	17.35	17.39	17.40	10.15	17.96	17.49
CH_2CH_2	27.44	24.80	24.33	24.40	24.47	24.43	24.36	24.28	24.33	24.35	12.95	23.44	24.38
CH_3CH_3	34.43	31.09	30.55	30.81	30.79	30.86	30.82	30.82	30.84	30.85	15.56	28.75	30.84
HCN	15.68	14.17	13.91	13.58	13.50	13.61	13.52	13.47	13.46	13.45	10.33	16.54	13.51
CO	13.02	11.70	11.39	11.22	11.22	11.11	11.28	11.19	11.17	11.17	3.17	10.12	11.22
HCO	14.41	12.78	12.44	12.16	12.21	12.14	12.04	12.05	12.06	12.09	3.91	11.75	12.01
CH_2O	18.87	16.78	16.43	16.25	16.24	16.24	16.22	16.17	16.19	16.22	6.14	15.52	16.20
CH_3OH	25.45	22.57	22.18	21.99	22.07	22.21	22.25	22.13	22.17	22.21	16.11	24.66	22.22
N_2	11.62	10.56	10.42	9.76	9.62	9.95	9.81	9.95	9.86	9.79	10.45	14.09	9.85
NH_2NH_2	22.19	19.49	19.24	18.50	18.48	19.09	18.81	18.91	18.90	18.90	19.16	25.42	18.82
NO	8.66	7.49	7.24	6.60	6.59	6.75	6.59	6.81	6.73	6.68	9.87	12.49	6.57
O_2	7.59	6.24	5.89	5.40	5.54	5.38	5.29	5.51	5.44	5.42	2.54	7.37	5.20
HOOH	14.47	12.19	11.93	11.23	11.44	11.54	11.52	11.42	11.46	11.52	12.66	16.74	11.62
F_2	3.34	2.25	2.09	1.55	1.68	1.57	1.40	1.61	1.54	1.52	0.23	2.17	1.67
CO_2	20.62	18.13	17.41	17.38	17.13	16.90	16.99	16.95	16.97	17.03	2.79	16.39	16.85
P_2	6.29	5.30	5.30	5.06	5.01	5.06	5.24	4.71	4.93	5.07	4.93	6.34	4.99
S_2	5.87	4.97	4.64	4.81	4.71	4.47	4.52	4.38	4.48	4.57	0.86	4.21	4.41
Cl_2	3.59	2.82	2.49	2.69	2.38	2.39	2.57	2.41	2.47	2.54	-1.54	1.31	2.53
NaCl	4.55	4.13	4.01	4.83	4.38	4.06	4.32	4.46	4.46	4.35	0.82	2.56	4.32
SiO	9.70	8.48	8.44	8.20	8.22	8.12	8.24	8.12	8.14	8.13	1.74	6.64	8.25
CS	8.79	7.79	7.48	7.56	7.52	7.22	7.33	7.17	7.22	7.28	3.31	6.78	7.37
ClO	4.54	3.53	3.24	2.97	2.88	2.88	2.81	2.81	2.85	2.90	4.64	6.10	2.74
ClF	4.13	3.12	2.89	2.65	2.63	2.62	2.69	2.67	2.66	2.68	6.50	7.06	2.68
SiH_3SiH_3	25.07	22.49	22.50	23.55	23.20	22.98	22.98	23.30	23.27	23.19	-6.49	7.29	23.19
CH_3Cl	19.40	17.35	16.90	17.16	17.01	17.02	17.11	17.07	17.09	17.10	6.50	14.66	17.08
CH_3SH	23.25	20.72	20.26	20.47	20.49	20.44	20.51	20.47	20.52	20.54	9.62	18.94	20.50
SO_2	14.54	12.09	11.48	11.21	11.06	10.87	10.90	10.92	10.99	11.07	-9.08	5.22	10.97
BF_3	23.88	20.93	20.36	20.33	20.53	20.22	20.63	20.37	20.35	20.30	-4.41	10.68	20.40
BCl_3	16.69	14.67	13.63	14.77	14.20	13.72	14.29	14.18	14.19	14.18	-9.02	4.00	14.02
$AlCl_3$	14.99	13.35	12.60	14.02	13.72	12.83	13.57	13.52	13.49	13.42	-15.10	-3.36	13.57

CF_4	26.13	21.94	20.75	20.69	20.69	20.45	21.01	21.00	20.91	20.82	-18.21	5.58	20.80
CCl_4	17.55	14.57	13.04	14.18	13.52	12.97	13.81	13.70	13.67	13.62	-9.11	5.44	13.59
OCS	17.81	15.64	14.93	15.15	14.87	14.50	14.61	14.47	14.53	14.63	5.31	14.89	14.45
CS_2	14.96	13.09	12.37	12.87	12.54	12.03	12.16	11.83	11.96	12.12	7.78	13.69	12.00
CF_2O	22.85	19.53	18.58	18.45	18.33	18.13	18.40	18.42	18.38	18.36	-6.99	11.27	18.21
SiF_4	28.28	24.58	24.05	24.22	24.82	23.96	24.69	24.59	24.44	24.24	-17.96	2.67	24.92
N_2O	15.75	13.51	12.89	12.25	11.88	12.00	11.63	11.89	11.82	11.82	9.66	18.74	11.66
NF_3	13.63	10.67	9.92	9.04	9.10	9.07	8.98	9.40	9.22	9.11	-7.69	4.90	8.94
PF_3	19.05	15.99	15.56	15.24	15.49	15.32	15.69	15.59	15.59	15.52	-9.92	4.55	15.64
O_3	10.50	8.04	7.41	6.33	6.43	6.09	5.58	6.00	5.95	6.01	2.66	10.31	6.26
F_2O	7.40	5.35	4.94	3.99	4.19	4.04	3.82	4.11	4.02	3.98	-1.17	4.18	4.04
ClF_3	9.95	7.12	6.41	5.66	5.80	5.53	5.33	5.60	5.54	5.54	-19.25	-5.94	5.43
CF_2CF_2	32.49	27.50	26.00	25.85	25.80	25.47	25.89	25.91	25.84	25.78	-28.32	2.89	25.54
CF_3CN	34.44	29.67	28.25	28.00	27.74	27.63	28.00	28.06	27.94	27.83	-10.05	17.83	27.77
CH_3CCH	34.78	31.26	30.41	30.70	30.57	30.45	30.54	30.39	30.43	30.42	16.56	30.76	30.43
CH_2CCH_2	34.95	31.42	30.57	30.75	30.73	30.57	30.54	30.39	30.45	30.48	16.87	31.04	30.40
$cylC_3H_4$	34.06	30.45	29.37	29.94	29.65	29.45	29.70	29.65	29.59	29.52	12.97	29.38	29.45
$cylC_3H_6$	42.03	37.68	36.54	37.20	36.92	36.87	37.12	37.15	37.09	37.02	16.45	35.55	36.91
$CH_3CH_2CH_3$	48.93	44.02	43.07	43.56	43.46	43.53	43.59	43.61	43.62	43.63	21.07	40.80	43.58
CH_3CCCH_3	49.54	44.48	43.21	43.70	43.43	43.34	43.48	43.37	43.39	43.37	24.19	44.18	43.32
$cylC_4H_6$	49.68	44.43	42.88	43.59	43.29	43.14	43.37	43.43	43.40	43.39	17.59	41.00	43.28
isobutane	63.50	56.98	55.58	56.31	56.29	56.18	56.40	56.44	56.42	56.42	26.09	52.50	56.37
benzene	68.31	61.17	58.88	59.76	59.47	59.07	59.35	59.19	59.26	59.29	27.20	58.81	59.14
CH_2F_2	22.51	19.62	19.04	18.86	18.94	18.93	19.08	19.08	19.04	19.01	4.26	16.18	18.99
CF_3H	24.36	20.84	19.97	19.79	19.85	19.74	20.06	20.07	20.01	19.94	-6.08	11.35	19.92
CH_2Cl_2	18.86	16.55	15.77	16.29	15.92	15.84	16.17	16.09	16.11	16.11	3.95	13.79	16.05
CCl_3H	18.25	15.61	14.46	15.26	14.73	14.46	15.04	14.95	14.94	14.91	-2.26	9.91	14.87
CH_3NO_2	32.34	27.91	26.85	26.25	26.11	26.19	26.01	26.29	26.24	26.22	12.46	29.97	26.01
CH_3SiH_3	29.93	26.95	26.73	27.38	27.18	27.12	27.13	27.26	27.26	27.22	4.71	17.89	27.22
HCOOH	25.79	22.50	21.80	21.47	21.47	21.47	21.60	21.49	21.54	21.58	10.06	23.05	21.49
CH_3CONH_2	43.90	38.87	37.78	37.56	37.47	37.63	37.61	37.70	37.69	37.69	19.30	38.82	37.48
$cylNHC_2H_4$	36.07	32.10	31.14	31.34	30.98	31.21	31.32	31.39	31.32	31.26	17.48	33.38	31.11
NCCN	26.12	23.39	22.60	22.18	21.76	21.88	21.73	21.68	21.64	21.62	15.52	29.78	21.59
CH_3NHCH_3	42.93	38.33	37.56	37.51	37.42	37.78	37.73	37.75	37.75	37.76	25.53	40.84	37.66
CH_2CO	27.29	24.26	23.47	23.52	23.41	23.20	23.24	23.13	23.17	23.22	-0.86	17.85	23.03
$cylOC_2H_4$	32.89	29.11	28.15	28.38	28.13	28.14	28.39	28.33	28.30	28.28	13.71	29.18	28.18
OCHCHO	32.74	28.84	27.86	27.63	27.52	27.40	27.49	27.47	27.48	27.49	2.56	23.49	27.39
CH_3CH_2OH	40.06	35.62	34.80	34.84	34.85	34.98	35.11	35.02	35.05	35.07	20.99	36.15	35.06
CH_3OCH_3	39.58	35.15	34.40	34.42	34.41	34.55	34.69	34.54	34.58	34.59	24.58	38.57	34.55
$cylSC_2H_4$	31.25	27.78	26.74	27.39	27.05	26.90	27.24	27.18	27.16	27.14	10.70	25.84	27.06
CH_3SOCH_3	42.99	37.82	36.64	36.94	36.92	36.73	36.92	36.92	36.96	36.99	9.16	32.20	36.89
CH_2CHF	28.84	25.62	24.92	24.89	24.95	24.85	24.89	24.84	24.85	24.85	10.34	23.43	24.81
CH_3CH_2Cl	34.04	30.42	29.56	30.06	29.85	29.83	30.03	30.00	30.02	30.01	13.61	28.14	29.96
CH_2CHCl	27.15	24.22	23.39	23.75	23.57	23.44	23.59	23.49	23.53	23.54	7.55	20.40	23.51
CH_3CClO	34.07	30.11	28.98	29.31	29.02	28.82	29.04	29.00	29.02	29.04	6.83	25.63	28.90
prplCl	48.52	43.35	42.06	42.75	42.49	42.44	42.74	42.75	42.74	42.73	18.16	38.97	42.65

NC_3H_9	57.32	51.08	49.88	50.07	50.05	50.23	50.34	50.35	50.33	50.32	32.76	53.92	50.20
$cylOC_4H_4$	50.63	44.80	42.98	43.38	43.15	42.90	43.25	43.07	43.12	43.14	20.68	45.19	42.99
$cylNHC_4H_4$	54.29	48.23	46.38	46.71	46.45	46.41	46.60	46.54	46.56	46.58	24.84	49.43	46.34
NO_2	14.10	11.75	11.07	10.31	10.18	10.14	9.75	10.14	10.07	10.08	1.56	12.57	9.80
SF_6	28.23	21.99	20.23	20.34	20.80	19.79	20.72	20.79	20.66	20.46	-57.93	-17.79	20.77
$CFCl_3$	19.60	16.35	14.94	15.69	15.19	14.75	15.46	15.42	15.37	15.30	-13.04	4.16	15.22
$CClF_3$	23.91	20.06	18.80	18.97	18.81	18.52	19.08	19.10	19.01	18.92	-18.87	3.44	18.85
$CBrF_3$	23.39	19.60	18.39	18.36	18.34	18.05	18.39	18.55	18.46	18.37	-21.34	1.29	18.34
HCCF	20.75	18.19	17.49	17.55	17.42	17.23	17.40	17.23	17.24	17.24	5.10	16.43	17.19
HCCCN	30.78	27.58	26.63	26.57	26.25	26.12	26.08	25.88	25.90	25.90	16.64	31.47	25.93
NCCCCN	41.41	36.94	35.47	35.36	34.67	34.60	34.50	34.26	34.27	34.27	19.34	45.43	34.15
C_2N_2	26.12	23.39	22.60	22.18	21.76	21.88	21.73	21.68	21.64	21.62	15.52	29.78	21.59
C_3O_2	35.52	31.24	29.80	30.01	29.53	29.04	29.06	28.77	28.88	29.03	-9.62	21.28	28.58
FCN	16.45	14.37	13.80	13.56	13.30	13.31	13.33	13.31	13.27	13.25	2.60	13.30	13.19
HCCCCH	35.22	31.55	30.43	30.74	30.52	30.15	30.25	29.89	29.97	30.00	17.39	32.77	30.05
H_2CS	16.25	14.45	14.07	14.15	14.16	14.02	14.06	13.92	14.00	14.06	6.74	13.51	14.07
$HCONH_2$	29.16	25.70	25.03	24.62	24.55	24.78	24.67	24.70	24.73	24.75	14.96	27.77	24.56
CH_2CHCHO	41.55	37.06	35.95	36.02	35.98	35.80	35.84	35.76	35.81	35.83	12.06	33.27	35.76
CH_2CCl_2	26.72	23.46	22.25	22.97	22.53	22.25	22.66	22.55	22.57	22.55	5.90	20.31	22.48
$CHFCF_2$	31.28	26.91	25.68	25.55	25.53	25.28	25.57	25.57	25.52	25.48	-12.33	11.61	25.31
CH_2CF_2	30.41	26.57	25.58	25.56	25.57	25.37	25.57	25.54	25.52	25.50	2.23	20.01	25.38
CH_3F	20.96	18.64	18.32	18.23	18.31	18.34	18.34	18.32	18.32	18.32	10.93	18.79	18.31
CF_2Cl_2	21.71	18.17	16.84	17.28	16.96	16.59	17.21	17.23	17.15	17.06	-16.41	3.41	16.97
SiF_2	14.87	12.95	12.79	12.66	12.93	12.59	12.85	12.86	12.79	12.67	2.17	9.27	12.93
MSE	3.75	0.84	0.13	0.17	0.07	-0.04	0.07	0.05	0.05	0.04	-15.24	-2.36	
MAE	3.75	0.88	0.36	0.27	0.14	0.16	0.12	0.12	0.10	0.10	15.53	4.81	
rms	4.22	1.06	0.48	0.36	0.20	0.23	0.16	0.15	0.13	0.14	20.02	7.44	

