Summary Tables of Calculated and Experimental Parameters of Diatomic, Triatomic, Organic, Silicon, Boron, Aluminum and Organometallic Molecules, Exemplary Results on Condensed Matter Physics, One-Through Twenty-Electron Atoms, Excited States of Helium, g Factor, and Fundamental Particle Masses

The closed-form derivations from Maxwell's equations given in *The Grand Unified Theory of Classical Physics* posted at http://www.blacklightpower.com/theory/bookdownload.shtml contain fundamental constants only. The nature of the chemical bond is given in Chapters 12 through 15. The atoms are solved exactly in Chapters 1, 7, and 10. The excited states of helium are solved exactly in Chapter 9. The electron g factor and relations between fundamental particles are given in Chapter 1 and Chapters 36, 37 and 38.

Tables summarizing the results of the calculated experimental parameters of 800 exemplary solved molecules follow. The closed-form derivations of these molecules can be found in The Grand Theory of Classical Physics posted at http://www.blacklightpower.com/theory/bookdownload.shtml Chapters 15–17, as well as Silicon in Chapter 20, Boron in Chapter 22, and Aluminum and Organometallics in Chapter 23. Condensed matter physics based on first principles with analytical solutions of (i) of the geometrical parameters and energies of the hydrogen bond of H_2O in the ice and steam phases, and of H_2O and NH_3; (ii) analytical solutions of the geometrical parameters and interplane van der Waals cohesive energy of graphite; (iii) analytical solutions of the geometrical parameters and interatomic van der Waals cohesive energy of liquid helium and solid neon, argon, krypton, and xenon are given in Chapter 16.

Table 1. The calculated and experimental parameters of H_2, D_2, H_2^+ and D_2^+.

Parameter	Calculated	Experimental	Eqs.
H_2 Bond Energy	4.478 eV	4.478 eV	261
D_2 Bond Energy	4.556 eV	4.556 eV	263
H_2^+ Bond Energy	2.654 eV	2.651 eV	230
D_2^+ Bond Energy	2.696 eV	2.691 eV	232
H_2 Total Energy	31.677 eV	31.675 eV	257
D_2 Total Energy	31.760 eV	31.760 eV	258
H_2 Ionization Energy	15.425 eV	15.426 eV	259
D_2 Ionization Energy	15.463 eV	15.466 eV	260
H_2^+ Ionization Energy	16.253 eV	16.250 eV	228
D_2^+ Ionization Energy	16.299 eV	16.294 eV	229
H_2^+ Magnetic Moment	$9.274\ X10^{-24}\ JT^{-1}$ μ_B	$9.274\ X10^{-24}\ JT^{-1}$ μ_B	328-334
Absolute H_2 Gas-Phase NMR Shift	-28.0 ppm	-28.0 ppm	345
H_2 Internuclear Distance[e]	0.748 Å $\sqrt{2}a_o$	0.741 Å	248
D_2 Internuclear Distance[e]	0.748 Å $\sqrt{2}a_o$	0.741 Å	248
H_2^+ Internuclear Distance[f]	1.058 Å $2a_o$	1.06 Å	217
D_2^+ Internuclear Distance[e]	1.058 Å $2a_o$	1.0559 Å	217
H_2 Vibrational Energy	0.517 eV	0.516 eV	269
D_2 Vibrational Energy	0.371 eV	0.371 eV	274
H_2 $\omega_e x_e$	120.4 cm^{-1}	121.33 cm^{-1}	271
D_2 $\omega_e x_e$	60.93 cm^{-1}	61.82 cm^{-1}	275
H_2^+ Vibrational Energy	0.270 eV	0.271 eV	238
D_2^+ Vibrational Energy	0.193 eV	0.196 eV	242
H_2 J=1 to J=0 Rotational Energy[e]	0.0148 eV	0.01509 eV	290
D_2 J=1 to J=0 Rotational Energy[e]	0.00741 eV	0.00755 eV	278-283, 290
H_2^+ J=1 to J=0 Rotational Energy[f]	0.00740 eV	0.00739 eV	286
D_2^+ J=1 to J=0 Rotational Energy[e]	0.00370 eV	0.003723 eV	278-286

[a] The experimental total energy of the hydrogen molecule is given by adding the first (15.42593 eV) [81] and second (16.2494 eV) ionization energies where the second ionization energy is given by the addition of the ionization energy of the hydrogen atom (13.59844 eV) [47] and the bond energy of H_2^+ (2.651 eV).

[b] The experimental total energy of the deuterium molecule is given by adding the first (15.466 eV) [80] and second (16.294 eV) ionization energies where the second ionization energy is given by the addition of the ionization energy of the deuterium atom

(13.603 eV) [37] and the bond energy of D_2^+ (2.692 eV).

[c] The experimental second ionization energy of the hydrogen molecule, IP_2, is given by the sum of the ionization energy of the hydrogen atom (13.59844 eV) [47] and the bond energy of H_2^+ (2.651 eV).

[d] The experimental second ionization energy of the deuterium molecule, IP_2, is given by the sum of the ionization energy of the deuterium atom (13.603 eV) [37] and the bond energy of D_2^+ (2.692 eV).

[e] The internuclear distances are not corrected for the reduction due to $\overline{E}_{osc}$.

[f] The internuclear distances are not corrected for the increase due to $\overline{E}_{osc}$.

Table 13.1. The calculated and experimental bond parameters of H_3^+, D_3^+, OH, OD, H_2O, D_2O, NH, ND, NH_2, ND_2, NH_3, ND_3, CH, CD, CH_2, CH_3, CH_4, N_2, O_2, F_2, Cl_2, CN, CO, and NO.

Parameter	Calculated	Experimental	Ref. for Exp.
H_3^+ Bond Energy	4.373 eV	4.373 eV	8
D_3^+ Bond Energy	4.374 eV		
OH Bond Energy	4.4104 eV	4.4117 eV	22
OD Bond Energy	4.4687 eV	4.454 eV	23
OH Bond Length	0.971651 Å	0.971 Å	13
OD Bond Length	0.971651 Å	0.971 Å	13
OH Vibrational Energy	0.4367 eV	0.4424 eV	16-17
OD Vibrational Energy	0.3219 eV	0.3263 eV	16-17
OH ω_e	3696.38 cm^{-1}	3735.21 cm^{-1}	14
OD ω_e	2689.51 cm^{-1}	2720.9 cm^{-1}	14
OH $\omega_e x_e$	87.18 cm^{-1}	82.81 cm^{-1}	14
OD $\omega_e x_e$	46.75 cm^{-1}	44.2 cm^{-1}	14
OH B_e	18.835 cm^{-1}	18.871 cm^{-1}	14
OD B_e	9.971 cm^{-1}	10.01 cm^{-1}	14
H_2O Bond Energy	5.1059 eV	5.0991 eV	26
D_2O Bond Energy	5.178 eV	5.191 eV	31-32
H_2O $O-H$ Bond Length	0.971574 Å	0.970 ± 0.005 Å	23
D_2O $O-D$ Bond Length	0.971574 Å	0.970 ± 0.005 Å	23
H_2O $H-H$ Distance	1.552 Å	1.55 ± 0.01 Å	13
D_2O $D-D$ Distance	1.552 Å	1.55 ± 0.01 Å	13
H_2O Bond Angle	106°	106°	23
D_2O Bond Angle	106°	106°	23
NH Bond Energy	3.47530 eV	3.47 eV	30
ND Bond Energy	3.52556 eV	3.5134 eV	31
NH Bond Length	1.04262 Å	1.0362 Å	28
ND Bond Length	1.04262 Å	1.0361 Å	28
NH Vibrational Energy	0.38581 eV	0.38752 eV	28
ND Vibrational Energy	0.28583 eV	0.28690 eV	28
NH ω_e	3284.58 cm^{-1}	3282.3 cm^{-1}	28
ND ω_e	2398.72 cm^{-1}	2398 cm^{-1}	28
NH $\omega_e x_e$	86.37 cm^{-1}	78.4 cm^{-1}	28
ND $\omega_e x_e$	47.40 cm^{-1}	42 cm^{-1}	28
NH B_e	16.495 cm^{-1}	16.993 cm^{-1}	28

Parameter	Calculated	Experimental	Ref. for Exp.
ND B_e	8.797 cm^{-1}	8.7913 cm^{-1}	28
NH_2 Bond Energy	3.9323 eV	3.9461 eV	35
ND_2 Bond Energy	3.9401 eV	3.9362 eV	33-35
NH_2 Bond Length	1.04262 Å	1.0240 Å	32
ND_2 Bond Length	1.04262 Å		
NH_2 Bond Angle	105.97	103.3°	32
ND_2 Bond Angle	105.97		
NH_3 Bond Energy	4.57913 eV	4.60155 eV	37
ND_3 Bond Energy	4.64499 eV	4.71252 eV	37
NH_3 Bond Length	1.0368 Å	1.012 Å	32
ND_3 Bond Length	1.0368 Å		
NH_3 Bond Angle	106.67	106.67°	36
ND_3 Bond Angle	106.67	106.70	36
CH Bond Energy	3.47404 eV	3.47 eV	14
CD Bond Energy	3.51673 eV	3.52 eV	14
CH Bond Length	1.1183 Å	1.1198 Å	14
CD Bond Length	1.1183 Å	1.118 Å	14
CH Vibrational Energy	0.33879 eV	0.33885 eV	14
CD Vibrational Energy	0.25173 eV	0.25189 eV	14
CH ω_e	2865.86 cm^{-1}	2861.6 cm^{-1}	14
CD ω_e	2102.97 cm^{-1}	2101.0 cm^{-1}	14
CH $\omega_e x_e$	66.624 cm^{-1}	64.3 cm^{-1}	14
CD $\omega_e x_e$	36.335 cm^{-1}	34.7 cm^{-1}	14
CH B_e	14.498 cm^{-1}	14.457 cm^{-1}	14
CD B_e	7.807 cm^{-1}	7.808 cm^{-1}	14
CH_2 Bond Energy	4.36968 eV	4.33064 eV	39
CH_2 Bond Length	1.1067 Å	1.111 Å	38
CH_2 Bond Angle	100.22	102.4°	38
CH_3 Bond Energy	4.70075 eV	4.72444 eV	40
CH_3 Bond Length	1.1029 Å	1.079 Å	38
CH_3 Bond Angle	120°	120°	38
CH_4 Bond Energy	4.4900 eV	4.48464 eV	40
CH_4 Bond Length	1.1010 Å	1.087 Å	41
CH_4 Bond Angle	109.5°	109.5°	41
N_2 Bond Energy	9.71181 eV	9.756 eV	43

Parameter	Calculated	Experimental	Ref. for Exp.
N_2 Bond Length	1.0955 Å	1.094 Å	43
O_2 Bond Energy	5.10711 eV	5.11665 eV	46
O_2 Bond Length	1.20862 Å	1.20752 Å	28
F_2 Bond Energy	1.62168 eV	1.606 eV	48
F_2 Bond Length	1.41114 Å	1.41193 Å	28
Cl_2 Bond Energy	2.52236 eV	2.51412 eV	49
Cl_2 Bond Length	1.988 Å	1.988 Å	28
Cl_2 ω_e	538.52 cm^{-1}	559.7 cm^{-1}	28
Cl_2 $\omega_e x_e$	3.41 cm^{-1}	2.68 cm^{-1}	28
Cl_2 B_e	0.2420 cm^{-1}	0.2440 cm^{-1}	28
CN Bond Energy	7.77526 eV	7.7731 eV	50
CN Bond Length	1.17231 Å	1.17181 Å	28
CO Bond Energy	11.16652 eV	11.15696 eV	49
CO Bond Length	1.13290 Å	1.12823 Å	28
NO Bond Energy	6.57092 eV	6.5353 eV	49
NO Bond Length	1.15733 Å	1.15077 Å	28

Table 14.1. The calculated and experimental bond parameters of CO_2, NO_2, CH_3CH_3, CH_2CH_2, $CHCH$, benzene, propane, butane, pentane, hexane, heptane, octane, nonane, decane, undecane, dodecane, and octadecane.

Parameter	Calculated	Experimental
CO_2 Bond Energy	5.49553 eV	5.51577 eV
CO_2 Bond Length	1.1616 Å	1.1600 Å
NO_2 Bond Energy	3.1532 eV	3.161 eV
NO_2 Bond Length	1.1872 Å	1.193 Å
NO_2 Bond Angle	131.012°	134.1°
H_3C-CH_3 Bond Energy	3.90245 eV	3.8969 eV
H_3C-CH_3 Bond Length	1.53635 Å	1.5351 Å
$H-CH_2CH_3$ Bond Length	1.10822 Å	1.0940 Å
Ethane $H-C-H$ Bond Angle	107.44°	107.4°
Ethane $C-C-H$ Bond Angle	111.44°	111.17°
$H_2C=CH_2$ Bond Energy	7.55681 eV	7.597 eV
$H_2C=CH_2$ Bond Length	1.3405 Å	1.339 Å
$H-CHCH_2$ Bond Length	1.0826 Å	1.087 Å
Ethylene $H-C-H$ Bond Angle	116.31°	116.6°
Ethylene $C=C-H$ Bond Angle	121.85°	121.7°
$HC\equiv CH$ Bond Energy	10.07212 eV	10.0014 eV
$HC\equiv CH$ Bond Length	1.2007 Å	1.203 Å
$H-CCH$ Bond Length	1.0538 Å	1.060 Å
Acetylene $C\equiv C-H$ Bond Angle	180°	180°
C_6H_6 Total Bond Energy	57.2601 eV	57.26 eV
Benzene $C=C$ Bond Length	1.3914 Å	1.399 Å
$H-C_6H_5$ Bond Length	1.0933 Å	1.101 Å
C_6H_6 $C=C=C$ Bond Angle	120°	120°
C_6H_6 $C=C-H$ Bond Angle	120°	120°
C_3H_8 Total Bond Energy	41.46896 eV	41.434 eV
Propane $C-C$ Bond Length	1.5428 Å	1.532 Å
Propane $C-H$ Bond Length	1.1097 Å	1.107 Å
Alkane $H-C-H$ Bond Angle	109.50°	109.3°
Alkane $C-C-H$ Bond Angle	109.44°	109.3°
C_4H_{10} Total Bond Energy	53.62666 eV	53.61 eV
Butane $C-C$ Bond Length	1.5428 Å	1.531 Å
Butane $C-H$ Bond Length	1.11713 Å	1.117 Å

Parameter	Calculated	Experimental
C_5H_{12} Total Bond Energy	65.78436 eV	65.77 eV
C_6H_{14} Total Bond Energy	77.94206 eV	77.93 eV
C_7H_{16} Total Bond Energy	90.09976 eV	90.09 eV
C_8H_{18} Total Bond Energy	102.25746 eV	102.25 eV
C_9H_{20} Total Bond Energy	114.41516 eV	114.40 eV
$C_{10}H_{22}$ Total Bond Energy	126.57286 eV	126.57 eV
$C_{11}H_{24}$ Total Bond Energy	138.73056 eV	138.736 eV
$C_{12}H_{26}$ Total Bond Energy	150.88826 eV	150.88 eV
$C_{18}H_{38}$ Total Bond Energy	223.83446 eV	223.85 eV

SUMMARY TABLES OF ORGANIC, SILICON, BORON, ORGANOMETALLIC, AND COORDNINATE MOLECULES

The results of the determination of the total bond energies with the experimental values are given in the following tables for a large array of functional groups and molecules per class for which the experimental data was available. Here, the total bond energies of exemplary organic, silicon, boron, organometallic, and coordinate molecules whose designation is based on the main functional group were calculated using the functional group composition and the corresponding energies derived previously [1] and compared to the experimental values. References for the experimental values are mainly from Ref. [2-5], and they are given for each compound in Ref. [1]. For each molecule, the calculated results is based on first principles and given in closed-form, exact equations containing fundamental constants and integers only. The agreement between the experimental and calculated results is excellent. And, unlike previous curve-fitting approaches, the exact geometric parameters, current densities, and energies are given for every electron.

Table 1. Summary results of n-alkanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_8	propane	41.46896	41.434	-0.00085
C_4H_{10}	butane	53.62666	53.61	-0.00036
C_5H_{12}	pentane	65.78436	65.77	-0.00017
C_6H_{14}	hexane	77.94206	77.93	-0.00019
C_7H_{16}	heptane	90.09976	90.09	-0.00013
C_8H_{18}	octane	102.25746	102.25	-0.00006
C_9H_{20}	nonane	114.41516	114.40	-0.00012
$C_{10}H_{22}$	decane	126.57286	126.57	-0.00003
$C_{11}H_{24}$	undecane	138.73056	138.736	0.00004
$C_{12}H_{26}$	dodecane	150.88826	150.88	-0.00008
$C_{18}H_{38}$	octadecane	223.83446	223.85	0.00008

Table 2. Summary results of branched alkanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_4H_{10}	isobutane	53.69922	53.695	-0.00007
C_5H_{12}	isopentane	65.85692	65.843	-0.00021
C_5H_{12}	neopentane	65.86336	65.992	0.00195
C_6H_{14}	2-methylpentane	78.01462	78.007	-0.00010
C_6H_{14}	3-methylpentane	78.01462	77.979	-0.00046
C_6H_{14}	2,2-dimethylbutane	78.02106	78.124	0.00132
C_6H_{14}	2,3-dimethylbutane	77.99581	78.043	0.00061
C_7H_{16}	2-methylhexane	90.17232	90.160	-0.00014
C_7H_{16}	3-methylhexane	90.17232	90.127	-0.00051
C_7H_{16}	3-ethylpentane	90.17232	90.108	-0.00072
C_7H_{16}	2,2-dimethylpentane	90.17876	90.276	0.00107
C_7H_{16}	2,2,3-trimethylbutane	90.22301	90.262	0.00044
C_7H_{16}	2,4-dimethylpentane	90.24488	90.233	-0.00013
C_7H_{16}	3,3-dimethylpentane	90.17876	90.227	0.00054
C_8H_{18}	2-methylheptane	102.33002	102.322	-0.00008
C_8H_{18}	3-methylheptane	102.33002	102.293	-0.00036
C_8H_{18}	4-methylheptane	102.33002	102.286	-0.00043
C_8H_{18}	3-ethylhexane	102.33002	102.274	-0.00055
C_8H_{18}	2,2-dimethylhexane	102.33646	102.417	0.00079
C_8H_{18}	2,3-dimethylhexane	102.31121	102.306	-0.00005
C_8H_{18}	2,4-dimethylhexane	102.40258	102.362	-0.00040
C_8H_{18}	2,5-dimethylhexane	102.40258	102.396	-0.00006
C_8H_{18}	3,3-dimethylhexane	102.33646	102.369	0.00032
C_8H_{18}	3,4-dimethylhexane	102.31121	102.296	-0.00015
C_8H_{18}	3-ethyl-2-methylpentane	102.31121	102.277	-0.00033
C_8H_{18}	3-ethyl-3-methylpentane	102.33646	102.317	-0.00019
C_8H_{18}	2,2,3-trimethylpentane	102.38071	102.370	-0.00010
C_8H_{18}	2,2,4-trimethylpentane	102.40902	102.412	0.00003
C_8H_{18}	2,3,3-trimethylpentane	102.38071	102.332	-0.00048
C_8H_{18}	2,3,4-trimethylpentane	102.29240	102.342	0.00049
C_8H_{18}	2,2,3,3-tetramethylbutane	102.41632	102.433	0.00016
C_9H_{20}	2,3,5-trimethylhexane	114.54147	114.551	0.00008
C_9H_{20}	3,3-diethylpentane	114.49416	114.455	-0.00034
C_9H_{20}	2,2,3,3-tetramethylpentane	114.57402	114.494	-0.00070
C_9H_{20}	2,2,3,4-tetramethylpentane	114.51960	114.492	-0.00024
C_9H_{20}	2,2,4,4-tetramethylpentane	114.57316	114.541	-0.00028
C_9H_{20}	2,3,3,4-tetramethylpentane	114.58266	114.484	-0.00086
$C_{10}H_{22}$	2-methylnonane	126.64542	126.680	0.00027
$C_{10}H_{22}$	5-methylnonane	126.64542	126.663	0.00014

