

Contents

List of tables	<i>page</i> vii
Preface	ix
Acknowledgements	xi
Introduction	1
1 Standard enthalpies of formation derived from experimental data	3
1.1 Data tables	3
1.2 Processing of experimental data	5
2 Prediction of standard enthalpies of formation	7
2.1 Component enthalpies	7
2.2 Determination of values for component enthalpies	9
2.3 Summary	19
2.4 Uncertainties on values for component enthalpies	20
2.5 Comparison of calculated and experimental values	20
3 Group interactions	52
3.1 Introduction	52
3.2 Derivation of values for group interactions	52
4 Interpretation of group interactions: prediction of unknown values for component enthalpies	64
4.1 Introduction	64
4.2 Alkanes	64
4.3 Alkenes and alkynes	67
4.4 Monofunctional compounds	69
4.5 Polyfunctional compounds	72
4.6 Summary	79
5 Future developments	81
5.1 Experimental data files	81
5.2 Parametric schemes	81
5.3 Software development	82
Appendix	83
Table 1.1 Selected values of $\Delta_f H^\ominus$	87

Table 1.2 Experimental thermochemical data	233
Table 1.3 Standard enthalpies of formation for inorganic compounds	617
References	621
Name index	661
Chemical Abstracts Service Registry Number Index	759