TABLE III: $-\epsilon_N(N)$ (in eV) of the IP131 database.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
H	-7.32	-7.59	-7.40	-7.92	-7.71	-8.77	-10.32	-11.91	-11.62	-11.06	-11.96	-11.45	13.60
He	-15.52	-15.76	-15.91	-16.53	-16.16	-18.00	-20.62	-21.13	-20.90	-20.26	-23.15	-22.22	24.59
Li	-3.16	-3.22	-3.03	-3.11	-3.20	-3.65	-4.18	-5.32	-5.31	-5.21	-5.24	-5.07	5.39
Be	-5.60	-5.61	-5.47	-5.71	-5.66	-6.32	-7.26	-8.76	-8.63	-8.29	-8.71	-8.40	9.32
B	-4.11	-4.17	-4.06	-4.45	-4.10	-5.17	-6.17	-7.91	-7.73	-7.24	-8.16	-7.76	8.30
C	-6.13	-6.10	-5.95	-6.36	-6.20	-7.34	-8.84	-10.36	-10.14	-9.57	-10.92	-10.50	11.26
N	-8.42	-8.31	-8.10	-8.79	-8.55	-9.79	-11.78	-12.94	-12.72	-12.14	-13.90	-13.49	14.53
O	-7.47	-7.60	-7.63	-8.00	-7.37	-9.28	-11.21	-12.38	-12.12	-11.49	-14.30	-13.18	13.62
F	-10.40	-10.32	-10.35	-10.73	-10.35	-12.32	-14.83	-15.43	-15.24	-14.63	-17.70	-16.72	17.42
Ne	-13.60	-13.38	-13.40	-14.06	-13.71	-15.69	-18.68	-18.73	-18.63	-18.08	-21.33	-20.52	21.57
Na	-3.08	-3.03	-2.90	-2.93	-2.81	-3.48	-4.18	-4.82	-4.91	-4.87	-5.53	-5.20	5.14
Mg	-4.77	-4.70	-4.57	-4.70	-4.66	-5.29	-6.18	-7.35	-7.31	-7.08	-7.85	-7.45	7.65
Al	-3.00	-3.09	-2.84	-3.02	-3.07	-3.62	-4.30	-5.88	-5.77	-5.47	-5.78	-5.56	5.99
Si	-4.56	-4.61	-4.32	-4.55	-4.73	-5.28	-6.25	-7.93	-7.72	-7.31	-7.84	-7.61	8.15
P	-6.30	-6.30	-5.97	-6.42	-6.51	-7.12	-8.36	-10.08	-9.78	-9.26	-10.01	-9.79	10.49
S	-6.16	-6.15	-6.05	-6.08	-6.13	-7.20	-8.51	-10.08	-9.83	-9.31	-10.95	-10.25	10.36
Cl	-8.22	-8.14	-8.03	-8.24	-8.25	-9.36	-10.96	-12.45	-12.15	-11.56	-13.27	-12.68	12.97
Ar	-10.41	-10.30	-10.16	-10.58	-10.53	-11.68	-13.57	-14.89	-14.56	-13.92	-15.75	-15.28	15.76
CH_3	-5.39	-5.42	-5.22	-5.63	-5.46	-6.47	-7.82	-9.42	-9.15	-8.59	-10.06	-9.57	9.84
CH_4	-9.48	-9.45	-9.39	-9.79	-9.59	-10.78	-12.42	-13.91	-13.60	-12.99	-14.36	-13.87	13.60
NH	-7.98	-7.92	-7.74	-8.27	-8.13	-9.37	-11.27	-12.49	-12.24	-11.65	-13.23	-12.83	13.49
NH_2	-7.21	-7.22	-7.17	-7.44	-7.24	-8.56	-10.28	-11.65	-11.36	-10.76	-12.64	-11.93	12.00
NH_3	-6.28	-6.18	-6.11	-6.46	-6.28	-7.51	-9.30	-10.64	-10.33	-9.73	-11.50	-10.84	10.82
OH	-7.43	-7.38	-7.38	-7.60	-7.37	-9.02	-11.08	-12.16	-11.89	-11.27	-13.65	-12.77	13.02
H_2O	-7.40	-7.24	-7.20	-7.53	-7.37	-8.83	-10.96	-12.02	-11.73	-11.11	-13.16	-12.46	12.62
HF	-9.83	-9.65	-9.64	-10.04	-9.85	-11.56	-14.08	-14.73	-14.50	-13.90	-16.38	-15.64	16.12
SiH_3	-5.31	-5.37	-5.13	-5.39	-5.43	-6.15	-7.22	-8.78	-8.59	-8.16	-9.10	-8.76	8.74
SiH_4	-8.53	-8.52	-8.44	-8.82	-8.69	-9.67	-11.08	-12.66	-12.37	-11.82	-12.92	-12.47	12.30
PH_3	-6.77	-6.72	-6.60	-6.85	-6.81	-7.68	-8.96	-10.49	-10.26	-9.77	-11.17	-10.67	10.59
SH_2	-6.40	-6.31	-6.16	-6.40	-6.42	-7.33	-8.77	-10.30	-10.01	-9.46	-10.88	-10.39	10.50
HCl	-8.16	-8.05	-7.92	-8.28	-8.20	-9.24	-10.91	-12.37	-12.05	-11.45	-13.00	-12.51	12.77
HCCH	-7.38	-7.20	-7.04	-7.39	-7.21	-8.20	-9.74	-11.21	-10.92	-10.36	-12.25	-11.62	11.49
CH_2CH_2	-6.93	-6.74	-6.58	-6.88	-6.73	-7.63	-9.10	-10.55	-10.28	-9.75	-11.85	-11.16	10.68
CH_3CH_3	-8.16	-8.17	-8.13	-8.50	-8.28	-9.45	-11.00	-12.43	-12.15	-11.59	-13.05	-12.58	11.99
HCN	-9.20	-9.02	-8.87	-9.24	-9.06	-10.14	-11.80	-13.26	-12.94	-12.35	-14.35	-13.81	13.61
CO	-9.13	-9.04	-9.01	-9.34	-9.22	-10.54	-12.29	-13.75	-13.44	-12.81	-14.36	-13.87	14.01
HCO	-5.12	-5.16	-5.10	-5.34	-5.21	-6.52	-8.05	-9.40	-9.17	-8.63	-10.42	-9.96	9.31
CH_2O	-6.35	-6.26	-6.23	-6.58	-6.35	-7.68	-9.52	-10.58	-10.36	-9.82	-11.85	-11.26	10.89
CH_3OH	-6.37	-6.26	-6.21	-6.55	-6.35	-7.72	-9.65	-10.75	-10.49	-9.92	-11.87	-11.25	10.96
N_2	-10.43	-10.28	-10.27	-10.53	-10.45	-11.98	-13.99	-15.17	-14.91	-14.29	-15.90	-15.48	15.58
NH_2NH_2	-5.36	-5.30	-5.24	-5.57	-5.40	-6.62	-8.38	-9.66	-9.38	-8.80	-10.66	-10.04	8.98
NO	-4.57	-4.52	-4.52	-4.68	-4.59	-6.19	-8.05	-9.15	-8.93	-8.36	-10.52	-10.01	9.26
O_2	-6.97	-6.84	-6.83	-7.30	-7.12	-8.75	-11.05	-11.79	-11.59	-11.01	-13.33	-12.84	12.30
HOOH	-6.61	-6.46	-6.43	-6.76	-6.59	-8.12	-10.29	-11.24	-10.98	-10.38	-12.60	-11.93	11.70

F_2	-9.69	-9.49	-9.50	-10.04	-9.72	-11.57	-14.23	-14.64	-14.47	-13.90	-16.75	-16.04	15.70
CO_2	-9.33	-9.09	-9.00	-9.38	-9.18	-10.47	-12.33	-13.41	-13.18	-12.65	-15.30	-14.66	13.78
P_2	-7.26	-7.15	-6.92	-7.21	-7.25	-7.86	-9.02	-10.49	-10.30	-9.90	-11.13	-10.75	10.62
S_2	-5.83	-5.83	-5.62	-5.83	-6.00	-6.81	-8.13	-9.70	-9.41	-8.88	-10.13	-9.86	9.55
Cl_2	-7.44	-7.33	-7.19	-7.51	-7.48	-8.48	-10.09	-11.50	-11.20	-10.63	-12.33	-11.89	11.49
NaCl	-5.44	-5.30	-5.19	-5.38	-5.35	-6.34	-7.83	-9.25	-8.96	-8.41	-9.82	-9.33	9.80
SiO	-7.61	-7.48	-7.37	-7.61	-7.61	-8.62	-10.10	-11.44	-11.25	-10.77	-12.06	-11.64	11.61
CS	-7.45	-7.40	-7.30	-7.56	-7.58	-8.68	-10.22	-11.78	-11.50	-10.92	-11.96	-11.60	11.34
ClO	-6.37	-6.30	-6.23	-6.41	-6.33	-7.74	-9.50	-10.73	-10.48	-9.91	-11.89	-11.29	11.01
ClF	-8.00	-7.86	-7.77	-8.12	-8.04	-9.24	-11.05	-12.33	-12.04	-11.45	-13.44	-12.94	12.77
SiH_3SiH_3	-7.26	-7.20	-7.05	-7.32	-7.41	-8.10	-9.27	-10.82	-10.59	-10.13	-11.28	-10.93	10.53
CH_3Cl	-7.20	-7.12	-6.99	-7.35	-7.23	-8.27	-9.89	-11.31	-11.00	-10.43	-12.04	-11.56	11.29
CH_3SH	-5.65	-5.57	-5.43	-5.69	-5.65	-6.58	-8.00	-9.49	-9.21	-8.68	-10.19	-9.70	9.44
SO_2	-8.28	-8.08	-8.01	-8.22	-8.19	-9.44	-11.15	-12.35	-12.13	-11.61	-13.67	-13.18	12.50
BF_3	-10.32	-10.07	-10.03	-10.49	-10.32	-11.96	-14.51	-15.01	-14.84	-14.28	-16.99	-16.29	15.96
BCl_3	-7.85	-7.72	-7.55	-7.95	-7.91	-8.86	-10.51	-11.90	-11.59	-11.02	-12.66	-12.22	11.64
$AlCl_3$	-8.17	-8.02	-7.85	-8.27	-8.22	-9.14	-10.77	-12.17	-11.86	-11.30	-12.86	-12.41	12.01
CF_4	-10.68	-10.42	-10.39	-10.92	-10.70	-12.37	-14.96	-15.43	-15.26	-14.69	-17.52	-16.82	16.20
CCl_4	-7.82	-7.69	-7.53	-7.93	-7.97	-8.84	-10.51	-11.90	-11.59	-11.01	-12.66	-12.22	11.69
OCS	-7.66	-7.50	-7.33	-7.66	-7.59	-8.47	-9.86	-11.22	-10.99	-10.53	-12.55	-12.05	11.19
CS_2	-6.94	-6.82	-6.62	-6.91	-6.91	-7.62	-8.83	-10.18	-9.97	-9.57	-11.38	-10.95	10.09
CF_2O	-8.77	-8.52	-8.46	-8.89	-8.68	-10.15	-12.31	-13.20	-12.97	-12.39	-15.01	-14.37	13.60
SiF_4	-10.96	-10.69	-10.64	-11.13	-10.97	-12.54	-15.02	-15.61	-15.42	-14.85	-17.53	-16.82	16.40
N_2O	-8.65	-8.40	-8.31	-8.65	-8.44	-9.64	-11.30	-12.44	-12.23	-11.74	-14.48	-13.86	12.89
NF_3	-8.63	-8.45	-8.44	-8.82	-8.69	-10.11	-12.14	-13.13	-12.90	-12.33	-15.22	-14.58	13.60
PF_3	-7.51	-7.36	-7.30	-7.57	-7.51	-8.58	-10.04	-11.44	-11.21	-10.70	-12.96	-12.48	12.20
O_3	-8.25	-8.02	-8.01	-8.29	-8.16	-9.72	-11.68	-12.78	-12.55	-11.97	-14.40	-13.78	12.73
F_2O	-7.91	-7.72	-7.75	-8.14	-7.95	-9.73	-12.21	-12.81	-12.62	-12.03	-14.72	-14.05	13.26
ClF_3	-8.18	-8.00	-7.95	-8.30	-8.23	-9.63	-11.72	-12.68	-12.44	-11.87	-14.39	-13.82	13.05
CF_2CF_2	-6.56	-6.31	-6.26	-6.50	-6.42	-7.61	-9.24	-10.42	-10.22	-9.71	-12.78	-12.12	10.69
CF_3CN	-9.77	-9.57	-9.44	-9.82	-9.67	-10.80	-12.55	-13.90	-13.60	-13.00	-15.26	-14.80	14.30
CH_3CCH	-6.64	-6.49	-6.34	-6.68	-6.47	-7.48	-8.99	-10.42	-10.14	-9.60	-11.49	-10.89	10.37
CH_2CCH_2	-6.72	-6.56	-6.42	-6.71	-6.55	-7.51	-8.96	-10.38	-10.12	-9.60	-11.58	-10.96	10.20
$cylC_3H_4$	-6.23	-6.11	-5.98	-6.26	-6.07	-7.04	-8.50	-9.88	-9.63	-9.11	-11.20	-10.58	9.86
$cylC_3H_6$	-7.23	-7.07	-6.94	-7.26	-7.14	-8.15	-9.60	-11.11	-10.83	-10.28	-12.04	-11.51	10.54
$CH_3CH_2CH_3$	-7.73	-7.75	-7.72	-8.07	-7.87	-9.00	-10.53	-11.93	-11.66	-11.11	-12.61	-12.13	11.51
CH_3CCCH_3	-6.06	-5.93	-5.79	-6.12	-5.89	-6.91	-8.38	-9.78	-9.51	-8.99	-10.90	-10.31	9.79
$cylC_4H_6$	-6.19	-6.04	-5.89	-6.17	-6.01	-6.92	-8.36	-9.74	-9.49	-8.99	-11.12	-10.45	9.43
isobutane	-7.59	-7.58	-7.53	-7.86	-7.75	-8.78	-10.27	-11.68	-11.42	-10.87	-12.39	-11.93	11.13
benzene	-6.54	-6.33	-6.14	-6.42	-6.28	-7.08	-8.42	-9.69	-9.49	-9.06	-11.44	-10.75	9.25
CH_2F_2	-8.25	-8.15	-8.15	-8.50	-8.32	-9.78	-11.77	-12.76	-12.54	-11.98	-14.23	-13.67	13.27
CF_3H	-9.51	-9.35	-9.35	-9.70	-9.58	-11.02	-13.05	-14.01	-13.79	-13.22	-15.72	-15.14	15.50
CH_2Cl_2	-7.48	-7.38	-7.26	-7.58	-7.54	-8.56	-10.18	-11.58	-11.29	-10.72	-12.33	-11.87	11.40
CCl_3H	-7.55	-7.42	-7.26	-7.66	-7.65	-8.56	-10.21	-11.60	-11.29	-10.71	-12.38	-11.93	11.50
CH_3NO_2	-7.11	-6.92	-6.86	-7.21	-7.07	-8.50	-10.63	-11.53	-11.30	-10.73	-12.86	-12.26	11.29
CH_3SiH_3	-8.01	-7.92	-7.79	-8.12	-8.07	-9.00	-10.37	-11.94	-11.67	-11.13	-12.45	-12.02	11.60

HCOOH	-6.92	-6.73	-6.68	-6.96	-6.84	-8.17	-10.13	-11.16	-10.92	-10.36	-12.52	-11.92	11.50
CH_3CONH_2	-5.95	-5.79	-5.72	-6.03	-5.93	-7.18	-9.09	-10.15	-9.91	-9.35	-11.28	-10.71	10.00
$cylNHC_2H_4$	-5.88	-5.78	-5.67	-6.03	-5.83	-6.97	-8.63	-9.94	-9.67	-9.12	-11.01	-10.40	9.85
NCCN	-9.64	-9.39	-9.23	-9.57	-9.40	-10.44	-12.01	-13.34	-13.07	-12.54	-14.91	-14.32	13.51
CH_3NHCH_3	-5.13	-5.06	-4.98	-5.32	-5.14	-6.27	-7.91	-9.20	-8.93	-8.39	-10.22	-9.61	8.95
CH_2CO	-6.09	-5.91	-5.79	-6.08	-5.91	-6.94	-8.39	-9.72	-9.50	-9.01	-11.29	-10.66	9.64
$cylOC_2H_4$	-6.39	-6.27	-6.20	-6.56	-6.34	-7.71	-9.71	-10.70	-10.46	-9.90	-11.87	-11.24	10.57
OCHCHO	-6.53	-6.39	-6.35	-6.64	-6.54	-7.77	-9.51	-10.62	-10.41	-9.88	-11.98	-11.45	10.60
CH_3CH_2OH	-6.27	-6.15	-6.11	-6.42	-6.28	-7.60	-9.50	-10.62	-10.37	-9.79	-11.69	-11.08	10.64
CH_3OCH_3	-5.93	-5.83	-5.77	-6.11	-5.92	-7.20	-9.05	-10.14	-9.90	-9.36	-11.28	-10.67	10.10
$cylSC_2H_4$	-5.46	-5.37	-5.22	-5.47	-5.42	-6.36	-7.82	-9.26	-8.98	-8.46	-10.03	-9.53	9.05
CH_3SOCH_3	-5.52	-5.38	-5.29	-5.49	-5.48	-6.51	-8.06	-9.29	-9.07	-8.58	-10.59	-10.04	9.10
CH_2CHF	-6.72	-6.52	-6.40	-6.71	-6.56	-7.55	-9.07	-10.43	-10.18	-9.66	-12.02	-11.34	10.63
CH_3CH_2Cl	-7.07	-6.97	-6.85	-7.21	-7.11	-8.13	-9.74	-11.16	-10.86	-10.29	-11.88	-11.39	11.06
CH_2CHCl	-6.59	-6.42	-6.27	-6.56	-6.47	-7.35	-8.79	-10.18	-9.92	-9.42	-11.50	-10.91	10.20
CH_3CClO	-7.29	-7.13	-7.02	-7.39	-7.27	-8.40	-10.14	-11.27	-11.04	-10.52	-12.51	-12.01	11.03
prplCl	-7.04	-6.94	-6.82	-7.18	-7.11	-8.09	-9.69	-11.12	-10.82	-10.25	-11.82	-11.34	10.88
NC_3H_9	-4.92	-4.85	-4.77	-5.07	-4.97	-6.00	-7.56	-8.83	-8.59	-8.07	-9.92	-9.32	8.54
$cylOC_4H_4$	-5.88	-5.67	-5.52	-5.77	-5.63	-6.50	-7.83	-9.20	-8.97	-8.51	-10.91	-10.23	8.90
$cylNHC_4H_4$	-5.33	-5.13	-4.97	-5.22	-5.08	-5.92	-7.25	-8.58	-8.36	-7.92	-10.26	-9.58	8.23
NO_2	-6.60	-6.50	-6.48	-6.68	-6.62	-8.18	-10.15	-11.16	-10.95	-10.37	-12.58	-12.09	11.23
SF_6	-10.40	-10.14	-10.11	-10.66	-10.52	-12.10	-14.71	-15.12	-14.96	-14.41	-17.28	-16.58	15.70
$CFCl_3$	-7.88	-7.75	-7.60	-7.99	-8.01	-8.92	-10.59	-11.97	-11.66	-11.08	-12.82	-12.38	11.76
$CClF_3$	-8.73	-8.56	-8.44	-8.84	-8.80	-9.86	-11.63	-12.97	-12.67	-12.06	-14.04	-13.55	13.08
$CBrF_3$	-8.00	-7.82	-7.68	-8.03	-8.00	-8.97	-10.56	-11.88	-11.64	-11.12	-13.06	-12.53	12.08
HCCF	-7.22	-7.02	-6.88	-7.22	-7.03	-8.12	-9.72	-11.09	-10.82	-10.28	-12.48	-11.86	11.50
HCCCN	-8.08	-7.87	-7.70	-8.03	-7.84	-8.81	-10.28	-11.62	-11.36	-10.87	-13.12	-12.52	11.75
NCCCCN	-8.68	-8.44	-8.26	-8.59	-8.40	-9.36	-10.80	-12.08	-11.83	-11.36	-13.81	-13.24	11.84
C_2N_2	-9.64	-9.39	-9.23	-9.57	-9.40	-10.44	-12.01	-13.34	-13.07	-12.54	-14.91	-14.32	13.51
C_3O_2	-7.50	-7.27	-7.13	-7.44	-7.25	-8.25	-9.66	-10.81	-10.63	-10.22	-12.96	-12.36	10.80
FCN	-8.97	-8.73	-8.61	-8.97	-8.78	-9.98	-11.71	-13.02	-12.74	-12.17	-14.61	-13.99	13.65
HCCCCH	-6.84	-6.64	-6.47	-6.77	-6.60	-7.51	-8.91	-10.24	-10.00	-9.52	-11.69	-11.09	10.30
H_2CS	-5.61	-5.53	-5.39	-5.62	-5.59	-6.53	-7.97	-9.40	-9.14	-8.62	-10.14	-9.68	9.38
$HCONH_2$	-6.17	-6.02	-5.96	-6.26	-6.13	-7.42	-9.35	-10.39	-10.15	-9.59	-11.60	-11.00	10.40
CH_2CHCHO	-6.15	-6.00	-5.94	-6.29	-6.14	-7.41	-9.31	-10.37	-10.14	-9.59	-11.43	-10.87	10.10
CH_2CCl_2	-6.61	-6.44	-6.28	-6.55	-6.52	-7.37	-8.80	-10.17	-9.92	-9.42	-11.54	-10.97	10.00
$CHFCF_2$	-6.45	-6.22	-6.15	-6.42	-6.30	-7.42	-8.99	-10.24	-10.02	-9.52	-12.36	-11.70	10.62
CH_2CF_2	-6.78	-6.57	-6.46	-6.76	-6.63	-7.67	-9.22	-10.54	-10.30	-9.78	-12.33	-11.66	10.70
CH_3F	-8.19	-8.09	-8.06	-8.47	-8.23	-9.69	-11.69	-12.70	-12.48	-11.91	-13.95	-13.38	13.04
CF_2Cl_2	-8.23	-8.08	-7.94	-8.33	-8.34	-9.29	-10.97	-12.35	-12.04	-11.45	-13.31	-12.86	12.24
SiF_2	-7.27	-7.14	-7.05	-7.29	-7.25	-8.16	-9.42	-10.88	-10.70	-10.24	-12.06	-11.58	11.08
MSE	-4.28	-4.40	-4.50	-4.17	-4.29	-3.15	-1.48	-0.24	-0.48	-1.01	0.90	0.35	
MAE	4.28	4.40	4.50	4.17	4.29	3.15	1.48	0.40	0.51	1.01	1.00	0.60	
rms	4.39	4.50	4.60	4.26	4.39	3.22	1.56	0.63	0.75	1.18	1.12	0.72	

