
Contents

Chapter one	Introduction	1
1.1	Comprehensive database of the BDEs	1
1.2	What is the BDE?	1
1.3	Why are reliable BDEs needed?	3
1.4	Scope of this book	3
1.5	On energy units	5
1.6	How to search for BDEs in this book	6
1.7	How to use the BDE data tables	7
Chapter two	Experimental methods for measuring BDEs	13
2.1	A summary of main experimental methods	13
2.2	The conversion between D_0 , D_e , and DH^0	16
2.2.1	Diatomic molecules	17
2.2.2	Polyatomic molecules	18
Chapter three	BDEs of C–H bonds	19
3.1	Chain saturated hydrocarbons	19
3.2	Chain unsaturated hydrocarbons	24
3.3	Cyclic hydrocarbons	31
3.4	Aromatic hydrocarbons	40
3.5	Halogenated hydrocarbons	61
3.6	Organic compounds containing heteroatom(s)	70
3.6.1	C–H BDEs with a-OH, -OR, -C(O), -C(O)OH, -C(O)OR, -OC(O)R and -OOR	70
3.6.1.1	C–H BDEs with a-OH	70
3.6.1.2	C–H BDEs with a-OR	73
3.6.1.3	C–H BDEs with α -C(O)	83
3.6.1.4	C–H BDEs with α -C(O)OH	93
3.6.1.5	C–H BDEs with α -C(O)OR, -OC(O)R and -OOR	96
3.6.2	C–H BDEs with α -N, -CN, -NC, -NO, -NO ₂ , -NN and in heterocyclic species	102
3.6.2.1	C–H BDEs with a-N	102
3.6.2.2	C–H BDEs with a-CN and -NC	106
3.6.2.3	C–H BDEs with α -NO, -NO ₂ , and -NN	109
3.6.2.4	C–H BDEs in heterocyclic species	112
3.6.3	C–H BDEs with α -O, -N and their groups	118

7.3	N-C bonds	403
7.4	N-S bonds	420
7.5	N-halogen bonds	422
7.6	N-B, N-Al, N-Ga, and N-In bonds	424
Chapter eight BDEs of S-, Se-, Te-, Po-X bonds		425
8.1	S-H bonds	425
8.2	S-S bonds	431
8.3	S-C bonds	436
8.4	S-halogen bonds	445
8.5	S-P, S-As, and S-Sb bonds	449
8.6	Se-X bonds	451
8.7	Te-X bonds	453
8.8	Po-X bonds	454
Chapter nine BDEs of Si-, Ge-, Sn-, and Pb-X bonds		455
9.1	Si-X BDEs	455
9.2	Ge-X bonds	467
9.3	Sn-X bonds	473
9.4	Pb-X bonds	478
Chapter ten BDEs of P-, As Sb-, Bi-X bonds		481
10.1	P-X bonds	481
10.2	As-X bonds	487
10.3	Sb-X bonds	489
10.4	Bi-X bonds	490
Chapter eleven BDEs of H(H [±])-, Li(Li [±])-, Na(Na [±])-, K(K [±])-, Rb(Rb [±])-, and Cs(Cs [±])-X bonds		493
11.1	H-, H ⁺ -, and H ⁻ -X bonds	493
11.2	Li- and Li [±] -X bonds	496
11.2.1	Li-X bonds	496
11.2.2	Li [±] -X bonds	500
