# ELECTRON AFFINITIES

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Electron affinity is defined as the energy difference between the lowest (ground) state of the neutral and the lowest state of the corresponding negative ion. The accuracy of electron affinity measurements has been greatly improved since the advent of laser photodetachment experiments with negative ions. Electron affinities can be determined with optical precision, though a detailed understanding of atomic and molecular states and splittings is required to specify the photodetachment threshold corresponding to the electron affinity.

Atomic and molecular electron affinities are discussed in two excellent articles reviewing photodetachment studies which appear in *Gas Phase Ion Chemistry*, Vol. 3, Bowers, M. T., Ed., Academic Press, Orlando, 1984: Chapter 21 by Drzaic, P. S., Marks, J., and Brauman, J. I., "Electron Photodetachment from Gas Phase Negative Ions", p. 167, and Chapter 22 by Mead, R. D., Stevens, A. E., and Lineberger, W. C., "Photodetachment in Negative Ion Beams", p. 213. Persons interested in photodetachment details should consult these articles and the critical review of Hotop, H., and Lineberger, W. C., *J. Phys. Chem. Ref. Data*, 14, 731, 1985. For simplicity in the tables below, any electron affinity which was discussed in the articles by Drzaic *et al*. or Hotop and Lineberger is referenced to these sources, where original references are given. A great many additional electron affinities have been provided here by G. B. Ellison, W. C. Lineberger, H. Hotop, D. G. Leopold, and K. H. Bowen. Electron affinities for the lanthanides and actinides have not been measured, but theoretical estimates have been made by Bratch, S. G., *Chem. Phys. Lett.*, 98, 113, 1983, and Bratch, S. G., and Lagowski, J. J., *Chem. Phys. Lett.*, 107, 136, 1984. The development of cluster-ion photodetachment apparatuses has brought an explosion of electron affinity estimates for atomic and molecular clusters. [See Arnold, S. T., Eaton, J. G., Patel-Mistra, D., Sarkas, H. W., and Bowen, K. H., in *Ion and Cluster Ion Spectroscopy and Structure*, Maier, J. P., Ed., Elsevier Science, New York, 1989, p. 417.] The policy in this tabulation is to list the electron affinities for the atoms, diatoms, and triatoms, if adiabatic electron affinities have been determined, but to refer the reader to original sources for higher-order clusters. Additional data on molecular electron affinities may be found in Lias, S. G., Bartmess, J. E., Liebman, J. F., Holmes, J. L., Levin, R. D., and Mallard, W. G., *Gas Phase Ion and Neutral Thermochemistry*, *J. Phys. Chem. Ref. Data*, 17, (Supplement No. 1), 1988.

For the present tabulation the value $e/hc = 8065.5410 \pm 0.0024$ cm$^{-1}$ eV$^{-1}$ (Cohen, E. R., and Taylor, B. N., *Rev. Mod. Phys.*, 59, 1121, 1987) has been used to convert electron affinities from the units used in spectroscopic work, cm$^{-1}$, into eV for these tables. The uncertainties in the electron affinities given in the tables do not include the 0.3 ppm uncertainty in $e/hc$; only in a few cases, *e.g.*, atomic oxygen, is this additional uncertainty significant.

Abbreviations used in the tables: calc = calculated value; PT = photodetachment threshold using a lamp as a light source; LPT = laser photodetachment threshold; LPES = laser photoelectron spectroscopy; DA = dissociative attachment; e-scat = electron scattering; CT = charge transfer; and CD = collisional detachment.

## Table 1
## Atomic Electron Affinities

| Atomic number | Atom | Electron affinity in eV | Uncertainty in eV | Method | Ref. |
|---|---|---|---|---|---|
| 1 | D | 0.754593 | 0.000074 | LPT | 89 |
| | H | 0.754195 | 0.000019 | LPT | 89 |
| | | 0.754209 | 0.000003 | calc | 1 |
| 2 | He | not stable | — | calc | 1 |
| 3 | Li | 0.6180 | 0.0005 | LPT | 1 |
| 4 | Be | not stable | — | calc | 1 |
| 5 | B | 0.277 | 0.010 | LPES | 1 |
| 6 | C | 1.2629 | 0.0003 | LPT | 1 |
| 7 | N | not stable | — | DA | 1 |
| 8 | O | 1.4611103 | 0.0000007 | LPT | 4 |
| 9 | F | 3.401190 | 0.000004 | LPT | 74 |
| 10 | Ne | not stable | — | calc | 1 |
| 11 | Na | 0.547926 | 0.000025 | LPT | 1 |
| 12 | Mg | not stable | — | e-scat | 1 |
| 13 | Al | 0.441 | 0.010 | LPES | 1 |
| 14 | Si | 1.385 | 0.005 | LPES | 1 |
| 15 | P | 0.7465 | 0.0003 | LPT | 1 |
| 16 | S | 2.077104 | 0.000001 | LPT | 1 |
| 17 | Cl | 3.61269 | 0.00006 | LPT | 52 |
| 18 | Ar | not stable | — | calc | 1 |
| 19 | K | 0.50147 | 0.00010 | LPT | 1 |
| 20 | Ca | 0.02455 | 0.00010 | LPT | 44 |
| 21 | Sc | 0.188 | 0.020 | LPES | 1 |
| 22 | Ti | 0.079 | 0.014 | LPES | 1 |
| 23 | V | 0.525 | 0.012 | LPES | 1 |
| 24 | Cr | 0.666 | 0.012 | LPES | 1 |
| 25 | Mn | not stable | — | calc | 1 |