TABLE IV: $-\epsilon_{N+1}(N+1)$ (in eV) of the EA131 database.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
H	1.87	1.97	2.05	1.64	1.98	1.21	0.32	-1.37	-1.21	-0.85	-0.80	-0.42	0.75
He	6.30	6.06	6.31	6.15	5.89	5.73	5.22	4.10	4.15	4.26	4.25	4.26	-2.63
Li	0.82	0.88	1.00	0.96	0.95	0.58	0.16	-0.69	-0.73	-0.70	-0.51	-0.34	0.62
Be	1.92	1.89	2.08	1.97	2.04	1.63	1.27	0.44	0.34	0.40	0.22	0.46	-0.36
B	2.08	2.14	2.32	2.20	2.33	1.60	0.77	-0.45	-0.42	-0.15	-0.42	-0.10	0.25
C	1.95	2.06	2.26	2.25	2.21	1.27	0.10	-1.28	-1.16	-0.74	-1.33	-0.94	1.25
N	3.53	3.49	3.51	3.53	3.79	2.57	1.59	-0.11	0.12	0.62	-0.75	0.11	-0.22
O	2.80	2.91	2.92	2.94	3.03	1.64	0.02	-1.44	-1.16	-0.55	-2.10	-1.30	1.45
F	1.74	1.96	1.96	1.89	1.86	0.35	-1.70	-2.87	-2.59	-1.94	-3.71	-3.01	3.44
Ne	9.80	9.77	10.00	10.12	10.14	9.28	7.98	7.28	7.29	7.53	6.35	6.77	-5.31
Na	0.80	0.85	0.98	0.92	0.89	0.56	0.13	-0.67	-0.71	-0.67	-0.60	-0.39	0.54
Mg	1.42	1.38	1.55	1.50	1.49	1.23	1.04	0.42	0.35	0.31	0.19	0.36	-0.23
Al	1.54	1.58	1.78	1.61	1.73	1.21	0.58	-0.48	-0.47	-0.31	-0.42	-0.18	0.45
Si	1.19	1.26	1.50	1.31	1.35	0.74	-0.11	-1.46	-1.35	-1.07	-1.33	-1.05	1.42
P	1.83	1.90	1.95	1.96	2.07	1.20	0.37	-1.01	-0.92	-0.63	-1.52	-0.90	0.74
S	1.09	1.20	1.28	1.14	1.24	0.33	-0.85	-2.34	-2.15	-1.71	-2.61	-2.06	2.10
Cl	0.16	0.31	0.41	0.05	0.25	-0.74	-2.21	-3.73	-3.46	-2.92	-3.92	-3.43	3.69
Ar	5.11	5.19	5.39	5.54	5.71	4.84	3.92	3.59	3.46	3.48	2.48	2.85	-2.81
CH_3	2.65	2.78	2.88	2.66	2.85	2.08	1.06	-0.36	-0.20	0.17	-0.72	-0.19	-0.07
CH_4	2.00	1.97	2.16	2.17	1.99	1.81	1.50	1.05	0.99	0.92	0.43	0.67	-0.62
NH	3.06	3.16	3.21	3.18	3.30	2.20	0.94	-0.60	-0.37	0.14	-1.11	-0.39	0.33
NH_2	2.66	2.84	2.91	2.76	2.86	1.85	0.46	-1.03	-0.78	-0.27	-1.37	-0.78	0.74
NH_3	2.19	2.18	2.39	2.27	2.18	1.98	1.57	1.02	0.97	0.90	0.41	0.68	-0.56
OH	2.36	2.56	2.60	2.49	2.53	1.27	-0.46	-1.84	-1.56	-0.96	-2.27	-1.64	1.83
H_2O	2.45	2.44	2.66	2.54	2.43	2.18	1.76	1.02	0.97	0.94	0.51	0.78	-0.56
HF	2.67	2.65	2.87	2.78	2.58	2.36	1.94	1.04	1.00	1.00	0.72	0.99	-0.63
SiH_3	1.49	1.61	1.72	1.62	1.62	1.01	0.14	-1.18	-1.09	-0.81	-1.61	-1.18	0.93
SiH_4	2.03	2.02	2.20	2.28	2.03	1.88	1.52	1.20	1.13	1.05	0.19	0.50	-1.11
PH_3	1.95	1.95	2.15	2.05	1.99	1.79	1.37	1.04	0.97	0.88	0.16	0.45	-1.21
SH_2	2.04	2.05	2.25	2.13	2.06	1.85	1.42	0.95	0.88	0.82	0.18	0.48	-0.49
HCl	2.33	2.37	2.54	2.39	2.46	2.08	1.55	0.91	0.85	0.85	0.30	0.62	-0.52
HCCH	1.85	1.81	1.98	2.03	1.81	1.68	1.48	1.18	1.13	1.04	1.36	1.79	-1.90
CH_2CH_2	2.08	2.05	2.25	2.27	1.99	1.91	1.58	1.22	1.17	1.09	0.45	1.23	-1.86
CH_3CH_3	1.89	1.89	2.06	2.19	1.84	1.74	1.44	1.09	1.03	0.95	0.18	0.47	-0.62
HCN	2.33	3.59	2.51	2.65	2.20	2.07	1.66	0.81	0.77	0.79	1.14	1.54	-0.48
CO	3.80	3.73	3.91	3.88	3.92	3.34	2.72	1.94	1.89	1.93	0.99	1.41	-1.50
HCO	2.87	2.94	2.97	2.77	3.02	2.21	1.11	-0.22	-0.06	0.33	-0.86	-0.35	0.02
CH_2O	2.59	2.45	2.64	2.67	2.13	1.93	2.11	1.02	1.12	1.40	0.01	0.51	-0.55
CH_3OH	1.91	1.89	2.07	2.13	1.88	1.72	1.47	0.94	0.90	0.84	0.20	0.48	-0.55
N_2	5.41	5.45	5.50	5.54	5.77	4.67	3.65	2.35	2.50	2.88	1.40	1.90	-2.24
NH_2NH_2	2.07	2.11	2.29	2.42	2.02	1.88	1.47	0.89	0.84	0.81	0.08	0.39	-0.45
NO	4.19	4.30	4.35	4.40	4.42	3.17	1.69	0.40	0.61	1.12	-0.37	0.11	-0.42
O_2	4.45	4.58	4.56	4.73	4.71	3.21	1.51	0.26	0.50	1.08	-0.89	-0.18	-0.08
HOOH	2.38	2.40	2.59	2.58	2.34	2.16	1.76	1.17	1.11	1.06	0.48	0.87	-0.92

F_2	4.32	4.43	4.43	4.42	4.29	2.88	0.83	-0.01	0.17	0.73	-1.35	-0.86	0.42
CO_2	2.57	2.60	2.78	2.77	2.64	2.33	1.88	1.28	1.22	1.19	2.20	2.56	-0.65
P_2	2.11	2.13	2.28	2.24	2.22	1.48	0.61	-0.89	-0.72	-0.35	-1.17	-0.84	0.48
S_2	1.57	1.67	1.77	1.76	1.73	0.83	-0.32	-1.72	-1.54	-1.12	-2.38	-1.89	1.53
Cl_2	2.11	2.20	2.30	2.35	2.32	1.48	0.46	-0.86	-0.68	-0.28	-1.78	-1.43	0.75
NaCl	0.80	0.83	0.96	0.80	0.90	0.53	0.14	-0.62	-0.65	-0.65	-0.87	-0.63	0.65
SiO	2.35	2.35	2.51	2.48	2.54	1.86	1.18	-0.07	0.01	0.25	-0.39	-0.08	0.03
CS	2.96	3.00	3.10	3.22	3.13	2.20	1.22	-0.26	-0.11	0.32	-0.70	-0.31	-0.09
ClO	1.79	1.97	2.03	1.87	1.97	0.73	-0.95	-2.18	-1.95	-1.41	-3.03	-2.46	2.19
ClF	2.86	2.95	3.03	3.22	3.04	2.09	0.96	-0.41	-0.22	0.23	-1.37	-0.97	0.44
SiH_3SiH_3	1.96	1.95	2.12	2.12	2.05	1.75	1.69	1.14	1.07	1.00	-0.23	0.14	-0.69
CH_3Cl	1.95	1.96	2.15	2.16	1.94	1.76	1.38	0.87	0.81	0.76	0.06	0.39	-0.51
CH_3SH	1.88	1.90	2.08	2.19	1.81	1.72	1.30	0.93	0.86	0.80	-0.04	0.30	-0.50
SO_2	2.72	2.78	2.86	2.92	2.80	1.71	0.42	-1.01	-0.80	-0.29	-1.89	-1.47	0.81
BF_3	2.38	2.44	2.60	2.76	2.24	2.18	1.69	1.31	1.24	1.18	1.04	0.50	-1.04
BCl_3	2.95	2.99	3.15	3.05	3.02	2.21	1.18	1.15	1.06	0.99	-1.35	-0.90	-0.17
$AlCl_3$	1.51	1.61	1.75	2.08	1.82	1.28	0.72	0.13	0.07	0.12	-1.58	-1.21	0.06
CF_4	2.92	2.98	3.13	3.51	2.95	2.75	2.27	1.96	1.90	1.83	0.60	0.95	-1.33
CCl_4	2.04	2.11	2.17	2.39	2.22	1.67	1.06	0.14	0.19	0.35	-2.12	-1.72	-0.46
OCS	2.44	2.47	2.61	3.24	2.34	2.13	1.57	1.38	1.29	1.22	0.14	0.58	-0.74
CS_2	2.56	2.59	2.68	2.86	2.73	1.88	0.95	-0.45	-0.30	0.10	-1.17	-0.77	0.01
CF_2O	2.69	2.74	2.90	3.10	2.73	2.47	1.99	1.51	1.44	1.40	0.78	1.32	-2.37
SiF_4	2.34	2.48	2.59	2.92	2.42	2.17	1.60	1.36	1.27	1.23	-0.49	-0.07	-0.81
N_2O	3.24	3.27	3.46	3.31	3.42	3.01	2.40	1.89	1.82	1.79	1.00	1.53	-2.01
NF_3	4.37	4.45	4.56	4.86	4.38	4.03	3.06	2.88	2.81	2.84	1.03	1.55	-2.06
PF_3	2.66	2.59	2.75	2.84	2.60	2.39	2.12	1.60	1.54	1.49	0.52	0.85	-1.23
O_3	2.16	2.29	2.29	2.23	2.15	0.65	-1.35	-2.39	-2.16	-1.56	-3.45	-2.89	1.93
F_2O	4.42	4.52	4.50	4.61	4.43	3.18	1.65	0.44	0.63	1.16	-1.20	-0.73	-0.31
ClF_3	2.51	2.61	2.66	2.73	2.55	1.48	0.07	-1.25	-1.02	-0.51	-2.67	-2.25	1.20
CF_2CF_2	2.57	2.65	2.79	3.12	2.47	2.40	1.98	1.67	1.60	1.54	1.19	0.38	-1.65
CF_3CN	3.47	2.71	2.82	3.34	2.23	2.26	1.85	1.49	1.45	1.39	0.08	0.11	-0.96
CH_3CCH	1.68	1.66	1.84	1.95	1.56	1.54	1.32	0.94	0.89	0.82	0.06	0.34	-1.13
CH_2CCH_2	1.83	1.82	2.00	2.18	1.76	1.70	1.41	1.10	1.06	0.98	0.31	0.39	-0.56
$cylC_3H_4$	1.89	1.88	2.05	2.22	1.82	1.75	1.53	1.12	1.07	1.00	0.57	1.09	-1.82
$cylC_3H_6$	1.98	1.97	2.16	2.32	1.87	1.84	1.54	1.22	1.17	1.09	0.22	0.50	-0.65
$CH_3CH_2CH_3$	1.76	1.77	1.93	2.09	1.68	1.63	1.36	1.10	1.04	0.96	-0.05	0.26	-0.60
CH_3CCCH_3	1.59	1.61	1.77	1.98	1.52	1.49	1.30	1.01	0.97	0.89	-0.32	0.01	-0.67
$cylC_4H_6$	1.80	1.81	1.97	2.31	1.71	1.68	1.41	1.14	1.08	1.01	0.04	0.34	-1.41
isobutane	1.66	1.69	1.85	2.05	1.58	1.55	1.30	1.04	0.99	0.91	-0.26	0.08	-0.56
benzene	3.70	1.60	1.75	2.00	1.50	1.48	1.32	1.08	1.03	0.94	-0.58	-0.06	-0.71
CH_2F_2	2.12	2.09	2.26	2.30	2.13	1.89	1.71	1.00	0.95	0.91	0.33	0.58	-0.58
CF_3H	2.43	2.43	2.58	2.97	2.36	2.19	1.90	1.02	0.99	1.01	0.40	0.66	-0.60
CH_2Cl_2	2.05	2.07	2.26	2.24	2.08	1.83	1.41	0.84	0.78	0.74	-0.42	-0.02	-0.49
CCl_3H	2.21	2.25	2.40	2.42	2.33	1.95	1.47	0.82	0.75	0.74	-1.18	-0.75	-0.83
CH_3NO_2	2.13	2.09	2.25	2.42	2.01	2.12	1.23	0.01	0.21	0.66	-1.34	-0.77	-0.37
CH_3SiH_3	1.86	1.88	2.06	2.19	1.76	1.71	1.35	0.97	0.91	0.84	-0.03	0.31	-0.53