Table 3. Summary results of alkenes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_6	propene	35.56033	35.63207	0.00201
C_4H_8	1-butene	47.71803	47.78477	0.00140
C_4H_8	trans-2-butene	47.93116	47.90395	-0.00057
C_4H_8	isobutene	47.90314	47.96096	0.00121
C_5H_{10}	1-pentene	59.87573	59.95094	0.00125
C_5H_{10}	trans-2-pentene	60.08886	60.06287	-0.00043
C_5H_{10}	2-methyl-1-butene	60.06084	60.09707	0.00060
C_5H_{10}	2-methyl-2-butene	60.21433	60.16444	-0.00083
C_5H_{10}	3-methyl-1-butene	59.97662	60.01727	0.00068
C_6H_{12}	1-hexene	72.03343	72.12954	0.00133
C_6H_{12}	trans-2-hexene	72.24656	72.23733	-0.00013
C_6H_{12}	trans-3-hexene	72.24656	72.24251	-0.00006
C_6H_{12}	2-methyl-1-pentene	72.21854	72.29433	0.00105
C_6H_{12}	2-methyl-2-pentene	72.37203	72.37206	0.00000
C_6H_{12}	3-methyl-1-pentene	72.13432	72.19173	0.00080
C_6H_{12}	4-methyl-1-pentene	72.10599	72.21038	0.00145
C_6H_{12}	3-methyl-trans-2-pentene	72.37203	72.33268	-0.00054
C_6H_{12}	4-methyl-trans-2-pentene	72.34745	72.31610	-0.00043
C_6H_{12}	2-ethyl-1-butene	72.21854	72.25909	0.00056
C_6H_{12}	2,3-dimethyl-1-butene	72.31943	72.32543	0.00008
C_6H_{12}	3,3-dimethyl-1-butene	72.31796	72.30366	-0.00020
C_6H_{12}	2,3-dimethyl-2-butene	72.49750	72.38450	-0.00156
C_7H_{14}	1-heptene	84.19113	84.27084	0.00095
C_7H_{14}	5-methyl-1-hexene	84.26369	84.30608	0.00050
C_7H_{14}	trans-3-methyl-3-hexene	84.52973	84.42112	-0.00129
C_7H_{14}	2,4-dimethyl-1-pentene	84.44880	84.49367	0.00053
C_7H_{14}	4,4-dimethyl-1-pentene	84.27012	84.47087	0.00238
C_7H_{14}	2,4-dimethyl-2-pentene	84.63062	84.54445	-0.00102
C_7H_{14}	trans-4,4-dimethyl-2-pentene	84.54076	84.54549	0.00006
C_7H_{14}	2-ethyl-3-methyl-1-butene	84.47713	84.44910	-0.00033
C_7H_{14}	2,3,3-trimethyl-1-butene	84.51274	84.51129	-0.00002
C_8H_{16}	1-octene	96.34883	96.41421	0.00068
C_8H_{16}	trans-2,2-dimethyl-3-hexene	96.69846	96.68782	-0.00011
C_8H_{16}	3-ethyl-2-methyl-1-pentene	96.63483	96.61113	-0.00025
C_8H_{16}	2,4,4-trimethyl-1-pentene	96.61293	96.71684	0.00107
C_8H_{16}	2,4,4-trimethyl-2-pentene	96.67590	96.65880	-0.00018
$C_{10}H_{20}$	1-decene	120.66423	120.74240	0.00065
$C_{12}H_{24}$	1-dodecene	144.97963	145.07163	0.00063
$C_{16}H_{32}$	1-hexadecene	193.61043	193.71766	0.00055

Table 4. Summary results of alkynes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_4	propyne	29.42932	29.40432	-0.00085
C_4H_6	1-butyne	41.58702	41.55495	-0.00077
C_4H_6	2-butyne	41.72765	41.75705	0.00070
C_9H_{16}	1-nonyne	102.37552	102.35367	-0.00021

Table 5. Summary results of alkyl fluorides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CF_4	tetrafluoromethane	21.07992	21.016	-0.00303
CHF_3	trifluoromethane	19.28398	19.362	0.00405
CH_2F_2	difluoromethane	18.22209	18.280	0.00314
C_3H_7F	1-fluoropropane	41.86745	41.885	0.00041
C_3H_7F	2-fluoropropane	41.96834	41.963	-0.00012

Table 6. Summary results of alkyl chlorides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CCl_4	tetrachloromethane	13.43181	13.448	0.00123
$CHCl_3$	trichloromethane	14.49146	14.523	0.00217
CH_2Cl_2	dichloromethane	15.37248	15.450	0.00499
CH_3Cl	chloromethane	16.26302	16.312	0.00299
C_2H_5Cl	chloroethane	28.61064	28.571	-0.00138
C_3H_7Cl	1-chloropropane	40.76834	40.723	-0.00112
C_3H_7Cl	2-chloropropane	40.86923	40.858	-0.00028
C_4H_9Cl	1-chlorobutane	52.92604	52.903	-0.00044
C_4H_9Cl	2-chlorobutane	53.02693	52.972	-0.00104
C_4H_9Cl	1-chloro-2-methylpropane	52.99860	52.953	-0.00085
C_4H_9Cl	2-chloro-2-methylpropane	53.21057	53.191	-0.00037
$C_5H_{11}Cl$	1-chloropentane	65.08374	65.061	-0.00034
$C_5H_{11}Cl$	1-chloro-3-methylbutane	65.15630	65.111	-0.00069
$C_5H_{11}Cl$	2-chloro-2-methylbutane	65.36827	65.344	-0.00037
$C_5H_{11}Cl$	2-chloro-3-methylbutane	65.16582	65.167	0.00002
$C_6H_{13}Cl$	2-chlorohexane	77.34233	77.313	-0.00038
$C_8H_{17}Cl$	1-chlorooctane	101.55684	101.564	0.00007
$C_{12}H_{25}Cl$	1-chlorododecane	150.18764	150.202	0.00009
$C_{18}H_{37}Cl$	1-chlorooctadecane	223.13384	223.175	0.00018

Table 7. Summary results of alkyl bromides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CBr_4	tetrabromomethane	11.25929	11.196	-0.00566
$CHBr_3$	tribromomethane	12.87698	12.919	0.00323
CH_3Br	bromomethane	15.67551	15.732	0.00360
C_2H_5Br	bromoethane	28.03939	27.953	-0.00308
C_3H_7Br	1-bromopropane	40.19709	40.160	-0.00093
C_3H_7Br	2-bromopropane	40.29798	40.288	-0.00024
$C_5H_{10}Br_2$	2,3-dibromo-2-methylbutane	63.53958	63.477	-0.00098
$C_6H_{13}Br$	1-bromohexane	76.67019	76.634	-0.00047
$C_7H_{15}Br$	1-bromoheptane	88.82789	88.783	-0.00051
$C_8H_{17}Br$	1-bromooctane	100.98559	100.952	-0.00033
$C_{12}H_{25}Br$	1-bromododecane	149.61639	149.573	-0.00029
$C_{16}H_{33}Br$	1-bromohexadecane	198.24719	198.192	-0.00028

Table 8. Summary results of alkyl iodides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CHI_3	triiodomethane	10.35888	10.405	0.00444
CH_2I_2	diiodomethane	12.94614	12.921	-0.00195
CH_3I	iodomethane	15.20294	15.163	-0.00263
C_2H_5I	iodoethane	27.36064	27.343	-0.00066
C_3H_7I	1-iodopropane	39.51834	39.516	-0.00006
C_3H_7I	2-iodopropane	39.61923	39.623	0.00009
C_4H_9I	2-iodo-2-methylpropane	51.96057	51.899	-0.00119

Table 9. Summary results of alkene halides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_3Cl	chloroethene	22.46700	22.505	0.00170
C_3H_5Cl	2-chloropropene	35.02984	35.05482	0.00071

Table 10. Summary results of alcohols.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_4O	methanol	21.11038	21.131	0.00097
C_2H_6O	ethanol	33.40563	33.428	0.00066
C_3H_8O	1-propanol	45.56333	45.584	0.00046
C_3H_8O	2-propanol	45.72088	45.766	0.00098
$C_4H_{10}O$	1-butanol	57.72103	57.736	0.00026
$C_4H_{10}O$	2-butanol	57.87858	57.922	0.00074
$C_4H_{10}O$	2-methyl-1-propananol	57.79359	57.828	0.00060
$C_4H_{10}O$	2-methyl-2-propananol	58.15359	58.126	-0.00048
$C_5H_{12}O$	1-pentanol	69.87873	69.887	0.00011
$C_5H_{12}O$	2-pentanol	70.03628	70.057	0.00029
$C_5H_{12}O$	3-pentanol	70.03628	70.097	0.00087
$C_5H_{12}O$	2-methyl-1-butananol	69.95129	69.957	0.00008
$C_5H_{12}O$	3-methyl-1-butananol	69.95129	69.950	-0.00002
$C_5H_{12}O$	2-methyl-2-butananol	70.31129	70.246	-0.00092
$C_5H_{12}O$	3-methyl-2-butananol	69.96081	70.083	0.00174
$C_6H_{14}O$	1-hexanol	82.03643	82.054	0.00021
$C_6H_{14}O$	2-hexanol	82.19398	82.236	0.00052
$C_7H_{16}O$	1-heptanol	94.19413	94.214	0.00021
$C_8H_{18}O$	1-octanol	106.35183	106.358	0.00006
$C_8H_{18}O$	2-ethyl-1-hexananol	106.42439	106.459	0.00032
$C_9H_{20}O$	1-nonanol	118.50953	118.521	0.00010
$C_{10}H_{22}O$	1-decanol	130.66723	130.676	0.00007
$C_{12}H_{26}O$	1-dodecanol	154.98263	154.984	0.00001
$C_{16}H_{34}O$	1-hexadecanol	203.61343	203.603	-0.00005

Table 11. Summary results of ethers.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_6O	dimethyl ether	32.84496	32.902	0.00174
C_3H_8O	ethyl methyl ether	45.19710	45.183	-0.00030
$C_4H_{10}O$	diethyl ether	57.54924	57.500	-0.00086
$C_4H_{10}O$	methyl propyl ether	57.35480	57.355	0.00000
$C_4H_{10}O$	isopropyl methyl ether	57.45569	57.499	0.00075
$C_6H_{14}O$	dipropyl ether	81.86464	81.817	-0.00059
$C_6H_{14}O$	diisopropyl ether	82.06642	82.088	0.00026
$C_6H_{14}O$	t-butyl ethyl ether	82.10276	82.033	-0.00085
$C_7H_{16}O$	t-butyl isopropyl ether	94.36135	94.438	0.00081
$C_8H_{18}O$	dibutyl ether	106.18004	106.122	-0.00055
$C_8H_{18}O$	di-sec-butyl ether	106.38182	106.410	0.00027
$C_8H_{18}O$	di-t-butyl ether	106.36022	106.425	0.00061
$C_8H_{18}O$	t-butyl isobutyl ether	106.65628	106.497	-0.00218

Table 12. Summary results of 1° amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_5N	methylamine	23.88297	23.857	-0.00110
C_2H_7N	ethylamine	36.04067	36.062	0.00060
C_3H_9N	propylamine	48.19837	48.243	0.00092
$C_4H_{11}N$	butylamine	60.35607	60.415	0.00098
$C_4H_{11}N$	sec-butylamine	60.45696	60.547	0.00148
$C_4H_{11}N$	t-butylamine	60.78863	60.717	-0.00118
$C_4H_{11}N$	isobutylamine	60.42863	60.486	0.00094

Table 13. Summary results of 2° amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_7N	dimethylamine	35.76895	35.765	-0.00012
$C_4H_{11}N$	diethylamine	60.22930	60.211	-0.00030
$C_6H_{15}N$	dipropylamine	84.54470	84.558	0.00016
$C_6H_{15}N$	diisopropylamine	84.74648	84.846	0.00117
$C_8H_{19}N$	dibutylamine	108.86010	108.872	0.00011
$C_8H_{19}N$	diisobutylamine	109.00522	109.106	0.00092

Table 14. Summary results of 3° amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9N	trimethylamine	47.83338	47.761	-0.00152
$C_6H_{15}N$	triethylamine	84.30648	84.316	0.00012
$C_9H_{21}N$	tripropylamine	120.77958	120.864	0.00070

Table 15. Summary results of aldehydes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_2O	formaldehyde	15.64628	15.655	0.00056
C_2H_4O	acetaldehyde	28.18711	28.198	0.00039
C_3H_6O	propanal	40.34481	40.345	0.00000
C_4H_8O	butanal	52.50251	52.491	-0.00022
C_4H_8O	isobutanal	52.60340	52.604	0.00001
$C_5H_{10}O$	pentanal	64.66021	64.682	0.00034
$C_7H_{14}O$	heptanal	88.97561	88.942	-0.00038
$C_8H_{16}O$	octanal	101.13331	101.179	0.00045
$C_8H_{16}O$	2-ethylhexanal	101.23420	101.259	0.00025

Table 16. Summary results of ketones.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_6O	acetone	40.68472	40.672	-0.00031
C_4H_8O	2-butanone	52.84242	52.84	-0.00005
$C_5H_{10}O$	2-pentanone	65.00012	64.997	-0.00005
$C_5H_{10}O$	3-pentanone	65.00012	64.988	-0.00005
$C_5H_{10}O$	3-methyl-2-butanone	65.10101	65.036	-0.00099
$C_6H_{12}O$	2-hexanone	77.15782	77.152	-0.00008
$C_6H_{12}O$	3-hexanone	77.15782	77.138	-0.00025
$C_6H_{12}O$	2-methyl-3-pentanone	77.25871	77.225	-0.00043
$C_6H_{12}O$	3,3-dimethyl-2-butanone	77.29432	77.273	-0.00028
$C_7H_{14}O$	3-heptanone	89.31552	89.287	-0.00032
$C_7H_{14}O$	4-heptanone	89.31552	89.299	-0.00018
$C_7H_{14}O$	2,2-dimethyl-3-pentanone	89.45202	89.458	0.00007
$C_7H_{14}O$	2,4-dimethyl-3-pentanone	89.51730	89.434	-0.00093
$C_8H_{16}O$	2,2,4-trimethyl-3-pentanone	101.71061	101.660	-0.00049
$C_9H_{18}O$	2-nonanone	113.63092	113.632	0.00001
$C_9H_{18}O$	5-nonanone	113.63092	113.675	0.00039
$C_9H_{18}O$	2,6-dimethyl-4-heptanone	113.77604	113.807	0.00027

Table 17. Summary results of carboxylic acids.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_2O_2	formic acid	21.01945	21.036	0.00079
$C_2H_4O_2$	acetic acid	33.55916	33.537	-0.00066
$C_3H_6O_2$	propanoic acid	45.71686	45.727	0.00022
$C_4H_8O_2$	butanoic acid	57.87456	57.883	0.00015
$C_5H_{10}O_2$	pentanoic acid	70.03226	69.995	-0.00053
$C_5H_{10}O_2$	3-methylbutanoic acid	70.10482	70.183	0.00111
$C_5H_{10}O_2$	2,2-dimethylpropanoic acid	70.31679	69.989	-0.00468
$C_6H_{12}O_2$	hexanoic acid	82.18996	82.149	-0.00050
$C_7H_{14}O_2$	heptanoic acid	94.34766	94.347	0.00000
$C_8H_{16}O_2$	octanoic acid	106.50536	106.481	-0.00022
$C_9H_{18}O_2$	nonanoic acid	118.66306	118.666	0.00003
$C_{10}H_{20}O_2$	decanoic acid	130.82076	130.795	-0.00020
$C_{12}H_{24}O_2$	dodecanoic acid	155.13616	155.176	0.00026
$C_{14}H_{28}O_2$	tetradecanoic acid	179.45156	179.605	0.00085
$C_{15}H_{30}O_2$	pentadecanoic acid	191.60926	191.606	-0.00002
$C_{16}H_{32}O_2$	hexadecanoic acid	203.76696	203.948	0.00089
$C_{18}H_{36}O_2$	stearic acid	228.08236	228.298	0.00094
$C_{20}H_{40}O_2$	eicosanoic acid	252.39776	252.514	0.00046

Table 18. Summary results of carboxylic acid esters.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_4O_2$	methyl formate	32.71076	32.762	0.00156
$C_3H_6O_2$	methyl acetate	45.24849	45.288	0.00087
$C_6H_{12}O_2$	methyl pentanoate	81.72159	81.726	0.00005
$C_7H_{14}O_2$	methyl hexanoate	93.87929	93.891	0.00012
$C_8H_{16}O_2$	methyl heptanoate	106.03699	106.079	0.00040
$C_9H_{18}O_2$	methyl octanoate	118.19469	118.217	0.00018
$C_{10}H_{20}O_2$	methyl nonanoate	130.35239	130.373	0.00016
$C_{11}H_{22}O_2$	methyl decanoate	142.51009	142.523	0.00009
$C_{12}H_{24}O_2$	methyl undecanoate	154.66779	154.677	0.00006
$C_{13}H_{26}O_2$	methyl dodecanoate	166.82549	166.842	0.00010
$C_{14}H_{28}O_2$	methyl tridecanoate	178.98319	179.000	0.00009
$C_{15}H_{30}O_2$	methyl tetradecanoate	191.14089	191.170	0.00015
$C_{16}H_{32}O_2$	methyl pentadecanoate	203.29859	203.356	0.00028
$C_4H_8O_2$	propyl formate	57.76366	57.746	-0.00030
$C_4H_8O_2$	ethyl acetate	57.63888	57.548	-0.00157
$C_5H_{10}O_2$	isopropyl acetate	69.89747	69.889	-0.00013
$C_5H_{10}O_2$	ethyl propanoate	69.79658	69.700	-0.00139
$C_6H_{12}O_2$	butyl acetate	81.95428	81.873	-0.00099
$C_6H_{12}O_2$	t-butyl acetate	82.23881	82.197	-0.00051
$C_6H_{12}O_2$	methyl 2,2-dimethylpropanoate	82.00612	81.935	-0.00087
$C_7H_{14}O_2$	ethyl pentanoate	94.11198	94.033	-0.00084
$C_7H_{14}O_2$	ethyl 3-methylbutanoate	94.18454	94.252	0.00072
$C_7H_{14}O_2$	ethyl 2,2-dimethylpropanoate	94.39651	94.345	-0.00054
$C_8H_{16}O_2$	isobutyl isobutanoate	106.44313	106.363	-0.00075
$C_8H_{16}O_2$	propyl pentanoate	106.26968	106.267	-0.00003
$C_8H_{16}O_2$	isopropyl pentanoate	106.37057	106.384	0.00013
$C_9H_{18}O_2$	butyl pentanoate	118.42738	118.489	0.00052
$C_9H_{18}O_2$	sec-butyl pentanoate	118.52827	118.624	0.00081
$C_9H_{18}O_2$	isobutyl pentanoate	118.49994	118.576	0.00064

Table 19. Summary results of amides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO	formamide	23.68712	23.697	0.00041
C_2H_5NO	acetamide	36.15222	36.103	-0.00135
C_3H_7NO	propanamide	48.30992	48.264	-0.00094
C_4H_9NO	butanamide	60.46762	60.449	-0.00030
C_4H_9NO	2-methylpropanamide	60.51509	60.455	-0.00099
$C_5H_{11}NO$	pentanamide	72.62532	72.481	-0.00200
$C_5H_{11}NO$	2,2-dimethylpropanamide	72.67890	72.718	0.00054
$C_6H_{13}NO$	hexanamide	84.78302	84.780	-0.00004
$C_8H_{17}NO$	octanamide	109.09842	109.071	-0.00025

Table 20. Summary results of N-alkyl and N,N-dialkyl amides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_7NO	N,N-dimethylformamide	47.679454	47.574	0.00221
C_4H_9NO	N,N-dimethylacetamide	60.14455	59.890	-0.00426
$C_6H_{13}NO$	N-butylacetamide	84.63649	84.590	-0.00055

Table 21. Summary results of urea.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_4N_2O	urea	31.35919	31.393	0.00108

Table 22. Summary results of acid halide.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_3ClO	acetyl chloride	28.02174	27.990	-0.00115

Table 23. Summary results of acid anhydrides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_4H_6O_3$	acetic anhydride	56.94096	56.948	0.00013
$C_6H_{10}O_3$	propanoic anhydride	81.25636	81.401	0.00177

Table 24. Summary results of nitriles.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_3N	acetonitrile	25.72060	25.77	0.00174
C_3H_5N	propanenitrile	37.87830	37.94	0.00171
C_4H_7N	butanenitrile	50.03600	50.08	0.00082
C_4H_7N	2-methylpropanenitrile	50.13689	50.18	0.00092
C_5H_9N	pentanenitrile	62.19370	62.26	0.00111
C_5H_9N	2,2-dimethylpropanenitrile	62.47823	62.40	-0.00132
$C_7H_{13}N$	heptanenitrile	86.50910	86.59	0.00089
$C_8H_{15}N$	octanenitrile	98.66680	98.73	0.00069
$C_{10}H_{19}N$	decanenitrile	122.98220	123.05	0.00057
$C_{14}H_{27}N$	tetradecanenitrile	171.61300	171.70	0.00052