## Table 1
## Atomic Electron Affinities (continued)

| Atomic number | Atom | Electron affinity in eV | Uncertainty in eV | Method | Ref. |
|---|---|---|---|---|---|
| 26 | Fe | 0.151 | 0.003 | LPES | 27 |
| 27 | Co | 0.662 | 0.003 | LPES | 27 |
| 28 | Ni | 1.156 | 0.010 | LPES | 1 |
| 29 | Cu | 1.235 | 0.005 | LPES | 37 |
| 30 | Zn | not stable | — | e-scat | 1 |
| 31 | Ga | 0.3 | 0.15 | PT | 1 |
| 32 | Ge | 1.233 | 0.003 | LPES | 28 |
| 33 | As | 0.81 | 0.03 | PT | 1 |
| 34 | Se | 2.020670 | 0.000025 | LPT | 1 |
| 35 | Br | 3.363590 | 0.000003 | LPT | 74 |
| 36 | Kr | not stable | — | calc | 1 |
| 37 | Rb | 0.48592 | 0.00002 | LPT | 1 |
| 38 | Sr | 0.048 | 0.006 | LPT | 122 |
| 39 | Y | 0.307 | 0.012 | LPES | 1 |
| 40 | Zr | 0.426 | 0.014 | LPES | 1 |
| 41 | Nb | 0.893 | 0.025 | LPES | 1 |
| 42 | Mo | 0.748 | 0.002 | LPES | 127 |
| 43 | Tc | 0.55 | 0.20 | calc | 1 |
| 44 | Ru | 1.05 | 0.15 | calc | 1 |
| 45 | Rh | 1.137 | 0.008 | LPES | 1 |
| 46 | Pd | 0.562 | 0.005 | LPES | 116 |
| 47 | Ag | 1.302 | 0.007 | LPES | 1 |
| 48 | Cd | not stable | — | e-scat | 1 |
| 49 | In | 0.3 | 0.2 | PT | 1 |
| 50 | Sn | 1.112 | 0.004 | LPES | 28 |
| 51 | Sb | 1.046 | 0.005 | LPES | 108 |
| 52 | Te | 1.9708 | 0.0003 | LPT | 1 |
| 53 | I | 3.059038 | 0.000010 | LPT | 92 |
| 54 | Xe | not stable | — | calc | 1 |
| 55 | Cs | 0.471626 | 0.000025 | LPT | 1 |
| 56 | Ba | 0.15 | — | calc | 57 |
| 57 | La | 0.5 | 0.3 | calc | 1 |
| 72 | Hf | ≈0 | — | calc | 1 |
| 73 | Ta | 0.322 | 0.012 | LPES | 1 |
| 74 | W | 0.815 | 0.002 | LPES | 37 |
| 75 | Re | 0.15 | 0.15 | calc | 1 |
| 76 | Os | 1.1 | 0.2 | calc | 1 |
| 77 | Ir | 1.5638 | 0.0005 | LPT | 141 |
| 78 | Pt | 2.128 | 0.002 | LPT | 1 |
| 79 | Au | 2.30863 | 0.00003 | LPT | 1 |
| 80 | Hg | not stable | — | e-scat | 1 |
| 81 | Tl | 0.2 | 0.2 | PT | 1 |
| 82 | Pb | 0.364 | 0.008 | LPES | 1 |
| 83 | Bi | 0.946 | 0.010 | LPES | 1 |
| 84 | Po | 1.9 | 0.3 | calc | 1 |
| 85 | At | 2.8 | 0.2 | calc | 1 |
| 86 | Rn | not stable | — | calc | 1 |
| 87 | Fr | 0.46 | — | calc | 82 |
| 118 | ekaradon | 0.056 | — | calc | 140 |

## Table 2
## Electron Affinities for Diatomic Molecules

| Molecule | Electron affinity in eV | Uncertainty in eV | Method | Ref. |
|---|---|---|---|---|
| $Ag_2$ | 1.023 | 0.007 | LPES | 37 |
| $Al_2$ | 1.10 | 0.15 | LPES | 68 |
| AlO | 2.60 | 0.02 | LPES | 143 |
| AlS | 2.60 | 0.03 | LPES | 129 |
| $As_2$ | 0 | — | PT | 2 |
| AsH | 1.0 | 0.1 | PT | 2 |
| $Au_2$ | 1.938 | 0.007 | LPES | 37 |
| BO | 3.12 | 0.09 | PT | 6 |
| BeH | 0.7 | 0.1 | PT | 2 |
| $Bi_2$ | 1.271 | 0.008 | LPES | 119 |
| $Br_2$ | 2.55 | 0.10 | CT | 2 |
| BrO | 2.353 | 0.006 | LPES | 88 |
| $C_2$ | 3.269 | 0.006 | LPES | 87 |
| CH | 1.238 | 0.008 | LPES | 2 |
| CN | 3.862 | 0.004 | LPES | 111 |
| CS | 0.205 | 0.021 | LPES | 2 |
| CaH | 0.93 | 0.05 | PT | 2 |
| $Cl_2$ | 2.38 | 0.10 | CT | 2 |
| ClO | 2.275 | 0.006 | LPES | 88 |
| $Co_2$ | 1.110 | 0.008 | LPES | 27 |
| CoD | 0.680 | 0.010 | LPES | 29 |
| CoH | 0.671 | 0.010 | LPES | 29 |
| $Cr_2$ | 0.505 | 0.005 | LPES | 114 |
| CrD | 0.568 | 0.010 | LPES | 29 |
| CrH | 0.563 | 0.010 | LPES | 29 |
| CrO | 1.221 | 0.006 | LPES | 5 |
| $Cs_2$ | 0.469 | 0.015 | LPES | 104 |
| CsCl | 0.455 | 0.010 | LPES | 30 |
| CsO | 0.273 | 0.012 | LPES | 133 |
| $Cu_2$ | 0.836 | 0.006 | LPES | 37 |
| CuO | 1.777 | 0.006 | LPES | 118 |
| $F_2$ | 3.08 | 0.10 | CT | 2 |
| FO | 2.272 | 0.006 | LPES | 88 |
| $Fe_2$ | 0.902 | 0.008 | LPES | 27 |
| FeD | 0.932 | 0.015 | LPES | 9 |
| FeH | 0.934 | 0.011 | LPES | 9 |
| FeO | 1.493 | 0.005 | LPES | 45 |
| $Ge_2$ | 2.035 | 0.001 | LPES | 123 |
| $I_2$ | 2.55 | 0.05 | CT | 2 |
| IBr | 2.55 | 0.10 | CT | 2 |
| IO | 2.378 | 0.006 | LPES | 88 |
| InP | 1.95 | 0.05 | LPES | 137 |
| $K_2$ | 0.497 | 0.012 | LPES | 104 |
| KBr | 0.642 | 0.010 | LPES | 30 |
| KCl | 0.582 | 0.010 | LPES | 30 |
| KCs | 0.471 | 0.020 | LPES | 104 |
| KI | 0.728 | 0.010 | LPES | 30 |
| KRb | 0.486 | 0.020 | LPES | 104 |
| LiCl | 0.593 | 0.010 | LPES | 30 |
| LiD | 0.337 | 0.012 | LPES | 102 |
| LiH | 0.342 | 0.012 | LPES | 102 |
| MgCl | 1.589 | 0.011 | LPES | 31 |
| MgH | 1.05 | 0.06 | PT | 2 |
| MgI | 1.899 | 0.018 | LPES | 31 |
| MnD | 0.866 | 0.010 | LPES | 9 |
| MnH | 0.869 | 0.010 | LPES | 9 |
| MoO | 1.290 | 0.006 | LPES | 127 |
| NH | 0.370 | 0.004 | LPT | 32 |
| NO | 0.026 | 0.005 | LPES | 73 |
| NS | 1.194 | 0.011 | LPES | 2 |
| $Na_2$ | 0.430 | 0.015 | LPES | 104 |
| NaBr | 0.788 | 0.010 | LPES | 30 |
| NaCl | 0.727 | 0.010 | LPES | 30 |
| NaF | 0.520 | 0.010 | LPES | 30 |
| NaI | 0.865 | 0.010 | LPES | 30 |
| NaK | 0.465 | 0.030 | LPES | 104 |
| $Ni_2$ | 0.926 | 0.010 | LPES | 112 |
| NiCu | 0.889 | 0.010 | LPES | 128 |
| NiAg | 0.979 | 0.010 | LPES | 128 |
| NiD | 0.477 | 0.007 | LPES | 29 |
| NiH | 0.481 | 0.007 | LPES | 29 |
| NiO | 1.470 | 0.003 | LPES | 146 |
| $O_2$ | 0.451 | 0.007 | LPES | 73 |
| OD | 1.825534 | 0.000037 | LPT | 142 |
| OH | 1.8276542 | 0.0000037 | LPT | 142 |
| $P_2$ | 0.589 | 0.025 | LPES | 42 |
| PH | 1.028 | 0.010 | LPES | 2 |
| PO | 1.092 | 0.010 | LPES | 2 |
| $Pb_2$ | 1.366 | 0.010 | LPES | 117 |
| PbO | 0.722 | 0.006 | LPES | 105 |
| $Pd_2$ | 1.685 | 0.008 | LPES | 112 |
| $Pt_2$ | 1.898 | 0.008 | LPES | 112 |
| PtN | 1.240 | 0.010 | LPES | 46 |
| $Rb_2$ | 0.498 | 0.015 | LPES | 104 |
| RbCl | 0.544 | 0.010 | LPES | 30 |
| RbCs | 0.478 | 0.020 | LPES | 104 |
| $Re_2$ | 1.571 | 0.008 | LPES | 33 |
| $S_2$ | 1.670 | 0.015 | LPES | 53 |
| SD | 2.315 | 0.002 | LPES | 10 |
| SF | 2.285 | 0.006 | LPES | 93 |
| SH | 2.314344 | 0.000004 | LPT | 47 |
| SO | 1.125 | 0.005 | LPES | 84 |
| $Sb_2$ | 1.282 | 0.008 | LPES | 108 |
| $Se_2$ | 1.94 | 0.07 | LPES | 38 |
| SeH | 2.212520 | 0.000025 | LPT | 48 |
| SeO | 1.456 | 0.020 | LPES | 41 |
| $Si_2$ | 2.201 | 0.010 | LPES | 100 |
| SiH | 1.277 | 0.009 | LPES | 2 |
| $Sn_2$ | 1.962 | 0.010 | LPES | 117 |
| SnPb | 1.569 | 0.008 | LPES | 117 |
| $Te_2$ | 1.92 | 0.07 | LPES | 38 |
| TeH | 2.102 | 0.015 | LPES | 39 |
| TeO | 1.697 | 0.022 | LPES | 40 |
| ZnH | $\leq$0.95 | — | PT | 2 |