HCOOH	2.11	2.06	2.23	2.24	2.07	2.39	1.84	1.02	0.98	2.17	0.82	1.33	-0.57
CH_3CONH_2	1.64	1.66	1.83	1.98	1.59	1.48	1.21	0.66	0.60	0.55	-0.38	-0.04	-0.31
$cylNHC_2H_4$	1.92	1.90	2.07	2.26	1.83	1.75	1.53	0.97	0.92	0.87	0.17	0.45	-0.56
NCCN	3.03	3.15	3.26	3.23	3.26	2.28	1.21	1.25	1.17	0.39	-1.63	-1.13	-0.19
CH_3NHCH_3	1.72	1.71	1.89	2.02	1.65	1.59	1.36	0.98	0.93	0.86	-0.04	0.26	-0.56
CH_2CO	2.02	2.45	2.60	2.59	1.96	1.83	1.53	1.00	0.94	0.88	0.03	0.48	-0.51
$cylOC_2H_4$	1.97	1.94	2.12	2.16	1.92	1.79	1.58	1.06	1.01	0.95	0.23	0.49	-0.86
OCHCHO	2.10	2.24	2.35	2.33	2.27	1.39	0.26	-1.05	-0.90	-0.50	-2.82	-2.23	0.69
CH_3CH_2OH	1.81	1.82	1.97	2.15	1.73	1.65	1.38	0.92	0.87	0.81	-0.09	0.23	-0.53
CH_3OCH_3	1.78	1.77	1.93	2.05	1.74	1.63	1.42	1.02	0.97	0.90	0.02	0.31	-0.58
$cylSC_2H_4$	1.95	1.93	2.13	2.16	1.81	1.78	1.47	1.03	0.98	0.91	0.09	0.46	-0.78
CH_3SOCH_3	1.65	1.67	1.82	2.03	1.58	1.50	1.20	0.77	0.71	0.68	-0.15	0.12	-0.40
CH_2CHF	2.06	2.03	2.21	2.48	1.97	1.88	1.61	1.08	1.03	0.99	0.71	1.21	-0.88
CH_3CH_2Cl	1.84	1.86	2.03	2.27	1.75	1.68	1.32	0.91	0.86	0.80	-0.02	0.32	-0.51
CH_2CHCl	1.91	1.91	2.09	2.32	1.81	1.76	1.42	1.00	0.94	0.90	0.09	0.61	-1.11
CH_3CClO	2.00	1.99	2.15	2.47	1.88	1.61	1.26	0.79	0.73	0.68	-0.72	-0.20	-0.85
prplCl	1.70	1.73	1.90	1.99	1.61	1.56	1.24	0.88	0.83	0.76	-0.51	-0.12	-0.48
NC_3H_9	1.62	1.64	1.81	2.01	1.59	1.52	1.30	1.00	0.95	0.88	-0.27	0.06	-0.54
$cylOC_4H_4$	1.69	1.68	1.84	3.99	1.65	1.56	1.38	1.03	0.98	0.91	-0.05	0.24	-0.74
$cylNHC_4H_4$	1.67	1.70	1.83	2.07	1.59	1.54	1.32	0.78	0.72	0.69	-0.22	0.09	-0.51
NO_2	2.25	2.44	2.43	2.79	2.44	1.29	-0.24	-1.51	-1.31	-0.77	-2.50	-1.95	1.44
SF_6	2.71	2.85	2.88	4.00	2.72	2.38	1.99	1.03	1.10	1.29	-1.96	-1.56	-1.05
$CFCl_3$	2.38	2.43	2.49	2.84	2.69	2.01	1.45	0.50	0.55	0.73	-1.56	-1.17	-0.68
$CClF_3$	2.71	2.76	2.90	3.65	2.50	2.52	2.04	1.60	1.54	1.56	0.26	0.59	-1.06
$CBrF_3$	2.73	2.73	2.86	3.33	2.87	2.51	2.07	1.11	1.13	1.27	-0.36	0.03	-0.81
HCCF	1.90	1.91	2.07	2.32	1.83	1.73	1.46	0.90	0.86	0.82	0.16	0.46	-0.55
HCCCN	2.94	3.01	2.12	2.07	1.66	2.43	1.25	0.57	0.49	0.49	-1.12	-0.62	-0.36
NCCCCN	1.60	1.75	1.90	1.79	1.87	1.04	0.10	-1.20	-1.06	-0.72	-3.11	-2.60	0.68
C_2N_2	3.03	3.15	3.26	3.23	3.26	2.28	1.21	1.25	1.17	0.39	-1.63	-1.13	-0.19
C_3O_2	3.92	3.04	3.04	4.13	4.15	3.04	1.59	1.40	1.31	1.23	-1.14	-0.64	-0.74
FCN	2.45	2.50	2.67	2.61	2.59	2.18	1.64	0.99	0.93	0.93	-0.02	0.36	-0.66
HCCCCH	3.11	1.68	1.83	2.24	1.47	1.43	1.36	1.03	0.98	0.90	-0.60	-0.10	-0.64
H_2CS	2.59	2.64	2.77	2.75	2.72	1.86	0.83	-0.65	-0.47	-0.04	-1.27	-0.83	0.28
$HCONH_2$	1.96	1.94	2.12	2.20	1.90	1.74	1.43	0.72	2.43	2.45	0.07	0.34	-0.35
CH_2CHCHO	2.77	2.88	3.00	3.02	2.98	2.18	1.19	-0.15	0.01	0.38	-1.80	-1.21	-0.46
CH_2CCl_2	2.05	1.96	2.10	2.53	1.92	1.77	1.46	0.99	0.93	0.89	-0.53	-0.01	-1.07
$CHFCF_2$	2.17	2.22	2.35	2.76	2.09	1.99	1.70	1.03	0.99	0.98	0.61	0.90	-0.54
CH_2CF_2	2.09	2.08	2.26	2.37	2.04	1.90	1.64	1.07	1.02	0.97	0.79	0.45	-1.03
CH_3F	2.02	1.99	2.17	2.14	2.01	1.81	1.60	0.98	0.93	0.87	0.41	0.61	-0.58
CF_2Cl_2	2.63	2.64	2.76	3.03	3.04	2.34	1.90	1.19	1.21	1.29	-0.75	-0.36	-0.90
SiF_2	2.35	2.36	2.51	2.54	2.52	1.85	1.11	-0.19	-0.09	0.19	-0.56	-0.27	0.10
MSE	-2.04	-2.05	-2.17	-2.28	-2.04	-1.59	-0.94	-0.17	-0.20	-0.32	0.75	0.37	
MAE	2.04	2.05	2.17	2.28	2.04	1.60	0.96	0.36	0.35	0.41	0.83	0.55	
rms	2.29	2.32	2.41	2.49	2.34	1.76	1.03	0.46	0.47	0.55	1.02	0.75	

TABLE V: $-\epsilon_{N+1}(N)$ (in eV) of the EA131 database.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
H	-2.60	0.51	-0.85	0.41	0.53	-1.12	0.52	0.52	0.53	0.53	-2.48	-2.45	0.75
He	2.49	2.29	2.02	2.54	2.67	2.39	2.67	4.55	4.64	4.30	-2.44	-2.22	-2.63
Li	-2.03	-1.34	-1.57	-1.14	-1.58	-1.48	-0.26	0.28	0.27	0.20	-7.79	-7.57	0.62
Be	-2.10	-2.02	-1.93	-1.67	-2.08	-1.43	-0.53	0.67	0.54	0.29	-5.36	-5.01	-0.36
B	-3.92	-3.62	-3.45	-2.84	-3.56	-2.69	-1.40	0.15	-0.12	-0.57	-8.32	-7.73	0.25
C	-6.06	-5.59	-5.34	-4.89	-5.35	-4.29	-2.72	-1.00	-1.38	-1.98	-11.44	-10.68	1.25
N	-4.40	-4.15	-4.44	-3.37	-3.82	-3.18	-1.70	0.15	-0.06	-0.51	-10.62	-9.46	-0.22
O	-7.18	-6.51	-6.70	-5.21	-6.11	-5.16	-3.04	-1.70	-1.94	-2.48	-14.58	-13.16	1.45
F	-10.28	-9.33	-9.43	-7.95	-9.00	-7.59	-4.77	-4.13	-4.32	-4.90	-18.51	-17.01	3.44
Ne	3.65	3.59	3.29	4.45	4.35	3.96	5.17	7.25	7.18	6.84	-2.57	-2.07	-5.31
Na	-2.17	-1.45	-1.92	-0.72	-1.12	-1.70	-0.16	0.29	0.29	0.24	-7.45	-7.24	0.54
Mg	-1.38	-1.34	-1.20	-0.95	-1.44	-0.92	-0.33	0.59	0.54	0.38	-4.17	-3.85	-0.23
Al	-2.91	-2.76	-2.55	-2.28	-2.81	-2.10	-1.25	0.08	-0.07	-0.36	-6.20	-5.80	0.45
Si	-4.59	-4.37	-4.11	-4.02	-4.30	-3.51	-2.38	-0.87	-1.11	-1.55	-8.36	-7.90	1.42
P	-4.13	-3.73	-3.95	-3.38	-3.74	-3.26	-2.39	-0.55	-0.84	-1.21	-9.37	-8.35	0.74
S	-6.11	-5.64	-5.73	-5.21	-5.76	-4.89	-3.51	-2.01	-2.34	-2.79	-11.59	-10.61	2.10
Cl	-8.30	-7.75	-7.77	-7.38	-7.70	-6.79	-5.10	-3.65	-4.03	-4.58	-14.03	-13.09	3.69
Ar	0.82	0.84	0.70	2.16	1.25	1.14	2.10	3.74	3.61	3.41	-3.91	-3.52	-2.81
CH_3	-3.60	-2.95	-3.06	-2.37	-2.99	-2.20	-1.19	0.55	0.29	-0.04	-9.39	-8.35	-0.07
CH_4	-0.27	-0.31	-0.42	-0.13	-0.01	-0.15	0.09	1.26	1.36	1.16	-4.28	-3.99	-0.62
NH	-4.88	-4.32	-4.51	-3.66	-4.19	-3.31	-1.78	-0.12	-0.38	-0.83	-11.23	-10.03	0.33
NH_2	-5.24	-4.54	-4.62	-3.68	-4.30	-3.45	-1.93	-0.36	-0.64	-1.11	-11.47	-10.33	0.74
NH_3	-0.64	-0.66	-0.77	-0.33	-0.32	-0.42	-0.08	1.28	1.35	1.12	-4.91	-4.56	-0.56
OH	-7.27	-6.46	-6.55	-5.33	-6.13	-5.05	-2.94	-1.72	-1.98	-2.53	-14.28	-12.99	1.83
H_2O	-0.83	-0.85	-0.99	-0.49	-0.45	-0.59	-0.16	1.28	1.35	1.10	-5.50	-5.10	-0.56
HF	-0.83	-0.87	-1.06	-0.50	-0.42	-0.61	-0.15	1.27	1.36	1.11	-5.98	-5.54	-0.63
SiH_3	-3.98	-3.54	-3.59	-3.29	-4.26	-3.01	-2.59	-1.11	-1.18	-1.31	-8.95	-8.18	0.93
SiH_4	-0.39	-0.37	-0.43	0.15	-0.15	-0.13	0.19	1.45	1.48	1.28	-4.48	-4.12	-1.11
PH_3	-0.64	-0.61	-0.67	0.06	-0.35	-0.36	0.03	1.27	1.28	1.09	-4.85	-4.34	-1.21
SH_2	-0.84	-0.79	-0.86	-0.14	-0.50	-0.51	-0.05	1.22	1.23	1.03	-5.32	-4.74	-0.49
HCl	-1.14	-1.08	-1.16	-0.59	-0.76	-0.69	-0.10	1.19	1.20	0.99	-5.95	-5.46	-0.52
HCCH	-0.60	-0.40	-0.33	-0.02	-0.14	0.11	0.24	1.27	1.38	1.21	-5.55	-4.88	-1.90
CH_2CH_2	-1.33	-1.12	-1.01	-0.81	-0.88	-0.36	0.19	1.46	1.56	1.35	-6.39	-5.67	-1.86
CH_3CH_3	-0.36	-0.38	-0.45	-0.18	-0.04	-0.17	0.05	1.29	1.38	1.18	-4.44	-4.10	-0.62
HCN	-1.33	-1.11	-1.06	-0.73	-0.86	-0.35	0.02	1.14	1.26	1.08	-6.63	-5.97	-0.48
CO	-2.26	-2.01	-1.95	-1.64	-1.76	-1.13	0.27	1.77	1.54	1.08	-7.82	-7.15	-1.50
HCO	-3.81	-3.46	-3.51	-3.34	-3.38	-2.72	-1.52	0.14	-0.12	-0.57	-9.45	-8.66	0.02
CH_2O	-2.94	-2.68	-2.59	-2.31	-2.44	-1.77	-0.36	1.16	0.92	0.46	-8.58	-7.83	-0.55
CH_3OH	-0.62	-0.61	-0.70	-0.33	-0.20	-0.35	-0.07	1.18	1.28	1.08	-5.17	-4.74	-0.55
N_2	-2.22	-1.96	-1.92	-1.65	-1.70	-1.02	0.63	2.10	1.81	1.29	-8.04	-7.36	-2.24
NH_2NH_2	-0.93	-0.91	-0.98	-0.54	-0.51	-0.60	-0.26	1.20	1.25	1.01	-5.33	-4.93	-0.45
NO	-4.61	-4.25	-4.17	-3.96	-4.08	-3.20	-1.48	0.03	-0.29	-0.87	-10.76	-10.06	-0.42
O_2	-4.91	-4.53	-4.54	-4.23	-4.18	-3.48	-1.66	-0.24	-0.56	-1.13	-11.52	-10.58	-0.08
HOOH	-1.95	-1.68	-1.68	-1.14	-1.39	-0.71	-0.08	1.42	1.50	1.25	-8.03	-7.34	-0.92

F_2	-6.28	-5.87	-5.83	-5.47	-5.76	-4.59	-2.26	-1.37	-1.59	-2.15	-13.51	-12.73	0.42
CO_2	-0.92	-0.86	-0.95	-0.39	-0.34	-0.53	-0.06	1.50	1.55	1.30	-6.80	-6.08	-0.65
P_2	-3.56	-3.43	-3.26	-3.15	-3.38	-2.80	-1.75	-0.42	-0.62	-0.95	-7.66	-7.19	0.48
S_2	-4.79	-4.53	-4.43	-4.24	-4.44	-3.87	-2.83	-1.29	-1.54	-1.94	-9.58	-8.90	1.53
Cl_2	-4.48	-4.27	-4.16	-3.98	-4.14	-3.46	-2.03	-0.63	-0.89	-1.34	-9.48	-9.04	0.75
NaCl	-2.14	-2.26	-2.38	-1.83	-1.72	-2.02	-1.65	-0.38	-0.28	-0.45	-6.47	-6.12	0.65
SiO	-3.00	-2.86	-2.75	-2.54	-2.84	-2.25	-1.21	0.20	0.01	-0.33	-7.32	-6.82	0.03
CS	-3.60	-3.42	-3.28	-3.13	-3.25	-2.63	-1.36	0.12	-0.12	-0.55	-8.34	-7.79	-0.09
ClO	-6.40	-5.98	-5.90	-5.68	-5.76	-4.98	-3.55	-2.04	-2.28	-2.79	-12.15	-11.36	2.19
ClF	-4.72	-4.47	-4.37	-4.13	-4.33	-3.52	-1.86	-0.53	-0.79	-1.27	-10.36	-9.81	0.44
SiH_3SiH_3	-0.70	-0.61	-0.60	-0.06	-0.43	-0.28	0.07	1.38	1.38	1.19	-4.92	-4.39	-0.69
CH_3Cl	-0.95	-0.87	-0.90	-0.54	-0.58	-0.47	-0.09	1.15	1.22	1.02	-5.76	-5.26	-0.51
CH_3SH	-0.88	-0.83	-0.85	-0.41	-0.54	-0.48	-0.10	1.19	1.24	1.03	-5.29	-4.82	-0.50
SO_2	-4.64	-4.42	-4.33	-4.25	-4.35	-3.76	-2.43	-0.95	-1.20	-1.66	-10.16	-9.57	0.81
BF_3	-0.77	-0.75	-0.85	-0.42	-0.23	-0.45	-0.10	1.49	1.56	1.32	-6.94	-6.16	-1.04
BCl_3	-3.00	-2.74	-2.57	-2.38	-2.49	-2.01	-0.95	0.67	0.43	0.03	-7.98	-7.35	-0.17
$AlCl_3$	-2.50	-2.23	-2.17	-1.62	-2.10	-1.70	-1.00	0.51	0.39	0.18	-7.13	-6.64	0.06
CF_4	0.00	-0.04	-0.16	0.08	0.59	0.22	0.46	2.23	2.31	2.04	-4.92	-4.56	-1.33
CCl_4	-2.92	-2.76	-2.65	-2.51	-2.76	-1.97	-0.69	0.79	0.56	0.14	-7.80	-7.36	-0.46
OCS	-2.15	-1.94	-1.83	-1.55	-1.71	-1.23	-0.02	1.45	1.21	0.81	-7.35	-6.77	-0.74
CS_2	-3.00	-2.85	-2.70	-2.52	-2.71	-2.24	-1.21	0.13	-0.05	-0.37	-7.64	-7.13	0.01
CF_2O	-2.14	-1.79	-1.75	-1.38	-1.49	-0.94	0.07	1.73	1.79	1.37	-8.62	-7.85	-2.37
SiF_4	-1.30	-1.15	-1.21	-0.67	-0.70	-0.72	-0.16	1.49	1.49	1.24	-6.65	-6.15	-0.81
N_2O	-1.84	-1.57	-1.54	-1.23	-1.30	-0.83	0.49	2.10	1.84	1.37	-7.92	-7.24	-2.01
NF_3	-1.35	-1.03	-1.08	-0.52	-0.73	0.01	1.32	3.05	2.85	2.36	-8.05	-7.46	-2.06
PF_3	-1.08	-0.88	-0.82	-0.46	-0.68	-0.30	0.37	1.82	1.82	1.54	-6.23	-5.69	-1.23
O_3	-6.52	-6.24	-6.20	-6.25	-6.20	-5.65	-4.16	-2.74	-3.00	-3.48	-12.94	-12.23	1.93
F_2O	-4.69	-4.32	-4.32	-3.97	-4.18	-3.24	-1.14	-0.02	-0.28	-0.82	-11.60	-10.90	-0.31
ClF_3	-5.16	-4.88	-4.83	-4.67	-4.84	-4.14	-2.55	-1.18	-1.43	-1.91	-11.37	-10.81	1.20
CF_2CF_2	-0.68	-0.50	-0.59	-0.18	-0.12	-0.19	0.15	1.87	1.91	1.67	-7.06	-6.31	-1.65
CF_3CN	-2.28	-1.96	-1.87	-1.56	-1.73	-1.15	0.17	1.73	1.48	1.03	-8.04	-7.37	-0.96
CH_3CCH	-0.43	-0.45	-0.53	-0.22	-0.10	-0.24	-0.02	1.16	1.25	1.07	-5.00	-4.35	-1.13
CH_2CCH_2	-1.03	-0.85	-0.76	-0.58	-0.59	-0.16	0.07	1.33	1.42	1.22	-6.03	-5.37	-0.56
$cylC_3H_4$	-1.33	-1.10	-0.99	-0.71	-0.80	-0.34	0.19	1.38	1.49	1.30	-6.42	-5.68	-1.82
$cylC_3H_6$	-0.26	-0.27	-0.33	-0.11	0.10	-0.04	0.13	1.45	1.54	1.33	-4.40	-4.03	-0.65
$CH_3CH_2CH_3$	-0.43	-0.42	-0.47	-0.21	-0.14	-0.19	0.03	1.29	1.36	1.17	-4.49	-4.13	-0.60
CH_3CCCH_3	-0.48	-0.48	-0.55	-0.24	-0.11	-0.27	-0.04	1.20	1.29	1.09	-4.69	-4.20	-0.67
$cylC_4H_6$	-0.85	-0.66	-0.55	-0.36	-0.39	-0.08	0.09	1.36	1.45	1.25	-5.92	-5.20	-1.41
isobutane	-0.54	-0.51	-0.54	-0.26	-0.39	-0.25	-0.01	1.25	1.32	1.13	-4.63	-4.24	-0.56
benzene	-1.46	-1.23	-1.08	-0.99	-0.96	-0.52	0.01	1.26	1.34	1.15	-6.48	-5.77	-0.71
CH_2F_2	-0.31	-0.34	-0.46	-0.23	0.06	-0.17	0.04	1.27	1.38	1.18	-4.85	-4.43	-0.58
CF_3H	-0.28	-0.30	-0.43	-0.19	0.13	-0.13	0.08	1.34	1.45	1.26	-4.94	-4.54	-0.60
CH_2Cl_2	-1.62	-1.46	-1.40	-1.10	-1.24	-0.80	-0.13	1.17	1.20	0.98	-6.53	-6.03	-0.49
CCl_3H	-2.23	-2.07	-1.98	-1.75	-1.96	-1.31	-0.21	1.17	1.08	0.75	-7.12	-6.64	-0.83
CH_3NO_2	-3.44	-3.18	-3.13	-2.98	-3.03	-2.44	-0.97	0.44	0.20	-0.26	-9.41	-8.71	-0.37
CH_3SiH_3	-0.70	-0.64	-0.65	-0.24	-0.41	-0.33	-0.02	1.24	1.30	1.10	-4.85	-4.42	-0.53