11.3	Na-, Na ⁺ -, and Na ⁻ -X bonds	516
11.3.1	Na-X bonds	516
11.3.2	Na ⁺ -X bonds	522
11.3.3	Na ⁻ -X bonds	541
11.4	K-, K ⁺ -, and K ⁻ -X bonds	541
11.4.1	K-X bonds	541
11.4.2	K ⁺ -X bonds	544
11.4.3	K ⁻ -X bonds	557
11.5	Rb-, Rb ⁺ -, and Rb ⁻ -X bonds	557
11.5.1	Rb-X bonds	557
11.5.2	Rb ⁺ -X bonds	559
11.5.3	Rb ⁻ -X bonds	562
11.6	Cs-, Cs ⁺ -, and Cs ⁻ -X bonds	563
11.6.1	Cs-X bonds	563
11.6.2	Cs ⁺ -X bonds	565
11.6.3	Cs ⁻ -X bonds	569

Chapter twelve	BDEs of Be(Be ⁺)-, Mg(Mg ⁺)-, Ca(Ca ⁺)-, Sr(Sr ⁺)-, Ba(Ba ⁺)-, and Ra-X bonds	571
12.1	Be- and Be ⁺ -X bonds	571
12.1.1	Be-X bonds	571
12.1.2	Be ⁺ -X bonds	573
12.2	Mg- and Mg ⁺ -X bonds	574
12.2.1	Mg-X bonds	574
12.2.2	Mg ⁺ -X bonds	579
12.3	Ca- and Ca ⁺ -X bonds	584
12.3.1	Ca-X bonds	584
12.3.2	Ca ⁺ -X bonds	587
12.4	Sr- and Sr ⁺ -X bonds	591
12.4.1	Sr-X bonds	591
12.4.2	Sr ⁺ -X bonds	593
12.5	Ba- and Ba ⁺ -X bonds	596
12.5.1	Ba-X bonds	596
12.5.2	Ba ⁺ -X bonds	598
12.6	Ra-X bonds	599
Chapter thirteen	BDEs of Sc(Sc ⁺)-, Y(Y ⁺)-, La(La ⁺)-, and Ac(Ac ⁺)-Xbonds	601
13.1	Sc- and Sc ⁺ -X bonds	601
13.1.1	Sc-X bonds	601
13.1.2	Sc ⁺ -X bonds	603
13.2	Y- and Y ⁺ -X bonds	607
13.2.1	Y- bonds	607
13.2.2	Y ⁺ -X bonds	610
13.3	La- and La ⁺ -X bonds	612
13.4	Ac- and Ac ⁺ -X bonds	643
Chapter fourteen	BDEs of Ti(Ti [±])-, Zr(Zr ⁺)-, and Hf(Hf ⁺)-X bonds	667
14.1	Ti- Ti ⁺ -, and Ti ⁻ -X bonds	667
14.1.1	Ti-X bonds	667
14.1.2	Ti ⁺ - and Ti ⁻ -X bonds	673
14.2	Zr- and Zr ⁺ -X bonds	679
14.2.1	Zr-X bonds	679
14.2.2	Zr ⁺ -X bonds	683
14.3	Hf- and Hf ⁺ -X bonds	685
Chapter fifteen	BDEs of V(V [±])-, Nb(Nb ⁺)-, and Ta(Ta ⁺)-X bonds	689
15.1	V-, V ⁺ -, and V ⁻ -X bonds	689
15.1.1	V-Xbonds	689
15.1.2	V ⁺ -X bonds	692
15.1.3	V ⁻ -X bonds	699
15.2	Nb- and Nb ⁺ -X bonds	700
15.2.1	Nb-X bonds	700
15.2.2	Nb ⁺ -X bonds	704
15.3	Ta- and Ta ⁺ -X bonds	708
15.3.1	Ta-X bonds	708
15.3.2	Ta ⁺ -X bonds	711

Chapter sixteen	BDEs of Cr(Cr [±])-, Mo(Mo [±])-, and W(W [±])-X bonds	713
16.1	Cr-, Cr ⁺ -, and Cr ⁻ -X bonds	713
16.1.1	Cr-X bonds	713
16.1.2	Cr ⁺ -X bonds	723
16.1.3	Cr ⁻ -X bonds	733
16.2	Mo-, Mo ⁺ -, and Mo ⁻ -X bonds	734
16.2.1	Mo-X bonds	734
16.2.2	Mo ⁺ -X bonds	746