## Table 3
## Electron Affinities for Triatomic Molecules

| Molecule | Electron affinity in eV | Uncertainty in eV | Method | Ref. | Molecule | Electron affinity in eV | Uncertainty in eV | Method | Ref. |
|---|---|---|---|---|---|---|---|---|---|
| $Ag_3$ | 2.32 | 0.05 | LPES | 37 | $Ge_3$ | 2.23 | 0.01 | LPES | 123 |
| $Al_3$ | 1.4 | 0.15 | LPES | 68 | $GeH_2$ | 1.097 | 0.015 | LPES | 28 |
| $AlO_2$ | 4.23 | 0.02 | LPES | 143 | HCO | 0.313 | 0.005 | LPES | 35 |
| $Al_2S$ | 0.80 | 0.12 | LPES | 129 | $HCl_2$ | 4.896 | 0.005 | LPES | 69 |
| $AsH_2$ | 1.27 | 0.03 | PT | 2 | HNO | 0.338 | 0.015 | LPES | 14 |
| $Au_3$ | 3.7 | 0.3 | LPES | 37 | $HO_2$ | 1.078 | 0.017 | LPES | 15 |
| $BO_2$ | 3.57 | 0.13 | CT | 6 | $InP_2$ | 1.61 | 0.05 | LPES | 137 |
| $BO_2$ | 4.3 | 0.2 | CT | 98 | $In_2P$ | 2.36 | 0.05 | LPES | 137 |
| $Bi_3$ | 1.60 | 0.03 | LPES | 119 | $K_3$ | 0.956 | 0.050 | LPES | 18 |
| $C_3$ | 1.981 | 0.020 | LPES | 11 | $MnD_2$ | 0.465 | 0.014 | LPES | 34 |
| $CCl_2$ | 1.591 | 0.010 | LPES | 95 | $MnH_2$ | 0.444 | 0.016 | LPES | 34 |
| $CD_2$ | 0.645 | 0.006 | LPES | 12 | $N_3$ | 2.70 | 0.12 | PT | 2 |
| CDF | 0.535 | 0.005 | LPES | 95 | NCN | 2.484 | 0.006 | LPES | 154 |
| $CF_2$ | 0.165 | 0.010 | LPES | 95 | NCND | 2.622 | 0.005 | LPES | 154 |
| $CH_2$ | 0.652 | 0.006 | LPES | 12 | NCNH | 2.622 | 0.005 | LPES | 154 |
| CHBr | 1.454 | 0.005 | LPES | 95 | NCO | 3.609 | 0.005 | LPES | 111 |
| CHCl | 1.210 | 0.005 | LPES | 95 | NCS | 3.537 | 0.005 | LPES | 111 |
| CHF | 0.542 | 0.005 | LPES | 95 | $NH_2$ | 0.771 | 0.005 | LPES | 58 |
| CHI | 1.42 | 0.17 | LPES | 95 | $N_2O$ | 0.22 | 0.10 | CT | 59 |
| $C_2H$ | 2.969 | 0.006 | LPES | 87 | $NO_2$ | 2.273 | 0.005 | LPES | 63 |
| $C_2O$ | 1.848 | 0.027 | LPES | 13 | (NO)R | R=Ar,Kr,Xe | — | LPES | 90 |
| COS | 0.46 | 0.20 | CD | 2 | $Na_3$ | 1.019 | 0.060 | LPES | 18 |
| $CS_2$ | 0.895 | 0.020 | LPES | 11 | $Ni_3$ | 1.41 | 0.05 | LPES | 55 |
| $C_2Ti$ | 1.542 | 0.020 | LPES | 147 | NiCO | 0.804 | 0.012 | LPES | 2 |
| $CoD_2$ | 1.465 | 0.013 | LPES | 34 | $NiD_2$ | 1.926 | 0.007 | LPES | 34 |
| $CoH_2$ | 1.450 | 0.014 | LPES | 34 | $NiH_2$ | 1.934 | 0.008 | LPES | 34 |
| $CrH_2$ | >2.5 | — | LPES | 34 | $O_3$ | 2.1028 | 0.0025 | LPT | 2 |
| $Cr_2D$ | 1.464 | 0.005 | LPES | 107 | $O_2Ar$ | 0.52 | 0.02 | LPES | 75 |
| $Cr_2H$ | 1.474 | 0.005 | LPES | 107 | OClO | 2.140 | 0.008 | LPES | 88 |
| $CrO_2$ | 2.413 | 0.008 | LPES | 144 | OIO | 2.577 | 0.008 | LPES | 88 |
| $Cs_3$ | 0.864 | 0.030 | LPES | 18 | $PH_2$ | 1.271 | 0.010 | LPES | 2 |
| $Cu_3$ | 2.11 | 0.05 | LPES | 37 | $PO_2$ | 3.42 | 0.01 | LPES | 124 |
| DCO | 0.301 | 0.005 | LPES | 35 | $Pt_3$ | 1.87 | 0.02 | LPES | 55 |
| DNO | 0.330 | 0.015 | LPES | 14 | $Pd_3$ | <1.5 | 0.1 | LPES | 55 |
| $DO_2$ | 1.089 | 0.017 | LPES | 15 | $Rb_3$ | 0.920 | 0.030 | LPES | 18 |
| $DS_2$ | 1.912 | 0.015 | LPES | 53 | $S_3$ | 2.093 | 0.025 | LPES | 16 |
| $HS_2$ | 1.907 | 0.015 | LPES | 53 | $SO_2$ | 1.107 | 0.008 | LPES | 16 |
| $Fe_3$ | 1.47 | 0.08 | LPES | 149 | $S_2O$ | 1.877 | 0.008 | LPES | 16 |
| FeCO | 1.157 | 0.005 | LPES | 103 | $Sb_3$ | 1.85 | 0.03 | LPES | 108 |
| $FeD_2$ | 1.038 | 0.013 | LPES | 34 | $SeO_2$ | 1.823 | 0.050 | LPES | 38 |
| $FeH_2$ | 1.049 | 0.014 | LPES | 34 | $SiH_2$ | 1.124 | 0.020 | LPES | 2 |
| $FeO_2$ | 2.358 | 0.030 | LPES | 130 | $VO_2$ | 2.3 | 0.2 | CT | 101 |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $Ag_n$ | $n$ = 1-10 | — | LPES | 37 | |
| $Al_n$ | $n$ = 3-32 | — | LPES | 68 | |
| $Al_nO_m$ | $n$=1,2 | $m$=1-5 | LPES | 143 | |
| $Al_3O$ | 1.00 | 0.15 | LPES | 68 | |
| $Al_nS_m$ | $n$ = 1-5 | $m$ = 1-3 | LPES | 129 | |
| $Ar(H_2O)_n$ | $n$ = 2,6,7 | — | LPES | 77 | |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules (continued)