HCOOH	-1.79	-1.51	-1.45	-1.13	-1.25	-0.66	0.02	1.39	1.47	1.25	-7.58	-6.83	-0.57
CH_3CONH_2	-0.98	-0.91	-0.96	-0.60	-0.63	-0.62	-0.33	0.98	1.05	0.85	-6.39	-5.67	-0.31
$cylNHC_2H_4$	-0.52	-0.50	-0.56	-0.29	-0.12	-0.24	-0.01	1.27	1.36	1.16	-4.89	-4.46	-0.56
NCCN	-3.81	-3.54	-3.41	-3.24	-3.30	-2.77	-1.45	0.00	-0.26	-0.69	-9.17	-8.54	-0.19
CH_3NHCH_3	-0.53	-0.51	-0.56	-0.25	-0.23	-0.26	-0.02	1.21	1.29	1.10	-4.70	-4.30	-0.56
CH_2CO	-2.37	-2.14	-2.05	-1.81	-1.84	-1.29	-0.01	1.29	1.33	0.87	-7.87	-7.19	-0.51
$cylOC_2H_4$	-0.30	-0.32	-0.41	-0.16	0.04	-0.12	0.08	1.33	1.43	1.23	-4.53	-4.17	-0.86
OCHCHO	-4.73	-4.44	-4.32	-4.14	-4.27	-3.59	-2.17	-0.69	-0.96	-1.43	-10.41	-9.68	0.69
CH_3CH_2OH	-0.63	-0.62	-0.69	-0.33	-0.24	-0.35	-0.08	1.19	1.28	1.08	-5.06	-4.64	-0.53
CH_3OCH_3	-0.46	-0.45	-0.51	-0.22	-0.21	-0.22	0.02	1.26	1.34	1.14	-4.65	-4.23	-0.58
$cylSC_2H_4$	-1.12	-0.97	-0.90	-0.61	-0.72	-0.35	0.04	1.34	1.41	1.21	-5.91	-5.33	-0.78
CH_3SOCH_3	-0.69	-0.67	-0.70	-0.40	-0.47	-0.42	-0.20	1.08	1.16	0.97	-5.25	-4.66	-0.40
CH_2CHF	-1.26	-1.02	-0.95	-0.74	-0.81	-0.31	0.13	1.38	1.48	1.28	-6.61	-5.89	-0.88
CH_3CH_2Cl	-0.75	-0.67	-0.69	-0.37	-0.39	-0.34	-0.07	1.20	1.28	1.08	-5.51	-4.98	-0.51
CH_2CHCl	-1.67	-1.45	-1.34	-1.15	-1.24	-0.72	0.08	1.30	1.39	1.20	-6.74	-6.05	-1.11
CH_3CClO	-2.57	-2.34	-2.22	-1.99	-2.09	-1.49	-0.19	1.10	1.09	0.64	-8.03	-7.35	-0.85
prplCl	-0.90	-0.81	-0.80	-0.49	-0.63	-0.43	-0.13	1.17	1.23	1.03	-5.57	-5.05	-0.48
NC_3H_9	-0.58	-0.55	-0.58	-0.25	-0.48	-0.28	-0.03	1.22	1.28	1.09	-4.62	-4.23	-0.54
$cylOC_4H_4$	-1.09	-0.87	-0.77	-0.64	-0.63	-0.19	0.09	1.29	1.39	1.20	-6.29	-5.60	-0.74
$cylNHC_4H_4$	-0.55	-0.57	-0.63	-0.34	-0.13	-0.32	-0.12	1.15	1.24	1.04	-5.41	-4.71	-0.51
NO_2	-5.47	-5.08	-5.09	-4.82	-4.87	-4.37	-3.06	-1.45	-1.71	-2.18	-11.66	-10.90	1.44
SF_6	-2.77	-2.43	-2.47	-1.98	-2.06	-1.63	-0.17	1.31	1.13	0.69	-9.56	-9.06	-1.05
$CFCl_3$	-2.67	-2.49	-2.39	-2.21	-2.42	-1.72	-0.46	1.06	0.82	0.40	-7.71	-7.25	-0.68
$CClF_3$	-1.55	-1.32	-1.30	-0.91	-1.11	-0.60	0.38	1.97	1.88	1.52	-7.16	-6.62	-1.06
$CBrF_3$	-2.16	-1.92	-1.91	-1.43	-1.73	-1.29	-0.16	1.46	1.25	0.86	-7.66	-7.11	-0.81
HCCF	-0.71	-0.67	-0.73	-0.28	-0.22	-0.31	0.05	1.16	1.26	1.09	-5.50	-5.07	-0.55
HCCCN	-2.92	-2.67	-2.54	-2.38	-2.43	-1.94	-0.77	0.69	0.46	0.07	-8.06	-7.42	-0.36
NCCCCN	-4.24	-3.97	-3.81	-3.72	-3.73	-3.29	-2.18	-0.76	-0.99	-1.37	-9.45	-8.82	0.68
C_2N_2	-3.81	-3.54	-3.41	-3.24	-3.30	-2.77	-1.45	0.00	-0.26	-0.69	-9.17	-8.54	-0.19
C_3O_2	-2.83	-2.55	-2.44	-2.30	-2.28	-1.92	-0.79	0.68	0.44	0.05	-8.49	-7.84	-0.74
FCN	-1.65	-1.52	-1.58	-0.96	-1.05	-1.02	-0.32	1.23	1.23	0.95	-6.85	-6.40	-0.66
HCCCCH	-2.06	-1.84	-1.70	-1.53	-1.59	-1.13	-0.08	1.19	1.18	0.82	-7.00	-6.35	-0.64
H_2CS	-3.81	-3.63	-3.48	-3.37	-3.48	-2.85	-1.67	-0.19	-0.41	-0.81	-8.66	-8.04	0.28
$HCONH_2$	-1.02	-0.77	-0.85	-0.50	-0.49	-0.52	-0.24	1.08	1.17	0.95	-6.59	-5.85	-0.35
CH_2CHCHO	-3.32	-3.07	-2.93	-2.81	-2.87	-2.27	-1.07	0.40	0.18	-0.23	-8.68	-7.95	-0.46
CH_2CCl_2	-1.92	-1.70	-1.58	-1.38	-1.50	-1.00	0.01	1.35	1.33	0.99	-6.96	-6.31	-1.07
$CHFCF_2$	-1.06	-0.77	-0.74	-0.46	-0.56	-0.22	0.03	1.35	1.45	1.25	-7.05	-6.32	-0.54
CH_2CF_2	-1.01	-0.75	-0.70	-0.41	-0.51	-0.16	0.07	1.38	1.47	1.27	-6.67	-5.95	-1.03
CH_3F	-0.31	-0.35	-0.47	-0.21	0.00	-0.18	0.03	1.23	1.34	1.14	-4.93	-4.39	-0.58
CF_2Cl_2	-2.17	-1.97	-1.90	-1.63	-1.84	-1.21	0.02	1.57	1.35	0.93	-7.44	-6.95	-0.90
SiF_2	-3.18	-3.01	-2.90	-2.76	-3.03	-2.40	-1.32	0.13	-0.07	-0.43	-7.80	-7.27	0.10
MSE	2.66	2.43	2.44	2.06	2.20	1.85	0.98	-0.39	-0.31	0.00	7.79	7.19	
MAE	2.66	2.45	2.44	2.08	2.22	1.85	1.02	0.49	0.52	0.54	7.79	7.19	
rms	2.97	2.72	2.70	2.37	2.55	2.07	1.11	0.59	0.62	0.63	8.06	7.43	

TABLE VI: HOMO-LUMO gaps (in eV) of the FG131 database.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
H	4.72	8.11	6.55	8.33	8.24	7.66	10.84	12.44	12.15	11.59	9.48	9.00	12.86
He	18.01	18.05	17.93	19.07	18.83	20.39	23.30	25.68	25.54	24.57	20.71	20.00	27.23
Li	1.13	1.88	1.46	1.97	1.61	2.17	3.93	5.60	5.57	5.41	-2.55	-2.50	4.22
Be	3.50	3.59	3.54	4.03	3.58	4.89	6.72	9.43	9.17	8.58	3.35	3.40	9.66
B	0.19	0.55	0.62	1.61	0.54	2.48	4.77	8.07	7.61	6.67	-0.16	0.03	7.99
C	0.08	0.52	0.61	1.47	0.86	3.05	6.12	9.37	8.75	7.59	-0.52	-0.18	9.97
N	4.02	4.17	3.65	5.42	4.74	6.61	10.08	13.09	12.67	11.64	3.28	4.03	14.74
O	0.29	1.10	0.93	2.79	1.26	4.12	8.18	10.68	10.18	9.01	-0.28	0.02	12.14
F	0.12	0.99	0.91	2.78	1.35	4.73	10.06	11.30	10.92	9.73	-0.81	-0.29	13.98
Ne	17.25	16.97	16.69	18.51	18.06	19.66	23.85	25.98	25.81	24.92	18.77	18.46	26.91
Na	0.91	1.58	0.98	2.21	1.69	1.78	4.01	5.11	5.20	5.12	-1.92	-2.04	4.14
Mg	3.39	3.36	3.36	3.74	3.22	4.37	5.85	7.93	7.85	7.46	3.68	3.60	7.76
Al	0.09	0.33	0.29	0.74	0.26	1.52	3.06	5.96	5.70	5.11	-0.41	-0.24	5.53
Si	-0.02	0.24	0.21	0.54	0.42	1.77	3.86	7.06	6.61	5.76	-0.52	-0.29	6.73
P	2.16	2.57	2.02	3.04	2.77	3.87	5.96	9.53	8.93	8.05	0.65	1.44	9.78
S	0.04	0.51	0.32	0.87	0.37	2.31	5.00	8.07	7.48	6.52	-0.64	-0.35	8.23
Cl	-0.07	0.39	0.26	0.87	0.55	2.57	5.86	8.79	8.12	6.98	-0.76	-0.41	9.30
Ar	11.23	11.14	10.86	12.74	11.78	12.82	15.67	18.64	18.16	17.33	11.85	11.76	18.65
CH_3	1.79	2.48	2.16	3.26	2.47	4.27	6.64	9.96	9.44	8.55	0.67	1.22	9.86
CH_4	9.21	9.14	8.97	9.66	9.58	10.63	12.51	15.18	14.96	14.16	10.08	9.88	15.06
NH	3.10	3.60	3.23	4.61	3.93	6.06	9.49	12.36	11.86	10.81	1.99	2.80	13.17
NH_2	1.97	2.68	2.55	3.76	2.93	5.11	8.35	11.29	10.71	9.65	1.17	1.60	11.34
NH_3	5.64	5.52	5.34	6.13	5.96	7.08	9.23	11.92	11.68	10.85	6.59	6.29	11.54
OH	0.16	0.92	0.83	2.27	1.24	3.97	8.14	10.44	9.91	8.74	-0.63	-0.22	11.27
H_2O	6.57	6.39	6.21	7.04	6.93	8.25	10.80	13.30	13.08	12.21	7.65	7.36	13.35
HF	9.00	8.78	8.58	9.55	9.44	10.95	13.93	16.00	15.86	15.01	10.40	10.09	16.91
SiH_3	1.32	1.83	1.54	2.10	1.17	3.13	4.63	7.68	7.41	6.85	0.15	0.58	7.95
SiH_4	8.14	8.15	8.01	8.97	8.54	9.54	11.27	14.11	13.85	13.10	8.43	8.36	14.03
PH_3	6.13	6.11	5.93	6.91	6.45	7.32	8.99	11.77	11.54	10.85	6.32	6.33	11.82
SH_2	5.57	5.52	5.30	6.26	5.93	6.82	8.72	11.52	11.24	10.49	5.56	5.65	11.00
HCl	7.02	6.97	6.76	7.70	7.43	8.55	10.81	13.56	13.25	12.43	7.06	7.05	13.36
HCCH	6.78	6.80	6.71	7.37	7.07	8.30	9.98	12.48	12.30	11.58	6.70	6.74	13.43
CH_2CH_2	5.60	5.62	5.56	6.07	5.85	7.26	9.29	12.02	11.83	11.10	5.46	5.49	12.57
CH_3CH_3	7.80	7.80	7.68	8.32	8.24	9.28	11.06	13.72	13.53	12.77	8.61	8.48	13.41
HCN	7.87	7.91	7.82	8.52	8.20	9.78	11.83	14.39	14.20	13.42	7.71	7.84	14.31
CO	6.87	7.04	7.06	7.70	7.46	9.41	12.56	15.52	14.98	13.89	6.54	6.72	15.57
HCO	1.31	1.69	1.59	2.00	1.82	3.80	6.52	9.54	9.05	8.06	0.97	1.30	9.56
CH_2O	3.41	3.58	3.64	4.27	3.91	5.91	9.16	11.74	11.28	10.28	3.27	3.43	11.56
CH_3OH	5.75	5.65	5.51	6.22	6.15	7.37	9.58	11.94	11.77	11.00	6.70	6.50	11.67
N_2	8.21	8.32	8.35	8.88	8.75	10.96	14.62	17.27	16.72	15.58	7.85	8.12	17.88
NH_2NH_2	4.44	4.39	4.27	5.03	4.88	6.02	8.12	10.86	10.63	9.81	5.33	5.11	10.29
NO	-0.04	0.28	0.35	0.71	0.51	3.00	6.57	9.18	8.64	7.48	-0.24	-0.05	10.11
O_2	2.06	2.31	2.29	3.07	2.94	5.27	9.38	11.55	11.03	9.88	1.81	2.26	12.52
HOOH	4.66	4.78	4.76	5.62	5.20	7.41	10.21	12.66	12.48	11.63	4.57	4.59	12.65

