

Contents

List of Figures	xiii
List of Tables	xv
List of Abbreviations and Nomenclature	xxi
Glossary	xxv
1 Introduction	1
2 Tools of Quantum Mechanics	3
2.1 The Born-Oppenheimer Approximation	4
2.2 Hartree-Fock Method	5
2.3 Post Hartree-Fock Methods	7
2.3.1 Perturbation Theory	8
2.3.2 Configurational Interaction	11
2.3.3 Coupled Cluster	12
2.4 Density Functional Theory	13
2.5 Basis Sets	16
2.5.1 Minimal Basis Sets	18
2.5.2 Split Valence Basis Sets	18
2.5.3 Polarized Basis Sets	18
2.5.4 Diffuse Basis Sets	18
2.5.5 Split Valence Basis Sets with Polarized and Diffuse Basis Functions	19
3 Dispersion Coefficients and Dispersion Interaction Energy	21
3.1 $C^{(6)}$ Coefficients from Dipole Oscillator Strength Distributions (DOSDs) and Pseudo DOSDs	24
3.2 $C^{(6)}$ Coefficients and Casimir-Polder Forces	26
3.3 $C^{(6)}$ Coefficients from Quantum Mechanics	27
3.3.1 Cartesian Tensor Expression	29
3.3.2 Spherical Harmonic Tensor Expression	35
3.4 $C^{(6)}$ Coefficients from London's Approximation	40
3.5 $C^{(6)}$ Coefficients from Scaling Methods	43

4	Equations of State	49
4.1	The Unlike Pair Interactions	50
4.2	Methods for Henry's Law Constant Calculations	53
4.2.1	Theory	53
5	Results and Discussion	61
5.1	Quantum Chemical Calculations	61
5.1.1	Static Polarizability	62
5.1.2	Pure Component Dispersion Coefficient	63
5.1.3	Binary Systems Dispersion Coefficient	64
5.1.4	Dispersion Coefficient Ratio	67
5.2	Prediction of Mixture Behavior	72
5.3	Henry's Law Constant	77
6	Summary	81
	Bibliography	83
A	Theory Supplements	92
A.1	Derivation of Frequency Dependent Dynamic Polarizability	92
A.2	Proof of the Identity Eq. (3.57)	93
B	Result Supplements	95
B.1	Code for the Calculation of the Dispersion Coefficient	95
B.2	32-point Gauss-Legendre Abscissas and Weights	100
B.3	Quantum Chemically Calculated Results	101
B.4	EOS Parameters	124