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $Au_n$ | $n$ = 2-5 | — | LPES | 37 | |
| $AuF_6$ | 7.5 | estimate | CT | 98 | |
| $BD_3$ | 0.027 | 0.014 | LPES | 62 | |
| $BH_3$ | 0.038 | 0.015 | LPES | 62 | |
| $Bi_4$ | 1.05 | 0.010 | LPES | 119 | |
| $Br(CO_2)$ | 3.582 | 0.017 | LPES | 131 | |
| $C_n$ | $n$ = 2-84 | — | LPES | 70 | |
| $(CO_2)_n$ | $n$ = 1,2 | — | LPES | 75 | |
| $(CS)_n$ | $n$ = 2 | — | LPES | 75 | |
| $(CS_2)_n$ | $n$ = 1,2 | — | LPES | 75 | |
| $CF_3Br$ | 0.91 | 0.2 | CD | 2 | |
| $CF_3I$ | 1.57 | 0.2 | CD | 2 | |
| $CDO_2$ | 3.510 | 0.015 | LPES | 109 | |
| $CHO_2$ | 3.498 | 0.015 | LPES | 109 | |
| $CH_2S$ | 0.465 | 0.023 | LPES | 53 | |
| $CH_3$ | 0.08 | 0.03 | LPES | 2 | |
| $CH_3I$ | 0.2 | 0.1 | CT | 2 | |
| $CH_3NO_2$ | 0.48 | 0.10 | CT | 61 | |
| $CH_3Si$ | 0.852 | 0.010 | LPES | 97 | $CH_3$-Si |
| $CH_3Si$ | 2.010 | 0.010 | LPES | 97 | $CH_2$ = SiH |
| $CD_3O$ | 1.552 | 0.022 | LPES | 2 | |
| $CH_3O$ | 1.570 | 0.022 | LPES | 2 | |
| $CD_3S$ | 1.856 | 0.006 | LPT | 2 | |
| $CH_3S$ | 1.861 | 0.004 | LPT | 2 | |
| $CD_3S_2$ | 1.748 | 0.022 | LPES | 53 | |
| $CH_3S_2$ | 1.757 | 0.022 | LPES | 53 | |
| $CH_3SiH_2$ | 1.19 | 0.04 | LPT | 65 | |
| $CFO_2$ | 4.277 | 0.030 | LPES | 131 | |
| $CO_3$ | 2.69 | 0.14 | LPES | 2 | |
| $CO_3(H_2O)$ | 2.1 | 0.2 | PT | 2 | |
| $C_2F_2$ | 2.255 | 0.006 | LPES | 106 | difluorovinylidene |
| $C_2DO$ | 2.350 | 0.020 | LPES | 13 | |
| $C_2HO$ | 2.350 | 0.020 | LPES | 13 | |
| $C_2D_2$ | 0.492 | 0.006 | LPES | 83 | vinylidene-$d_2$ |
| $C_2HD$ | 0.489 | 0.006 | LPES | 83 | vinylidene-$d_1$ |
| $C_2HF$ | 1.718 | 0.006 | LPES | 106 | monofluorovinylidene |
| $C_2H_2$ | 0.490 | 0.006 | LPES | 83 | vinylidene |
| $C_2H_2FO$ | 2.22 | 0.09 | PT | 2 | acetyl fluoride enolate |
| $C_2D_2N$ | 1.538 | 0.012 | LPES | 21 | cyanomethyl-$d_2$ radical |
| $C_2D_2N$ | 1.070 | 0.024 | LPES | 21 | isocyanomethyl-$d_2$ radical |
| $C_2H_2N$ | 1.543 | 0.014 | LPES | 21 | cyanomethyl radical |
| $C_2H_2N$ | 1.059 | 0.024 | LPES | 21 | isocyanomethyl radical |
| $C_2H_3$ | 0.667 | 0.024 | LPES | 90 | vinyl |
| $C_2D_3O$ | 1.81897 | 0.00012 | LPT | 22 | acetaldehyde-$d_3$ enolate |
| $C_2H_3O$ | 1.82476 | 0.00012 | LPT | 22 | acetaldehyde enolate |
| $C_2H_5N$ | 0.56 | 0.01 | PT | 2 | ethyl nitrine |
| $C_2D_5O$ | 1.702 | 0.033 | LPES | 23 | ethoxide-$d_3$ |
| $C_2H_5O$ | 1.726 | 0.033 | LPES | 23 | ethoxide |
| $C_2H_5S$ | 1.953 | 0.006 | LPT | 2 | ethyl sulfide |
| $C_2H_5S$ | 0.868 | 0.051 | LPES | 53 | $CH_3SCH_2$ |
| $C_2H_7O_2$ | 2.26 | 0.08 | PT | 50 | MeOHOMe |
| $C_3Fe$ | 1.69 | 0.08 | LPES | 132 | |
| $C_3H$ | 1.858 | 0.023 | LPES | 11 | |
| $C_3HFe$ | 1.58 | 0.06 | LPES | 132 | |
| $C_3H_2$ | 1.794 | 0.008 | LPES | 153 | |
| $C_3H_2F_3O$ | 2.625 | 0.010 | LPT | 113 | 1,1,1-trifluoroacetone enolate |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules (continued)