F_2	3.42	3.62	3.67	4.57	3.97	6.98	11.97	13.27	12.88	11.75	3.24	3.31	15.53
CO_2	8.41	8.23	8.04	8.99	8.84	9.94	12.27	14.91	14.73	13.95	8.51	8.58	14.58
P_2	3.71	3.71	3.65	4.06	3.87	5.06	7.27	10.06	9.69	8.96	3.46	3.56	10.19
S_2	1.05	1.30	1.20	1.59	1.56	2.95	5.30	8.41	7.87	6.95	0.55	0.96	7.96
Cl_2	2.96	3.06	3.03	3.53	3.34	5.03	8.06	10.87	10.31	9.30	2.85	2.86	10.93
NaCl	3.30	3.04	2.82	3.55	3.62	4.32	6.19	8.87	8.68	7.96	3.35	3.21	8.64
SiO	4.61	4.62	4.62	5.07	4.76	6.37	8.89	11.64	11.26	10.44	4.74	4.82	11.60
CS	3.85	3.98	4.02	4.42	4.33	6.05	8.86	11.90	11.37	10.37	3.62	3.81	11.58
ClO	-0.03	0.32	0.33	0.72	0.57	2.76	5.95	8.69	8.20	7.13	-0.26	-0.06	8.85
ClF	3.28	3.40	3.40	3.99	3.71	5.72	9.19	11.80	11.26	10.19	3.08	3.14	12.43
SiH_3SiH_3	6.56	6.58	6.45	7.26	6.99	7.82	9.34	12.19	11.97	11.32	6.37	6.53	11.33
CH_3Cl	6.25	6.24	6.09	6.81	6.65	7.80	9.79	12.46	12.23	11.45	6.28	6.30	12.01
CH_3SH	4.76	4.74	4.58	5.28	5.11	6.10	7.90	10.69	10.45	9.72	4.89	4.88	10.01
SO_2	3.64	3.66	3.68	3.96	3.83	5.67	8.72	11.40	10.93	9.94	3.51	3.61	11.74
BF_3	9.55	9.32	9.18	10.07	10.09	11.51	14.41	16.50	16.40	15.59	10.04	10.12	17.22
BCl_3	4.85	4.98	4.98	5.57	5.41	6.85	9.56	12.58	12.02	11.05	4.68	4.87	12.07
$AlCl_3$	5.66	5.79	5.68	6.66	6.12	7.43	9.77	12.68	12.25	11.48	5.73	5.76	12.13
CF_4	10.68	10.37	10.22	11.00	11.30	12.60	15.43	17.66	17.57	16.74	12.60	12.26	17.85
CCl_4	4.90	4.93	4.88	5.42	5.22	6.87	9.82	12.69	12.15	11.14	4.86	4.86	11.97
OCS	5.51	5.56	5.50	6.11	5.87	7.23	9.85	12.67	12.21	11.34	5.20	5.29	12.13
CS_2	3.94	3.97	3.92	4.39	4.21	5.38	7.63	10.32	9.92	9.20	3.74	3.81	10.19
CF_2O	6.63	6.74	6.71	7.51	7.18	9.21	12.39	14.93	14.76	13.76	6.39	6.52	16.08
SiF_4	9.66	9.54	9.43	10.46	10.26	11.82	14.86	17.10	16.90	16.09	10.87	10.66	16.95
N_2O	6.81	6.84	6.77	7.42	7.14	8.80	11.79	14.54	14.07	13.11	6.56	6.62	15.01
NF_3	7.28	7.42	7.36	8.29	7.95	10.11	13.46	16.18	15.75	14.69	7.17	7.11	15.76
PF_3	6.43	6.48	6.48	7.12	6.83	8.28	10.41	13.26	13.04	12.24	6.72	6.79	13.00
O_3	1.72	1.79	1.80	2.05	1.96	4.07	7.52	10.04	9.55	8.49	1.46	1.55	11.06
F_2O	3.22	3.40	3.43	4.17	3.77	6.49	11.06	12.80	12.34	11.20	3.13	3.15	13.82
ClF_3	3.02	3.12	3.13	3.63	3.39	5.49	9.17	11.50	11.01	9.96	3.02	3.01	11.79
CF_2CF_2	5.88	5.81	5.67	6.32	6.30	7.42	9.40	12.30	12.13	11.38	5.72	5.81	12.45
CF_3CN	7.49	7.61	7.57	8.26	7.94	9.65	12.72	15.63	15.08	14.04	7.22	7.43	15.39
CH_3CCH	6.21	6.04	5.82	6.46	6.37	7.24	8.97	11.57	11.39	10.67	6.49	6.54	11.69
CH_2CCH_2	5.69	5.71	5.66	6.13	5.96	7.35	9.03	11.71	11.54	10.82	5.55	5.60	10.83
$cylC_3H_4$	4.90	5.01	4.99	5.55	5.27	6.71	8.70	11.26	11.11	10.41	4.79	4.90	11.87
$cylC_3H_6$	6.97	6.80	6.61	7.15	7.24	8.11	9.73	12.56	12.37	11.61	7.64	7.48	11.64
$CH_3CH_2CH_3$	7.30	7.33	7.25	7.86	7.73	8.81	10.56	13.22	13.02	12.28	8.12	8.00	12.72
CH_3CCCH_3	5.58	5.45	5.24	5.88	5.78	6.64	8.34	10.98	10.79	10.08	6.21	6.12	10.46
$cylC_4H_6$	5.33	5.38	5.34	5.82	5.62	6.84	8.45	11.11	10.94	10.24	5.20	5.25	11.14
isobutane	7.04	7.06	6.99	7.60	7.36	8.53	10.25	12.93	12.74	12.00	7.77	7.69	12.28
benzene	5.08	5.10	5.06	5.43	5.32	6.56	8.43	10.95	10.83	10.21	4.96	4.98	10.16
CH_2F_2	7.94	7.81	7.69	8.27	8.37	9.61	11.80	14.03	13.92	13.16	9.39	9.24	14.15
CF_3H	9.23	9.05	8.92	9.51	9.71	10.89	13.13	15.34	15.24	14.48	10.78	10.60	15.44
CH_2Cl_2	5.86	5.92	5.86	6.49	6.30	7.76	10.05	12.75	12.49	11.70	5.80	5.84	12.18
CCl_3H	5.31	5.36	5.29	5.91	5.69	7.25	10.00	12.76	12.37	11.47	5.26	5.29	12.38
CH_3NO_2	3.67	3.74	3.73	4.23	4.04	6.07	9.66	11.98	11.50	10.47	3.44	3.55	11.94
CH_3SiH_3	7.30	7.27	7.14	7.88	7.66	8.67	10.35	13.18	12.96	12.23	7.60	7.60	12.35

HCOOH	5.13	5.22	5.23	5.83	5.58	7.51	10.15	12.55	12.39	11.60	4.95	5.09	11.98
CH_3CONH_2	4.98	4.88	4.76	5.43	5.30	6.56	8.77	11.14	10.97	10.20	4.89	5.04	10.05
$cylNHC_2H_4$	5.36	5.28	5.11	5.74	5.71	6.74	8.62	11.21	11.03	10.28	6.12	5.94	10.44
NCCN	5.83	5.85	5.82	6.33	6.09	7.67	10.56	13.34	12.81	11.85	5.74	5.79	13.90
CH_3NHCH_3	4.60	4.55	4.43	5.07	4.91	6.02	7.88	10.40	10.22	9.49	5.52	5.31	9.65
CH_2CO	3.72	3.76	3.74	4.27	4.07	5.65	8.38	11.02	10.83	9.88	3.42	3.47	10.32
$cylOC_2H_4$	6.10	5.95	5.79	6.40	6.38	7.59	9.79	12.03	11.89	11.13	7.34	7.06	11.68
OCHCHO	1.80	1.94	2.03	2.50	2.26	4.18	7.34	9.93	9.45	8.46	1.57	1.77	10.04
CH_3CH_2OH	5.64	5.54	5.42	6.09	6.04	7.25	9.43	11.82	11.64	10.87	6.63	6.43	11.38
CH_3OCH_3	5.47	5.38	5.26	5.89	5.71	6.98	9.06	11.40	11.24	10.50	6.64	6.44	10.79
$cylSC_2H_4$	4.34	4.39	4.32	4.86	4.71	6.01	7.86	10.60	10.40	9.67	4.13	4.20	9.93
CH_3SOCH_3	4.83	4.71	4.59	5.09	5.01	6.09	7.86	10.38	10.23	9.54	5.34	5.38	9.54
CH_2CHF	5.46	5.50	5.45	5.97	5.75	7.24	9.20	11.80	11.66	10.94	5.41	5.45	11.55
CH_3CH_2Cl	6.31	6.31	6.16	6.84	6.73	7.79	9.67	12.37	12.14	11.37	6.36	6.41	11.74
CH_2CHCl	4.92	4.97	4.93	5.41	5.23	6.63	8.86	11.48	11.30	10.61	4.76	4.86	11.35
CH_3CClO	4.72	4.79	4.80	5.40	5.18	6.91	9.96	12.37	12.13	11.16	4.49	4.67	11.97
prplCl	6.13	6.14	6.01	6.69	6.48	7.66	9.56	12.29	12.05	11.28	6.25	6.29	11.63
NC_3H_9	4.34	4.30	4.19	4.82	4.50	5.71	7.54	10.05	9.87	9.16	5.30	5.09	9.10
$cylOC_4H_4$	4.79	4.80	4.75	5.13	5.00	6.30	7.92	10.49	10.36	9.71	4.62	4.63	9.82
$cylNHC_4H_4$	4.79	4.57	4.34	4.88	4.94	5.60	7.14	9.72	9.60	8.96	4.85	4.86	8.89
NO_2	1.13	1.42	1.39	1.86	1.75	3.82	7.09	9.70	9.23	8.20	0.93	1.19	9.79
SF_6	7.63	7.70	7.64	8.68	8.46	10.47	14.54	16.42	16.10	15.10	7.71	7.52	16.98
$CFCl_3$	5.21	5.26	5.20	5.79	5.58	7.20	10.13	13.03	12.48	11.48	5.11	5.13	12.61
$CClF_3$	7.18	7.24	7.13	7.93	7.69	9.26	12.00	14.94	14.55	13.59	6.89	6.92	14.27
$CBrF_3$	5.84	5.91	5.77	6.60	6.27	7.69	10.40	13.35	12.89	11.98	5.39	5.42	12.97
HCCF	6.50	6.35	6.15	6.94	6.81	7.81	9.77	12.25	12.08	11.36	6.98	6.79	12.04
HCCCN	5.17	5.19	5.16	5.65	5.42	6.87	9.51	12.31	11.83	10.94	5.06	5.11	12.20
NCCCCN	4.44	4.47	4.45	4.87	4.67	6.07	8.63	11.31	10.84	9.99	4.37	4.42	11.52
C_2N_2	5.83	5.85	5.82	6.33	6.09	7.67	10.56	13.34	12.81	11.85	5.74	5.79	13.90
C_3O_2	4.67	4.71	4.69	5.15	4.97	6.33	8.87	11.49	11.07	10.27	4.47	4.52	11.64
FCN	7.31	7.21	7.04	8.02	7.73	8.96	11.39	14.25	13.97	13.12	7.76	7.59	14.33
HCCCCH	4.77	4.80	4.77	5.25	5.01	6.37	8.83	11.43	11.18	10.34	4.69	4.74	11.00
H_2CS	1.80	1.91	1.92	2.25	2.11	3.68	6.29	9.21	8.73	7.81	1.48	1.63	9.18
$HCONH_2$	5.15	5.25	5.11	5.76	5.64	6.90	9.10	11.47	11.32	10.54	5.00	5.14	10.81
CH_2CHCHO	2.82	2.94	3.01	3.48	3.26	5.13	8.24	10.78	10.32	9.36	2.75	2.92	10.70
CH_2CCl_2	4.69	4.74	4.70	5.17	5.02	6.37	8.81	11.53	11.25	10.41	4.58	4.67	11.17
$CHFCF_2$	5.39	5.45	5.41	5.96	5.74	7.20	9.02	11.59	11.48	10.77	5.31	5.37	11.11
CH_2CF_2	5.77	5.81	5.76	6.35	6.11	7.51	9.29	11.92	11.78	11.05	5.66	5.72	11.81
CH_3F	7.88	7.74	7.59	8.26	8.23	9.50	11.72	13.94	13.81	13.06	9.02	8.98	14.09
CF_2Cl_2	6.06	6.12	6.04	6.70	6.49	8.08	10.99	13.92	13.39	12.39	5.87	5.91	13.33
SiF_2	4.09	4.13	4.15	4.53	4.22	5.76	8.11	11.02	10.63	9.81	4.26	4.31	11.04
MSE	-7.05	-6.94	-7.05	-6.34	-6.60	-5.11	-2.57	0.04	-0.27	-1.12	-6.99	-6.94	
MAE	7.05	6.94	7.05	6.34	6.60	5.11	2.57	0.49	0.57	1.16	6.99	6.94	
rms	7.27	7.15	7.25	6.53	6.81	5.26	2.66	0.65	0.77	1.41	7.29	7.20	

TABLE VII: $\epsilon_{N+1}(N+1) - \epsilon_N(N)$ (in eV) of the FG131 database.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
H	9.19	9.56	9.46	9.56	9.69	9.99	10.64	10.54	10.41	10.21	11.16	11.03	12.86
He	21.81	21.82	22.22	22.68	22.05	23.73	25.85	25.22	25.05	24.53	27.40	26.47	27.23
Li	3.98	4.10	4.03	4.07	4.15	4.23	4.35	4.63	4.57	4.51	4.72	4.73	4.22
Be	7.51	7.50	7.55	7.68	7.71	7.95	8.53	9.21	8.97	8.69	8.93	8.86	9.66
B	6.19	6.31	6.38	6.65	6.44	6.77	6.94	7.46	7.32	7.09	7.74	7.66	7.99
C	8.08	8.16	8.20	8.62	8.41	8.62	8.94	9.08	8.98	8.83	9.59	9.56	9.97
N	11.94	11.81	11.60	12.32	12.34	12.37	13.38	12.83	12.85	12.76	13.15	13.60	14.74
O	10.27	10.51	10.55	10.94	10.40	10.92	11.23	10.95	10.96	10.94	12.20	11.88	12.14
F	12.13	12.28	12.31	12.62	12.21	12.67	13.13	12.55	12.64	12.68	13.99	13.70	13.98
Ne	23.40	23.15	23.41	24.18	23.85	24.98	26.66	26.01	25.92	25.61	27.69	27.30	26.91
Na	3.88	3.88	3.88	3.85	3.70	4.05	4.31	4.14	4.20	4.20	4.93	4.81	4.14
Mg	6.20	6.08	6.12	6.19	6.15	6.52	7.21	7.77	7.66	7.39	8.04	7.81	7.76
Al	4.54	4.67	4.62	4.62	4.81	4.83	4.89	5.40	5.30	5.16	5.37	5.38	5.53
Si	5.76	5.87	5.82	5.86	6.08	6.02	6.14	6.47	6.37	6.24	6.52	6.56	6.73
P	8.13	8.20	7.93	8.38	8.58	8.33	8.72	9.07	8.86	8.63	8.49	8.89	9.78
S	7.25	7.35	7.34	7.23	7.37	7.53	7.67	7.74	7.67	7.60	8.34	8.19	8.23
Cl	8.38	8.45	8.44	8.30	8.50	8.61	8.75	8.72	8.69	8.64	9.35	9.24	9.30
Ar	15.52	15.49	15.55	16.12	16.24	16.52	17.49	18.48	18.01	17.40	18.23	18.13	18.65
CH_3	8.04	8.21	8.10	8.29	8.31	8.55	8.88	9.05	8.96	8.76	9.35	9.39	9.86
CH_4	11.47	11.42	11.55	11.96	11.57	12.59	13.92	14.96	14.59	13.91	14.78	14.54	15.06
NH	11.04	11.09	10.94	11.44	11.42	11.57	12.22	11.89	11.87	11.79	12.11	12.44	13.17
NH_2	9.87	10.05	10.08	10.19	10.10	10.41	10.74	10.63	10.57	10.49	11.27	11.15	11.34
NH_3	8.47	8.36	8.49	8.73	8.46	9.49	10.87	11.66	11.29	10.63	11.91	11.53	11.54
OH	9.79	9.94	9.97	10.09	9.90	10.28	10.61	10.32	10.33	10.30	11.38	11.13	11.27
H_2O	9.85	9.69	9.86	10.07	9.81	11.02	12.72	13.04	12.70	12.05	13.66	13.24	13.35
HF	12.50	12.30	12.51	12.82	12.43	13.92	16.02	15.77	15.50	14.90	17.10	16.62	16.91
SiH_3	6.80	6.98	6.86	7.02	7.05	7.15	7.37	7.60	7.50	7.35	7.49	7.58	7.95
SiH_4	10.55	10.54	10.64	11.11	10.73	11.55	12.60	13.86	13.51	12.87	13.11	12.97	14.03
PH_3	8.72	8.68	8.75	8.90	8.80	9.47	10.33	11.53	11.22	10.65	11.34	11.13	11.82
SH_2	8.44	8.36	8.41	8.52	8.49	9.18	10.19	11.25	10.89	10.29	11.06	10.87	11.00
HCl	10.49	10.43	10.46	10.67	10.65	11.32	12.46	13.28	12.90	12.30	13.30	13.13	13.36
HCCH	9.23	9.01	9.02	9.42	9.02	9.88	11.22	12.39	12.05	11.41	13.61	13.41	13.43
CH_2CH_2	9.01	8.79	8.82	9.15	8.73	9.54	10.68	11.77	11.45	10.84	12.30	12.39	12.57
CH_3CH_3	10.06	10.07	10.20	10.69	10.12	11.18	12.44	13.52	13.18	12.54	13.24	13.05	13.41
HCN	11.53	12.62	11.38	11.89	11.26	12.20	13.46	14.07	13.72	13.14	15.48	15.35	14.31
CO	12.93	12.77	12.92	13.22	13.14	13.88	15.01	15.69	15.33	14.74	15.35	15.28	15.57
HCO	7.99	8.09	8.06	8.11	8.23	8.73	9.15	9.17	9.11	8.97	9.56	9.61	9.56
CH_2O	8.94	8.72	8.87	9.24	8.48	9.61	11.63	11.60	11.48	11.23	11.86	11.77	11.56
CH_3OH	8.28	8.15	8.27	8.68	8.23	9.44	11.12	11.70	11.39	10.76	12.07	11.72	11.67
N_2	15.84	15.72	15.77	16.07	16.22	16.66	17.63	17.52	17.41	17.18	17.30	17.38	17.88
NH_2NH_2	7.44	7.41	7.53	7.99	7.41	8.50	9.85	10.55	10.21	9.61	10.74	10.43	10.29
NO	8.76	8.82	8.88	9.08	9.01	9.36	9.75	9.55	9.54	9.48	10.15	10.12	10.11
O_2	11.42	11.42	11.39	12.03	11.83	11.96	12.56	12.05	12.09	12.09	12.44	12.65	12.52
HOOH	8.99	8.85	9.02	9.34	8.94	10.28	12.05	12.41	12.09	11.44	13.08	12.80	12.65