16.2.3	Mo ⁻ -X bonds	751
16.3	W-, W ⁺ -, and W ⁻ -X bonds	751
16.3.1	W-X bonds	751
16.3.2	W ⁺ -X bonds	778
16.3.3	W ⁻ -X bonds	780
Chapter seventeen	BDEs of Mn(Mn [±])-, Tc(Tc [±]), and Re(Re [±])-X bonds	781
17.1	Mn-, Mn ⁺ -, and Mn ⁻ -X bonds	781
17.1.1	Mn-X bonds	781
17.1.2	Mn ⁺ -X bonds	787
17.1.3	Mn ⁻ -X bonds	793
17.2	Tc-X and Tc ⁺ -X bonds	795
17.2.1	Tc-X bonds	795
17.2.2	Tc ⁺ -X bonds	795
17.3	Re-, Re ⁺ -, and Re ⁻ -X bonds	796
17.3.1	Re-X bonds	796
17.3.2	Re ⁺ -X bonds	799
17.3.3	Re ⁻ -X bonds	801
Chapter eighteen	BDEs of Fe(Fe [±])-, Ru(Ru [±])-, and Os(Os [±])-X bonds	803
18.1	Fe-, Fe ⁺ -, and Fe ⁻ -X bonds	803
18.1.1	Fe-X bonds	803
18.1.2	Fe ⁺ -X bonds	815
18.1.3	Fe ⁻ -X bonds	838
18.2	Ru- and Ru ⁺ -X bonds	840
18.2.1	Ru-X bonds	840
18.2.2	Ru ⁺ -X bonds	849
18.3	Os- and Os ⁺ -X bonds	851
18.3.1	Os-X bonds	851
18.3.2	Os ⁺ -X bonds	853
Chapter nineteen	BDEs of Co(Co [±])-, Rh(Rh [±])-, and Ir(Ir [±])-X bonds	855
19.1	Co-, Co ⁺ -, and Co ⁻ -X bonds	855
19.1.1	Co-X bonds	855
19.1.2	Co ⁺ -X bonds	868
19.1.3	Co ⁻ -X bonds	881
19.2	Rh- and Rh ⁺ -X bonds	882
19.2.1	Rh-X bonds	882
19.2.2	Rh ⁺ -X bonds	892
19.3	Ir- and Ir ⁺ -X bonds	895
19.3.1	Ir-X bonds	895
19.3.2	Ir ⁺ -X bonds	901

Chapter twenty	BDEs of Ni(Ni [±])-, Pd(Pd [±])-, and Pt(Pt [±])-X bonds	903
20.1	Ni-, Ni ⁺ -, and Ni ⁻ -X bonds	903
20.1.1	Ni-X bonds	903
20.1.2	Ni ⁺ - and Ni ⁻ -X bonds	921
20.1.3	Ni ⁻ -X bonds	931
20.2	Pd-, Pd ⁺ -, and Pd ⁻ -X bonds	932
20.2.1	Pd-X bonds	932
20.2.2	Pd ⁺ -X bonds	939
20.2.3	Pd ⁻ -X bonds	941
20.3	Pt-, Pt ⁺ -, and Pt ⁻ -X bonds	941
20.3.1	Pt-X bonds	941
20.3.2	Pt ⁺ -X bonds	963
20.3.3	Pt ⁻ -X bonds	965
Chapter twenty-one	BDEs of Cu(Cu [±])-, Ag(Ag [±])-, and Au(Au [±])-X bonds	967
21.1	Cu-, Cu ⁺ -, and Cu ⁻ -X bonds	967
21.1.1	Cu-X bonds	967
21.1.2	Cu ⁺ -X bonds	982
21.1.3	Cu ⁻ -X bonds	989
21.2	Ag-, Ag ⁺ -, and Ag ⁻ -X bonds	990
21.2.1	Ag-X bonds	990
21.2.2	Ag ⁺ -X bonds	999
21.2.3	Ag ⁻ -X bonds	1009
21.3	Au-, Au ⁺ -, and Au ⁻ -X bonds	1009
21.3.1	Au-X bonds	1009
21.3.2	Au ⁺ -X bonds	1021
21.3.3	Au ⁻ -X bonds	1025
Chapter twenty-two	BDEs of Zn(Zn ⁺)-, Cd(Cd ⁺)-, and Hg(Hg ⁺)-X bonds	1027