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $C_3H_3$ | 0.893 | 0.025 | LPES | 24 | propargyl radical |
| $C_3H_2D$ | 0.88 | 0.15 | LPES | 24 | propargyl-$d_1$ radical |
| $C_3D_2H$ | 0.907 | 0.023 | LPES | 24 | propargyl-$d_2$ radical |
| $C_3H_3N$ | 1.247 | 0.012 | LPES | 21 | $CH_3CH$-CN |
| $C_3D_5$ | 0.464 | 0.006 | LPES | 138 | allyl-$d_5$ |
| $C_3H_5$ | 0.481 | 0.008 | LPES | 138 | allyl |
| $C_3H_4D$ | 0.373 | 0.019 | LPES | 25 | allyl-$d_1$ |
| $C_3H_5O$ | 1.758 | 0.019 | LPT | 113 | acetone enolate |
| $C_3H_5O$ | 1.621 | 0.006 | LPT | 113 | propionaldehyde enolate |
| $C_3H_5O_2$ | 1.80 | 0.06 | PT | 2 | methyl acetate enolate |
| $C_3H_7O$ | 1.789 | 0.033 | LPES | 23 | *n*-propyl oxide |
| $C_3H_7O$ | 1.839 | 0.029 | LPES | 23 | isopropyl oxide |
| $C_3H_7S$ | 2.00 | 0.02 | PT | 2 | *n*-propyl sulfide |
| $C_3H_7S$ | 2.02 | 0.02 | PT | 2 | isopropyl sulfide |
| $C_3O$ | 1.34 | 0.15 | LPES | 11 | |
| $C_3O_2$ | 0.85 | 0.15 | LPES | 11 | |
| $C_3Ti$ | 1.561 | 0.015 | LPES | 147 | |
| $C_4F_4O_3$ | 0.5 | 0.2 | CD | 2 | tetrafluorosuccinic anhydride |
| $C_4Fe$ | ≤2.2 | 0.2 | LPES | 132 | |
| $C_4HFe$ | 1.67 | 0.06 | LPES | 132 | |
| $C_4H_2O_3$ | 1.44 | 0.10 | CT | 61 | maleic anhydride |
| $C_4D_4$ | 0.909 | 0.015 | LPES | 125 | vinylvinylidene-$d_4$ |
| $C_4H_4$ | 0.914 | 0.015 | LPES | 125 | vinylvinylidene |
| $C_4H_4N$ | 2.39 | 0.13 | PT | 2 | pyrrolate |
| $C_4H_5O$ | 1.801 | 0.008 | LPT | 113 | cyclobutanone enolate |
| $C_4H_6$ | 0.431 | 0.006 | LPES | 135 | trimethylenemethane |
| $C_4H_6O_2$ | 0.69 | 0.10 | CT | 61 | 2,3-butanedione |
| $C_4H_6D$ | 0.493 | 0.008 | LPES | 138 | 2-methylallyl-$d_7$ |
| $C_4H_7$ | 0.505 | 0.006 | LPES | 138 | 2-methylallyl |
| $C_4H_7O$ | 1.67 | 0.05 | PT | 2 | butyraldehyde enolate |
| $C_4H_5DO$ | 1.67 | 0.05 | PT | 2 | 2-butanone-3-$d_1$ enolate |
| $C_4H_5D_2O$ | 1.75 | 0.06 | PT | 2 | 2-butanone-3,3-$d_2$ enolate |
| $C_4H_9O$ | 1.912 | 0.054 | LPES | 23 | *t*-butoxyl |
| $C_4H_9S$ | 2.03 | 0.02 | PT | 2 | *n*-butyl sulfide |
| $C_4H_9S$ | 2.07 | 0.02 | PT | 2 | *t*-butyl sulfide |
| $C_4O$ | 2.05 | 0.15 | LPES | 11 | |
| $C_4O_2$ | 2.0 | 0.2 | LPES | 11 | |
| $C_4Ti$ | 1.494 | 0.020 | LPES | 147 | |
| $C_5$ | 2.853 | 0.001 | LPT | 99 | |
| $C_5F_5N$ | 0.68 | 0.11 | CT | 67 | pentafluoropyridine |
| $C_5F_6O_3$ | 1.5 | 0.2 | CD | 2 | hexafluoroglutaric anhydride |
| $C_5D_5$ | 1.790 | 0.008 | LPES | 11 | cyclopentadienyl-$d_5$ |
| $C_5H_5$ | 1.804 | 0.007 | LPES | 11 | cyclopentadienyl |
| $C_5H_7$ | 0.91 | 0.03 | PT | 2 | pentadienyl |
| $C_5H_7O$ | 1.598 | 0.007 | LPT | 113 | cyclopentanone enolate |
| $C_5H_9O$ | 1.69 | 0.05 | PT | 2 | 3-penanone enolate |
| $C_5H_{11}O$ | 1.93 | 0.05 | LPT | 2 | neopentoxyl |
| $C_5H_{11}S$ | 2.09 | 0.02 | PT | 2 | *n*-pentyl sulfide |
| $C_5O_2$ | 1.2 | 0.2 | LPES | 11 | |
| $C_5Ti$ | 1.748 | 0.050 | LPES | 147 | |
| $C_6$ | 4.180 | 0.001 | LPT | 8 | |
| $C_6Br_4O_2$ | 2.44 | 0.20 | CT | 2 | tetrabromo-BQ |
| $C_6Cl_4O_2$ | 2.78 | 0.10 | CT | 61 | tetrachloro-BQ |
| $C_6F_4O_2$ | 2.70 | 0.10 | CT | 61 | tetrafluoro-BQ |
| $C_6F_5Br$ | 1.15 | 0.11 | CT | 67 | pentafluorobromobenzene |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules (continued)