F_2	14.02	13.92	13.93	14.47	14.01	14.45	15.07	14.63	14.65	14.63	15.40	15.18	15.53
CO_2	11.90	11.69	11.78	12.16	11.82	12.80	14.21	14.69	14.40	13.84	17.51	17.22	14.58
P_2	9.37	9.28	9.20	9.45	9.47	9.34	9.63	9.60	9.58	9.55	9.96	9.92	10.19
S_2	7.40	7.50	7.39	7.59	7.73	7.65	7.82	7.98	7.87	7.76	7.75	7.97	7.96
Cl_2	9.55	9.53	9.49	9.85	9.80	9.96	10.55	10.64	10.52	10.36	10.55	10.46	10.93
NaCl	6.24	6.13	6.15	6.18	6.25	6.87	7.98	8.63	8.31	7.75	8.95	8.71	8.64
SiO	9.96	9.83	9.88	10.10	10.14	10.48	11.28	11.37	11.26	11.02	11.67	11.55	11.60
CS	10.42	10.40	10.40	10.77	10.71	10.89	11.44	11.53	11.39	11.24	11.26	11.30	11.58
ClO	8.16	8.27	8.26	8.28	8.30	8.46	8.56	8.54	8.53	8.50	8.86	8.83	8.85
ClF	10.86	10.81	10.80	11.34	11.08	11.34	12.02	11.92	11.82	11.68	12.07	11.97	12.43
SiH_3SiH_3	9.22	9.14	9.17	9.43	9.47	9.85	10.97	11.96	11.66	11.13	11.05	11.07	11.33
CH_3Cl	9.16	9.07	9.14	9.51	9.17	10.03	11.27	12.18	11.82	11.19	12.09	11.94	12.01
CH_3SH	7.53	7.46	7.51	7.88	7.47	8.29	9.30	10.42	10.08	9.48	10.14	9.99	10.01
SO_2	10.99	10.86	10.88	11.13	10.99	11.15	11.57	11.34	11.34	11.31	11.78	11.71	11.74
BF_3	12.70	12.51	12.63	13.25	12.56	14.14	16.20	16.32	16.08	15.46	18.03	16.79	17.22
BCl_3	10.80	10.71	10.70	11.01	10.93	11.07	11.69	13.05	12.65	12.01	11.31	11.33	12.07
$AlCl_3$	9.67	9.64	9.59	10.35	10.04	10.42	11.49	12.30	11.93	11.42	11.28	11.20	12.13
CF_4	13.60	13.40	13.52	14.43	13.65	15.12	17.23	17.39	17.16	16.53	18.12	17.76	17.85
CCl_4	9.86	9.80	9.70	10.32	10.19	10.52	11.57	12.05	11.77	11.35	10.54	10.50	11.97
OCS	10.09	9.97	9.94	10.91	9.93	10.60	11.43	12.60	12.29	11.75	12.69	12.63	12.13
CS_2	9.50	9.41	9.30	9.77	9.65	9.50	9.78	9.74	9.67	9.66	10.21	10.18	10.19
CF_2O	11.46	11.26	11.36	12.00	11.41	12.61	14.30	14.71	14.41	13.79	15.78	15.69	16.08
SiF_4	13.30	13.17	13.23	14.05	13.39	14.71	16.62	16.97	16.69	16.08	17.03	16.74	16.95
N_2O	11.89	11.68	11.77	11.96	11.86	12.64	13.71	14.33	14.06	13.54	15.49	15.38	15.01
NF_3	13.00	12.90	13.00	13.67	13.06	14.14	15.20	16.00	15.71	15.17	16.25	16.13	15.76
PF_3	10.17	9.95	10.05	10.41	10.11	10.97	12.16	13.04	12.76	12.18	13.48	13.32	13.00
O_3	10.40	10.32	10.30	10.53	10.31	10.37	10.33	10.39	10.39	10.41	10.95	10.89	11.06
F_2O	12.34	12.24	12.25	12.75	12.37	12.91	13.85	13.25	13.25	13.19	13.52	13.32	13.82
ClF_3	10.69	10.61	10.62	11.03	10.78	11.11	11.80	11.43	11.42	11.37	11.72	11.57	11.79
CF_2CF_2	9.13	8.96	9.05	9.62	8.89	10.02	11.23	12.10	11.82	11.25	13.97	12.50	12.45
CF_3CN	13.24	12.28	12.27	13.16	11.90	13.06	14.40	15.39	15.05	14.40	15.33	14.91	15.39
CH_3CCH	8.32	8.15	8.19	8.63	8.03	9.02	10.31	11.35	11.03	10.42	11.54	11.22	11.69
CH_2CCH_2	8.55	8.39	8.42	8.89	8.31	9.21	10.36	11.48	11.17	10.58	11.89	11.35	10.83
$cylC_3H_4$	8.13	7.99	8.03	8.48	7.89	8.79	10.03	11.01	10.70	10.11	11.77	11.67	11.87
$cylC_3H_6$	9.21	9.04	9.10	9.58	9.01	9.98	11.14	12.33	12.00	11.37	12.26	12.02	11.64
$CH_3CH_2CH_3$	9.49	9.52	9.65	10.15	9.55	10.63	11.88	13.03	12.70	12.07	12.56	12.40	12.72
CH_3CCCH_3	7.65	7.54	7.56	8.10	7.41	8.39	9.68	10.79	10.48	9.88	10.58	10.33	10.46
$cylC_4H_6$	7.99	7.85	7.86	8.49	7.72	8.60	9.77	10.88	10.57	10.00	11.15	10.79	11.14
isobutane	9.25	9.27	9.38	9.92	9.33	10.34	11.56	12.72	12.41	11.78	12.13	12.01	12.28
benzene	10.24	7.93	7.89	8.42	7.78	8.56	9.75	10.78	10.51	10.00	10.86	10.69	10.16
CH_2F_2	10.37	10.24	10.42	10.80	10.45	11.67	13.48	13.76	13.49	12.88	14.57	14.25	14.15
CF_3H	11.94	11.78	11.93	12.67	11.94	13.20	14.95	15.03	14.78	14.23	16.11	15.80	15.44
CH_2Cl_2	9.53	9.45	9.52	9.82	9.62	10.39	11.59	12.42	12.07	11.45	11.91	11.85	12.18
CCl_3H	9.75	9.67	9.67	10.08	9.98	10.51	11.68	12.42	12.04	11.46	11.20	11.18	12.38
CH_3NO_2	9.25	9.01	9.11	9.63	9.08	10.63	11.85	11.54	11.51	11.39	11.52	11.48	11.94
CH_3SiH_3	9.87	9.79	9.85	10.31	9.83	10.72	11.72	12.91	12.58	11.97	12.42	12.33	12.35

HCOOH	9.03	8.79	8.91	9.20	8.91	10.56	11.96	12.17	11.89	12.53	13.35	13.25	11.98
CH_3CONH_2	7.59	7.46	7.55	8.01	7.53	8.66	10.30	10.82	10.51	9.91	10.91	10.66	10.05
$cylNHC_2H_4$	7.80	7.68	7.74	8.29	7.66	8.72	10.16	10.91	10.59	9.99	11.18	10.85	10.44
NCCN	12.67	12.54	12.49	12.80	12.66	12.71	13.22	14.59	14.24	12.93	13.28	13.19	13.90
CH_3NHCH_3	6.85	6.78	6.87	7.34	6.79	7.86	9.27	10.18	9.86	9.25	10.18	9.87	9.65
CH_2CO	8.11	8.36	8.38	8.67	7.87	8.76	9.91	10.72	10.44	9.89	11.32	11.14	10.32
$cylOC_2H_4$	8.37	8.21	8.32	8.72	8.26	9.50	11.29	11.76	11.47	10.85	12.10	11.73	11.68
OCHCHO	8.63	8.62	8.70	8.97	8.80	9.16	9.77	9.57	9.52	9.39	9.16	9.22	10.04
CH_3CH_2OH	8.07	7.97	8.08	8.58	8.01	9.25	10.88	11.54	11.23	10.61	11.60	11.31	11.38
CH_3OCH_3	7.71	7.60	7.71	8.16	7.67	8.84	10.46	11.16	10.87	10.26	11.31	10.98	10.79
$cylSC_2H_4$	7.41	7.30	7.35	7.63	7.23	8.14	9.29	10.29	9.96	9.37	10.12	9.99	9.93
CH_3SOCH_3	7.17	7.05	7.11	7.52	7.06	8.01	9.26	10.07	9.79	9.25	10.44	10.16	9.54
CH_2CHF	8.78	8.55	8.60	9.19	8.53	9.43	10.68	11.51	11.21	10.65	12.73	12.56	11.55
CH_3CH_2Cl	8.90	8.83	8.88	9.47	8.87	9.81	11.06	12.08	11.72	11.09	11.85	11.71	11.74
CH_2CHCl	8.50	8.34	8.35	8.88	8.28	9.11	10.21	11.18	10.86	10.31	11.59	11.52	11.35
CH_3CClO	9.29	9.12	9.18	9.86	9.15	10.01	11.40	12.06	11.77	11.20	11.80	11.82	11.97
prplCl	8.74	8.67	8.71	9.18	8.72	9.66	10.92	12.00	11.65	11.01	11.31	11.22	11.63
NC_3H_9	6.55	6.49	6.58	7.08	6.56	7.52	8.87	9.83	9.54	8.95	9.66	9.39	9.10
$cylOC_4H_4$	7.57	7.35	7.36	9.76	7.28	8.06	9.22	10.23	9.95	9.42	10.87	10.47	9.82
$cylNHC_4H_4$	7.00	6.83	6.80	7.28	6.67	7.47	8.58	9.36	9.08	8.61	10.04	9.67	8.89
NO_2	8.85	8.94	8.91	9.47	9.06	9.47	9.91	9.65	9.64	9.61	10.08	10.14	9.79
SF_6	13.12	12.98	12.99	14.66	13.24	14.48	16.70	16.14	16.06	15.70	15.32	15.02	16.98
$CFCl_3$	10.26	10.18	10.08	10.83	10.70	10.93	12.04	12.47	12.21	11.81	11.26	11.21	12.61
$CClF_3$	11.44	11.32	11.33	12.49	11.30	12.38	13.67	14.58	14.20	13.63	14.30	14.14	14.27
$CBrF_3$	10.74	10.55	10.54	11.36	10.87	11.48	12.63	12.99	12.78	12.40	12.69	12.56	12.97
HCCF	9.12	8.93	8.95	9.54	8.86	9.85	11.18	11.99	11.68	11.09	12.64	12.32	12.04
HCCCN	11.03	10.88	9.82	10.10	9.50	11.24	11.53	12.19	11.85	11.35	12.00	11.90	12.20
NCCCCN	10.28	10.19	10.17	10.38	10.27	10.40	10.90	10.87	10.77	10.64	10.70	10.64	11.52
C_2N_2	12.67	12.54	12.49	12.80	12.66	12.71	13.22	14.59	14.24	12.93	13.28	13.19	13.90
C_3O_2	11.42	10.31	10.17	11.57	11.40	11.29	11.25	12.21	11.94	11.45	11.82	11.72	11.64
FCN	11.41	11.23	11.28	11.58	11.37	12.15	13.35	14.01	13.67	13.09	14.59	14.34	14.33
HCCCCH	9.94	8.32	8.30	9.01	8.06	8.93	10.27	11.28	10.98	10.42	11.09	10.99	11.00
H_2CS	8.20	8.17	8.16	8.37	8.31	8.39	8.79	8.75	8.67	8.58	8.87	8.85	9.18
$HCONH_2$	8.13	7.96	8.08	8.46	8.03	9.16	10.77	11.11	12.58	12.04	11.67	11.34	10.81
CH_2CHCHO	8.91	8.89	8.94	9.31	9.12	9.59	10.50	10.23	10.15	9.96	9.63	9.66	10.70
CH_2CCl_2	8.66	8.40	8.39	9.09	8.44	9.14	10.26	11.16	10.85	10.31	11.01	10.96	11.17
$CHFCF_2$	8.62	8.44	8.50	9.18	8.39	9.41	10.69	11.26	11.01	10.50	12.97	12.59	11.11
CH_2CF_2	8.87	8.65	8.72	9.13	8.67	9.57	10.86	11.61	11.32	10.75	13.12	12.12	11.81
CH_3F	10.21	10.08	10.23	10.61	10.24	11.50	13.28	13.68	13.41	12.79	14.36	13.99	14.09
CF_2Cl_2	10.86	10.72	10.70	11.36	11.37	11.64	12.88	13.54	13.24	12.74	12.56	12.50	13.33
SiF_2	9.62	9.49	9.56	9.83	9.77	10.01	10.53	10.69	10.61	10.43	11.50	11.30	11.04
MSE	-2.35	-2.46	-2.44	-2.00	-2.36	-1.67	-0.65	-0.17	-0.38	-0.80	0.05	-0.12	
MAE	2.35	2.46	2.44	2.00	2.36	1.67	0.66	0.45	0.50	0.83	0.50	0.43	
rms	2.57	2.68	2.64	2.21	2.60	1.82	0.79	0.60	0.66	0.96	0.69	0.61	

TABLE VIII: IP(N) − EA(N) values (in eV) of the FG131 database.

