

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.

| Molecule | IP131 | EA131 | FG131 | AE113 |
|---|--------------|----------|-------------|-------------|
| | Experimental | CCSD(T) | CCSD(T) | CCSD(T) |
| | Vertical | Vertical | Fundamental | Atomization |
| | Ionization | Electron | Gap | Energy |
| | Potential | Affinity | | |
| 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) (3Σ ⁻) | 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 ₂ O (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 ₂ S (Hydrogen sulfide) | 10.50 | -0.49 | 11.00 | 7.94 |
| HCl (Hydrogen chloride) | 12.77 | -0.52 | 13.36 | 4.65 |
| C ₂ H ₂ (Acetylene) | 11.49 | -1.90 | 13.43 | 17.49 |
| C ₂ H ₄ (Ethylene) | 10.68 | -1.87 | 12.57 | 24.38 |

| | | | | |
|---|-------|--------------------|--------------------|-------|
| C ₂ H 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 (Formyl radical) | 9.31 | 0.02 | 9.56 | 12.01 |
| H ₂ CO (Formaldehyde) | 10.89 | -0.55 | 11.56 | 16.20 |
| CH ₃ OH (Methyl alcohol) | 10.96 | -0.55 | 11.67 | 22.22 |
| N ₂ (Nitrogen diatomic) | 15.58 | -2.24 | 17.88 | 9.85 |
| N ₂ H 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 ₂ O 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 ₂ H ₆ (Disilane) | 10.53 | -0.69 | 11.33 | 23.19 |
| CH ₃ Cl (Methyl chloride) | 11.29 | -0.51 | 12.01 | 17.08 |
| CH ₃ SH (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 ₂ O (Carbonic difluoride) | 13.60 | -2.37 | 16.08 | 18.22 |
| SiF ₄ (Silicon tetrafluoride) | 16.40 | -0.81 | 16.95 | 24.92 |
| N ₂ O (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 ₂ O (Difluorine monoxide) | 13.26 | -0.31 | 13.82 | 4.04 |
| ClF ₃ (Chlorine trifluoride) | 13.05 | 1.20 | 11.79 | 5.43 |
| C ₂ F ₄ (Tetrafluoroethylene) | 10.69 | -1.65 | 12.45 | 25.54 |
| CF ₃ CN (Acetonitrile, trifluoro-) | 14.30 | -0.96 ^b | 15.40 ^b | 27.77 |
| CH ₃ CCH (Propyne) | 10.37 | -1.13 | 11.70 | 30.44 |

| | | | | |
|--|-------|--------------------|--------------------|-------|
| CH ₂ CCH ₂ (Allene) | 10.20 | -0.56 | 10.83 | 30.40 |
| C ₃ H ₄ (Cyclopropene) | 9.86 | -1.82 | 11.87 | 29.45 |
| C ₃ H ₆ (Cyclopropane) | 10.54 | -0.65 | 11.64 | 36.91 |
| C ₃ H ₈ (Propane) | 11.51 | -0.60 ^b | 12.72 ^b | 43.58 |
| CH ₃ CCCH ₃ (2-Butyne) | 9.79 | -0.68 ^b | 10.46 ^b | 43.32 |
| C ₄ H ₆ (Cyclobutene) | 9.43 | -1.41 ^b | 11.14 ^b | 43.28 |
| CH ₃ CH(CH ₃)CH ₃ (Isobutane) | 11.13 | -0.56 ^b | 12.28 ^b | 56.37 |
| C ₆ H ₆ (Benzene) | 9.25 | -0.71 ^b | 10.16 ^b | 59.14 |
| CH ₂ F ₂ (Methane, difluoro-) | 13.27 | -0.58 | 14.15 | 18.99 |
| CHF ₃ (Methane, trifluoro-) | 15.50 | -0.60 | 15.44 | 19.92 |
| CH ₂ Cl ₂ (Methylene chloride) | 11.40 | -0.49 | 12.18 | 16.05 |
| CHCl ₃ (Chloroform) | 11.50 | -0.83 | 12.38 | 14.87 |
| CH ₃ NO ₂ (Methane, nitro-) | 11.29 | -0.37 | 11.95 | 26.01 |
| CH ₃ SiH ₃ (Methyl silane) | 11.60 | -0.53 | 12.35 | 27.23 |
| HCOOH (Formic acid) | 11.50 | -0.57 | 11.98 | 21.49 |
| CH ₃ CONH ₂ (Acetamide) | 10.00 | -0.31 | 10.05 | 37.48 |
| C ₂ H ₅ N (Aziridine) | 9.85 | -0.56 ^b | 10.44 ^b | 31.11 |
| C ₂ N ₂ (Cyanogen) | 13.51 | -0.19 | 13.90 | 21.60 |
| CH ₃ NHCH ₃ (Dimethylamine) | 8.95 | -0.56 ^b | 9.65 ^b | 37.66 |
| CH ₂ CO (Ketene) | 9.64 | -0.51 | 10.32 | 23.03 |
| C ₂ H ₄ O (Ethylene oxide) | 10.57 | -0.86 | 11.68 | 28.18 |
| C ₂ H ₂ O ₂ (Ethanedial) | 10.60 | 0.69 | 10.04 | 27.39 |
| CH ₃ CH ₂ OH (Ethanol) | 10.64 | -0.53 | 11.38 | 35.06 |
| CH ₃ OCH ₃ (Dimethyl ether) | 10.10 | -0.58 | 10.79 | 34.56 |
| C ₂ H ₄ S (Thiirane) | 9.05 | -0.78 | 9.93 | 27.06 |
| CH ₃ SOCH ₃ (Dimethyl sulfoxide) | 9.10 | -0.40 ^b | 9.54 ^b | 36.89 |
| CH ₂ CHF (Ethene, fluoro-) | 10.63 | -0.88 | 11.55 | 24.81 |
| CH ₃ CH ₂ Cl (Ethyl chloride) | 11.06 | -0.51 | 11.74 | 29.96 |
| CH ₂ CHCl (Ethene, chloro-) | 10.20 | -1.12 | 11.35 | 23.51 |
| CH ₃ COCl (Acetyl Chloride) | 11.03 | -0.85 | 11.97 | 28.90 |
| CH ₂ ClCH ₂ CH 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 ₄ H ₄ O (Furan) | 8.90 | -0.74 ^b | 9.82 ^b | 42.99 |
| C ₄ H ₅ N (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 ₃ Cl (Methane, chlorotrifluoro-) | 13.08 | -1.06 | 14.27 | 18.85 |
| CF ₃ Br (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 ₄ N ₂ (2-Butynedinitrile) | 11.84 | 0.68 | 11.52 | 34.15 |
| C ₂ N ₂ (Cyanogen) | 13.51 | -0.19 | 13.90 | 21.60 |

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|---|-------|--------------------|--------------------|-------|
| C ₃ O ₂ (Carbon suboxide) | 10.80 | -0.74 | 11.64 | 28.58 |
| FCN (Cyanogen fluoride) | 13.65 | -0.66 | 14.33 | 13.19 |
| C ₄ H ₂ (Diacetylene) | 10.30 | -0.64 | 11.00 | 30.05 |
| H ₂ CS (Thioformaldehyde) | 9.38 | 0.28 | 9.18 | 14.07 |
| CHONH ₂ (Formamide) | 10.40 | -0.35 | 10.81 | 24.56 |
| CH ₂ CHCHO (Acrolein) | 10.10 | -0.46 ^b | 10.70 ^b | 35.76 |
| CH ₂ CCl ₂ (Ethene, 1,1-dichloro-) | 10.00 | -1.07 | 11.17 | 22.48 |
| C ₂ HF ₃ (Trifluoroethylene) | 10.62 | -0.54 | 11.11 | 25.31 |
| CH ₂ CF ₂ (Ethene, 1,1-difluoro-) | 10.70 | -1.03 | 11.81 | 25.38 |
| CH ₃ F (Methyl fluoride) | 13.04 | -0.58 | 14.09 | 18.31 |
| CF ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | 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 ₂ CH 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 ₃ CH 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 ₂ O | 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 ₃ OH | 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 ₂ NH 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 ₃ SiH 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 ₃ Cl | 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 ₃ SH | 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 |

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|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|