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $C_6F_5Cl$ | 0.82 | 0.11 | CT | 67 | pentafluorochlorobenzene |
| $C_6F_5I$ | 1.41 | 0.11 | CT | 67 | pentafluoroiodobenzene |
| $C_6F_5NO_2$ | 1.52 | 0.11 | CT | 67 | pentafluoro-NB |
| $C_6F_6$ | 0.52 | 0.10 | CT | 51 | hexafluorobenzene |
| $C_6F_{10}$ | >1.4 | 0.3 | CT | 2 | perfluorocyclohexene |
| $C_6H_2Cl_2O_2$ | 2.48 | 0.10 | CT | 61 | 2,6-dichloro-BQ |
| $C_6H_3F_2NO_2$ | 1.17 | 0.10 | CT | 61 | 2,4-difluoro-NB |
| $C_6D_4$ | 0.551 | 0.010 | LPES | 36 | *o*-benzyne-$d_4$ |
| $C_6H_4$ | 0.560 | 0.010 | LPES | 36 | *o*-benzyne |
| $C_6H_4BrNO_2$ | 1.16 | 0.10 | CT | 61 | *o*-bromo-NB |
| $C_6H_4BrNO_2$ | 1.32 | 0.10 | CT | 61 | *m*-bromo-NB |
| $C_6H_4BrNO_2$ | 1.29 | 0.10 | CT | 61 | *p*-bromo-NB |
| $C_6H_4ClNO_2$ | 1.14 | 0.10 | CT | 61 | *o*-chloro-NB |
| $C_6H_4ClNO_2$ | 1.28 | 0.10 | CT | 61 | *m*-chloro-NB |
| $C_6H_4ClNO_2$ | 1.26 | 0.10 | CT | 61 | *p*-chloro-NB |
| $C_6H_4ClO$ | $\leq$2.58 | 0.08 | PT | 2 | *o*-chloroperoxide |
| $C_6H_4FNO_2$ | 1.07 | 0.10 | CT | 61 | *o*-fluoro-NB |
| $C_6H_4FNO_2$ | 1.23 | 0.10 | CT | 61 | *m*-fluoro-NB |
| $C_6H_4FNO_2$ | 1.12 | 0.10 | CT | 61 | *p*-fluoro-NB |
| $C_6H_4N_2O_4$ | 1.65 | 0.10 | CT | 61 | *o*-diNB |
| $C_6H_4N_2O_4$ | 1.65 | 0.10 | CT | 61 | *m*-diNB |
| $C_6H_4N_2O_4$ | 2.00 | 0.10 | CT | 61 | *p*-diNB |
| $C_6H_4O_2$ | 1.91 | 0.10 | CT | 61 | 1,4-benzoquinone (BQ) |
| $C_6D_5$ | 1.092 | 0.020 | LPES | 26 | phenyl-$d_5$ |
| $C_6D_5N$ | 1.44 | 0.02 | LPES | 96 | phenylnitrene-$d_5$ |
| $C_6H_5$ | 1.096 | 0.006 | LPES | 26 | phenyl |
| $C_6H_5N$ | 1.429 | 0.011 | LPT | 115 | phenylnitrene |
| $C_6H_5NO_2$ | 1.01 | 0.10 | CT | 61 | nitrobenzene (NB) |
| $C_6H_5O$ | 2.253 | 0.006 | LPES | 26 | phenoxyl |
| $C_6H_5S$ | $\leq$2.47 | 0.06 | PT | 2 | thiophenoxide |
| $C_6H_5NH$ | 1.70 | 0.03 | PT | 2 | anilide |
| $C_6H_7$ | <1.67 | 0.04 | PT | 2 | methylchylopentadienyl |
| $C_6H_8Si$ | 1.435 | 0.004 | LPT | 65 | $C_6H_5SiH_3$ |
| $C_6H_9O$ | 1.526 | 0.010 | LPT | 113 | cyclohexanone enolate |
| $C_6H_{10}$ | 0.645 | 0.015 | LPES | 126 | *t*-butyl vinylidene |
| $C_6H_{11}O$ | 1.755 | +0.05/-0.005 | LPT | 113 | pinacolone enolate |
| $C_6H_{11}O$ | 1.82 | 0.06 | PT | 2 | 3,3-dimethylbutananl enolate |
| $C_6N_4$ | 2.3 | 0.3 | PT | 2 | TCNE |
| $C_7F_5N$ | 1.11 | 0.11 | CT | 67 | pentafluorobenzonitrile |
| $C_7F_8$ | 0.86 | 0.11 | CT | 67 | octafluorotoluene |
| $C_7F_{14}$ | 1.08 | 0.10 | CT | 61 | perfluoromethylcyclohexane |
| $C_7HF_5O$ | 1.10 | 0.11 | CT | 67 | pentafluorobenzaldehyde |
| $C_7H_3N_3O_4$ | 2.16 | 0.10 | CT | 61 | 3,5-$(NO_2)_2$-benzonitrile |
| $C_7H_4F_3NO_2$ | 1.41 | 0.10 | CT | 61 | *m*-trifluoromethyl-NB |
| $C_7H_4N_2O_2$ | 1.61 | 0.10 | CT | 61 | *o*-cyano-NB |
| $C_7H_4N_2O_2$ | 1.56 | 0.10 | CT | 61 | *m*-cyno-NB |
| $C_7H_4N_2O_2$ | 1.72 | 0.10 | CT | 61 | *p*-cyano-NB |
| $C_7H_6FO$ | 2.218 | 0.010 | LPT | 2 | *m*-fluoroacetophenone enolate |
| $C_7H_6FO$ | 2.176 | 0.010 | LPT | 2 | *p*-fluoroacetophenone enolate |
| $C_7H_6FeO_3$ | 0.990 | 0.10 | CT | 120 | $\eta^4$-1,3-butadiene-$Fe(CO)_3$ |
| $C_7H_6N_2O_4$ | 1.77 | 0.05 | PT | 60 | 3,4-dintrotoluene |
| $C_7H_6N_2O_4$ | 1.77 | 0.05 | PT | 60 | 2,3-dinitrotoluene |
| $C_7H_6N_2O_4$ | 1.60 | 0.05 | PT | 60 | 2,4-dinitrotoluene |
| $C_7H_6N_2O_4$ | 1.55 | 0.05 | PT | 60 | 2,6-dinitrotoluene |
| $C_7H_7$ | 0.912 | 0.006 | LPES | 26 | benzyl |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules (continued)

