Summary Tables of Organic, Silicon, Boron, Aluminum and Organometallic Molecules and Exemplary Results on Condensed Matter Physics

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.

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

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