Table 25. Summary results of thiols.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
HS	hydrogen sulfide	3.77430	3.653	-0.03320
H_2S	dihydrogen sulfide	7.56058	7.605	0.00582
CH_4S	methanethiol	19.60264	19.575	-0.00141
C_2H_6S	ethanethiol	31.76034	31.762	0.00005
C_3H_8S	1-propanethiol	43.91804	43.933	0.00035
C_3H_8S	2-propanethiol	44.01893	44.020	0.00003
$C_4H_{10}S$	1-butanethiol	56.07574	56.089	0.00024
$C_4H_{10}S$	2-butanethiol	56.17663	56.181	0.00009
$C_4H_{10}S$	2-methyl-1-propanethiol	56.14830	56.186	0.00066
$C_4H_{10}S$	2-methyl-2-propanethiol	56.36027	56.313	-0.00084
$C_5H_{12}S$	2-methyl-1-butanethiol	68.30600	68.314	0.00012
$C_5H_{12}S$	1-pentanethiol	68.23344	68.264	0.00044
$C_5H_{12}S$	2-methyl-2-butanethiol	68.51797	68.441	-0.00113
$C_5H_{12}S$	3-methyl-2-butanethiol	68.31552	68.381	0.00095
$C_5H_{12}S$	2,2-dimethyl-1-propanethiol	68.16441	68.461	0.00433
$C_6H_{14}S$	1-hexanethiol	80.39114	80.416	0.00031
$C_6H_{14}S$	2-methyl-2-pentanethiol	80.67567	80.607	-0.00085
$C_7H_{16}S$	1-heptanethiol	92.54884	92.570	0.00023
$C_{10}H_{22}S$	1-decanethiol	129.02194	129.048	0.00020

Table 25. Summary results of sulfides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_6S	dimethyl sulfide	31.65668	31.672	0.00048
C_3H_8S	ethyl methyl sulfide	43.81438	43.848	0.00078
$C_4H_{10}S$	diethyl sulfide	55.97208	56.043	0.00126
$C_4H_{10}S$	methyl propyl sulfide	55.97208	56.029	0.00102
$C_4H_{10}S$	isopropyl methyl sulfide	56.07297	56.115	0.00075
$C_5H_{12}S$	butyl methyl sulfide	68.12978	68.185	0.00081
$C_5H_{12}S$	t-butyl methyl sulfide	68.28245	68.381	0.00144
$C_5H_{12}S$	ethyl propyl sulfide	68.12978	68.210	0.00117
$C_5H_{12}S$	ethyl isopropyl sulfide	68.23067	68.350	0.00174
$C_6H_{14}S$	diisopropyl sulfide	80.48926	80.542	0.00065
$C_6H_{14}S$	butyl ethyl sulfide	80.28748	80.395	0.00133
$C_6H_{14}S$	methyl pentyl sulfide	80.28748	80.332	0.00056
$C_8H_{18}S$	dibutyl sulfide	104.60288	104.701	0.00094
$C_8H_{18}S$	di-sec-butyl sulfide	104.80466	104.701	-0.00099
$C_8H_{18}S$	di-t-butyl sulfide	104.90822	104.920	0.00011
$C_8H_{18}S$	diisobutyl sulfide	104.74800	104.834	0.00082
$C_{10}H_{22}S$	dipentyl sulfide	128.91828	128.979	0.00047
$C_{10}H_{22}S$	diisopentyl sulfide	129.06340	129.151	0.00068

Table 27. Summary results of disulfides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6S_2$	dimethyl disulfide	34.48127	34.413	-0.00199
$C_4H_{10}S_2$	diethyl disulfide	58.79667	58.873	0.00129
$C_6H_{14}S_2$	dipropyl disulfide	83.11207	83.169	0.00068
$C_8H_{18}S_2$	di-t-butyl disulfide	107.99653	107.919	-0.00072

Table 28. Summary results of sulfoxides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_6SO	dimethyl sulfoxide	35.52450	35.435	-0.00253
$C_4H_{10}SO$	diethyl sulfoxide	59.83990	59.891	0.00085
$C_6H_{14}SO$	dipropyl sulfoxide	84.15530	84.294	0.00165

Table 29. Summary results of sulfones.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6SO_2$	dimethyl sulfone	40.27588	40.316	0.00100

Table 30. Summary results of sulfites.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6SO_3$	dimethyl sulfite	43.95058	44.042	0.00207
$C_4H_{10}SO_3$	diethyl sulfite	68.54939	68.648	0.00143
$C_8H_{18}SO_3$	dibutyl sulfite	117.18019	117.191	0.00009

Table 31. Summary results of sulfates.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_2H_6SO_4$	dimethyl sulfate	48.70196	48.734	0.00067
$C_4H_{10}SO_4$	diethyl sulfate	73.30077	73.346	0.00061
$C_6H_{14}SO_4$	dipropyl sulfate	97.61617	97.609	-0.00008

Table 32. Summary results of nitro alkanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO_2	nitromethane	25.14934	25.107	-0.00168
$C_2H_5NO_2$	nitroethane	37.30704	37.292	-0.00040
$C_3H_7NO_2$	1-nitropropane	49.46474	49.451	-0.00028
$C_3H_7NO_2$	2-nitropropane	49.56563	49.602	0.00074
$C_4H_9NO_2$	1-nitrobutane	61.62244	61.601	-0.00036
$C_4H_9NO_2$	2-nitroisobutane	61.90697	61.945	0.00061
$C_5H_{11}NO_2$	1-nitropentane	73.78014	73.759	-0.00028

Table 33. Summary results of nitrite.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO_2	methyl nitrite	24.92328	24.955	0.00126

Table 34. Summary results of nitrate.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_3NO_3	methyl nitrate	28.18536	28.117	-0.00244
$C_2H_5NO_3$	ethyl nitrate	40.34306	40.396	0.00131
$C_3H_7NO_3$	propyl nitrate	52.50076	52.550	0.00093
$C_3H_7NO_3$	isopropyl nitrate	52.60165	52.725	0.00233

Table 35. Summary results of conjugated alkenes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_5H_8	cyclopentene	54.83565	54.86117	0.00047
C_4H_6	1,3 butadiene	42.09159	42.12705	0.00084
C_5H_8	1,3 pentadiene	54.40776	54.42484	0.00031
C_5H_8	1,4 pentadiene	54.03745	54.11806	0.00149
C_5H_6	1,3 cyclopentadiene	49.27432	49.30294	0.00058

Table 36 Summary results of aromatics and heterocyclic aromatics.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_6H_6	benzene	57.26008	57.26340	0.00006
C_6H_5Cl	fluorobenzene	57.93510	57.887	-0.00083
C_6H_5Cl	chlorobenzene	56.55263	56.581	0.00051
$C_6H_4Cl_2$	m-dichlorobenzene	55.84518	55.852	0.00012
$C_6H_3Cl_3$	1,2,3-trichlorobenzene	55.13773	55.077	-0.00111
$C_6H_3Cl_3$	1,3,5-trichlorbenzene	55.29542	55.255	-0.00073
C_6Cl_6	hexachlorobenzene	52.57130	52.477	-0.00179
C_6H_5Br	bromobenzene	56.17932	56.391[a]	0.00376
C_6H_5I	iodobenzene	55.25993	55.261	0.00001
$C_6H_5NO_2$	nitrobenzene	65.18754	65.217	0.00046
C_7H_8	toluene	69.48425	69.546	0.00088
$C_7H_6O_2$	benzoic acid	73.76938	73.762	-0.00009
$C_7H_5ClO_2$	2-chlorobenzoic acid	73.06193	73.082	0.00027
$C_7H_5ClO_2$	3-chlorobenzoic acid	73.26820	73.261	-0.00010
C_6H_7N	aniline	64.43373	64.374	-0.00093
C_7H_9N	2-methylaniline	76.62345	76.643	-0.00025
C_7H_9N	3-methylaniline	76.62345	76.661	0.00050
C_7H_9N	4-methylaniline	76.62345	76.654	0.00040
$C_6H_6N_2O_2$	2-nitroaniline	72.47476	72.424	-0.00070
$C_6H_6N_2O_2$	3-nitroaniline	72.47476	72.481	-0.00009
$C_6H_6N_2O_2$	4-nitroaniline	72.47476	72.476	-0.00002
$C_7H_7NO_2$	aniline-2-carboxylic acid	80.90857	80.941	0.00041
$C_7H_7NO_2$	aniline-3-carboxylic acid	80.90857	80.813	-0.00118
$C_7H_7NO_2$	aniline-4-carboxylic acid	80.90857	80.949	0.00050
C_6H_6O	phenol	61.75817	61.704	-0.00087
$C_6H_4N_2O_5$	2,4-dinitrophenol	77.61308	77.642	0.00037
C_6H_8O	anisole	73.39006	73.355	-0.00047
$C_{10}H_8$	naphthalene	90.74658	90.79143	0.00049
C_4H_5N	pyrrole	44.81090	44.785	-0.00057
C_4H_4O	furan	41.67782	41.692	0.00033
C_4H_4S	thiophene	40.42501	40.430	0.00013
$C_3H_4N_2$	imidazole	39.76343	39.74106	-0.00056
C_5H_5N	pyridine	51.91802	51.87927	-0.00075
$C_4H_4N_2$	pyrimidine	46.57597	46.51794	-0.00125
$C_4H_4N_2$	pyrazine	46.57597	46.51380	0.00095
C_9H_7N	quinoline	85.40453	85.48607	0.00178
C_9H_7N	isoquinoline	85.40453	85.44358	0.00046
C_8H_7N	indole	78.52215	78.514	-0.00010

[a] Liquid.

Table 37. Summary results of DNA bases.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_5H_5N_5$	adenine	70.85416	70.79811	-0.00079
$C_5H_6N_2O_2$	thymine	69.08792	69.06438	-0.00034
$C_5H_5N_5O$	guanine	76.88212	77.41849	-0.00055
$C_4H_5N_3O$	cytosine	59.53378	60.58056	0.01728

Table 38. Summary results of alkyl phosphines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9P	trimethylphosphine	45.80930	46.87333	0.02270
$C_6H_{15}P$	triethylphosphine	82.28240	82.24869	-0.00041
$C_{18}H_{15}P$	triphenylphosphine	168.40033	167.46591	-0.00558

Table 39. Summary results of alkyl phosphites.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_3H_9O_3P$	trimethyl phosphite	61.06764	60.94329	-0.00204
$C_6H_{15}O_3P$	triethyl phosphite	98.12406	97.97947	-0.00148
$C_9H_{21}O_3P$	tri-isopropyl phosphite	134.89983	135.00698	0.00079

Table 40. Summary results of alkyl phosphine oxides.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9PO	trimethylphosphine oxide	53.00430	52.91192	-0.00175

Table 41. Summary results of alkyl phosphates.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_6H_{15}O_4P$	triethyl phosphate	105.31906	104.40400	-0.00876
$C_9H_{21}O_4P$	tri-n-propyl phosphate	141.79216	140.86778	-0.00656
$C_9H_{21}O_4P$	tri-isopropyl phosphate	142.09483	141.42283	-0.00475
$C_9H_{27}O_4P$	tri-n-butyl phosphate	178.26526	178.07742	-0.00105

Table 42. Summary results of monosaccharides of DNA and RNA.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_5H_{10}O_4$	2-deoxy-D-ribose	77.25842		
$C_5H_{10}O_5$	D-ribose	81.51034	83.498[a]	0.02381
$C_5H_{10}O_4$	alpha-2-deoxy-D-ribose	77.46684		
$C_5H_{10}O_5$	alpha-D-ribose	82.31088		

[a] Crystal

Table 43. Summary results of amino acids.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_4H_7NO_4$	aspartic acid	68.98109	70.843[a]	0.02628
$C_5H_9NO_4$	glutamic acid	81.13879	83.167[a]	0.02438
$C_3H_7NO_4S$	cysteine	55.02457	56.571[a]	0.02733
$C_6H_{14}N_2O_2$	lysine	95.77799	98.194[a]	0.02461
$C_6H_{14}N_2O_2$	arginine	105.07007	107.420[a]	0.02188
$C_6H_9N_3O_2$	histidine	88.10232	89.599[a]	0.01671
$C_4H_8N_2O_2$	asparagine	71.57414	73.513[a]	0.02637
$C_5H_{10}N_2O_2$	glutamine	83.73184	85.843[a]	0.02459
$C_4H_9NO_3$	threonine	68.95678	71.058[a]	0.02956
$C_9H_{11}NO_3$	tyrosine	109.40427	111.450[a]	0.01835
$C_3H_7NO_3$	serine	56.66986	58.339[a]	0.02861
$C_{11}H_{12}N_2O_2$	tryptophan	126.74291	128.084[a]	0.01047
$C_9H_{11}NO_2$	phenylalanine	104.90618	105.009	0.00098
$C_5H_9NO_2$	proline	71.76826	71.332	-0.00611
$C_5H_9NO_2$	methionine	79.23631	79.214	-0.00028
$C_6H_{13}NO_2$	leucine	89.12115	89.047	-0.00083
$C_6H_{13}NO_2$	isoleucine	89.02978	90.612	0.01746
$C_6H_{13}NO_2$	valine	76.87208	76.772	-0.00130
$C_3H_7NO_2$	alanine	52.57549	52.991	0.00785
$C_2H_5NO_2$	glycine	40.28857	40.280	-0.00021

[a] Crystal

Table 44. Summary results of allotropes of carbon.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_n	diamond	3.74829	3.704	-0.01
C_{60}	fullerene	419.75539	419.73367	-0.00005
C_n	graphite	4.91359	4.89866	-0.00305

Table 45. Summary results of silanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
SiH	silylidyne	3.07526	3.02008	-0.01827
SiH_2	silylene	6.15052	6.35523	0.03221
SiH_3	silyl	9.22578	9.36494	0.01486
SiH_4	silane	13.57257	13.34577	-0.01699
Si_2H_6	disilane	21.76713	22.05572	0.01308
Si_3H_8	trisilane	31.23322	30.81334	-0.01363

Table 46. Summary results of alkyl silanes and disilanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_6Si	methylsilane	25.37882	25.99491	0.02370
C_2H_8Si	dimethylsilane	38.45660	38.64819	0.00496
$C_3H_{10}Si$	trimethylsilane	51.53438	51.33567	-0.00387
$C_4H_{12}Si$	tetramethylsilane	64.61216	64.22319	-0.00606
$C_4H_{12}Si$	diethylsilane	62.77200	63.37771	0.00956
$C_6H_{16}Si$	triethylsilane	88.00748	87.46141	-0.00624
$C_8H_{20}Si$	tetraethylsilane	113.24296	112.06547	-0.01051
CH_8Si_2	methyldisilane	34.56739	34.73920	0.00495
$C_2H_{10}Si_2$	1,1-dimethyldisilane	47.36764	47.42283	0.00116
$C_2H_{10}Si_2$	1,2-dimethyldisilane	47.36764	47.42283	0.00116
$C_3H_{12}Si_2$	1,1,1-trimethyldisilane	60.16789	60.10646	-0.00102
$C_3H_{12}Si_2$	1,1,2-trimethyldisilane	60.16789	60.10646	-0.00102
$C_4H_{14}Si_2$	1,1,1,2-tetramethyldisilane	72.96815	72.79442	-0.00239
$C_4H_{14}Si_2$	1,1,2,2-tetramethyldisilane	72.96815	72.79442	-0.00239
$C_5H_{16}Si_2$	1,1,1,2,2-pentamethyldisilane	85.76840	85.47805	-0.00340
$C_6H_{18}Si_2$	hexamethyldisilane	98.56865	98.32646	-0.00246

Table 47. Summary results of silicon oxides, silicic acids, silanols, siloxanes, and disiloxanes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
SiO	silicon oxide	8.30876	8.29905	-0.00117
SiO_2	silicon dioxide	12.94190	12.98073	0.00299
SiH_4O	H_3SiOH	18.67184	19.00701[a]	0.01763
SiH_4O_2	$H_2Si(OH)_2$	25.04264	25.04264 [a]	0.00563
SiH_4O_3	$HSi(OH)_3$	31.41344	31.47012[a]	0.00180
SiH_4O_4	$Si(OH)_4$	37.78423	38.03638	0.00663
$C_3H_{10}SiO$	trimethylsilanol	57.31895	57.30073	-0.00032
C_2H_6SiO	vinylsilanol	37.33784		
CH_6SiO_4	$(HO)_3SiOCH_3$	47.45144	49.28171[a]	0.03714
$C_4H_{12}SiO_4$	tetramethoxysilioxane	83.48783	84.04681	0.00665
$C_6H_{16}SiO_3$	triethoxysilioxane	102.74755	102.57961	-0.00164
$C_8H_{20}SiO_4$	tetraethoxysilioxane	132.89639	133.23177	0.00252
$C_6H_{18}Si_3O_3$	$((CH_3)_2SiO)_3$	123.61510	123.22485	-0.00317
$C_8H_{24}Si_4O_4$	$((CH_3)_2SiO)_4$	164.82014	164.79037	-0.00018
$C_{10}H_{30}Si_5O_5$	$((CH_3)_2SiO)_5$	206.02517	206.35589	0.00160
$C_6H_{18}Si_2O$	hexamethyldisiloxane	105.24639	105.20196	-0.00042

[a] theory

Table 48. Summary results of boranes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
BB	diboron	3.12475	3.10405	-0.00667
B_2H_6	diborane	24.94229	24.89030	-0.00209
B_4H_{10}	tetraborane(10)	44.92160	45.33134	0.00904
B_5H_9	pentaborane(9)	48.25462	48.85411	0.01227
B_5H_{11}	pentaborane(11)	54.00546	53.06086	-0.01780
B_6H_{10}	hexaborane(10)	56.55063	56.74739	0.00347
B_9H_{15}	nonaborane(15)	85.61380	84.95008	-0.00781
$B_{10}H_{14}$	decaborane(14)	89.73467	89.69790	-0.00041

Table 49. Summary results of alkyl boranes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CH_5B	methylborane	24.60991	24.49350	-0.00475
C_2H_7B	dimethylborane	37.08821	37.17713	0.00239
B_2CH_8	methyldiborane	37.42060	37.58259	0.00431
$B_2C_2H_{10}$	ethyldiborane	49.57830	49.50736	-0.00143
C_3H_9B	trimethylboron	49.56652	49.76102	0.00391
$B_2C_2H_{10}$	1,1-dimethyldiborane	49.89890	50.20118	0.00602
$B_2C_2H_{10}$	1,2-dimethyldiborane	49.89890	50.20118	0.00602
B_4CH_{12}	methyltetraborane	57.39990	57.74604	0.00599
B_5CH_{11}	methylpentaborane	60.73292	61.51585	0.01273
$B_2C_3H_{12}$	trimethyldiborane	62.37721	62.88481	0.00807
$B_4C_2H_{14}$	ethyltetraborane	69.55760	69.99603	0.00626
$B_5C_2H_{13}$	ethylpentaborane	72.89062	73.76585	0.01186
$B_2C_4H_{14}$	1,1-diethyldiborane	74.21430	74.34420	0.00175
$B_2C_4H_{14}$	tetramethyldiborane	74.85551	75.48171	0.00830
$B_5C_3H_{15}$	propylpentaborane	85.04832	85.84239	0.00925
$C_6H_{15}B$	triethylboron	86.03962	86.12941	0.00104
$B_2C_6H_{18}$	triethyldiborane	98.85031	98.59407	-0.00260
$B_{10}CH_{16}$	methyldecaborane	102.21298	101.91775	-0.00290
$C_8H_{17}B$	n-butylboracyclopentane	105.35916	105.69874[a]	0.00321
$B_{10}C_2H_{18}$	ethyldecaborane	114.37068	113.56066	-0.00713
$C_9H_{21}B$	tripropylboron	122.51272	122.59753	0.00069
$C_9H_{21}B$	tri-isopropylboron	122.81539	122.75798	-0.00047
$B_2C_8H_{22}$	tetraethyldiborane	123.48631	123.74017	0.00205
$B_{10}C_3H_{20}$	propyldecaborane	126.52838	125.94075	-0.00467
$C_{12}H_{27}B$	tri-s-butylboron	159.28849	158.50627	-0.00493
$C_{12}H_{27}B$	tributylboron	158.98582	159.03530	0.00031
$C_{12}H_{27}B$	tri-isobutylboron	159.20350	159.34318	0.00088
$C_{18}H_{15}B$	triphenylboron	172.15755	172.09681	-0.00035
$C_{15}H_{33}B$	tri-3-methylbutylboron	195.67660	195.78095	0.00053
$C_{18}H_{33}B$	tricyclohexylboron	217.24711	218.23763	0.00454
$C_{18}H_{39}B$	tri-n-hexylboron	231.93202	231.76340	-0.00073
$C_{21}H_{45}B$	tri-n-heptylboron	268.40512	268.22285	-0.00068
$C_{24}H_{51}B$	tri-s-octylboron	305.18089	304.61292	-0.00186
$C_{24}H_{51}B$	tri-n-octylboron	304.87822	304.68230	-0.00064

[a] Crystal.

