

Contents

I Introduction	1
I.1 Background	1
I.2 Focus of the review	2
I.3 Review procedure and results	3
I.4 The NEA-TDB data base system	4
I.5 Presentation of the selected data	6
II Standards and Conventions	9
II.1 Symbols, terminology and nomenclature	9
II.1.1 Abbreviations	9
II.1.2 Symbols and terminology	9
II.1.3 Chemical formulae and nomenclature	9
II.1.4 Phase designators	13
II.1.5 Processes	14
II.1.6 Equilibrium constants	14
II.1.7 Order of formulae	20
II.1.8 Reference codes	20
II.2 Units and conversion factors	22
II.3 Standard and reference conditions	24
II.3.1 Standard state	24
II.3.2 Standard state pressure	24
II.3.3 Reference temperature	28
II.4 Fundamental physical constants	28
III Selected uranium data	29
IV Selected auxiliary data	63
V Discussion of data selection	85
V.1 Elemental uranium	85
V.1.1 Uranium metal	85
V.1.2 Uranium gas	86
V.2 Simple uranium aqua ions	86
V.2.1 UO_2^{2+}	86
V.2.2 UO_2^+	88
V.2.3 U^{4+}	91
V.2.4 U^{3+}	96
V.2.5 U^{2+}	97
V.3 Oxygen and hydrogen compounds and complexes	97
V.3.1 Gaseous uranium oxides	97
V.3.2 Aqueous uranium hydroxide complexes	98
V.3.3 Crystalline and amorphous uranium oxides and hydroxides	131

V.3.4 Uranium hydrides	148
V.4 Group 17 (halogen) compounds and complexes	150
V.4.1 Fluorine compounds and complexes	150
V.4.2 Chlorine compounds and complexes	185
V.4.3 Bromine compounds and complexes	213
V.4.4 Iodine compounds and complexes	226
V.4.5 Mixed halogen compounds	232
V.5 Group 16 (chalcogen) compounds and complexes	236
V.5.1 Sulphur compounds and complexes	236
V.5.2 Selenium compounds and complexes	256
V.5.3 Tellurium compounds	260
V.6 Group 15 compounds and complexes	261
V.6.1 Nitrogen compounds and complexes	261
V.6.2 Phosphorus compounds and complexes	279
V.6.3 Arsenic compounds	301
V.6.4 Antimony compounds	304
V.7 Group 14 compounds and complexes	306
V.7.1 Carbon compounds and complexes	306
V.7.2 Silicon compounds and complexes	334
V.7.3 Lead compounds	336
V.8 Actinide complexes	336
V.8.1 Actinide-actinide interactions	336
V.8.2 Mixed U(VI), Np(VI) and Pu(VI) carbonate complexes	337
V.9 Group 2 (alkaline-earth) compounds	337
V.9.1 Beryllium compounds	337
V.9.2 Magnesium compounds	338
V.9.3 Calcium compounds	340
V.9.4 Strontium compounds	342
V.9.5 Barium compounds	345
V.10 Group 1 (alkali) compounds	347
V.10.1 Lithium compounds	347
V.10.2 Sodium compounds	349
V.10.3 Potassium compounds	358
V.10.4 Rubidium compounds	359
V.10.5 Caesium compounds	360
VI Discussion of auxiliary data selection	365
VI.1 Group 17 (halogen) auxiliary species	366
VI.1.1 Fluorine auxiliary species	366
VI.1.2 Chlorine auxiliary species	368
VI.1.3 Bromine auxiliary species	371
VI.1.4 Iodine auxiliary species	373
VI.2 Group 16 (chalcogen) auxiliary species	374
VI.2.1 Sulphur auxiliary species	374
VI.2.2 Selenium auxiliary species	380
VI.2.3 Tellurium	383
VI.3 Group 15 auxiliary species	384
VI.3.1 Nitrogen auxiliary species	384
VI.3.2 Phosphorus auxiliary species	386
VI.3.3 Arsenic auxiliary species	389
VI.3.4 Antimony	391
VI.4 Group 14 auxiliary species	392
VI.4.1 Carbon auxiliary species	392
VI.4.2 Silicon auxiliary species	394

VI.5 Other auxiliary species	400
VI.5.1 Strontium auxiliary species	400
VI.5.2 Barium auxiliary species	400
VII Reference list	403
VIII Authors list	485
IX Formula list	519
X Alphabetical name list	549
Appendix A: Discussion of publications	555
Appendix B: Ionic strength corrections	683
B.1 The specific ion interaction theory	684
B.1.1 Background	684
B.1.2 Estimation of ion interaction coefficients	688
B.1.3 On the magnitude of ion interaction coefficients	691
B.2 Ion interaction coefficients and equilibrium constants for ion pairs	692
B.3 Tables of ion interaction coefficients	692
Appendix C: Assigned uncertainties	699
C.1 One source datum	699
C.2 Two or more independent source data	700
C.3 Several data at different ionic strengths	704
C.4 Procedures for data handling	708
C.4.1 Correction to zero ionic strength	708
C.4.2 Propagation of errors	709
C.4.3 Rounding	710
C.4.4 Significant digits	711
Appendix D: The estimation of entropies	713