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $C_7H_7$ | 0.868 | 0.006 | LPES | 136 | 1-quadricyclanide |
| $C_7H_7$ | 0.962 | 0.006 | LPES | 136 | 2-quadricyclanide |
| $C_7H_7$ | 1.286 | 0.006 | LPES | 136 | norbornadienide |
| $C_7H_7$ | 0.39 | 0.04 | LPES | 136 | cycloheptatrienide |
| $C_7H_7$ | 3.046 | 0.006 | LPES | 136 | 1-(1,6-heptadiynide) |
| $C_7H_7$ | ≥1.140 | 0.006 | LPES | 136 | 3-(1,6-heptadiynide) |
| $C_7H_7NO_2$ | 0.92 | 0.10 | CT | 61 | *o*-methyl-NB |
| $C_7H_7NO_2$ | 0.99 | 0.10 | CT | 61 | *m*-methyl-NB |
| $C_7H_7NO_2$ | 0.95 | 0.10 | CT | 61 | *p*-methyl-NB |
| $C_7H_7NO_3$ | 1.04 | 0.10 | CT | 61 | *m*-$OCH_3$-NB |
| $C_7H_7NO_3$ | 0.91 | 0.10 | CT | 61 | *p*-$OCH_3$-NB |
| $C_7H_7O$ | ≤2.36 | 0.06 | PT | 2 | *o*-methyl phenoxide |
| $C_7H_7O$ | 2.14 | 0.02 | PT | 50 | benzyloxide |
| $C_7H_7O_2$ | 1.85 | 0.10 | CT | 61 | *o*-$CH_3$-BQ |
| $C_7H_8FO$ | <3.05 | 0.06 | PT | 50 | $PhCH_2OHF$ |
| $C_7H_9$ | 1.27 | 0.03 | PT | 2 | heptatrienyl |
| $C_7H_9O$ | 1.61 | 0.05 | PT | 2 | 2-norbornanone enolate |
| $C_7H_9Si$ | 1.33 | 0.04 | LPT | 65 | $C_6H_5(CH_3)SiH$ |
| $C_7H_{11}O$ | 1.598 | 0.007 | LPT | 113 | cycloheptanone enolate |
| $C_7H_{11}O$ | 1.49 | 0.04 | PT | 2 | 2,5-dimethylcyclopentanone enolate |
| $C_7H_{13}O$ | 1.72 | 0.06 | PT | 2 | 4-heptanone enolate |
| $C_7H_{13}O$ | 1.46 | 0.04 | PT | 2 | di-isopropyl ketone enolate |
| $C_8F_{14}N_2$ | 1.89 | 0.10 | CT | 51 | 1,4-$(CN)_2C_6F_4$ |
| $C_8H_3F_5O$ | 0.88 | 0.11 | CT | 67 | pentafluoroacetophenone |
| $C_8H_3F_6NO_2$ | 1.79 | 0.10 | CT | 61 | 3,5-$(CF_3)_2$-NB |
| $C_8H_4O_3$ | 1.21 | 0.10 | CT | 61 | phthalic anhydride |
| $C_8H_6$ | 1.044 | 0.008 | LPES | 148 | |
| $C_8H_7$ | 1.091 | 0.008 | LPES | 134 | |
| $C_8H_7O$ | 2.057 | 0.010 | PT | 2 | acetophenone enolate |
| $C_8H_7O$ | 2.10 | 0.08 | LPT | 2 | phenylacetaldehyde enolate |
| $C_8H_8$ | 0.55 | 0.02 | CT | 134 | cycooctatetraene |
| $C_8H_8$ | 0.65 | 0.04 | LPES | 134 | cycooctatetraene |
| $C_8H_8$ | 0.919 | 0.008 | LPES | 139 | *m*-xylylene |
| $C_8H_9NO_2$ | 1.21 | 0.05 | PT | 60 | 3,5-dimethyl-NB |
| $C_8H_9NO_2$ | 2.61 | 0.05 | PT | 60 | 2,6-dimethyl-NB |
| $C_8H_9NO_2$ | 0.86 | 0.10 | CT | 61 | 2,3-dimethyl-NB |
| $C_8H_{13}O$ | 1.63 | 0.06 | PT | 2 | cyclooctanone enolate |
| $C_9H_8FeO_3$ | 0.76 | 0.10 | CT | 120 | $\eta^4$-1,3-cyclohexadiene-$Fe(CO)_3$ |
| $C_9H_9O$ | 2.030 | 0.010 | LPT | 2 | *m*-methylacetophenone enolate |
| $C_9H_9SiN$ | 1.43 | 0.10 | PT | 2 | trimethylsilylnitrene |
| $C_9H_{11}NO_2$ | 0.70 | 0.10 | CT | 61 | 2,4,6-trimethyl-NB |
| $C_9H_{15}O$ | 1.69 | 0.06 | PT | 2 | cyclononanone enolate |
| $C_{10}H_4Cl_2O_2$ | 2.19 | 0.10 | CT | 61 | 2,3-dichloro-1,4-naphthoquinone |
| $C_{10}H_6N_2O_4$ | 1.78 | 0.10 | CT | 61 | 1,3-dinitronaphthalene |
| $C_{10}H_6N_2O_4$ | 1.77 | 0.10 | CT | 61 | 1,5-dinitronaphthalene |
| $C_{10}H_6O_2$ | 1.81 | 0.10 | CT | 61 | 1,4-naphthoquinone |
| $C_{10}H_7NO_2$ | 1.23 | 0.10 | CT | 61 | 1-nitronaphthalene |
| $C_{10}H_7NO_2$ | 1.18 | 0.10 | CT | 61 | 2-nitronaphthalene |
| $C_{10}H_8$ | 0.69 | 0.10 | CT | 61 | azulene |
| $C_{10}H_8CrO_3$ | 0.93 | 0.10 | CT | 120 | $\eta^4$-1,3,5-cycloheptatriene $Cr(CO)_3$ |
| $C_{10}H_8FeO_3$ | 0.98 | 0.10 | CT | 120 | $\eta^4$-1,3,5-cycloheptatriene-$Fe(CO)_3$ |
| $C_{10}H_{17}O$ | 1.83 | 0.06 | PT | 2 | cyclodecanone enolate |
| $C_{11}H_8FeO_3$ | 1.29 | 0.10 | CT | 120 | $\eta^4$-1,3-butadiene-$Fe(CO)_3$ |
| $C_{12}F_{10}$ | 0.82 | 0.11 | CT | 67 | decafluorobiphenyl |
| $C_{12}H_4N_4$ | 2.8 | 0.3 | CD | 2 | TCNQ |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules (continued)