Table 50. Summary results of alkoxy boranes and borinic acids.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
BH_3O	hydroxyborane	18.29311	18.22572	-0.00370
BH_3O_2	dihydroxyborane	24.45460	24.43777	-0.00069
BH_3O_3	boric acid	30.61610	30.68431	0.00222
$BC_2H_7O_2$	dimethoxyborane	47.75325	47.72358	-0.00062
$BC_3H_9O_3$	trimethyl borate	65.56408	65.53950	-0.00037
$C_5H_{11}OB$	methoxyboracyclopentane	71.24858	74.47566[a]	0.00345
$C_6H_7O_2B$	phenylborinic acid	77.79659	78.86121[a]	0.01350
$C_6H_{15}O_2B$	di-isoproxyborane	96.97471	97.41737[a]	0.00454
$BC_6H_{15}O_3$	triethyl borate	102.62050	102.50197	-0.00116
$C_8H_{19}OB$	di-n-butylborinic acid	116.19591	116.45117	0.00219
$BC_9H_{21}O_3$	tri-n-propyl borate	139.09360	139.11319	0.00014
$C_{12}H_{27}OB$	N-butyl di-n-butylborinate	164.51278	165.29504[a]	0.00473
$C_{12}H_{27}O_2B$	di-n-butyl n-butylboronate	170.03974	170.86964[a]	0.00486
$BC_{12}H_{27}O_3$	tri-n-butyl borate	175.56670	175.62901	0.00035
$C_{18}H_{15}O_3B_3$	phenylborinic anhydride	204.75082	205.96548[a]	0.00590
$C_{16}H_{36}OB_2$	di-n-butylborinic anhydride	222.84551	223.70232[a]	0.00383
$C_{24}H_{20}OB_2$	diphenylborinic anhydride	240.40782	241.38941[a]	0.00407

[a] Crystal.

Table 51. Summary results of tertiary and quaternary amino boranes and borane amines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
B_2H_7N	aminodiborane	32.36213	31.99218	-0.01156
$B_2C_2H_{11}N$	N-dimethylaminodiborane	57.21517	57.52855	0.00545
$C_6H_{18}N_3B$	tris(dimethylamino)borane	108.95023	108.64490	-0.00281
$C_8H_{20}NB$	di-n-butylboronamine	117.45425	119.49184 [a]	0.01705
$C_{12}H_{28}NB$	di-n-butylboron-n-butylamine	166.49595	167.83269 [a]	0.00796
$C_2H_{10}NB$	dimethylaminoborane	49.30740	49.52189	0.00433
$BC_3H_{12}N$	trimethylaminoborane	61.37183	61.05205	-0.00524
$BC_3H_{12}N$	ammonia-trimethylborane	62.91857	62.52207	-0.00634
$C_6H_{18}NB$	triethylaminoborane	97.84493	97.42044	-0.00436
$BC_6H_{18}N$	trimethylaminotrimethylborane	98.80674	98.27036	-0.00546

[a] Crystal.

Table 52. Summary results of halidoboranes.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
HBF_2	difluoroboron	17.55666	17.41845	-0.00793
BF_3	boron trifluoride	20.26918	20.09744	-0.00855
BF_2HO	difluoroborinic acid	23.71816	23.64784	-0.00297
BFH_2O_2	fluoroboronic acid	27.16713	27.18135	0.00052
BCH_3F_2	difluoro-methyl-borane	30.03496	30.33624	0.00993
$BC_2H_3F_2$	vinyldifluoroborane	36.21893	36.54981	0.00905
$BC_3H_9NF_3$	trimethylamine-trifluoroborane	69.50941	69.11368	-0.00573
$HBCl_2$	dichloroboron	13.21640	13.25291	0.00276
BCl_3	boron trichloride	13.75879	13.80748	0.00353
BCl_2F	dichlorofluoroborane	15.92892	15.87507	-0.00339
$BClF_2$	chlorodifluoroborane	18.09905	17.98169	-0.00653
$C_2H_5OCl_2B$	ethoxydichloroborane	43.37936	43.55732	0.00409
$C_2H_4O_2ClB$	2-chloro-1,3,2-dioxaborolan	43.68867	43.99361[a]	0.00693
$C_2H_6NCI_2B$	dimethylaminodichloroborane	45.48927	45.73940	0.00547
$BC_2ClH_60_2$	dimethoxychloroborane	48.29565	48.40390	0.00224
$C_3H_6O_2ClB$	4-methyl-2-chloro-1,3,2-dioxaborolan	55.94726	56.39537[a]	0.00795
$BC_6H_5Cl_2$	phenylboron dichloride	66.55838	66.97820	0.00627
$C_4H_8O_2ClB$	4,5-dimethyl-2-chloro-1,3,2-dioxaborolan	68.23418	68.72342[a]	0.00712
$C_4H_{10}O_2ClB$	diethoxychloroborane	72.99993	73.07735	0.00106
$C_4H_{12}N_2ClB$	bis(dimethlamino) chloroborane	77.21975	77.38078	0.00208
$C_8H_{18}ClB$	di-n-butylchloroborane	110.57681	110.99317	0.00375
$C_{12}H_{10}ClB$	diphenylchloroborane	119.35796	119.79335	0.00363

[a] Crystal.

Table 53. Summary results of organoaluminum.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_2H_7Al	dimethylaluminum hydride	34.31171	34.37797[a]	0.00193
C_3H_9Al	trimethyl aluminum	47.10960	46.95319	-0.00333
$C_4H_{11}Al$	diethylaluminum hydride	58.62711	60.10948[b]	0.02466
$C_6H_{15}Al$	triethylaluminum hydride	83.58270	83.58176	-0.00001
$C_6H_{15}Al$	di-n-propylaluminum hydride	82.94251	84.40566[b]	0.01733
$C_9H_{21}Al$	tri-n-propyl aluminum	120.05580	121.06458[b]	0.00833
$C_8H_{19}Al$	di-n-butylaluminum hydride	107.25791	108.71051[b]	0.01336
$C_8H_{19}Al$	di-isobutylaluminum hydride	107.40303	108.77556[b]	0.01262
$C_{12}H_{27}Al$	tri-n-butyl aluminum	156.52890	157.42429[b]	0.00569
$C_{12}H_{27}Al$	tri-isobutyl aluminum	156.74658	157.58908[b]	0.00535

[a] Estimated.
[b] Crystal

Table 54. Summary results of scandium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
ScF	scandium fluoride	6.34474	6.16925	-0.02845
ScF_2	scandium difluoride	12.11937	12.19556	0.00625
ScF_3	scandium trifluoride	19.28412	19.27994	-0.00022
ScCl	scandium chloride	4.05515	4.00192	-0.01330
ScO	scandium oxide	7.03426	7.08349	0.00695

Table 55. Summary results of titanium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
TiF	titanium fluoride	6.44997	6.41871	-0.00487
TiF_2	titanium difluoride	13.77532	13.66390	-0.00815
TiF_3	titanium trifluoride	19.63961	19.64671	0.00036
TiF_4	titanium tetrafluoride	24.66085	24.23470	-0.01758
TiCl	titanium chloride	4.56209	4.56198	-0.00003
$TiCl_2$	titanium dichoride	10.02025	9.87408	-0.01517
$TiCl_3$	titanium trichloride	14.28674	14.22984	-0.00400
$TiCl_4$	titanium tetrachloride	17.94949	17.82402	-0.00704
TiBr	titanium bromide	3.77936	3.78466	0.00140
$TiBr_2$	titanium dibromide	8.91650	8.93012	0.00153
$TiBr_3$	titanium tribromide	12.07765	12.02246	-0.00459
$TiBr_4$	titanium tetrabromide	14.90122	14.93239	0.00209
TiI	titanium iodide	3.16446	3.15504	-0.00299
TiI_2	titanium diiodide	7.35550	7.29291	-0.00858
TiI_3	titanium triiodide	9.74119	9.71935	-0.00225
TiI_4	titanium tetraiodide	12.10014	12.14569	0.00375
TiO	titanium oxide	7.02729	7.00341	-0.00341
TiO_2	titanium dioxide	13.23528	13.21050	-0.00188
TiOF	titanium fluoride oxide	12.78285	12.77353	-0.00073
$TiOF_2$	titanium difluoride oxide	18.94807	18.66983	-0.01490
TiOCl	titanium chloride oxide	11.10501	11.25669	0.01347
$TiOCl_2$	titanium dichloride oxide	15.59238	15.54295	-0.00318

Table 56. Summary results of vanadium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
VF_5	vanadium pentafluoride	24.06031	24.24139	0.00747
VCl_4	vanadium tetrachloride	15.84635	15.80570	-0.00257
VN	vanadium nitride	4.85655	4.81931	-0.00775
VO	vanadium oxide	6.37803	6.60264	0.03402
VO_2	vanadium dioxide	12.75606	12.89729	0.01095
$VOCl_3$	vanadium trichloride oxide	18.26279	18.87469	0.03242
$V(CO)_6$	vanadium hexacarbonyl	75.26791	75.63369	0.00484
$V(C_6H_6))_2$	dibenzene vanadium	119.80633	121.20193[a]	0.01151

[a] Liquid.

Table 57. Summary results of chromium coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CrF_2	chromium difluoride	10.91988	10.92685	0.00064
$CrCl_2$	chromium dichloride	7.98449	7.96513	-0.00243
CrO	chromium oxide	4.73854	4.75515	0.00349
CrO_2	chromium dioxide	10.02583	10.04924	0.00233
CrO_3	chromium trioxide	14.83000	14.85404	0.00162
CrO_2Cl_2	chromium dichloride dioxide	17.46158	17.30608	-0.00899
$Cr(CO)_6$	chromium hexacarbonyl	74.22588	74.61872	0.00526
$Cr(C_6H_6)_2$	dibenzene chromium	117.93345	117.97971	0.00039
$Cr((CH_3)_3C_6H_3)_2$	di-(1,2,4-trimethylbenzene) chromium	191.27849	192.42933[a]	0.00598

[a] Liquid.

Table 58. Summary results of manganese coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
MnF	manganese fluoride	4.03858	3.97567	-0.01582
MnCl	manganese chloride	3.74528	3.73801	-0.00194
$Mn_2(CO)_{10}$	dimanganese decacarbonyl	123.78299	122.70895	-0.00875

Table 59. Summary results of iron coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
FeF	iron fluoride	4.65726	4.63464	-0.00488
FeF_2	iron difluoride	10.03188	9.98015	-0.00518
FeF_3	iron trifluoride	15.31508	15.25194	-0.00414
FeCl	iron chloride	2.96772	2.97466	0.00233
$FeCl_2$	iron dichoride	8.07880	8.28632	0.02504
$FeCl_3$	iron trichloride	10.82348	10.70065	-0.01148
FeO	iron oxide	4.09983	4.20895	0.02593
$Fe(CO)_5$	iron pentacarbonyl	61.75623	61.91846	0.00262
$Fe(C_5H_5)_2$	bis-cylopentadienyl iron (ferrocene)	98.90760	98.95272	0.00046

Table 60. Summary results of cobalt coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CoF_2	cobalt difluoride	9.45115	9.75552	0.03120
CoCl	cobalt chloride	3.66504	3.68049	0.00420
CoI_2	cobalt dichloride	7.98467	7.92106	-0.00803
$CoCl_3$	cobalt trichloride	9.83521	9.87205	0.00373
$CoH(CO)_4$	cobalt tetracarbonyl hydride	50.33217	50.36087	0.00057

Table 61. Summary results of nickel coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
NiCl	nickel chloride	3.84184	3.82934	-0.00327
$NiCl_2$	nickel dichloride	7.76628	7.74066	-0.00331
$Ni(CO)_4$	nickel tetracarbonyl	50.79297	50.77632	-0.00033
$Ni(C_5H_5)_2$	bis-cylopentadienyl nickel (nickelocene)	97.73062	97.84649	0.00118

Table 62. Summary results of copper coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
CuF	copper fluoride	4.39399	4.44620	0.01174
CuF_2	copper difluoride	7.91246	7.89040	-0.00280
CuCl	copper chloride	3.91240	3.80870	-0.02723
CuO	copper oxide	2.93219	2.90931	-0.00787

Table 63. Summary results of zinc coordinate compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
ZnCl	zinc chloride	2.56175	2.56529	0.00138
$ZnCl_2$	zinc dichloride	6.68749	6.63675	-0.00764
$Zn(CH_3)_2$	dimethylzinc	29.35815	29.21367	-0.00495
$(CH_3CH_2)_2Zn$	diethylzinc	53.67355	53.00987	-0.01252
$(CH_3CH_2CH_2)_2Zn$	di-n-propylzinc	77.98895	77.67464	-0.00405
$(CH_3CH_2CH_2CH_2)_2Zn$	di-n-butylzinc	102.30435	101.95782	-0.00340

Table 64. Summary results of germanium compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_8H_{20}Ge$	tetraethylgermanium	109.99686	110.18166	0.00168
$C_{12}H_{28}Ge$	tetra-n-propylgermanium	158.62766	158.63092	0.00002
$C_{12}H_{30}Ge_2$	hexaethyldigermanium	167.88982	167.89836	0.00005

Table 65. Summary results of tin compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$SnCl_4$	tin tetrachloride	12.95756	13.03704	0.00610
CH_3Cl_3Sn	methyltin trichloride	24.69530	25.69118[a]	0.03876
$C_2H_6Cl_2Sn$	dimethyltin dichloride	36.43304	37.12369	0.01860
C_3H_9ClSn	trimethylin chloride	48.17077	49.00689	0.01706
$SnBr_4$	tin tetrabromide	10.98655	11.01994	0.00303
C_3H_9BrSn	trimethyltin bromide	47.67802	48.35363	0.01397
$C_{12}H_{10}Br_2Sn$	diphenyltin dibromide	117.17489	117.36647[a]	0.00163
$C_{12}H_{27}BrSn$	tri-n-butyltin bromide	157.09732	157.26555[a]	0.00107
$C_{18}H_{15}BrSn$	triphenyltin bromide	170.26905	169.91511[a]	-0.00208
SnI_4	tin tetraiodide	9.71697	9.73306	0.00165
C_3H_9ISn	trimethyltin iodide	47.36062	47.69852	0.00708
$C_{18}H_{15}SnI$	triphenyltin iodide	169.95165	167.87948[a]	-0.01234
SnO	tin oxide	5.61858	5.54770	-0.01278
SnH_4	stannane	10.54137	10.47181	-0.00664
C_2H_8Sn	dimethylstannane	35.22494	35.14201	-0.00236
$C_3H_{10}Sn$	trimethylstannane	47.56673	47.77353	0.00433
$C_4H_{12}Sn$	diethylstannane	59.54034	59.50337	-0.00062
$C_4H_{12}Sn$	tetramethyltin	59.90851	60.13973	0.00384
$C_5H_{12}Sn$	trimethylvinyltin	66.08296	66.43260	0.00526
$C_5H_{14}Sn$	trimethylethyltin	72.06621	72.19922	0.00184
$C_6H_{16}Sn$	trimethylisopropyltin	84.32480	84.32346	-0.00002
$C_8H_{12}Sn$	tetravinyltin	84.64438	86.53803[a]	0.02188
$C_6H_{18}Sn_2$	hexamethyldistannane	91.96311	91.75569	-0.00226
$C_7H_{18}Sn$	trimethyl-t-butyltin	96.81417	96.47805	-0.00348
$C_9H_{14}Sn$	trimethylphenyltin	100.77219	100.42716	-0.00344
$C_8H_{18}Sn$	triethylvinyltin	102.56558	102.83906[a]	-0.00266
$C_8H_{20}Sn$	tetraethyltin	108.53931	108.43751	-0.00094
$C_{10}H_{16}Sn$	trimethylbenzyltin	112.23920	112.61211	0.00331
$C_{10}H_{14}O_2Sn$	trimethyltin benzoate	117.28149	119.31199[a]	0.01702
$C_{10}H_{20}Sn$	tetra-allyltin	133.53558	139.20655[a]	0.04074
$C_{12}H_{28}Sn$	tetra-n-propyltin	157.17011	157.01253	-0.00100
$C_{12}H_{28}Sn$	tetraisopropyltin	157.57367	156.9952	-0.00366
$C_{12}H_{30}Sn_2$	hexaethyldistannane	164.90931	164.76131[a]	-0.00090
$C_{19}H_{18}Sn$	triphenylmethyltin	182.49954	180.97881[a]	-0.00840
$C_{20}H_{20}Sn$	triphenylethyltin	194.65724	192.92526[a]	-0.00898
$C_{16}H_{36}Sn$	tetra-n-butyltin	205.80091	205.60055	-0.00097
$C_{16}H_{36}Sn$	tetraisobutyltin	206.09115	206.73234	0.00310
$C_{21}H_{24}Sn_2$	triphenyl-trimethyldistannane	214.55414	212.72973[a]	-0.00858
$C_{24}H_{20}Sn$	tetraphenyltin	223.36322	221.61425	-0.00789
$C_{24}H_{44}Sn$	tetracyclohexyltin	283.70927	284.57603	0.00305
$C_{36}H_{30}Sn_2$	hexaphenyldistannane	337.14517	333.27041	-0.01163

[a] Crystal.

Table 66. Summary results of lead compounds.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
$C_4H_{12}Pb$	tetramethyl-lead	57.55366	57.43264	-0.00211
$C_8H_{20}Pb$	tetraethyl-lead	106.18446	105.49164	-0.00657

Table 67. Summary results of alkyl arsines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9As	trimethylarsine	44.73978	45.63114	0.01953
$C_6H_{15}As$	triethylarsine	81.21288	81.01084	-0.00249
$C_{18}H_{15}As$	triphenylarsine	167.33081	166.49257	-0.00503

Table 68. Summary results of alkyl stibines.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9Sb	trimethylstibine	44.73078	45.02378	0.00651
$C_6H_{15}Sb$	triethylstibine	81.20388	80.69402	-0.00632
$C_{18}H_{15}Sb$	triphenylstibine	167.32181	165.81583	-0.00908

Table 69. Summary results of alkyl bismuths.

Formula	Name	Calculated Total Bond Energy (eV)	Experimental Total Bond Energy (eV)	Relative Error
C_3H_9Bi	trimethylbismuth	42.07387	42.79068	0.01675
$C_6H_{15}Bi$	triethylbismuth	78.54697	78.39153	-0.00198
$C_{18}H_{15}Bi$	triphenylbismuth	164.66490	163.75184	-0.00558

Table 70. The calculated and experimental geometrical and energy parameters of the H bond of water of Type I ice.

Parameter	Calculated	Experimental
H Bond Length $2c'_{O\cdots H}$	1.78219 Å	1.78 Å
Nearest Neighbor Separation Distance $2c'_{O\cdots HO}$	2.75377 Å	2.75 Å
H_2O Lattice Parameter a_l	4.49768 Å	4.49 Å 4.5212 Å
H_2O Lattice Parameter c_l	7.34077 Å	7.31 Å 7.3666 Å
Energy of Vaporization of Water at 0 °C	46.934 kJ/mole	45.054 kJ/mole

Table 71. The calculated and experimental geometrical and energy parameters of the H bond of steam.

Parameter	Calculated	Experimental
H Bond Length $2c'_{O\cdots H}$	2.04501 Å	2.02 Å 2.05 Å
Nearest Neighbor Separation Distance $2c'_{O\cdots HO}$	3.01658 Å	3.02 Å

Table 72. The calculated and experimental geometrical and energy parameters of the H-bonded ammonia-water vapor molecular dimer.

Parameter	Calculated	Experimental
H Bond Length $2c'_{N\cdots H}$	2.08186 Å	2.02 Å
Nearest Neighbor Separation Distance $2c'_{N\cdots HO}$	3.05343 Å	2.99 Å
$N\cdots H$ Bond Dissociation Energy	29.48 kJ/mole	29 kJ/mole

Table 73. The calculated and experimental geometrical parameters and interplane van der Waals cohesive energy of graphite.

Parameter	Calculated	Experimental
Graphite Interplane Distance $2c'_{C\cdots C}$	3.51134 Å	3.5 Å
van der Waals Energy per Carbon Atom	0.04968 eV	0.052 eV

Table 74. The calculated and experimental geometrical parameters and interatomic van der Waals cohesive energy of liquid helium.

Parameter	Calculated	Experimental
Liquid Helium Interatomic Distance $2c'_{C\cdots C}$	3.70593 Å	3.72 Å (T=4.24 K) 3.70 (T<2.25K)
Roton Length Scale	3.70593 Å	3.7-4.0 Å
van der Waals Energy per Helium Atom (4.221 K)	0.000799 eV	0.000859 eV
Roton Energy	0.000799 eV	0.00075 eV

Table 75. The calculated and experimental geometrical parameters and interatomic van der Waals cohesive energy of solid neon.

Parameter	Calculated	Experimental
Solid Neon Interatomic Distance $2c'_{C\cdots C}$	3.36683 Å	3.21 Å (T=24.48 K)
van der Waals Energy per Neon Atom	0.02368 eV	0.02125 eV

Table 76. The calculated and experimental geometrical parameters and interatomic van der Waals cohesive energy of solid argon.

Parameter	Calculated	Experimental
Solid Argon Interatomic Distance $2c'_{C\cdots C}$	3.62167 Å (T=0 K)	3.71 Å (T=4.2 K)
van der Waals Energy per Argon Atom	0.07977 eV (T=4.2 K)	0.08022 eV (T=0 K)

Table 77. The calculated and experimental geometrical parameters and interatomic van der Waals cohesive energy (0 K) of solid krypton.