| 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 ₂ O | 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 ₂ O | 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 ₂ O | 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 ₂ CF 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 ₃ CN | 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 ₃ CCH | 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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | 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 ₂ Cl 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 ₃ H | 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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 ₂ H 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 ₃ NHCH 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 ₂ CO | 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 ₂ H 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 ₃ CH ₂ OH | 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 ₃ OCH 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 ₂ H 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 ₃ SOCH 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 ₂ CHF | 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 ₃ CH ₂ Cl | 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 ₂ CHCl | 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 ₃ CClO | 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 |
| prpCl | 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 ₃ H 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 |
| cyIOC ₄ H 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 |
| cyINH ₄ C ₄ H 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 |
| CCIF 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 ₂ N 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 ₃ O 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 ₂ CS | 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 ₂ CHCHO | 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 ₂ CCl 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 |
| CHF ₂ CF 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 ₂ CF 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 ₃ F | 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 ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | -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 ₂ CH 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 ₃ CH 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 ₂ O | -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 ₃ OH | -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 ₂ NH 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 ₃ SiH 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 ₃ Cl | -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 ₃ SH | -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 ₂ O | -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 ₂ O | -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 ₂ O | -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 ₂ CF 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 ₃ CN | -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 ₃ CCH | -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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | -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 ₂ Cl 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 ₃ H | -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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 ₂ H 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 ₃ NHCH 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 ₂ CO | -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 ₂ H 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 ₃ CH ₂ OH | -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 ₃ OCH 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 ₂ H 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 ₃ SOCH 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 ₂ CHF | -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 ₃ CH ₂ Cl | -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 ₂ CHCl | -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 ₃ CClO | -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 ₃ H 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 ₄ H 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 ₄ H 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 ₂ N 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 ₃ O 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 ₂ CS | -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 ₂ CHCHO | -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 ₂ CCl 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 ₂ CF 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 ₃ F | -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 ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | 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 ₂ CH 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 ₃ CH 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 ₂ O | 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 ₃ OH | 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 ₂ NH 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 ₃ SiH 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 ₃ Cl | 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 ₃ SH | 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 ₂ O | 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 ₂ O | 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 ₂ O | 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 ₂ CF 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 ₃ CN | 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 ₃ CCH | 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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | 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 ₂ Cl 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 ₃ H | 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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 |
| cyINH ₂ C ₂ H 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 ₃ NHCH 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 ₂ CO | 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 |
| cyIOC ₂ H 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 ₃ CH ₂ OH | 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 ₃ OCH 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 |