22.1	Zn- and Zn ⁺ -X bonds	1027
22.1.1	Zn-X bonds	1027
22.1.2	Zn ⁺ -X bonds	1031
22.2	Cd- and Cd ⁺ -X bonds	1033
22.2.1	Cd-X bonds	1033
22.2.2	Cd ⁺ -X bonds	1035
22.3	Hg- and Hg ⁺ -X bonds	1036
22.3.1	Hg-X bonds	1036
22.3.2	Hg ⁺ -X bonds	1039
Chapter twenty-three	BDEs of B(B [±])-, Al(Al [±])-, Ga(Ga [±])-, In(In [±])-, and Tl(Tl [±])-X bonds	1041
23.1	B-, B ⁺ -, and B ⁻ -X bonds	1041
23.1.1	B-X bonds	1041
23.1.2	B ⁺ -X bonds	1049
23.1.3	B ⁻ -X bonds	1051
23.2	Al-, and Al [±] -X bonds	1052
23.2.1	Al-X bonds	1052
23.2.2	Al ⁺ - and Al ⁻ -X bonds	1062

26.3	Selenium clusters/complexes	1341
26.4	Tellurium clusters/complexes	1346
Chapter twenty-seven BDEs in the halogenated molecules, clusters and complexes		1351
27.1	F-, F ⁺ -, and F ⁻ -X bonds	1351
27.1.1	F-X bonds	1351
27.1.2	F ⁺ -X bonds	1355
27.1.3	F ⁻ -X bonds	1355
27.2	Cl-, Cl ⁺ -, and Cl ⁻ -X bonds	1374
27.2.1	Cl-X bonds	1374
27.2.2	Cl ⁺ -X bonds	1377
27.2.3	Cl ⁻ -X bonds	1379
27.3	Br-, Br ⁺ -, and Br ⁻ -X bonds	1399
27.3.1	Br-X bonds	1399
27.3.2	Br ⁺ -X bonds	1401
27.3.3	Br ⁻ -X bonds	1402
27.4	I-, I ⁺ -, and I ⁻ -X bonds	1414
27.4.1	I-X bonds	1414
27.4.2	I ⁺ -X bonds	1416
27.4.3	I ⁻ -X bonds	1417
27.5	At-X bonds	1427
Chapter twenty-eight BDEs in rare gas atom/ion clusters		1429
28.1	Rare gas atom clusters	1429
28.1.1	Diatomic clusters	1429
28.1.2	Polyatomic clusters	1436
28.2	Rare gas ion clusters	1446
Chapter twenty-nine Heats of formation of atoms, radicals, and ions		1453
29.1	Gaseous atoms	1453
29.2	Small inorganic radicals in the gas-phase	1455
29.2.1	Metallic radicals	1455
29.2.2	Non-metallic radicals	1459
29.3	Organic radicals in the gas-phase	1461
29.3.1	C-centered radicals	1461
29.3.2	O-centered radicals	1471
29.3.3	N-centered radicals	1474
29.3.4	S-centered radicals	1475
29.3.5	Si, Ge-, Sn-, and Pb-centered radicals	1476
29.4	Group additivity values for organic radicals	1478
29.5	Enthalpy of formation of monoatomic cations	1481
29.6	Enthalpy of formation of monoatomic anions	1484
References		1487
1946-1964		1487
1965-1969		1489
1970-1974		1494
1975-1979		1502
1980-1984		1511