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $C_{12}H_9$ | 1.07 | 0.10 | PT | 2 | perinaphthenyl |
| $C_{12}H_{15}O$ | 2.032 | 0.010 | LPT | 2 | *t*-butylacetophenone enolate |
| $C_{12}H_{21}O$ | 1.90 | 0.07 | PT | 2 | cyclododecanone enolate |
| $C_{13}F_{10}O$ | 1.52 | 0.11 | CT | 67 | decafluorobenzophenone |
| $C_{13}H_9FO$ | 0.64 | 0.10 | CT | 61 | 4-fluorobenzophenone |
| $C_{13}H_{10}O$ | 0.62 | 0.10 | CT | 61 | benzophenone |
| $C_{14}H_9NO_2$ | 1.43 | 0.10 | CT | 61 | 9-nitroanthracene |
| $C_{14}H_{10}$ | 0.57 | 0.10 | CT | 66 | anthracene |
| $C_{18}H_{12}$ | 1.04 | 0.10 | CT | 66 | tetracene |
| $C_{20}H_{12}$ | 0.79 | 0.10 | CT | 66 | benz[*a*]pyrene |
| $C_{20}H_{12}$ | 0.97 | 0.10 | CT | 66 | perylene |
| $C_{22}H_{14}$ | 1.35 | 0.10 | CT | 66 | pentacene |
| $CeF_4$ | 3.8 | 0.4 | CT | 98 | |
| $Cl(CO_2)$ | 3.907 | 0.010 | LPES | 131 | |
| $CoF_4$ | 6.4 | 0.3 | CT | 98 | |
| $Cr(CO)_3$ | 1.349 | 0.006 | LPES | 94 | |
| $CrO_3$ | 3.6 | 0.2 | CT | 98 | |
| $Cu_n$ | $n$ = 1-41 | — | LPES | 37 | |
| $Fe_n$ | n=3-24 | — | LPES | 149 | |
| $Fe(CO)_2$ | 1.22 | 0.02 | LPES | 2 | |
| $Fe(CO)_3$ | 1.8 | 0.2 | LPES | 2 | |
| $Fe(CO)_4$ | 2.4 | 0.3 | LPES | 2 | |
| $FeF_3$ | 3.6 | 0.1 | CT | 98 | |
| $FeF_4$ | 6.0 | estimate | CT | 98 | |
| $Fe_nO_m$ | $n$=1-4 | $m$=1-6 | LPES | 152 | |
| $Ge_n$ | $n$ = 3-15 | — | LPES | 71 | |
| $Ge_xAs_y$ | $n$ = 5-30 | $n = x + y$ | LPES | 72 | |
| $GeH_3$ | $\leq$1.74 | 0.04 | PT | 2 | |
| $H(NH_3)_n$ | $n$ = 1,2 | — | LPES | 76 | |
| $HNO_3$ | 0.57 | 0.15 | CD | 2 | |
| $(H_2O)_n$ | $n$ = 2-19 | — | LPES | 77 | |
| $I(CO_2)$ | 3.225 | 0.001 | LPES | 131 | |
| $In_xP_y$ | $n$ = 2-8 | $n = x + y$ | LPES | 137 | |
| $IrF_4$ | 4.7 | 0.3 | CT | 98 | |
| $IrF_6$ | 6.5 | 0.4 | CT | 98 | |
| $K_n$ | $n$ = 2-7 | — | LPES | 18 | |
| $MnF_4$ | 5.5 | 0.2 | CT | 98 | |
| $Mo(CO)_3$ | 1.337 | 0.006 | LPES | 94 | |
| $MoF_5$ | 3.5 | 0.2 | CT | 98 | |
| $MoF_6$ | 3.8 | 0.2 | CT | 98 | |
| $MoO_3$ | 2.9 | 0.2 | CT | 98 | |
| $(NH_3)_n$ | $n$ = 41-1100 | — | LPES | 77 | |
| $NH_2(NH_3)_n$ | $n$ = 1,2 | — | LPES | 78 | |
| $NO(H_2O)_n$ | $n$ = 1,2 | — | LPES | 75 | |
| $NO_3$ | 3.937 | 0.014 | LPES | 85 | |
| $NO(N_2O)_n$ | $n$ = 1,2 | — | LPES | 79 | |
| $(NO)_2$ | $\geq$2.1 | — | LPES | 75 | |
| $(N_2O)_n$ | $n$ = 1,2 | — | LPES | 81 | |
| $Na_n$ | $n$ = 2-5 | — | LPES | 18 | |
| $(NaF)_n$ | $n$ = 1-7,12 | — | LPES | 64 | |
| $Na(NaF)_n$ | $n$ = 5,7-12 | — | LPES | 64 | |
| $Ni(CO)_2$ | 0.643 | 0.014 | LPES | 2 | |
| $Ni(CO)_3$ | 1.077 | 0.013 | LPES | 2 | |
| $NiO_2$ | 3.05 | 0.01 | LPES | 145 | ONiO |
| $NiO_2$ | 0.82 | 0.03 | LPES | 145 | $Ni(O_2)$ |

## Table 4
## Electron Affinities for Larger Polyatomic Molecules (continued)

| Molecule | Electron Affinity in eV | Uncertainty in eV | Method | Ref. | Name |
|---|---|---|---|---|---|
| $OH(H_2O)$ | <2.95 | 0.15 | PT | 2 | |
| $OsF_4$ | 3.9 | 0.3 | CT | 98 | |
| $OsF_6$ | 6.0 | 0.3 | CT | 98 | |
| $PBr_3$ | 1.59 | 0.15 | CD | 2 | |
| $PBr_2Cl$ | 1.63 | 0.20 | CD | 2 | |
| $PCl_2Br$ | 1.52 | 0.20 | CD | 2 | |
| $PCl_3$ | 0.82 | 0.10 | CD | 2 | |
| $PF_5$ | 0.75 | 0.15 | CT | 121 | |
| $PO_3$ | 4.5 | 0.5 | CT | 98 | |
| $POCl_2$ | 3.83 | 0.25 | CD | 2 | |
| $POCl_3$ | 1.41 | 0.20 | CD | 2 | |
| $PtF_4$ | 5.5 | 0.3 | CT | 98 | |
| $PtF_6$ | 7.0 | 0.4 | CT | 98 | |
| $ReF_6$ | 4.7 | estimate | CT | 98 | |
| $RhF_4$ | 5.4 | 0.3 | CT | 98 | |
| $RuF_4$ | 4.8 | 0.3 | CT | 98 | |
| $RuF_5$ | 5.2 | 0.4 | CT | 98 | |
| $RuF_6$ | 7.5 | 0.3 | CT | 98 | |
| $SF_4$ | 1.5 | 0.2 | CT | 91 | |
| $SF_6$ | 1.05 | 0.10 | CT | 56 | |
| $SO_3$ | ≥1.70 | 0.15 | CD | 2 | |
| $(SO_2)_2$ | 0.6 | 0.2 | LPES | 80 | |
| $SeF_6$ | 2.9 | 0.2 | CD | 2 | |
| $Si_4$ | 2.17 | 0.01 | LPES | 110 | |
| $Si_n$ | $n$ = 3-20 | — | LPES | 71 | |
| $SiD_3$ | 1.386 | 0.022 | LPES | 43 | |
| $SiF_3$ | ≤2.95 | 0.10 | PT | 17 | |
| $SiH_3$ | 1.406 | 0.014 | LPES | 43 | |
| $TeF_6$ | 3.34 | 0.17 | CD | 2 | |
| $Ti_n$ | $n$=3-65 | — | LPES | 151 | |
| $UF_5$ | 3.7 | 0.2 | CT | 98 | |
| $UF_6$ | 5.1 | 0.2 | CT | 98 | |
| $UO_3$ | <2.1 | — | CT | 98 | |
| $V_n$ | $n$=3-65 | — | LPES | 150 | |
| $VF_4$ | 3.5 | 0.2 | CT | 98 | |
| $V_4O_{10}$ | 4.2 | 0.6 | CT | 101 | |
| $W(CO)_3$ | 1.859 | 0.006 | LPES | 94 | |
| $WF_5$ | 1.25 | 0.3 | CD | 18 | |
| $WF_6$ | 3.36 | +0.04/-0.20 | CT | 19 | |
| $WO_3$ | 3.33 | +0.04/-0.15 | LPT | 86 | |
| $WO_3$ | 3.9 | 0.2 | CT | 98 | |

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