| cyISC ₂ H 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 ₃ SOCH 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 ₂ CHF | 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 ₃ CH ₂ Cl | 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 ₂ CHCl | 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 ₃ CClO | 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 ₃ H 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 |
| cyIOC ₄ H 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 |
| cyINH ₂ C ₄ H 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 ₂ N 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 ₃ O 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 ₂ CS | 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 ₂ CHCHO | 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 ₂ CCl 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 |
| CHF ₂ CF 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 ₂ CF 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 ₃ F | 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 ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | -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 ₂ CH 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 ₃ CH 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 ₂ O | -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 ₃ OH | -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 ₂ NH 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 ₃ SiH 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 ₃ Cl | -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 ₃ SH | -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 ₂ O | -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 ₂ O | -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 ₂ O | -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 ₂ CF 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 ₃ CN | -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 ₃ CCH | -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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | -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 ₂ Cl 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 ₃ H | -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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 ₂ H 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 ₃ NHCH 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 ₂ CO | -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 ₂ H 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 ₃ CH ₂ OH | -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 ₃ OCH 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 ₂ H 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 ₃ SOCH 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 ₂ CHF | -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 ₃ CH ₂ Cl | -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 ₂ CHCl | -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 ₃ CClO | -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 ₃ H 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 ₄ H 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 ₄ H 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 ₂ N 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 ₃ O 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 ₂ CS | -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 ₂ CHCHO | -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 ₂ CCl 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 ₂ CF 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 ₃ F | -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 ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | 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 ₂ CH 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 ₃ CH 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 ₂ O | 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 ₃ OH | 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 ₂ NH 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 ₃ SiH 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 ₃ Cl | 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 ₃ SH | 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 ₂ O | 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 ₂ O | 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 ₂ O | 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 ₂ CF 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 ₃ CN | 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 ₃ CCH | 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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | 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 ₂ Cl 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 ₃ H | 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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 ₂ H 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 ₃ NHCH 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 ₂ CO | 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 ₂ H 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 ₃ CH ₂ OH | 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 ₃ OCH 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 ₂ H 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 ₃ SOCH 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 ₂ CHF | 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 ₃ CH ₂ Cl | 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 ₂ CHCl | 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 ₃ CClO | 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 ₃ H 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 ₄ H 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 ₄ H 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 ₂ N 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 ₃ O 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 ₂ CS | 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 ₂ CHCHO | 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 ₂ CCl 