Parameter	Calculated	Experimental
Solid Krypton Interatomic Distance $2c'_{C\cdots C}$	4.08688 Å	3.992 Å
van der Waals Energy per Krypton Atom	0.11890 eV	0.11561 eV

Table 78. The calculated and experimental geometrical parameters and interatomic van der Waals cohesive energy of solid xenon.

Parameter	Calculated	Experimental
Solid Xenon Interatomic Distance $2c'_{C\cdots C}$	4.4884 Å (T=0 K)	4.492 Å (T=161.35K)
van der Waals Energy per Xenon Atom (0 K)	0.18037 eV	0.16608 eV

REFERENCES

1. R. Mills, *The Grand Unified Theory of Classical Physics*; June 2008 Edition, posted at http://www.blacklightpower.com/theory/bookdownload.shtml.
2. D. R. Lide, *CRC Handbook of Chemistry and Physics*, 86th Edition, CRC Press, Taylor & Francis, Boca Raton, (2005-6), pp. 10-202 to 10-204.
3. D. R. Lide, *CRC Handbook of Chemistry and Physics*, 86th Edition, CRC Press, Taylor & Francis, Boca Raton, (2005-6), pp. 9-63; 5-18 to 5-42.
4. M. W. Chase, Jr., C. A. Davies, J. R. Downey, Jr., D. J. Frurip, R. A. McDonald, A. N. Syverud, JANAF Thermochemical Tables, Third Edition, Part I, Al-Co & Part II, Cr-Zr, J. Phys. Chem. Ref. Data, Vol. 14, Suppl. 1, (1985).
5. J. D. Cox, G. Pilcher, *Thermochemistry of Organometallic Compounds*, Academic Press, New York, (1970), p. 478.

Table 1.5. Relativistic ionization energies for some one-electron atoms.

One e Atom	Z	β (Eq. (1.267))	Theoretical Ionization Energies (eV) (Eq. (1.272))	Experimental Ionization Energies (eV) [a]	Relative Difference between Experimental and Calculated [b]
H	1	0.00730	13.59847	13.59844	-0.000002
He^{+}	2	0.01459	54.41826	54.41778	-0.000009
Li^{2+}	3	0.02189	122.45637	122.45429	-0.000017
Be^{3+}	4	0.02919	217.72427	217.71865	-0.000026
B^{4+}	5	0.03649	340.23871	340.2258	-0.000038
C^{5+}	6	0.04378	490.01759	489.99334	-0.000049
N^{6+}	7	0.05108	667.08834	667.046	-0.000063
O^{7+}	8	0.05838	871.47768	871.4101	-0.000078
F^{8+}	9	0.06568	1103.220	1103.1176	-0.000093
Ne^{9+}	10	0.07297	1362.348	1362.1995	-0.000109
Na^{10+}	11	0.08027	1648.910	1648.702	-0.000126
Mg^{11+}	12	0.08757	1962.945	1962.665	-0.000143
Al^{12+}	13	0.09486	2304.512	2304.141	-0.000161
Si^{13+}	14	0.10216	2673.658	2673.182	-0.000178
P^{14+}	15	0.10946	3070.451	3069.842	-0.000198
S^{15+}	16	0.11676	3494.949	3494.1892	-0.000217
Cl^{16+}	17	0.12405	3947.228	3946.296	-0.000236
Ar^{17+}	18	0.13135	4427.363	4426.2296	-0.000256
K^{18+}	19	0.13865	4935.419	4934.046	-0.000278
Ca^{19+}	20	0.14595	5471.494	5469.864	-0.000298
Sc^{20+}	21	0.15324	6035.681	6033.712	-0.000326
Ti^{21+}	22	0.16054	6628.064	6625.82	-0.000339
V^{22+}	23	0.16784	7248.745	7246.12	-0.000362
Cr^{23+}	24	0.17514	7897.827	7894.81	-0.000382
Mn^{24+}	25	0.18243	8575.426	8571.94	-0.000407
Fe^{25+}	26	0.18973	9281.650	9277.69	-0.000427
Co^{26+}	27	0.19703	10016.63	10012.12	-0.000450
Ni^{27+}	28	0.20432	10780.48	10775.4	-0.000471
Cu^{28+}	29	0.21162	11573.34	11567.617	-0.000495
Zn^{29+}	30	0.21892	12395.35	12388.93	-0.000518
Ga^{30+}	31	0.22622	13246.66	13239.49	-0.000542
Ge^{31+}	32	0.23351	14127.41	14119.43	-0.000565
As^{32+}	33	0.24081	15037.75	15028.62	-0.000608
Se^{33+}	34	0.24811	15977.86	15967.68	-0.000638
Kr^{35+}	36	0.26270	17948.05	17936.21	-0.000660

Rb^{36+}	37	0.27000	18978.49	18964.99	-0.000712
Mo^{41+}	42	0.30649	24592.04	24572.22	-0.000807
Xe^{53+}	54	0.39406	41346.76	41299.7	-0.001140
U^{91+}	92	0.67136	132279.32	131848.5	-0.003268

[a] From theoretical calculations, interpolation of H isoelectronic and Rydberg series, and experimental data [42-45].
[b] (Experimental-theoretical)/experimental.

Table 7.1. Relativistically corrected ionization energies for some two-electron atoms.

2 e Atom	Z	r_1 (a_o) [a]	Electric Energy [b] (eV)	Magnetic Energy [c] (eV)	Velocity (m/s) [d]	γ^* [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
He	2	0.566987	23.996467	0.590536	3.85845E+06	1.000021	24.58750	24.58741	-0.000004
Li^+	3	0.35566	76.509	2.543	6.15103E+06	1.00005	75.665	75.64018	-0.0003
Be^{2+}	4	0.26116	156.289	6.423	8.37668E+06	1.00010	154.699	153.89661	-0.0052
B^{3+}	5	0.20670	263.295	12.956	1.05840E+07	1.00016	260.746	259.37521	-0.0053
C^{4+}	6	0.17113	397.519	22.828	1.27836E+07	1.00024	393.809	392.087	-0.0044
N^{5+}	7	0.14605	558.958	36.728	1.49794E+07	1.00033	553.896	552.0718	-0.0033
O^{6+}	8	0.12739	747.610	55.340	1.71729E+07	1.00044	741.023	739.29	-0.0023
F^{7+}	9	0.11297	963.475	79.352	1.93649E+07	1.00057	955.211	953.9112	-0.0014
Ne^{8+}	10	0.10149	1206.551	109.451	2.15560E+07	1.00073	1196.483	1195.8286	-0.0005
Na^{9+}	11	0.09213	1476.840	146.322	2.37465E+07	1.00090	1464.871	1465.121	0.0002
Mg^{10+}	12	0.08435	1774.341	190.652	2.59364E+07	1.00110	1760.411	1761.805	0.0008
Al^{11+}	13	0.07778	2099.05	243.13	2.81260E+07	1.00133	2083.15	2085.98	0.0014
Si^{12+}	14	0.07216	2450.98	304.44	3.03153E+07	1.00159	2433.13	2437.63	0.0018
P^{13+}	15	0.06730	2830.11	375.26	3.25043E+07	1.00188	2810.42	2816.91	0.0023
S^{14+}	16	0.06306	3236.46	456.30	3.46932E+07	1.00221	3215.09	3223.78	0.0027
Cl^{15+}	17	0.05932	3670.02	548.22	3.68819E+07	1.00258	3647.22	3658.521	0.0031
Ar^{16+}	18	0.05599	4130.79	651.72	3.90705E+07	1.00298	4106.91	4120.8857	0.0034
K^{17+}	19	0.05302	4618.77	767.49	4.12590E+07	1.00344	4594.25	4610.8	0.0036
Ca^{18+}	20	0.05035	5133.96	896.20	4.34475E+07	1.00394	5109.38	5128.8	0.0038
Sc^{19+}	21	0.04794	5676.37	1038.56	4.56358E+07	1.00450	5652.43	5674.8	0.0039
Ti^{20+}	22	0.04574	6245.98	1195.24	4.78241E+07	1.00511	6223.55	6249	0.0041
V^{21+}	23	0.04374	6842.81	1366.92	5.00123E+07	1.00578	6822.93	6851.3	0.0041
Cr^{22+}	24	0.04191	7466.85	1554.31	5.22005E+07	1.00652	7450.76	7481.7	0.0041
Mn^{23+}	25	0.04022	8118.10	1758.08	5.43887E+07	1.00733	8107.25	8140.6	0.0041
Fe^{24+}	26	0.03867	8796.56	1978.92	5.65768E+07	1.00821	8792.66	8828	0.0040
Co^{25+}	27	0.03723	9502.23	2217.51	5.87649E+07	1.00917	9507.25	9544.1	0.0039
Ni^{26+}	28	0.03589	10235.12	2474.55	6.09529E+07	1.01022	10251.33	10288.8	0.0036
Cu^{27+}	29	0.03465	10995.21	2750.72	6.31409E+07	1.01136	11025.21	11062.38	0.0034

[a] From Equation (7.19).

[b] From Equation (7.29).

[c] From Equation (7.30).

[d] From Equations (7.31).

[e] From Equation (1.250) with the velocity given by Eq. (7.31).

[f] From Equations (7.28) and (7.47) with $E(electric)$ of Eq. (7.29) relativistically corrected by γ^* according to Eq.(1.251) except that the electron-nuclear electrodynamic relativistic factor corresponding to the reduced mass of Eqs. (1.213-1.223) was not included.

[g] From theoretical calculations for ions Ne^{8+} to Cu^{28+}.

[h] (Experimental-theoretical)/experimental.

Table 10.1. Ionization energies for some three-electron atoms.

3 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	Electric Energy [c] (eV)	Δv [d] (m/s)	ΔE_T [e] (eV)	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
Li	3	0.35566	2.55606	5.3230	1.6571E+04	1.5613E-03	5.40381	5.39172	-0.00224
Be^{+}	4	0.26116	1.49849	18.1594	4.4346E+04	1.1181E-02	18.1706	18.21116	0.00223
B^{2+}	5	0.20670	1.07873	37.8383	7.4460E+04	3.1523E-02	37.8701	37.93064	0.00160
C^{3+}	6	0.17113	0.84603	64.3278	1.0580E+05	6.3646E-02	64.3921	64.4939	0.00158
N^{4+}	7	0.14605	0.69697	97.6067	1.3782E+05	1.0800E-01	97.7160	97.8902	0.00178
O^{5+}	8	0.12739	0.59299	137.6655	1.7026E+05	1.6483E-01	137.8330	138.1197	0.00208
F^{6+}	9	0.11297	0.51621	184.5001	2.0298E+05	2.3425E-01	184.7390	185.186	0.00241
Ne^{7+}	10	0.10149	0.45713	238.1085	2.3589E+05	3.1636E-01	238.4325	239.0989	0.00279
Na^{8+}	11	0.09213	0.41024	298.4906	2.6894E+05	4.1123E-01	298.9137	299.864	0.00317
Mg^{9+}	12	0.08435	0.37210	365.6469	3.0210E+05	5.1890E-01	366.1836	367.5	0.00358
Al^{10+}	13	0.07778	0.34047	439.5790	3.3535E+05	6.3942E-01	440.2439	442	0.00397
Si^{11+}	14	0.07216	0.31381	520.2888	3.6868E+05	7.7284E-01	521.0973	523.42	0.00444
P^{12+}	15	0.06730	0.29102	607.7792	4.0208E+05	9.1919E-01	608.7469	611.74	0.00489
S^{13+}	16	0.06306	0.27132	702.0535	4.3554E+05	1.0785E+00	703.1966	707.01	0.00539
Cl^{14+}	17	0.05932	0.25412	803.1158	4.6905E+05	1.2509E+00	804.4511	809.4	0.00611
Ar^{15+}	18	0.05599	0.23897	910.9708	5.0262E+05	1.4364E+00	912.5157	918.03	0.00601
K^{16+}	19	0.05302	0.22552	1025.6241	5.3625E+05	1.6350E+00	1027.3967	1033.4	0.00581
Ca^{17+}	20	0.05035	0.21350	1147.0819	5.6993E+05	1.8468E+00	1149.1010	1157.8	0.00751
Sc^{18+}	21	0.04794	0.20270	1275.3516	6.0367E+05	2.0720E+00	1277.6367	1287.97	0.00802
Ti^{19+}	22	0.04574	0.19293	1410.4414	6.3748E+05	2.3106E+00	1413.0129	1425.4	0.00869
V^{20+}	23	0.04374	0.18406	1552.3606	6.7135E+05	2.5626E+00	1555.2398	1569.6	0.00915
Cr^{21+}	24	0.04191	0.17596	1701.1197	7.0530E+05	2.8283E+00	1704.3288	1721.4	0.00992
Mn^{22+}	25	0.04022	0.16854	1856.7301	7.3932E+05	3.1077E+00	1860.2926	1879.9	0.01043
Fe^{23+}	26	0.03867	0.16172	2019.2050	7.7342E+05	3.4011E+00	2023.1451	2023	-0.00007
Co^{24+}	27	0.03723	0.15542	2188.5585	8.0762E+05	3.7084E+00	2192.9020	2219	0.01176
Ni^{25+}	28	0.03589	0.14959	2364.8065	8.4191E+05	4.0300E+00	2369.5803	2399.2	0.01235
Cu^{26+}	29	0.03465	0.14418	2547.9664	8.7630E+05	4.3661E+00	2553.1987	2587.5	0.01326

[a] Radius of the paired inner electrons of three-electron atoms from Eq. (10.49).

[b] Radius of the unpaired outer electron of three-electron atoms from Eq. (10.50).

[c] Electric energy of the outer electron of three-electron atoms from Eq. (10.43).

[d] Change in the velocity of the paired inner electrons due to the unpaired outer electron of three-electron atoms from Eq. (10.46).

[e] Change in the kinetic energy of the paired inner electrons due to the unpaired outer electron of three-electron atoms from Eq. (10.47).

[f] Calculated ionization energies of three-electron atoms from Eq. (10.48) for $Z > 3$ and Eq. (10.25) for Li.

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.2. Ionization energies for some four-electron atoms.

4 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	Electric Energy [c] (eV)	Magnetic Energy [d] (eV)	Δv [e] (m/s X 10^{-5})	ΔE_T [f] (eV)	Theoretical Ionization Energies [g] (eV)	Experimental Ionization Energies [h] (eV)	Relative Error [i]
Be	4	0.26116	1.52503	8.9178	0.03226	0.4207	0.0101	9.28430	9.32263	0.0041
B^{+}	5	0.20670	1.07930	25.2016	0.0910	0.7434	0.0314	25.1627	25.15484	-0.0003
C^{2+}	6	0.17113	0.84317	48.3886	0.1909	1.0688	0.0650	48.3125	47.8878	-0.0089
N^{3+}	7	0.14605	0.69385	78.4029	0.3425	1.3969	0.1109	78.2765	77.4735	-0.0104
O^{4+}	8	0.12739	0.59020	115.2148	0.5565	1.7269	0.1696	115.0249	113.899	-0.0099
F^{5+}	9	0.11297	0.51382	158.8102	0.8434	2.0582	0.2409	158.5434	157.1651	-0.0088
Ne^{6+}	10	0.10149	0.45511	209.1813	1.2138	2.3904	0.3249	208.8243	207.2759	-0.0075
Na^{7+}	11	0.09213	0.40853	266.3233	1.6781	2.7233	0.4217	265.8628	264.25	-0.0061
Mg^{8+}	12	0.08435	0.37065	330.2335	2.2469	3.0567	0.5312	329.6559	328.06	-0.0049
Al^{9+}	13	0.07778	0.33923	400.9097	2.9309	3.3905	0.6536	400.2017	398.75	-0.0036
Si^{10+}	14	0.07216	0.31274	478.3507	3.7404	3.7246	0.7888	477.4989	476.36	-0.0024
P^{11+}	15	0.06730	0.29010	562.5555	4.6861	4.0589	0.9367	561.5464	560.8	-0.0013
S^{12+}	16	0.06306	0.27053	653.5233	5.7784	4.3935	1.0975	652.3436	652.2	-0.0002
Cl^{13+}	17	0.05932	0.25344	751.2537	7.0280	4.7281	1.2710	749.8899	749.76	-0.0002
Ar^{14+}	18	0.05599	0.23839	855.7463	8.4454	5.0630	1.4574	854.1849	854.77	0.0007
K^{15+}	19	0.05302	0.22503	967.0007	10.0410	5.3979	1.6566	965.2283	968	0.0029
Ca^{16+}	20	0.05035	0.21308	1085.0167	11.8255	5.7329	1.8687	1083.0198	1087	0.0037
Sc^{17+}	21	0.04794	0.20235	1209.7940	13.8094	6.0680	2.0935	1207.5592	1213	0.0045
Ti^{18+}	22	0.04574	0.19264	1341.3326	16.0032	6.4032	2.3312	1338.8465	1346	0.0053
V^{19+}	23	0.04374	0.18383	1479.6323	18.4174	6.7384	2.5817	1476.8813	1486	0.0061
Cr^{20+}	24	0.04191	0.17579	1624.6929	21.0627	7.0737	2.8450	1621.6637	1634	0.0075
Mn^{21+}	25	0.04022	0.16842	1776.5144	23.9495	7.4091	3.1211	1773.1935	1788	0.0083
Fe^{22+}	26	0.03867	0.16165	1935.0968	27.0883	7.7444	3.4101	1931.4707	1950	0.0095
Co^{23+}	27	0.03723	0.15540	2100.4398	30.4898	8.0798	3.7118	2096.4952	2119	0.0106
Ni^{24+}	28	0.03589	0.14961	2272.5436	34.1644	8.4153	4.0264	2268.2669	2295	0.0116
Cu^{25+}	29	0.03465	0.14424	2451.4080	38.1228	8.7508	4.3539	2446.7858	2478	0.0126

[a] Radius of the paired inner electrons of four-electron atoms from Eq. (10.51).

[b] Radius of the paired outer electrons of four-electron atoms from Eq. (10.62).

[c] Electric energy of the outer electrons of four-electron atoms from Eq. (10.63).

[d] Magnetic energy of the outer electrons of four-electron atoms upon unpairing from Eq. (7.30) and Eq. (10.64).

[e] Change in the velocity of the paired inner electrons due to the unpaired outer electron of four-electron atoms during ionization from Eq. (10.46).

[f] Change in the kinetic energy of the paired inner electrons due to the unpaired outer electron of four-electron atoms during ionization from Eq. (10.47).

[g] Calculated ionization energies of four-electron atoms from Eq. (10.68) for $Z > 4$ and Eq. (10.66) for Be.

[h] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[i] (Experimental-theoretical)/experimental.

Table 10.3. Ionization energies for some five-electron atoms.

5 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_5 (a_o) [c]	Theoretical Ionization Energies [d] (eV)	Experimental Ionization Energies [e] (eV)	Relative Error [f]
B	5	0.20670	1.07930	1.67000	8.30266	8.29803	-0.00056
C^{+}	6	0.17113	0.84317	1.12092	24.2762	24.38332	0.0044
N^{2+}	7	0.14605	0.69385	0.87858	46.4585	47.44924	0.0209
O^{3+}	8	0.12739	0.59020	0.71784	75.8154	77.41353	0.0206
F^{4+}	9	0.11297	0.51382	0.60636	112.1922	114.2428	0.0179
Ne^{5+}	10	0.10149	0.45511	0.52486	155.5373	157.93	0.0152
Na^{6+}	11	0.09213	0.40853	0.46272	205.8266	208.5	0.0128
Mg^{7+}	12	0.08435	0.37065	0.41379	263.0469	265.96	0.0110
Al^{8+}	13	0.07778	0.33923	0.37425	327.1901	330.13	0.0089
Si^{9+}	14	0.07216	0.31274	0.34164	398.2509	401.37	0.0078
P^{10+}	15	0.06730	0.29010	0.31427	476.2258	479.46	0.0067
S^{11+}	16	0.06306	0.27053	0.29097	561.1123	564.44	0.0059
Cl^{12+}	17	0.05932	0.25344	0.27090	652.9086	656.71	0.0058
Ar^{13+}	18	0.05599	0.23839	0.25343	751.6132	755.74	0.0055
K^{14+}	19	0.05302	0.22503	0.23808	857.2251	861.1	0.0045
Ca^{15+}	20	0.05035	0.21308	0.22448	969.7435	974	0.0044
Sc^{16+}	21	0.04794	0.20235	0.21236	1089.1678	1094	0.0044
Ti^{17+}	22	0.04574	0.19264	0.20148	1215.4975	1221	0.0045
V^{18+}	23	0.04374	0.18383	0.19167	1348.7321	1355	0.0046
Cr^{19+}	24	0.04191	0.17579	0.18277	1488.8713	1496	0.0048
Mn^{20+}	25	0.04022	0.16842	0.17466	1635.9148	1644	0.0049
Fe^{21+}	26	0.03867	0.16165	0.16724	1789.8624	1799	0.0051
Co^{22+}	27	0.03723	0.15540	0.16042	1950.7139	1962	0.0058
Ni^{23+}	28	0.03589	0.14961	0.15414	2118.4690	2131	0.0059
Cu^{24+}	29	0.03465	0.14424	0.14833	2293.1278	2308	0.0064

[a] Radius of the first set of paired inner electrons of five-electron atoms from Eq. (10.51).