Molecule	LSDA	PBE	BLYP	M06L	VS98	B3LYP	M06-2X	ωB97	ωB97X	ωB97X-D	LB94	LBα	Ref.
H	12.15	12.95	12.76	13.10	13.03	12.80	12.98	13.00	12.92	12.90	10.96	11.48	12.86
He	28.23	28.27	28.74	28.75	28.51	28.78	28.47	28.85	28.78	28.73	32.23	31.11	27.23
Li	4.87	5.06	5.06	4.51	4.87	5.06	4.89	4.91	4.81	4.85	4.53	4.64	4.22
Be	9.17	9.16	9.28	9.26	9.45	9.34	9.52	9.46	9.31	9.18	9.71	10.01	9.66
B	7.97	8.13	8.27	8.35	8.06	8.33	8.10	8.30	8.29	8.23	9.07	8.78	7.99
C	9.92	9.99	10.09	10.10	10.17	10.19	10.09	10.19	10.17	10.13	9.96	10.10	9.97
N	14.80	14.57	14.26	15.00	15.08	14.52	14.81	14.63	14.69	14.74	9.87	12.57	14.74
O	12.07	12.41	12.47	12.59	12.20	12.56	12.41	12.36	12.37	12.38	14.29	13.43	12.14
F	13.97	14.14	14.18	14.37	14.06	14.31	14.41	14.07	14.15	14.19	15.01	14.65	13.98
Ne	28.76	28.32	28.32	28.74	29.02	28.35	28.32	28.82	28.68	28.60	30.72	31.72	26.91
Na	4.74	4.80	4.85	4.06	4.42	4.84	4.59	4.35	4.30	4.44	6.12	5.95	4.14
Mg	7.89	7.76	7.94	7.87	7.83	7.95	8.18	8.14	8.03	7.81	13.31	13.09	7.76
Al	5.47	5.57	5.60	5.59	5.56	5.64	5.53	5.75	5.72	5.67	5.27	5.45	5.53
Si	6.67	6.74	6.75	6.71	6.87	6.80	6.75	6.89	6.86	6.82	6.09	6.42	6.73
P	9.54	9.64	9.31	9.86	9.94	9.44	9.49	9.69	9.58	9.54	5.56	7.65	9.78
S	8.18	8.28	8.30	8.20	8.25	8.36	8.31	8.38	8.34	8.33	8.41	8.26	8.23
Cl	9.26	9.33	9.34	9.17	9.43	9.39	9.35	9.36	9.35	9.35	9.33	9.30	9.30
Ar	18.82	18.70	18.61	19.31	19.37	18.75	18.83	19.33	19.19	19.09	17.55	18.85	18.65
CH_3	9.79	10.05	9.87	10.15	10.10	9.98	9.91	9.94	9.92	9.90	7.98	8.78	9.86
CH_4	14.78	14.68	14.72	15.27	14.61	14.93	15.22	15.31	15.26	15.15	11.89	13.78	15.06
NH	13.28	13.33	13.10	13.50	13.56	13.29	13.41	13.29	13.31	13.34	9.76	11.57	13.17
NH_2	11.23	11.43	11.50	11.48	11.57	11.59	11.40	11.55	11.48	11.47	10.49	10.64	11.34
NH_3	11.92	11.66	11.71	11.98	11.64	11.72	11.87	12.05	11.99	11.88	10.24	11.73	11.54
OH	11.28	11.45	11.50	11.62	11.45	11.60	11.57	11.47	11.49	11.50	11.94	11.70	11.27
H_2O	13.87	13.52	13.58	13.83	13.53	13.55	13.73	13.85	13.77	13.68	13.25	14.53	13.35
HF	17.55	17.12	17.19	17.37	17.16	17.13	17.24	17.36	17.29	17.20	18.07	19.19	16.91
SiH_3	7.80	8.04	7.91	8.13	7.93	8.01	8.09	7.96	7.97	7.96	5.35	6.08	7.95
SiH_4	12.90	12.92	12.94	13.68	13.04	13.30	13.57	14.10	14.01	13.85	8.43	10.17	14.03
PH_3	11.22	11.13	11.16	11.69	11.23	11.26	11.30	11.60	11.57	11.50	8.74	10.06	11.82
SH_2	11.17	11.00	10.99	11.47	11.12	11.07	11.26	11.43	11.39	11.32	8.84	10.25	11.00
HCl	13.55	13.34	13.33	13.79	13.54	13.42	13.65	13.71	13.67	13.60	11.89	13.16	13.36
HCCH	12.47	12.10	12.09	12.24	11.91	12.11	12.32	12.43	12.43	12.36	10.28	11.84	13.43
CH_2CH_2	11.76	11.44	11.42	11.77	11.20	11.41	11.49	11.67	11.67	11.60	8.82	10.33	12.57
CH_3CH_3	12.59	12.61	12.63	13.37	12.51	13.02	13.45	13.68	13.58	13.38	8.45	10.35	13.41
HCN	14.79	15.49	14.75	14.65	14.29	14.80	14.91	14.89	14.86	14.80	13.18	14.65	14.31
CO	15.33	15.17	15.28	15.29	15.53	15.53	15.76	16.21	16.14	15.68	14.44	14.60	15.57
HCO	9.63	9.80	9.74	9.89	9.87	9.98	9.95	9.98	9.98	9.96	8.70	9.23	9.56
CH_2O	11.43	11.31	11.36	11.67	11.40	11.63	11.99	11.94	11.88	11.82	9.52	10.51	11.56
CH_3OH	11.43	11.27	11.31	11.80	11.21	11.53	11.92	11.96	11.90	11.79	9.42	10.85	11.67
N_2	17.57	17.45	17.47	17.73	17.72	17.83	18.40	18.17	18.14	18.06	19.48	19.36	17.88
NH_2NH_2	10.01	9.95	9.97	10.64	9.96	10.24	10.65	10.72	10.65	10.51	8.31	9.67	10.29
NO	10.09	10.17	10.22	10.30	10.23	10.41	10.47	10.32	10.37	10.38	10.16	10.13	10.11
O_2	12.78	12.78	12.74	13.19	13.18	13.06	13.26	12.99	13.04	13.08	10.67	11.79	12.52
HOOH	12.26	12.07	12.11	12.81	12.14	12.48	12.97	12.96	12.92	12.79	12.80	12.94	12.65

F_2	15.01	14.91	14.91	15.31	14.93	15.25	15.89	15.27	15.34	15.37	15.15	14.75	15.53
CO_2	14.83	14.54	14.50	15.18	14.61	14.70	15.16	15.20	15.13	15.02	13.18	15.35	14.58
P_2	10.13	9.96	9.93	10.14	10.04	10.15	10.32	10.19	9.73	10.22	8.55	9.01	10.19
S_2	8.01	8.12	8.02	8.32	8.32	8.16	8.17	8.33	8.24	8.20	5.89	6.92	7.96
Cl_2	10.38	10.34	10.30	10.64	10.50	10.54	10.95	10.95	10.86	10.78	9.43	9.70	10.93
NaCl	8.85	8.56	8.56	8.91	8.63	8.55	8.75	8.67	8.69	8.65	8.54	9.34	8.64
SiO	11.41	11.22	11.28	11.44	11.36	11.38	11.63	11.61	11.58	11.51	14.04	13.92	11.60
CS	11.33	11.22	11.29	11.26	11.43	11.35	11.47	11.48	11.40	11.40	8.83	9.30	11.58
ClO	8.72	8.84	8.83	8.90	8.87	9.00	9.01	8.99	9.01	9.01	8.64	8.68	8.85
ClF	11.96	11.87	11.87	12.18	12.04	12.11	12.59	12.30	12.29	12.29	11.64	11.50	12.43
SiH_3SiH_3	11.08	11.00	11.01	11.66	11.25	11.17	11.60	11.69	11.65	11.55	5.20	6.76	11.33
CH_3Cl	11.76	11.65	11.64	12.17	11.67	11.87	12.21	12.30	12.25	12.14	9.38	10.49	12.01
CH_3SH	9.92	9.80	9.79	10.36	9.75	9.95	10.21	10.36	10.33	10.25	7.25	8.35	10.01
SO_2	11.55	11.40	11.42	11.59	11.44	11.50	11.77	11.62	11.62	11.61	10.27	10.86	11.74
BF_3	15.53	15.29	15.29	16.36	15.44	16.08	17.13	16.98	16.90	16.69	14.80	16.29	17.22
BCl_3	10.96	10.90	10.90	11.30	11.17	11.30	11.82	13.14	12.91	12.59	6.51	8.11	12.07
$AlCl_3$	10.67	10.64	10.58	11.42	11.03	11.16	11.83	12.55	12.26	11.89	6.97	7.98	12.13
CF_4	16.20	15.97	15.98	17.27	16.09	16.99	18.14	17.95	17.91	17.70	16.76	17.11	17.85
CCl_4	10.38	10.34	10.27	10.80	10.60	10.95	11.87	12.30	12.05	11.67	6.86	7.59	11.97
OCS	12.31	12.13	12.06	12.60	12.17	12.24	12.46	12.67	12.64	12.59	9.12	10.20	12.13
CS_2	10.18	10.04	9.98	10.29	10.15	9.93	10.10	9.83	9.86	9.96	7.30	8.02	10.19
CF_2O	14.47	14.19	14.18	15.08	14.24	14.52	15.04	15.06	15.02	14.92	11.22	13.28	16.08
SiF_4	15.35	15.18	15.16	16.55	15.55	16.13	17.47	17.40	17.27	16.99	13.55	13.94	16.95
N_2O	14.64	14.37	14.32	14.93	14.34	14.42	14.63	14.80	14.76	14.69	11.54	13.13	15.01
NF_3	15.34	15.19	15.16	16.13	15.40	15.75	16.36	16.44	16.39	16.25	13.33	14.58	15.76
PF_3	12.61	12.36	12.44	12.92	12.55	12.77	13.06	13.25	13.24	13.11	15.11	14.96	13.00
O_3	10.86	10.76	10.74	10.65	10.74	10.75	10.98	10.77	10.77	10.77	8.29	9.12	11.06
F_2O	13.08	13.01	13.00	13.36	13.06	13.47	14.21	13.62	13.66	13.66	14.27	13.66	13.82
ClF_3	11.04	10.98	10.97	11.34	11.10	11.39	12.05	11.72	11.70	11.64	10.52	10.72	11.79
CF_2CF_2	11.39	11.17	11.18	12.14	11.15	11.59	12.12	12.14	12.16	12.07	10.86	11.16	12.45
CF_3CN	14.91	14.49	14.44	15.30	14.40	15.28	15.69	15.92	15.91	15.79	12.45	13.63	15.39
CH_3CCH	10.99	10.77	10.75	11.14	10.47	10.88	11.20	11.22	11.22	11.13	6.94	8.79	11.69
CH_2CCH_2	10.89	10.69	10.65	11.18	10.48	10.84	11.07	11.20	11.20	11.11	7.63	8.49	10.83
$cylC_3H_4$	10.67	10.46	10.45	10.80	10.13	10.57	10.85	10.92	10.89	10.79	7.72	9.17	11.87
$cylC_3H_6$	11.72	11.51	11.48	12.15	11.17	11.65	11.96	12.11	12.07	11.96	7.39	9.57	11.64
$CH_3CH_2CH_3$	11.67	11.72	11.76	12.53	11.64	12.23	12.73	13.08	13.00	12.82	5.51	7.98	12.72
CH_3CCCH_3	9.97	9.82	9.79	10.38	9.50	9.99	10.41	10.50	10.48	10.37	2.88	5.04	10.46
$cylC_4H_6$	10.30	10.10	10.06	10.54	9.76	10.17	10.41	10.57	10.55	10.46	5.35	7.38	11.14
isobutane	11.49	11.30	11.32	12.09	11.26	11.76	12.28	12.59	12.50	12.30	4.31	6.66	12.28
benzene	10.76	9.79	9.70	10.26	9.54	9.85	10.28	10.37	10.35	10.25	7.18	4.20	10.16
CH_2F_2	13.26	13.11	13.20	13.73	13.24	13.75	14.42	14.23	14.19	14.04	13.21	14.31	14.15
CF_3H	14.58	14.36	14.46	15.01	14.57	15.06	15.80	15.52	15.46	15.31	14.44	15.56	15.44
CH_2Cl_2	11.24	11.19	11.16	11.77	11.35	11.65	12.25	12.59	12.41	12.13	8.49	9.37	12.18
CCl_3H	10.90	10.85	10.78	11.39	11.10	11.36	12.10	12.57	12.33	11.98	7.30	8.33	12.38
CH_3NO_2	11.22	11.07	11.07	11.47	11.16	11.55	12.12	11.97	11.91	11.71	8.26	9.36	11.94
CH_3SiH_3	11.84	11.85	11.88	12.61	11.82	12.24	12.55	12.71	12.66	12.54	6.83	8.63	12.35

HCOOH	12.13	11.81	11.84	12.09	11.74	12.12	12.49	12.37	12.31	13.14	10.49	11.80	11.98
CH_3CONH_2	10.20	9.99	10.00	10.50	9.95	10.19	10.57	10.64	10.57	10.44	5.24	7.15	10.05
$cylNHC_2H_4$	10.43	10.26	10.26	10.75	10.08	10.42	10.80	10.82	10.76	10.65	9.02	10.68	10.44
NCCN	13.15	13.00	12.96	13.09	13.05	13.05	13.50	14.73	14.65	13.20	10.79	11.80	13.90
CH_3NHCH_3	9.46	9.34	9.37	9.91	9.16	9.55	9.90	10.02	9.96	9.84	5.97	7.70	9.65
CH_2CO	10.66	10.43	10.42	10.60	10.22	10.50	10.79	10.79	10.77	10.70	7.98	9.13	10.32
$cylOC_2H_4$	11.37	11.16	11.18	11.65	10.97	11.35	11.72	11.77	11.72	11.61	9.34	11.07	11.68
OCHCHO	8.94	8.95	9.03	9.26	9.13	9.42	9.90	9.92	9.83	9.67	7.55	8.05	10.04
CH_3CH_2OH	10.82	10.74	10.78	11.35	10.69	11.12	11.57	11.65	11.58	11.44	7.13	8.68	11.38
CH_3OCH_3	10.46	10.33	10.36	10.93	10.21	10.60	11.00	11.11	11.05	10.92	7.14	8.72	10.79
$cylSC_2H_4$	9.77	9.59	9.58	10.11	9.38	9.72	10.00	10.11	10.09	10.01	7.52	8.24	9.93
CH_3SOCH_3	9.41	9.25	9.25	9.78	9.12	9.42	9.73	9.85	9.80	9.69	6.12	7.35	9.54
CH_2CHF	11.44	11.13	11.14	11.54	10.95	11.26	11.50	11.49	11.49	11.42	9.51	10.78	11.55
CH_3CH_2Cl	11.28	11.23	11.23	11.90	11.20	11.56	11.94	12.08	12.03	11.89	8.15	9.30	11.74
CH_2CHCl	10.73	10.51	10.47	10.97	10.35	10.65	10.97	11.09	11.03	10.91	8.66	9.79	11.35
CH_3CClO	11.26	11.11	11.09	11.55	11.16	11.46	11.85	11.98	11.90	11.77	8.02	9.24	11.97
prplCl	10.86	10.83	10.82	11.54	10.85	11.22	11.77	11.96	11.85	11.68	5.61	6.99	11.63
NC_3H_9	8.87	8.77	8.79	9.40	8.60	8.97	9.33	9.48	9.43	9.31	3.96	5.81	9.10
$cylOC_4H_4$	9.81	9.51	9.46	10.85	9.24	9.57	9.93	9.97	9.95	9.85	5.13	7.04	9.82
$cylNHC_4H_4$	9.00	8.73	8.68	9.11	8.51	8.77	9.18	9.10	9.07	8.98	3.23	5.26	8.89
NO_2	9.94	10.05	10.01	10.31	10.16	10.31	10.42	10.28	10.31	10.33	9.24	9.64	9.79
SF_6	14.35	14.22	14.18	15.53	14.69	15.37	17.07	16.59	16.51	16.24	10.97	12.30	16.98
$CFCl_3$	11.06	11.00	10.92	11.50	11.28	11.52	12.37	12.76	12.51	12.16	7.64	8.55	12.61
$CClF_3$	13.83	13.63	13.59	14.34	13.84	14.08	14.57	14.75	14.67	14.52	11.72	12.58	14.27
$CBrF_3$	12.64	12.45	12.41	12.74	12.69	12.75	13.00	13.17	13.11	13.02	13.58	13.45	12.97
HCCF	12.10	11.78	11.77	12.14	11.66	11.93	12.30	12.14	12.15	12.09	11.03	11.85	12.04
HCCCN	11.85	11.69	11.45	11.68	11.61	11.77	12.35	12.22	12.01	12.06	8.94	10.01	12.20
NCCCCN	10.52	10.42	10.40	10.55	10.48	10.57	11.05	10.94	10.86	10.77	8.62	9.48	11.52
C_2N_2	13.15	13.00	12.96	13.09	13.05	13.05	13.50	14.73	14.65	13.20	10.79	11.80	13.90
C_3O_2	11.69	11.44	11.39	11.64	11.58	11.44	12.05	12.18	12.17	12.11	8.28	9.66	11.64
FCN	14.17	13.91	13.87	14.50	14.01	14.05	14.47	14.40	14.38	14.30	13.75	14.39	14.33
HCCCCH	10.91	10.40	10.33	10.70	10.25	10.57	11.07	11.10	11.06	10.95	7.52	8.61	11.00
H_2CS	8.97	8.87	8.89	8.96	8.92	8.88	9.06	8.85	8.88	8.93	7.06	7.65	9.18
$HCONH_2$	11.50	10.70	10.74	11.09	10.65	10.82	11.14	11.13	12.77	12.63	8.37	10.11	10.81
CH_2CHCHO	9.86	9.79	9.84	9.96	9.88	9.96	10.25	10.18	10.13	10.07	7.57	8.45	10.70
CH_2CCl_2	10.38	10.20	10.15	10.59	10.16	10.43	10.85	10.99	10.91	10.77	7.13	8.29	11.17
$CHFCF_2$	11.03	10.75	10.78	11.29	10.71	11.08	11.50	11.32	11.34	11.27	10.10	10.99	11.11
CH_2CF_2	11.43	11.11	11.14	11.55	11.02	11.34	11.69	11.61	11.62	11.54	9.77	11.00	11.81
CH_3F	13.52	13.38	13.44	13.96	13.41	13.79	14.24	14.21	14.17	14.04	12.34	13.72	14.09
CF_2Cl_2	12.27	12.16	12.08	12.73	12.55	12.63	13.40	13.74	13.54	13.25	9.04	10.10	13.33
SiF_2	10.87	10.66	10.79	10.94	10.91	10.90	10.93	11.07	11.02	10.96	15.42	15.05	11.04
MSE	-0.34	-0.45	-0.46	-0.05	-0.42	-0.22	0.11	0.18	0.14	0.03	-2.20	-1.27	
MAE	0.50	0.58	0.59	0.38	0.57	0.40	0.29	0.34	0.32	0.30	2.73	1.83	
rms	0.69	0.77	0.78	0.50	0.75	0.54	0.39	0.44	0.45	0.44	3.26	2.32	