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 ₂ CF 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 ₃ F | 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 ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | 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 ₂ CH 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 ₃ CH 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 ₂ O | 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 ₃ OH | 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 ₂ NH 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 ₃ SiH 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 ₃ Cl | 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 ₃ SH | 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 ₂ O | 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 ₂ O | 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 ₂ O | 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 ₂ CF 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 ₃ CN | 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 ₃ CCH | 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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | 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 ₂ Cl 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 ₃ H | 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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 ₂ H 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 ₃ NHCH 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 ₂ CO | 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 ₂ H 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 ₃ CH ₂ OH | 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 ₃ OCH 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 ₂ H 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 ₃ SOCH 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 ₂ CHF | 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 ₃ CH ₂ Cl | 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 ₂ CHCl | 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 ₃ CClO | 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 ₃ H 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 ₄ H 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 ₄ H 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 |
| CFC 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 ₂ N 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 ₃ O 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 ₂ CS | 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 ₂ CHCHO | 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 ₂ CCl 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 ₂ CF 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 ₃ F | 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 ₂ Cl 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 | ω B97 | ω B97X | ω B97X-D | LB94 | LB α | 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 ₂ O | 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 ₂ CH 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 ₃ CH 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 ₂ O | 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 ₃ OH | 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 ₂ NH 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 ₃ SiH 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 ₃ Cl | 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 ₃ SH | 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 ₂ O | 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 ₂ O | 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 ₂ O | 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 ₂ CF 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 ₃ CN | 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 ₃ CCH | 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 ₂ CCH 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 ₃ H 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 ₃ H 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 ₃ CH ₂ CH 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 ₃ CCCH 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 ₄ H 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 ₂ F 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 ₃ H | 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 ₂ Cl 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 ₃ H | 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 ₃ NO 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 ₃ SiH 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 ₃ CONH 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 ₂ H 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 ₃ NHCH 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 ₂ CO | 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 ₂ H 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 ₃ CH ₂ OH | 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 ₃ OCH 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 ₂ H 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 ₃ SOCH 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 ₂ CHF | 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 ₃ CH ₂ Cl | 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 ₂ CHCl | 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 ₃ CClO | 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 ₃ H 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 ₄ H 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 ₄ H 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 ₂ N 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 ₃ O 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 ₂ CS | 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 ₂ CHCHO | 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 ₂ CCl 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 |
| CHF ₂ CF 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 ₂ CF 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 ₃ F | 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 ₂ Cl 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 | |