[b] Radius of the second set of paired inner electrons of five-electron atoms from Eq. (10.62).

[c] Radius of the outer electron of five-electron atoms from Eq. (10.113) for $Z > 5$ and Eq. (10.101) for B.

[d] Calculated ionization energies of five-electron atoms given by the electric energy (Eq. (10.114)) for $Z > 5$ and Eq. (10.104) for B.

[e] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[f] (Experimental-theoretical)/experimental.

Table 10.4. Ionization energies for some six-electron atoms.

6 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_6 (a_o) [c]	Theoretical Ionization Energies [d] (eV)	Experimental Ionization Energies [e] (eV)	Relative Error [f]
C	6	0.17113	0.84317	1.20654	11.27671	11.2603	-0.0015
N^{+}	7	0.14605	0.69385	0.90119	30.1950	29.6013	-0.0201
O^{2+}	8	0.12739	0.59020	0.74776	54.5863	54.9355	0.0064
F^{3+}	9	0.11297	0.51382	0.63032	86.3423	87.1398	0.0092
Ne^{4+}	10	0.10149	0.45511	0.54337	125.1986	126.21	0.0080
Na^{5+}	11	0.09213	0.40853	0.47720	171.0695	172.18	0.0064
Mg^{6+}	12	0.08435	0.37065	0.42534	223.9147	225.02	0.0049
Al^{7+}	13	0.07778	0.33923	0.38365	283.7121	284.66	0.0033
Si^{8+}	14	0.07216	0.31274	0.34942	350.4480	351.12	0.0019
P^{9+}	15	0.06730	0.29010	0.32081	424.1135	424.4	0.0007
S^{10+}	16	0.06306	0.27053	0.29654	504.7024	504.8	0.0002
Cl^{11+}	17	0.05932	0.25344	0.27570	592.2103	591.99	-0.0004
Ar^{12+}	18	0.05599	0.23839	0.25760	686.6340	686.1	-0.0008
K^{13+}	19	0.05302	0.22503	0.24174	787.9710	786.6	-0.0017
Ca^{14+}	20	0.05035	0.21308	0.22772	896.2196	894.5	-0.0019
Sc^{15+}	21	0.04794	0.20235	0.21524	1011.3782	1009	-0.0024
Ti^{16+}	22	0.04574	0.19264	0.20407	1133.4456	1131	-0.0022
V^{17+}	23	0.04374	0.18383	0.19400	1262.4210	1260	-0.0019
Cr^{18+}	24	0.04191	0.17579	0.18487	1398.3036	1396	-0.0017
Mn^{19+}	25	0.04022	0.16842	0.17657	1541.0927	1539	-0.0014
Fe^{20+}	26	0.03867	0.16165	0.16899	1690.7878	1689	-0.0011
Co^{21+}	27	0.03723	0.15540	0.16203	1847.3885	1846	-0.0008
Ni^{22+}	28	0.03589	0.14961	0.15562	2010.8944	2011	0.0001
Cu^{23+}	29	0.03465	0.14424	0.14970	2181.3053	2182	0.0003

[a] Radius of the first set of paired inner electrons of six-electron atoms from Eq. (10.51).

[b] Radius of the second set of paired inner electrons of six-electron atoms from Eq. (10.62).

[c] Radius of the two unpaired outer electrons of six-electron atoms from Eq. (10.132) for $Z > 6$ and Eq. (10.122) for C.

[d] Calculated ionization energies of six-electron atoms given by the electric energy (Eq. (10.133)).

[e] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[f] (Experimental-theoretical)/experimental.

Table 10.5. Ionization energies for some seven-electron atoms.

7 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_7 (a_o) [c]	Theoretical Ionization Energies [d] (eV)	Experimental Ionization Energies [e] (eV)	Relative Error [f]
N	7	0.14605	0.69385	0.93084	14.61664	14.53414	-0.0057
O^+	8	0.12739	0.59020	0.78489	34.6694	35.1173	0.0128
F^{2+}	9	0.11297	0.51382	0.67084	60.8448	62.7084	0.0297
Ne^{3+}	10	0.10149	0.45511	0.57574	94.5279	97.12	0.0267
Na^{4+}	11	0.09213	0.40853	0.50250	135.3798	138.4	0.0218
Mg^{5+}	12	0.08435	0.37065	0.44539	183.2888	186.76	0.0186
Al^{6+}	13	0.07778	0.33923	0.39983	238.2017	241.76	0.0147
Si^{7+}	14	0.07216	0.31274	0.36271	300.0883	303.54	0.0114
P^{8+}	15	0.06730	0.29010	0.33191	368.9298	372.13	0.0086
S^{9+}	16	0.06306	0.27053	0.30595	444.7137	447.5	0.0062
Cl^{10+}	17	0.05932	0.25344	0.28376	527.4312	529.28	0.0035
Ar^{11+}	18	0.05599	0.23839	0.26459	617.0761	618.26	0.0019
K^{12+}	19	0.05302	0.22503	0.24785	713.6436	714.6	0.0013
Ca^{13+}	20	0.05035	0.21308	0.23311	817.1303	817.6	0.0006
Sc^{14+}	21	0.04794	0.20235	0.22003	927.5333	927.5	0.0000
Ti^{15+}	22	0.04574	0.19264	0.20835	1044.8504	1044	-0.0008
V^{16+}	23	0.04374	0.18383	0.19785	1169.0800	1168	-0.0009
Cr^{17+}	24	0.04191	0.17579	0.18836	1300.2206	1299	-0.0009
Mn^{18+}	25	0.04022	0.16842	0.17974	1438.2710	1437	-0.0009
Fe^{19+}	26	0.03867	0.16165	0.17187	1583.2303	1582	-0.0008
Co^{20+}	27	0.03723	0.15540	0.16467	1735.0978	1735	-0.0001
Ni^{21+}	28	0.03589	0.14961	0.15805	1893.8726	1894	0.0001
Cu^{22+}	29	0.03465	0.14424	0.15194	2059.5543	2060	0.0002

[a] Radius of the first set of paired inner electrons of seven-electron atoms from Eq. (10.51).

[b] Radius of the second set of paired inner electrons of seven-electron atoms from Eq. (10.62).

[c] Radius of the three unpaired paired outer electrons of seven-electron atoms from Eq. (10.152) for $Z > 7$ and Eq. (10.142) for N.

[d] Calculated ionization energies of seven-electron atoms given by the electric energy (Eq. (10.153)).

[e] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[f] (Experimental-theoretical)/experimental.

Table 10.6. Ionization energies for some eight-electron atoms.

8 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_8 (a_o) [c]	Theoretical Ionization Energies [d] (eV)	Experimental Ionization Energies [e] (eV)	Relative Error [f]
O	8	0.12739	0.59020	1.00000	13.60580	13.6181	0.0009
F^+	9	0.11297	0.51382	0.7649	35.5773	34.9708	-0.0173
Ne^{2+}	10	0.10149	0.45511	0.6514	62.6611	63.45	0.0124
Na^{3+}	11	0.09213	0.40853	0.5592	97.3147	98.91	0.0161
Mg^{4+}	12	0.08435	0.37065	0.4887	139.1911	141.27	0.0147
Al^{5+}	13	0.07778	0.33923	0.4338	188.1652	190.49	0.0122
Si^{6+}	14	0.07216	0.31274	0.3901	244.1735	246.5	0.0094
P^{7+}	15	0.06730	0.29010	0.3543	307.1791	309.6	0.0078
S^{8+}	16	0.06306	0.27053	0.3247	377.1579	379.55	0.0063
Cl^{9+}	17	0.05932	0.25344	0.2996	454.0940	455.63	0.0034
Ar^{10+}	18	0.05599	0.23839	0.2782	537.9756	538.96	0.0018
K^{11+}	19	0.05302	0.22503	0.2597	628.7944	629.4	0.0010
Ca^{12+}	20	0.05035	0.21308	0.2434	726.5442	726.6	0.0001
Sc^{13+}	21	0.04794	0.20235	0.2292	831.2199	830.8	-0.0005
Ti^{14+}	22	0.04574	0.19264	0.2165	942.8179	941.9	-0.0010
V^{15+}	23	0.04374	0.18383	0.2051	1061.3351	1060	-0.0013
Cr^{16+}	24	0.04191	0.17579	0.1949	1186.7691	1185	-0.0015
Mn^{17+}	25	0.04022	0.16842	0.1857	1319.1179	1317	-0.0016
Fe^{18+}	26	0.03867	0.16165	0.1773	1458.3799	1456	-0.0016
Co^{19+}	27	0.03723	0.15540	0.1696	1604.5538	1603	-0.0010
Ni^{20+}	28	0.03589	0.14961	0.1626	1757.6383	1756	-0.0009
Cu^{21+}	29	0.03465	0.14424	0.1561	1917.6326	1916	-0.0009

[a] Radius of the first set of paired inner electrons of eight-electron atoms from Eq. (10.51).

[b] Radius of the second set of paired inner electrons of eight-electron atoms from Eq. (10.62).

[c] Radius of the two paired and two unpaired outer electrons of eight-electron atoms from Eq. (10.172) for $Z > 8$ and Eq. (10.162) for O.

[d] Calculated ionization energies of eight-electron atoms given by the electric energy (Eq. (10.173)).

[e] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[f] (Experimental-theoretical)/experimental.

Table 10.7. Ionization energies for some nine-electron atoms.

9 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_9 (a_o) [c]	Theoretical Ionization Energies [d] (eV)	Experimental Ionization Energies [e] (eV)	Relative Error [f]
F	9	0.11297	0.51382	0.78069	17.42782	17.42282	-0.0003
Ne^{+}	10	0.10149	0.45511	0.64771	42.0121	40.96328	-0.0256
Na^{2+}	11	0.09213	0.40853	0.57282	71.2573	71.62	0.0051
Mg^{3+}	12	0.08435	0.37065	0.50274	108.2522	109.2655	0.0093
Al^{4+}	13	0.07778	0.33923	0.44595	152.5469	153.825	0.0083
Si^{5+}	14	0.07216	0.31274	0.40020	203.9865	205.27	0.0063
P^{6+}	15	0.06730	0.29010	0.36283	262.4940	263.57	0.0041
S^{7+}	16	0.06306	0.27053	0.33182	328.0238	328.75	0.0022
Cl^{8+}	17	0.05932	0.25344	0.30571	400.5466	400.06	-0.0012
Ar^{9+}	18	0.05599	0.23839	0.28343	480.0424	478.69	-0.0028
K^{10+}	19	0.05302	0.22503	0.26419	566.4968	564.7	-0.0032
Ca^{11+}	20	0.05035	0.21308	0.24742	659.8992	657.2	-0.0041
Sc^{12+}	21	0.04794	0.20235	0.23266	760.2415	756.7	-0.0047
Ti^{13+}	22	0.04574	0.19264	0.21957	867.5176	863.1	-0.0051
V^{14+}	23	0.04374	0.18383	0.20789	981.7224	976	-0.0059
Cr^{15+}	24	0.04191	0.17579	0.19739	1102.8523	1097	-0.0053
Mn^{16+}	25	0.04022	0.16842	0.18791	1230.9038	1224	-0.0056
Fe^{17+}	26	0.03867	0.16165	0.17930	1365.8746	1358	-0.0058
Co^{18+}	27	0.03723	0.15540	0.17145	1507.7624	1504.6	-0.0021
Ni^{19+}	28	0.03589	0.14961	0.16427	1656.5654	1648	-0.0052
Cu^{20+}	29	0.03465	0.14424	0.15766	1812.2821	1804	-0.0046

[a] Radius of the first set of paired inner electrons of nine-electron atoms from Equation (10.51).

[b] Radius of the second set of paired inner electrons of nine-electron atoms from Equation (10.62).

[c] Radius of the one unpaired and two sets of paired outer electrons of nine-electron atoms from Eq. (10.192) for $Z > 9$ and Eq. (10.182) for F.

[d] Calculated ionization energies of nine-electron atoms given by the electric energy (Eq. (10.193)).

[e] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[f] (Experimental-theoretical)/experimental.

Table 10.8. Ionization energies for some ten-electron atoms.

10 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	Theoretical Ionization Energies [d] (eV)	Experimental Ionization Energies [e] (eV)	Relative Error [f]
Ne	10	0.10149	0.45511	0.63659	21.37296	21.56454	0.00888
Na^{+}	11	0.09213	0.40853	0.560945	48.5103	47.2864	-0.0259
Mg^{2+}	12	0.08435	0.37065	0.510568	79.9451	80.1437	0.0025
Al^{3+}	13	0.07778	0.33923	0.456203	119.2960	119.992	0.0058
Si^{4+}	14	0.07216	0.31274	0.409776	166.0150	166.767	0.0045
P^{5+}	15	0.06730	0.29010	0.371201	219.9211	220.421	0.0023
S^{6+}	16	0.06306	0.27053	0.339025	280.9252	280.948	0.0001
Cl^{7+}	17	0.05932	0.25344	0.311903	348.9750	348.28	-0.0020
Ar^{8+}	18	0.05599	0.23839	0.288778	424.0365	422.45	-0.0038
K^{9+}	19	0.05302	0.22503	0.268844	506.0861	503.8	-0.0045
Ca^{10+}	20	0.05035	0.21308	0.251491	595.1070	591.9	-0.0054
Sc^{11+}	21	0.04794	0.20235	0.236251	691.0866	687.36	-0.0054
Ti^{12+}	22	0.04574	0.19264	0.222761	794.0151	787.84	-0.0078
V^{13+}	23	0.04374	0.18383	0.210736	903.8853	896	-0.0088
Cr^{14+}	24	0.04191	0.17579	0.19995	1020.6910	1010.6	-0.0100
Mn^{15+}	25	0.04022	0.16842	0.19022	1144.4276	1134.7	-0.0086
Fe^{16+}	26	0.03867	0.16165	0.181398	1275.0911	1266	-0.0072
Co^{17+}	27	0.03723	0.15540	0.173362	1412.6783	1397.2	-0.0111
Ni^{18+}	28	0.03589	0.14961	0.166011	1557.1867	1541	-0.0105
Cu^{19+}	29	0.03465	0.14424	0.159261	1708.6139	1697	-0.0068
Zn^{20+}	30	0.03349	0.13925	0.153041	1866.9581	1856	-0.0059

[a] Radius of the first set of paired inner electrons of ten-electron atoms from Equation (10.51).

[b] Radius of the second set of paired inner electrons of ten-electron atoms from Equation (10.62).

[c] Radius of three sets of paired outer electrons of ten-electron atoms from Eq. (10.212)) for $Z > 10$ and Eq. (10.202) for Ne.

[d] Calculated ionization energies of ten-electron atoms given by the electric energy (Eq. (10.213)).

[e] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[f] (Experimental-theoretical)/experimental.

Table 10.10. Ionization energies for some eleven-electron atoms.

11 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{11} (a_o) [d]	Theoretical Ionization Energies [e] (eV)	Experimental Ionization Energies [f] (eV)	Relative Error [g]
Na	11	0.09213	0.40853	0.560945	2.65432	5.12592	5.13908	0.0026
Mg^{+}	12	0.08435	0.37065	0.510568	1.74604	15.5848	15.03528	-0.0365
Al^{2+}	13	0.07778	0.33923	0.456203	1.47399	27.6918	28.44765	0.0266
Si^{3+}	14	0.07216	0.31274	0.409776	1.25508	43.3624	45.14181	0.0394
P^{4+}	15	0.06730	0.29010	0.371201	1.08969	62.4299	65.0251	0.0399
S^{5+}	16	0.06306	0.27053	0.339025	0.96226	84.8362	88.0530	0.0365
Cl^{6+}	17	0.05932	0.25344	0.311903	0.86151	110.5514	114.1958	0.0319
Ar^{7+}	18	0.05599	0.23839	0.288778	0.77994	139.5577	143.460	0.0272
K^{8+}	19	0.05302	0.22503	0.268844	0.71258	171.8433	175.8174	0.0226
Ca^{9+}	20	0.05035	0.21308	0.251491	0.65602	207.3998	211.275	0.0183
Sc^{10+}	21	0.04794	0.20235	0.236251	0.60784	246.2213	249.798	0.0143
Ti^{11+}	22	0.04574	0.19264	0.222761	0.56631	288.3032	291.500	0.0110
V^{12+}	23	0.04374	0.18383	0.210736	0.53014	333.6420	336.277	0.0078
Cr^{13+}	24	0.04191	0.17579	0.19995	0.49834	382.2350	384.168	0.0050
Mn^{14+}	25	0.04022	0.16842	0.19022	0.47016	434.0801	435.163	0.0025
Fe^{15+}	26	0.03867	0.16165	0.181398	0.44502	489.1753	489.256	0.0002
Co^{16+}	27	0.03723	0.15540	0.173362	0.42245	547.5194	546.58	-0.0017
Ni^{17+}	28	0.03589	0.14961	0.166011	0.40207	609.1111	607.06	-0.0034
Cu^{18+}	29	0.03465	0.14424	0.159261	0.38358	673.9495	670.588	-0.0050
Zn^{19+}	30	0.03349	0.13925	0.153041	0.36672	742.0336	738	-0.0055

[a] Radius of the first set of paired inner electrons of eleven-electron atoms from Eq. (10.51).

[b] Radius of the second set of paired inner electrons of eleven-electron atoms from Eq. (10.62).

[c] Radius of three sets of paired inner electrons of eleven-electron atoms from Eq. (10.212)).

[d] Radius of unpaired outer electron of eleven-electron atoms from Eq. (10.235)) for $Z > 11$ and Eq. (10.226) for Na.

[e] Calculated ionization energies of eleven-electron atoms given by the electric energy (Eq. (10.236)).

[f] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[g] (Experimental-theoretical)/experimental.

Table 10.11. Ionization energies for some twelve-electron atoms.

12 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	Theoretical Ionization Energies [e] (eV)	Experimental Ionization Energies [f] (eV)	Relative Error [g]
Mg	12	0.08435	0.37065	0.51057	1.79386	7.58467	7.64624	0.0081
Al^{+}	13	0.07778	0.33923	0.45620	1.41133	19.2808	18.82856	-0.0240
Si^{2+}	14	0.07216	0.31274	0.40978	1.25155	32.6134	33.49302	0.0263
P^{3+}	15	0.06730	0.29010	0.37120	1.09443	49.7274	51.4439	0.0334
S^{4+}	16	0.06306	0.27053	0.33902	0.96729	70.3296	72.5945	0.0312
Cl^{5+}	17	0.05932	0.25344	0.31190	0.86545	94.3266	97.03	0.0279
Ar^{6+}	18	0.05599	0.23839	0.28878	0.78276	121.6724	124.323	0.0213
K^{7+}	19	0.05302	0.22503	0.26884	0.71450	152.3396	154.88	0.0164
Ca^{8+}	20	0.05035	0.21308	0.25149	0.65725	186.3102	188.54	0.0118
Sc^{9+}	21	0.04794	0.20235	0.23625	0.60857	223.5713	225.18	0.0071
Ti^{10+}	22	0.04574	0.19264	0.22276	0.56666	264.1138	265.07	0.0036
V^{11+}	23	0.04374	0.18383	0.21074	0.53022	307.9304	308.1	0.0006
Cr^{12+}	24	0.04191	0.17579	0.19995	0.49822	355.0157	354.8	-0.0006
Mn^{13+}	25	0.04022	0.16842	0.19022	0.46990	405.3653	403.0	-0.0059
Fe^{14+}	26	0.03867	0.16165	0.18140	0.44466	458.9758	457	-0.0043
Co^{15+}	27	0.03723	0.15540	0.17336	0.42201	515.8442	511.96	-0.0076
Ni^{16+}	28	0.03589	0.14961	0.16601	0.40158	575.9683	571.08	-0.0086
Cu^{17+}	29	0.03465	0.14424	0.15926	0.38305	639.3460	633	-0.0100
Zn^{18+}	30	0.03349	0.13925	0.15304	0.36617	705.9758	698	-0.0114

[a] Radius of the first set of paired inner electrons of twelve-electron atoms from Eq. (10.51).

[b] Radius of the second set of paired inner electrons of twelve-electron atoms from Eq. (10.62).

[c] Radius of three sets of paired inner electrons of twelve-electron atoms from Eq. (10.212)).

[d] Radius of paired outer electrons of twelve-electron atoms from Eq. (10.255)) for $Z > 12$ and Eq. (10.246) for Mg.

[e] Calculated ionization energies of twelve-electron atoms given by the electric energy (Eq. (10.256)).

[f] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[g] (Experimental-theoretical)/experimental.

Table 10.12. Ionization energies for some thirteen-electron atoms.

13 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{13} (a_o) [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
Al	13	0.07778	0.33923	0.45620	1.41133	2.28565	5.98402	5.98577	0.0003
Si^{+}	14	0.07216	0.31274	0.40978	1.25155	1.5995	17.0127	16.34585	-0.0408
P^{2+}	15	0.06730	0.29010	0.37120	1.09443	1.3922	29.3195	30.2027	0.0292
S^{3+}	16	0.06306	0.27053	0.33902	0.96729	1.1991	45.3861	47.222	0.0389
Cl^{4+}	17	0.05932	0.25344	0.31190	0.86545	1.0473	64.9574	67.8	0.0419
Ar^{5+}	18	0.05599	0.23839	0.28878	0.78276	0.9282	87.9522	91.009	0.0336
K^{6+}	19	0.05302	0.22503	0.26884	0.71450	0.8330	114.3301	117.56	0.0275
Ca^{7+}	20	0.05035	0.21308	0.25149	0.65725	0.7555	144.0664	147.24	0.0216
Sc^{8+}	21	0.04794	0.20235	0.23625	0.60857	0.6913	177.1443	180.03	0.0160
Ti^{9+}	22	0.04574	0.19264	0.22276	0.56666	0.6371	213.5521	215.92	0.0110
V^{10+}	23	0.04374	0.18383	0.21074	0.53022	0.5909	253.2806	255.7	0.0095
Cr^{11+}	24	0.04191	0.17579	0.19995	0.49822	0.5510	296.3231	298.0	0.0056
Mn^{12+}	25	0.04022	0.16842	0.19022	0.46990	0.5162	342.6741	343.6	0.0027
Fe^{13+}	26	0.03867	0.16165	0.18140	0.44466	0.4855	392.3293	392.2	-0.0003
Co^{14+}	27	0.03723	0.15540	0.17336	0.42201	0.4583	445.2849	444	-0.0029
Ni^{15+}	28	0.03589	0.14961	0.16601	0.40158	0.4341	501.5382	499	-0.0051
Cu^{16+}	29	0.03465	0.14424	0.15926	0.38305	0.4122	561.0867	557	-0.0073
Zn^{17+}	30	0.03349	0.13925	0.15304	0.36617	0.3925	623.9282	619	-0.0080

[a] Radius of the paired 1s inner electrons of thirteen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of thirteen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of thirteen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of thirteen-electron atoms from Eq. (10.255)).

[e] Radius of the unpaired 3p outer electron of thirteen-electron atoms from Eq. (10.288) for $Z > 13$ and Eq. (10.276) for Al.

[f] Calculated ionization energies of thirteen-electron atoms given by the electric energy (Eq. (10.289)) for $Z > 13$ and Eq. (10.279) for Al.

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.13. Ionization energies for some fourteen-electron atoms.

14 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{14} (a_o) [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
Si	14	0.07216	0.31274	0.40978	1.25155	1.67685	8.11391	8.15169	0.0046
P^+	15	0.06730	0.29010	0.37120	1.09443	1.35682	20.0555	19.7694	-0.0145
S^{2+}	16	0.06306	0.27053	0.33902	0.96729	1.21534	33.5852	34.790	0.0346
Cl^{3+}	17	0.05932	0.25344	0.31190	0.86545	1.06623	51.0426	53.4652	0.0453
Ar^{4+}	18	0.05599	0.23839	0.28878	0.78276	0.94341	72.1094	75.020	0.0388
K^{5+}	19	0.05302	0.22503	0.26884	0.71450	0.84432	96.6876	99.4	0.0273
Ca^{6+}	20	0.05035	0.21308	0.25149	0.65725	0.76358	124.7293	127.2	0.0194
Sc^{7+}	21	0.04794	0.20235	0.23625	0.60857	0.69682	156.2056	158.1	0.0120
Ti^{8+}	22	0.04574	0.19264	0.22276	0.56666	0.64078	191.0973	192.10	0.0052
V^{9+}	23	0.04374	0.18383	0.21074	0.53022	0.59313	229.3905	230.5	0.0048
Cr^{10+}	24	0.04191	0.17579	0.19995	0.49822	0.55211	271.0748	270.8	-0.0010
Mn^{11+}	25	0.04022	0.16842	0.19022	0.46990	0.51644	316.1422	314.4	-0.0055
Fe^{12+}	26	0.03867	0.16165	0.18140	0.44466	0.48514	364.5863	361	-0.0099
Co^{13+}	27	0.03723	0.15540	0.17336	0.42201	0.45745	416.4021	411	-0.0131
Ni^{14+}	28	0.03589	0.14961	0.16601	0.40158	0.43277	471.5854	464	-0.0163
Cu^{15+}	29	0.03465	0.14424	0.15926	0.38305	0.41064	530.1326	520	-0.0195
Zn^{16+}	30	0.03349	0.13925	0.15304	0.36617	0.39068	592.0410	579	-0.0225

[a] Radius of the paired 1s inner electrons of fourteen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of fourteen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of fourteen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of fourteen-electron atoms from Eq. (10.255)).

[e] Radius of the two unpaired 3p outer electrons of fourteen-electron atoms from Eq. (10.309) for $Z > 14$ and Eq. (10.297) for Si .

[f] Calculated ionization energies of fourteen-electron atoms given by the electric energy (Eq. (10.310)).

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.14. Ionization energies for some fifteen-electron atoms.

15 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{15} (a_o) [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
P	15	0.06730	0.29010	0.37120	1.09443	1.28900	10.55536	10.48669	-0.0065
S^+	16	0.06306	0.27053	0.33902	0.96729	1.15744	23.5102	23.3379	-0.0074
Cl^{2+}	17	0.05932	0.25344	0.31190	0.86545	1.06759	38.2331	39.61	0.0348
Ar^{3+}	18	0.05599	0.23839	0.28878	0.78276	0.95423	57.0335	59.81	0.0464
K^{4+}	19	0.05302	0.22503	0.26884	0.71450	0.85555	79.5147	82.66	0.0381
Ca^{5+}	20	0.05035	0.21308	0.25149	0.65725	0.77337	105.5576	108.78	0.0296
Sc^{6+}	21	0.04794	0.20235	0.23625	0.60857	0.70494	135.1046	138.0	0.0210
Ti^{7+}	22	0.04574	0.19264	0.22276	0.56666	0.64743	168.1215	170.4	0.0134
V^{8+}	23	0.04374	0.18383	0.21074	0.53022	0.59854	204.5855	205.8	0.0059
Cr^{9+}	24	0.04191	0.17579	0.19995	0.49822	0.55652	244.4799	244.4	-0.0003
Mn^{10+}	25	0.04022	0.16842	0.19022	0.46990	0.52004	287.7926	286.0	-0.0063
Fe^{11+}	26	0.03867	0.16165	0.18140	0.44466	0.48808	334.5138	330.8	-0.0112
Co^{12+}	27	0.03723	0.15540	0.17336	0.42201	0.45985	384.6359	379	-0.0149
Ni^{13+}	28	0.03589	0.14961	0.16601	0.40158	0.43474	438.1529	430	-0.0190
Cu^{14+}	29	0.03465	0.14424	0.15926	0.38305	0.41225	495.0596	484	-0.0229
Zn^{15+}	30	0.03349	0.13925	0.15304	0.36617	0.39199	555.3519	542	-0.0246

[a] Radius of the paired 1s inner electrons of fifteen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of fifteen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of fifteen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of fifteen-electron atoms from Eq. (10.255)).

[e] Radius of the three unpaired 3p outer electrons of fifteen-electron atoms from Eq. (10.331) for $Z > 15$ and Eq. (10.319) for P.

[f] Calculated ionization energies of fifteen-electron atoms given by the electric energy (Eq. (10.332)).

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.15. Ionization energies for some sixteen-electron atoms.

16 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{16} (a_o) [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
S	16	0.06306	0.27053	0.33902	0.96729	1.32010	10.30666	10.36001	0.0051
Cl^+	17	0.05932	0.25344	0.31190	0.86545	1.10676	24.5868	23.814	-0.0324
Ar^{2+}	18	0.05599	0.23839	0.28878	0.78276	1.02543	39.8051	40.74	0.0229
K^{3+}	19	0.05302	0.22503	0.26884	0.71450	0.92041	59.1294	60.91	0.0292
Ca^{4+}	20	0.05035	0.21308	0.25149	0.65725	0.82819	82.1422	84.50	0.0279
Sc^{5+}	21	0.04794	0.20235	0.23625	0.60857	0.75090	108.7161	110.68	0.0177
Ti^{6+}	22	0.04574	0.19264	0.22276	0.56666	0.68622	138.7896	140.8	0.0143
V^{7+}	23	0.04374	0.18383	0.21074	0.53022	0.63163	172.3256	173.4	0.0062
Cr^{8+}	24	0.04191	0.17579	0.19995	0.49822	0.58506	209.2996	209.3	0.0000
Mn^{9+}	25	0.04022	0.16842	0.19022	0.46990	0.54490	249.6938	248.3	-0.0056
Fe^{10+}	26	0.03867	0.16165	0.18140	0.44466	0.50994	293.4952	290.2	-0.0114
Co^{11+}	27	0.03723	0.15540	0.17336	0.42201	0.47923	340.6933	336	-0.0140
Ni^{12+}	28	0.03589	0.14961	0.16601	0.40158	0.45204	391.2802	384	-0.0190
Cu^{13+}	29	0.03465	0.14424	0.15926	0.38305	0.42781	445.2492	435	-0.0236
Zn^{14+}	30	0.03349	0.13925	0.15304	0.36617	0.40607	502.5950	490	-0.0257

[a] Radius of the paired 1s inner electrons of sixteen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of sixteen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of sixteen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of sixteen-electron atoms from Eq. (10.255)).

[e] Radius of the two paired and two unpaired 3p outer electrons of sixteen-electron atoms from Eq. (10.353) for $Z > 16$ and Eq. (10.341) for S.

[f] Calculated ionization energies of sixteen-electron atoms given by the electric energy (Eq. (10.354)).

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.16. Ionization energies for some seventeen-electron atoms.

17 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{17} (a_o) [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
Cl	17	0.05932	0.25344	0.31190	0.86545	1.05158	12.93841	12.96764	0.0023
Ar^+	18	0.05599	0.23839	0.28878	0.78276	0.98541	27.6146	27.62967	0.0005
K^{2+}	19	0.05302	0.22503	0.26884	0.71450	0.93190	43.8001	45.806	0.0438
Ca^{3+}	20	0.05035	0.21308	0.25149	0.65725	0.84781	64.1927	67.27	0.0457
Sc^{4+}	21	0.04794	0.20235	0.23625	0.60857	0.77036	88.3080	91.65	0.0365
Ti^{5+}	22	0.04574	0.19264	0.22276	0.56666	0.70374	116.0008	119.53	0.0295
V^{6+}	23	0.04374	0.18383	0.21074	0.53022	0.64701	147.2011	150.6	0.0226
Cr^{7+}	24	0.04191	0.17579	0.19995	0.49822	0.59849	181.8674	184.7	0.0153
Mn^{8+}	25	0.04022	0.16842	0.19022	0.46990	0.55667	219.9718	221.8	0.0082
Fe^{9+}	26	0.03867	0.16165	0.18140	0.44466	0.52031	261.4942	262.1	0.0023
Co^{10+}	27	0.03723	0.15540	0.17336	0.42201	0.48843	306.4195	305	-0.0047
Ni^{11+}	28	0.03589	0.14961	0.16601	0.40158	0.46026	354.7360	352	-0.0078
Cu^{12+}	29	0.03465	0.14424	0.15926	0.38305	0.43519	406.4345	401	-0.0136
Zn^{13+}	30	0.03349	0.13925	0.15304	0.36617	0.41274	461.5074	454	-0.0165

[a] Radius of the paired 1s inner electrons of seventeen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of seventeen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of seventeen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of seventeen-electron atoms from Eq. (10.255)).

[e] Radius of the two sets of paired and an unpaired 3p outer electron of seventeen-electron atoms from Eq. (10.376) for $Z > 17$ and Eq. (10.363) for Cl.

[f] Calculated ionization energies of seventeen-electron atoms given by the electric energy (Eq. (10.377)).

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.17. Ionization energies for some eighteen-electron atoms.

18 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{18} (a_o) [e]	Theoretical Ionization Energies [f] (eV)	Experimental Ionization Energies [g] (eV)	Relative Error [h]
Ar	18	0.05599	0.23839	0.28878	0.78276	0.86680	15.69651	15.75962	0.0040
K^+	19	0.05302	0.22503	0.26884	0.71450	0.85215	31.9330	31.63	-0.0096
Ca^{2+}	20	0.05035	0.21308	0.25149	0.65725	0.82478	49.4886	50.9131	0.0280
Sc^{3+}	21	0.04794	0.20235	0.23625	0.60857	0.76196	71.4251	73.4894	0.0281
Ti^{4+}	22	0.04574	0.19264	0.22276	0.56666	0.70013	97.1660	99.30	0.0215
V^{5+}	23	0.04374	0.18383	0.21074	0.53022	0.64511	126.5449	128.13	0.0124
Cr^{6+}	24	0.04191	0.17579	0.19995	0.49822	0.59718	159.4836	160.18	0.0043
Mn^{7+}	25	0.04022	0.16842	0.19022	0.46990	0.55552	195.9359	194.5	-0.0074
Fe^{8+}	26	0.03867	0.16165	0.18140	0.44466	0.51915	235.8711	233.6	-0.0097
Co^{9+}	27	0.03723	0.15540	0.17336	0.42201	0.48720	279.2670	275.4	-0.0140
Ni^{10+}	28	0.03589	0.14961	0.16601	0.40158	0.45894	326.1070	321.0	-0.0159
Cu^{11+}	29	0.03465	0.14424	0.15926	0.38305	0.43379	376.3783	369	-0.0200
Zn^{12+}	30	0.03349	0.13925	0.15304	0.36617	0.41127	430.0704	419.7	-0.0247

[a] Radius of the paired 1s inner electrons of eighteen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of eighteen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of eighteen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of eighteen-electron atoms from Eq. (10.255)).

[e] Radius of the three sets of paired 3p outer electrons of eighteen-electron atoms from Eq. (10.399) for $Z > 18$ and Eq. (10.386) for Ar.

[f] Calculated ionization energies of eighteen-electron atoms given by the electric energy (Eq. (10.400)).

[g] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[h] (Experimental-theoretical)/experimental.

Table 10.19. Ionization energies for some nineteen-electron atoms.

19 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{18} (a_o) [e]	r_{19} (a_o) [f]	Theoretical Ionization Energies [g] (eV)	Experimental Ionization Energies [h] (eV)	Relative Error [i]
K	19	0.05302	0.22503	0.26884	0.71450	0.85215	3.14515	4.32596	4.34066	0.0034
Ca^{+}	20	0.05035	0.21308	0.25149	0.65725	0.82478	2.40060	11.3354	11.87172	0.0452
Sc^{2+}	21	0.04794	0.20235	0.23625	0.60857	0.76196	1.65261	24.6988	24.75666	0.0023
Ti^{3+}	22	0.04574	0.19264	0.22276	0.56666	0.70013	1.29998	41.8647	43.2672	0.0324
V^{4+}	23	0.04374	0.18383	0.21074	0.53022	0.64511	1.08245	62.8474	65.2817	0.0373
Cr^{5+}	24	0.04191	0.17579	0.19995	0.49822	0.59718	0.93156	87.6329	90.6349	0.0331
Mn^{6+}	25	0.04022	0.16842	0.19022	0.46990	0.55552	0.81957	116.2076	119.203	0.0251
Fe^{7+}	26	0.03867	0.16165	0.18140	0.44466	0.51915	0.73267	148.5612	151.06	0.0165
Co^{8+}	27	0.03723	0.15540	0.17336	0.42201	0.48720	0.66303	184.6863	186.13	0.0078
Ni^{9+}	28	0.03589	0.14961	0.16601	0.40158	0.45894	0.60584	224.5772	224.6	0.0001
Cu^{10+}	29	0.03465	0.14424	0.15926	0.38305	0.43379	0.55797	268.2300	265.3	-0.0110
Zn^{11+}	30	0.03349	0.13925	0.15304	0.36617	0.41127	0.51726	315.6418	310.8	-0.0156

[a] Radius of the paired 1s inner electrons of nineteen-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of nineteen-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of nineteen-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of nineteen-electron atoms from Eq. (10.255)).

[e] Radius of the three sets of paired 3p inner electrons of nineteen-electron atoms from Eq. (10.399).

[f] Radius of the unpaired 4s outer electron of nineteen-electron atoms from Eq. (10.425) for $Z > 19$ and Eq. (10.414) for K.

[g] Calculated ionization energies of nineteen-electron atoms given by the electric energy (Eq. (10.426)).

[h] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[i] (Experimental-theoretical)/experimental.

Table 10.20. Ionization energies for some twenty-electron atoms.

20 e Atom	Z	r_1 (a_o) [a]	r_3 (a_o) [b]	r_{10} (a_o) [c]	r_{12} (a_o) [d]	r_{18} (a_o) [e]	r_{20} (a_o) [f]	Theoretical Ionization Energies [g] (eV)	Experimental Ionization Energies [h] (eV)	Relative Error [i]
Ca	20	0.05035	0.21308	0.25149	0.65725	0.82478	2.23009	6.10101	6.11316	0.0020
Sc^{+}	21	0.04794	0.20235	0.23625	0.60857	0.76196	2.04869	13.2824	12.79967	-0.0377
Ti^{2+}	22	0.04574	0.19264	0.22276	0.56666	0.70013	1.48579	27.4719	27.4917	0.0007
V^{3+}	23	0.04374	0.18383	0.21074	0.53022	0.64511	1.19100	45.6956	46.709	0.0217
Cr^{4+}	24	0.04191	0.17579	0.19995	0.49822	0.59718	1.00220	67.8794	69.46	0.0228
Mn^{5+}	25	0.04022	0.16842	0.19022	0.46990	0.55552	0.86867	93.9766	95.6	0.0170
Fe^{6+}	26	0.03867	0.16165	0.18140	0.44466	0.51915	0.76834	123.9571	124.98	0.0082
Co^{7+}	27	0.03723	0.15540	0.17336	0.42201	0.48720	0.68977	157.8012	157.8	0.0000
Ni^{8+}	28	0.03589	0.14961	0.16601	0.40158	0.45894	0.62637	195.4954	193	-0.0129
Cu^{9+}	29	0.03465	0.14424	0.15926	0.38305	0.43379	0.57401	237.0301	232	-0.0217
Zn^{10+}	30	0.03349	0.13925	0.15304	0.36617	0.41127	0.52997	282.3982	274	-0.0307

[a] Radius of the paired 1s inner electrons of twenty-electron atoms from Eq. (10.51).

[b] Radius of the paired 2s inner electrons of twenty-electron atoms from Eq. (10.62).

[c] Radius of the three sets of paired 2p inner electrons of twenty-electron atoms from Eq. (10.212)).

[d] Radius of the paired 3s inner electrons of twenty-electron atoms from Eq. (10.255)).

[e] Radius of the three sets of paired 3p inner electrons of twenty-electron atoms from Eq. (10.399).

[f] Radius of the paired 4s outer electrons of twenty-electron atoms from Eq. (10.445) for $Z > 20$ and Eq. (10.436) for Ca.

[g] Calculated ionization energies of twenty-electron atoms given by the electric energy (Eq. (10.446)).

[h] From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [2-3].

[i] (Experimental-theoretical)/experimental.

The agreement between the experimental and calculated values of Table 10.20 is well within the experimental capability of the spectroscopic determinations including the values at large Z which relies on X-ray spectroscopy. In this case, the experimental capability is about three to four significant figures which is consistent with the last column. Ionization energies are difficult to determine since the cut-off of the Rydberg series of lines at the ionization energy is often not observed. Thus, the calcium atom isoelectronic series given in Table 10.20 [2-3] relies on theoretical calculations and interpolation of the Ca isoelectronic and Rydberg series as well as direct experimental data to extend the precision beyond the capability of X-ray spectroscopy. But, no assurances can be given that these techniques are correct, and they may not improve the results. The error given in the last column is very reasonable given the quality of the data.

References

2. C. E. Moore, "Ionization Potentials and Ionization Limits Derived from the Analyses of Optical Spectra, Nat. Stand. Ref. Data Ser.-Nat. Bur. Stand. (U.S.), No. 34, 1970.
3. Robert C. Weast, CRC Handbook of Chemistry and Physics, 58 Edition, CRC Press, West Palm Beach, Florida, (1977), p. E-68.

Table 9.5. Calculated and experimental energies of states of helium.

n	ℓ	r_1 (a_{He}) [a]	r_2 (a_{He}) [b]	**Term Symbol**	E_{ele} CP He I Energy Levels [c] (eV)	NIST He I Energy Levels [d] (eV)	Difference CP-NIST (eV)	Relative Difference [e] (CP-NIST)
1	0	0.56699	0.566987	$1s^2\ ^1S$	-24.58750	-24.58741	-0.000092	0.0000038
2	0	0.506514	1.42265	$1s2s\ ^3S$	-4.78116	-4.76777	-0.0133929	0.0028090
2	0	0.501820	1.71132	$1s2s\ ^1S$	-3.97465	-3.97161	-0.0030416	0.0007658
2	1	0.500571	1.87921	$1s2p\ ^3P^0_2$	-3.61957	-3.6233	0.0037349	-0.0010308
2	1	0.500571	1.87921	$1s2p\ ^3P^0_1$	-3.61957	-3.62329	0.0037249	-0.0010280
2	1	0.500571	1.87921	$1s2p\ ^3P^0_0$	-3.61957	-3.62317	0.0036049	-0.0009949
2	1	0.499929	2.01873	$1s2p\ ^1P^0$	-3.36941	-3.36936	-0.0000477	0.0000141
3	0	0.500850	2.42265	$1s3s\ ^3S$	-1.87176	-1.86892	-0.0028377	0.0015184
3	0	0.500302	2.71132	$1s3s\ ^1S$	-1.67247	-1.66707	-0.0054014	0.0032401
3	1	0.500105	2.87921	$1s3p\ ^3P^0_2$	-1.57495	-1.58031	0.0053590	-0.0033911
3	1	0.500105	2.87921	$1s3p\ ^3P^0_1$	-1.57495	-1.58031	0.0053590	-0.0033911
3	1	0.500105	2.87921	$1s3p\ ^3P^0_0$	-1.57495	-1.58027	0.0053190	-0.0033659
3	2	0.500011	2.98598	$1s3d\ ^3D_3$	-1.51863	-1.51373	-0.0049031	0.0032391
3	2	0.500011	2.98598	$1s3d\ ^3D_2$	-1.51863	-1.51373	-0.0049031	0.0032391
3	2	0.500011	2.98598	$1s3d\ ^3D_1$	-1.51863	-1.51373	-0.0049031	0.0032391
3	2	0.499999	3.00076	$1s3d\ ^1D$	-1.51116	-1.51331	0.0021542	-0.0014235
3	1	0.499986	3.01873	$1s3p\ ^1P^0$	-1.50216	-1.50036	-0.0017999	0.0011997
4	0	0.500225	3.42265	$1s4s\ ^3S$	-0.99366	-0.99342	-0.0002429	0.0002445
4	0	0.500088	3.71132	$1s4s\ ^1S$	-0.91637	-0.91381	-0.0025636	0.0028054
4	1	0.500032	3.87921	$1s4p\ ^3P^0_2$	-0.87671	-0.87949	0.0027752	-0.0031555
4	1	0.500032	3.87921	$1s4p\ ^3P^0_1$	-0.87671	-0.87949	0.0027752	-0.0031555
4	1	0.500032	3.87921	$1s4p\ ^3P^0_0$	-0.87671	-0.87948	0.0027652	-0.0031442
4	2	0.500003	3.98598	$1s4d\ ^3D_3$	-0.85323	-0.85129	-0.0019398	0.0022787
4	2	0.500003	3.98598	$1s4d\ ^3D_2$	-0.85323	-0.85129	-0.0019398	0.0022787
4	2	0.500003	3.98598	$1s4d\ ^3D_1$	-0.85323	-0.85129	-0.0019398	0.0022787
4	2	0.500000	4.00076	$1s4d\ ^1D$	-0.85008	-0.85105	0.0009711	-0.0011411
4	3	0.500000	3.99857	$1s4f\ ^3F^0_3$	-0.85054	-0.85038	-0.0001638	0.0001926
4	3	0.500000	3.99857	$1s4f\ ^3F^0_4$	-0.85054	-0.85038	-0.0001638	0.0001926
4	3	0.500000	3.99857	$1s4f\ ^3F^0_2$	-0.85054	-0.85038	-0.0001638	0.0001926
4	3	0.500000	4.00000	$1s4f\ ^1F^0$	-0.85024	-0.85037	0.0001300	-0.0001529
4	1	0.499995	4.01873	$1s4p\ ^1P^0$	-0.84628	-0.84531	-0.0009676	0.0011446
5	0	0.500083	4.42265	$1s5s\ ^3S$	-0.61519	-0.61541	0.0002204	-0.0003582

5	0	0.500035	4.71132	$1s5s\ ^1S$	-0.57750	-0.57617	-0.0013253	0.0023002
5	1	0.500013	4.87921	$1s5p\ ^3P^0_2$	-0.55762	-0.55916	0.0015352	-0.0027456
5	1	0.500013	4.87921	$1s5p\ ^3P^0_1$	-0.55762	-0.55916	0.0015352	-0.0027456
5	1	0.500013	4.87921	$1s5p\ ^3P^0_0$	-0.55762	-0.55915	0.0015252	-0.0027277
5	2	0.500001	4.98598	$1s5d\ ^3D_3$	-0.54568	-0.54472	-0.0009633	0.0017685
5	2	0.500001	4.98598	$1s5d\ ^3D_2$	-0.54568	-0.54472	-0.0009633	0.0017685
5	2	0.500001	4.98598	$1s5d\ ^3D_1$	-0.54568	-0.54472	-0.0009633	0.0017685
5	2	0.500000	5.00076	$1s5d\ ^1D$	-0.54407	-0.54458	0.0005089	-0.0009345
5	3	0.500000	4.99857	$1s5f\ ^3F^0_3$	-0.54431	-0.54423	-0.0000791	0.0001454
5	3	0.500000	4.99857	$1s5f\ ^3F^0_4$	-0.54431	-0.54423	-0.0000791	0.0001454
5	3	0.500000	4.99857	$1s5f\ ^3F^0_2$	-0.54431	-0.54423	-0.0000791	0.0001454
5	3	0.500000	5.00000	$1s5f\ ^1F^0$	-0.54415	-0.54423	0.0000764	-0.0001404
5	4	0.500000	4.99988	$1s5g\ ^3G_4$	-0.54417	-0.54417	0.0000029	-0.0000054
5	4	0.500000	4.99988	$1s5g\ ^3G_5$	-0.54417	-0.54417	0.0000029	-0.0000054
5	4	0.500000	4.99988	$1s5g\ ^3G_3$	-0.54417	-0.54417	0.0000029	-0.0000054
5	4	0.500000	5.00000	$1s5g\ ^1G$	-0.54415	-0.54417	0.0000159	-0.0000293
5	1	0.499998	5.01873	$1s5p\ ^1P^0$	-0.54212	-0.54158	-0.0005429	0.0010025
6	0	0.500038	5.42265	$1s6s\ ^3S$	-0.41812	-0.41838	0.0002621	-0.0006266
6	0	0.500016	5.71132	$1s6s\ ^1S$	-0.39698	-0.39622	-0.0007644	0.0019291
6	1	0.500006	5.87921	$1s6p\ ^3P^0_2$	-0.38565	-0.38657	0.0009218	-0.0023845
6	1	0.500006	5.87921	$1s6p\ ^3P^0_1$	-0.38565	-0.38657	0.0009218	-0.0023845
6	1	0.500006	5.87921	$1s6p\ ^3P^0_0$	-0.38565	-0.38657	0.0009218	-0.0023845
6	2	0.500001	5.98598	$1s6d\ ^3D_3$	-0.37877	-0.37822	-0.0005493	0.0014523
6	2	0.500001	5.98598	$1s6d\ ^3D_2$	-0.37877	-0.37822	-0.0005493	0.0014523
6	2	0.500001	5.98598	$1s6d\ ^3D_1$	-0.37877	-0.37822	-0.0005493	0.0014523
6	2	0.500000	6.00076	$1s6d\ ^1D$	-0.37784	-0.37813	0.0002933	-0.0007757
6	3	0.500000	5.99857	$1s6f\ ^3F^0_3$	-0.37797	-0.37793	-0.0000444	0.0001176
6	3	0.500000	5.99857	$1s6f\ ^3F^0_4$	-0.37797	-0.37793	-0.0000444	0.0001176
6	3	0.500000	5.99857	$1s6f\ ^3F^0_2$	-0.37797	-0.37793	-0.0000444	0.0001176
6	3	0.500000	6.00000	$1s6f\ ^1F^0$	-0.37788	-0.37793	0.0000456	-0.0001205
6	4	0.500000	5.99988	$1s6g\ ^3G_4$	-0.37789	-0.37789	-0.0000023	0.0000060
6	4	0.500000	5.99988	$1s6g\ ^3G_5$	-0.37789	-0.37789	-0.0000023	0.0000060
6	4	0.500000	5.99988	$1s6g\ ^3G_3$	-0.37789	-0.37789	-0.0000023	0.0000060
6	4	0.500000	6.00000	$1s6g\ ^1G$	-0.37788	-0.37789	0.0000053	-0.0000140
6	5	0.500000	5.99999	$1s6h\ ^3H^0_4$	-0.37789	-0.37788	-0.0000050	0.0000133
6	5	0.500000	5.99999	$1s6h\ ^3H^0_5$	-0.37789	-0.37788	-0.0000050	0.0000133
6	5	0.500000	5.99999	$1s6h\ ^3H^0_6$	-0.37789	-0.37788	-0.0000050	0.0000133
6	5	0.500000	6.00000	$1s6h\ ^1H^0$	-0.37788	-0.37788	-0.0000045	0.0000119

6	1	0.499999	6.01873	$1s6p\ ^1P^0$	-0.37671	-0.37638	-0.0003286	0.0008730
7	0	0.500019	6.42265	$1s7s\ ^3S$	-0.30259	-0.30282	0.0002337	-0.0007718
7	0	0.500009	6.71132	$1s7s\ ^1S$	-0.28957	-0.2891	-0.0004711	0.0016295
7	1	0.500003	6.87921	$1s7p\ ^3P^0_2$	-0.28250	-0.28309	0.0005858	-0.0020692
7	1	0.500003	6.87921	$1s7p\ ^3P^0_1$	-0.28250	-0.28309	0.0005858	-0.0020692
7	1	0.500003	6.87921	$1s7p\ ^3P^0_0$	-0.28250	-0.28309	0.0005858	-0.0020692
7	2	0.500000	6.98598	$1s7d\ ^3D_3$	-0.27819	-0.27784	-0.0003464	0.0012468
7	2	0.500000	6.98598	$1s7d\ ^3D_2$	-0.27819	-0.27784	-0.0003464	0.0012468
7	2	0.500000	6.98598	$1s7d\ ^3D_1$	-0.27819	-0.27784	-0.0003464	0.0012468
7	2	0.500000	7.00076	$1s7d\ ^1D$	-0.27760	-0.27779	0.0001907	-0.0006864
7	3	0.500000	6.99857	$1s7f\ ^3F^0_3$	-0.27769	-0.27766	-0.0000261	0.0000939
7	3	0.500000	6.99857	$1s7f\ ^3F^0_4$	-0.27769	-0.27766	-0.0000261	0.0000939
7	3	0.500000	6.99857	$1s7f\ ^3F^0_2$	-0.27769	-0.27766	-0.0000261	0.0000939
7	3	0.500000	7.00000	$1s7f\ ^1F^0$	-0.27763	-0.27766	0.0000306	-0.0001102
7	4	0.500000	6.99988	$1s7g\ ^3G_4$	-0.27763	-0.27763	-0.0000043	0.0000155
7	4	0.500000	6.99988	$1s7g\ ^3G_5$	-0.27763	-0.27763	-0.0000043	0.0000155
7	4	0.500000	6.99988	$1s7g\ ^3G_3$	-0.27763	-0.27763	-0.0000043	0.0000155
7	4	0.500000	7.00000	$1s7g\ ^1G$	-0.27763	-0.27763	0.0000004	-0.0000016
7	5	0.500000	6.99999	$1s7h\ ^3H^0_5$	-0.27763	-0.27763	0.0000002	-0.0000009
7	5	0.500000	6.99999	$1s7h\ ^3H^0_6$	-0.27763	-0.27763	0.0000002	-0.0000009
7	5	0.500000	6.99999	$1s7h\ ^3H^0_4$	-0.27763	-0.27763	0.0000002	-0.0000009
7	5	0.500000	7.00000	$1s7h\ ^1H^0$	-0.27763	-0.27763	0.0000006	-0.0000021
7	6	0.500000	7.00000	$1s7\ i^3I_5$	-0.27763	-0.27762	-0.0000094	0.0000339
7	6	0.500000	7.00000	$1s7i\ ^3I6$	-0.27763	-0.27762	-0.0000094	0.0000339
7	6	0.500000	6.78349	$1s7i\ ^3I_7$	-0.27763	-0.27762	-0.0000094	0.0000339
7	6	0.500000	7.00000	$1s7i\ ^1I$	-0.27763	-0.27762	-0.0000094	0.0000338
7	1	0.500000	7.01873	$1s7p\ ^1P^0$	-0.27689	-0.27667	-0.0002186	0.0007900
8	0	0.500011	7.42265	$1s8s\ ^3S$	-0.22909	-0.22928	0.0001866	-0.0008139
8	0	0.500005	7.71132	$1s8s\ ^1S$	-0.22052	-0.2202	-0.0003172	0.0014407
9	0	0.500007	8.42265	$1s9s\ ^3S$	-0.17946	-0.17961	0.0001489	-0.0008291
9	0	0.500003	8.71132	$1s9s\ ^1S$	-0.17351	-0.1733	-0.0002141	0.0012355
10	0	0.500004	9.42265	$1s10s\ ^3S$	-0.14437	-0.1445	0.0001262	-0.0008732
10	0	0.500002	9.71132	$1s10s\ ^1S$	-0.14008	-0.13992	-0.0001622	0.0011594
11	0	0.500003	10.42265	$1s11s\ ^3S$	-0.11866	-0.11876	0.0001037	-0.0008734
11	0	0.500001	10.71132	$1s11s\ ^1S$	-0.11546	-0.11534	-0.0001184	0.0010268
						Avg.	**-0.000112**	**0.0000386**

[a] Radius of the inner electron 1 of singlet excited states with $\ell = 0$ from Eq. (9.29); triplet excited states with $\ell = 0$ from Eq. (9.37); singlet excited states with $\ell \neq 0$ from Eq. (9.60) for $\ell = 1$ or $\ell = 2$ and Eq. (9.61) for $\ell = 3$, and Eq. (9.62) for $\ell = 4, 5, 6...$; triplet excited states with $\ell \neq 0$ from Eq. (9.69), and $1s^2\ ^1S$ from Eq. (7.19).

[b] Radius of the outer electron 2 of singlet excited states with $\ell = 0$ from Eq. (9.11); triplet excited states with $\ell = 0$ from Eq. (9.32); singlet excited states with $\ell \neq 0$ from Eq. (9.53); triplet excited states with $\ell \neq 0$ from Eq. (9.64), and $1s^2\ ^1S$ from Eq. (7.19).

[e] Classical Physics (CP) calculated excited-state energy levels given by the electric energy (Eq. (9.12)) and the energy level of $1s^2\ ^1S$ is given by Eqs. (7.28-7.30).

[d] Experimental NIST levels [6] with the ionization potential defined as zero.

[e] (Theoretical-Experimental)/Experimental.

STERN-GERLACH EXPERIMENT

The Stern-Gerlach experiment implies a magnetic moment of one Bohr magneton and an associated angular momentum quantum number of 1/2. Historically, this quantum number is called the spin quantum number, s ($s = \frac{1}{2}; m_s = \pm\frac{1}{2}$). The superposition of the vector projection of the orbitsphere angular momentum on the z-axis is $\frac{\hbar}{2}$ with an orthogonal component of $\frac{\hbar}{4}$. Excitation of a resonant Larmor precession gives rise to $\hbar$ on an axis $\mathbf{S}$ that precesses about the z-axis called the spin axis at the Larmor frequency at an angle of $\theta = \frac{\pi}{3}$ to give a perpendicular projection of

$$\mathbf{S}_{\perp} = \pm\sqrt{\frac{3}{4}}\hbar \tag{1}$$

and a projection onto the axis of the applied magnetic field of

$$\mathbf{S}_{\parallel} = \pm\frac{\hbar}{2} \tag{2}$$

The superposition of the $\frac{\hbar}{2}$, z-axis component of the orbitsphere angular momentum and the $\frac{\hbar}{2}$, z-axis component of $\mathbf{S}$ gives $\hbar$ corresponding to the observed electron magnetic moment of a Bohr magneton, μ_B.

ELECTRON g FACTOR

Conservation of angular momentum of the orbitsphere permits a discrete change of its "kinetic angular momentum" ($\mathbf{r} \times m\mathbf{v}$) by the applied magnetic field of $\frac{\hbar}{2}$, and concomitantly the "potential angular momentum" ($\mathbf{r} \times e\mathbf{A}$) must change by $-\frac{\hbar}{2}$.

$$\Delta\mathbf{L} = \frac{\hbar}{2} - \mathbf{r} \times e\mathbf{A} \tag{3}$$

$$= \left[\frac{\hbar}{2} - \frac{e\phi}{2\pi}\right]\hat{z} \tag{4}$$

In order that the change of angular momentum, $\Delta\mathbf{L}$, equals zero, ϕ must be $\Phi_0 = \frac{h}{2e}$, the magnetic flux quantum. The magnetic moment of the electron is parallel or antiparallel to the applied field only. During the spin-flip transition, power must be conserved. Power flow is governed by the Poynting power theorem,

$$\nabla \bullet (\mathbf{E} \times \mathbf{H}) = -\frac{\partial}{\partial t}\left[\frac{1}{2}\mu_o \mathbf{H} \bullet \mathbf{H}\right] - \frac{\partial}{\partial t}\left[\frac{1}{2}\varepsilon_o \mathbf{E} \bullet \mathbf{E}\right] - \mathbf{J} \bullet \mathbf{E} \tag{5}$$

Eq. (6) gives the total energy of the flip transition which is the sum of the energy of reorientation of the magnetic moment (1st term), the magnetic energy (2nd term), the electric energy (3rd term), and the dissipated energy of a fluxon treading the orbitsphere (4th term), respectively,

$$\Delta E_{mag}^{spin} = 2\left(1 + \frac{\alpha}{2\pi} + \frac{2}{3}\alpha^2\left(\frac{\alpha}{2\pi}\right) - \frac{4}{3}\left(\frac{\alpha}{2\pi}\right)^2\right)\mu_B B \tag{6}$$

$$\Delta E_{mag}^{spin} = g\mu_B B \tag{7}$$

where the stored magnetic energy corresponding to the $\frac{\partial}{\partial t}\left[\frac{1}{2}\mu_o \mathbf{H} \bullet \mathbf{H}\right]$ term increases, the stored electric energy corresponding to the $\frac{\partial}{\partial t}\left[\frac{1}{2}\varepsilon_o \mathbf{E} \bullet \mathbf{E}\right]$ term increases, and the $\mathbf{J} \bullet \mathbf{E}$ term is dissipative. The spin-flip transition can be considered as involving a magnetic moment of g times that of a Bohr magneton. The g factor is redesignated the fluxon g factor as opposed to the anomalous g factor. Using $\alpha^{-1} = 137.03603(82)$, the calculated value of $\frac{g}{2}$ is **1.001 159 652 137**. The experimental value [1] of $\frac{g}{2}$ is **1.001 159 652 188(4)**.

References

1. R. S. Van Dyck, Jr., P. Schwinberg, H. Dehmelt, "New high precision comparison of electron and positron g factors", Phys. Rev. Lett., Vol. 59, (1987), p. 26-29.

RELATIONS BETWEEN FUNDAMENTAL PARTICLES

The relations between the lepton masses and neutron to electron mass ratio which are independent of the definition of the imaginary time ruler *ti* including the contribution of the fields due to charge production are given in terms of the dimensionless fine structure constant α only:

$$\frac{m_\mu}{m_e} = \left(\frac{\alpha^{-2}}{2\pi}\right)^{\frac{2}{3}} \frac{\left(1+2\pi\frac{\alpha^2}{2}\right)}{\left(1+\frac{\alpha}{2}\right)} = 206.76828 \qquad (206.76827)^{a}$$

$$\frac{m_\tau}{m_\mu} = \left(\frac{\alpha^{-1}}{2}\right)^{\frac{2}{3}} \frac{\left(1+\frac{\alpha}{2}\right)}{\left(1-4\pi\alpha^2\right)} = 16.817 \qquad (16.817)$$

$$\frac{m_\tau}{m_e} = \left(\frac{\alpha^{-3}}{4\pi}\right)^{\frac{2}{3}} \frac{\left(1+2\pi\frac{\alpha^2}{2}\right)}{\left(1-4\pi\alpha^2\right)} = 3477.2 \qquad (3477.3)$$

$$\frac{m_N}{m_e} = \frac{12\pi^2}{1-\alpha}\sqrt{\frac{\sqrt{3}}{\alpha}}\frac{\left(1+2\pi\frac{\alpha^2}{2}\right)}{\left(1-2\pi\frac{\alpha^2}{2}\right)} = 1838.67 \qquad (1838.68)$$

[a] Experimental according to the 1998 CODATA and the Particle Data Group [K. Hagiwara et al., Phys. Rev. D 66, 010001 (2002); http://pdg.lbl.gov/2002/s035.pdf; P. J. Mohr and B. N. Taylor, "CODATA recommended values of the fundamental physical constants: 1998", Reviews of Modern Physics, Vol. 72, No. 2, April, (2000), pp. 351-495].