

Contents

1 Reverse Dative Bond in Organic Compounds, Molecular Complexes and Inconsistency of the sp^3-Hybridization Model with Respect to Carbon Atom	1
1.1 Introduction	1
1.2 Some Problems of Liquid Molecular Complexes and Solutions	2
1.3 Contradiction of Thermodynamic Properties of Organoelemental Compounds to the sp^3 -Hybridization Model	4
1.4 Reverse Dative Bond in Organometallic and Organoelemental Compounds	7
1.5 Electronic Configurations of Alkyl Compounds and Inconsistency of the sp^3 -Hybridization Model	11
1.6 Reverse Dative Bond and Steric Effect in Alkyls and Molecular Complexes	16
References	25
2 Nontraditional Approaches to Thermodynamic Analysis of Liquid Organic Compounds	29
2.1 Consequences of the Essentially Unshared $2s^2$ -Electron Pair of Carbon Atom	29
2.2 Specific Interactions of Liquid Alkyls and Their Energies	32
2.3 Novel Approaches to the Thermodynamic Analysis of Liquid Functional Solvents and Energies of Specific Interaction	38
2.4 Energy of Specific Interactions in Liquid Acetonitrile and Dimethyl Sulfoxide	51
2.5 Hydrogen Bonds and Specific Interactions of <i>N,N</i> -Dimethylformamide in Solvents	54
References	58

3	Types and Energies of Specific Intermolecular Interactions in Ethers and Organic Cyclic Oxides	63
3.1	The Structure and Specific Intermolecular Interaction in Liquid Ethers	63
3.2	Energy of Specific Intermolecular Interaction in Solid Ethers	70
3.3	Energies of Specific Intermolecular Interaction in Vinyl Ethers	76
3.4	Energies of Specific Intermolecular Interaction in Methoxy, Ethoxy, and 1,2-Epoxy Compounds	81
3.5	The Energies of Hydrogen Bonds and Specific Intermolecular Interaction of Liquid and Solid Organic Cyclic Oxides	87
3.5.1	Saturated Organic Cyclic Oxides	87
3.5.2	Unsaturated Organic Cyclic Oxides	93
3.5.3	Energies of H-bonds in 1,4-Dioxane-2,5-dione, Ethylene Ozonide, Diethyl Peroxide, and Furaldehyde	97
3.5.4	Crystalline Saturated Organic Cyclic Oxides. Energies of H-bonds	105
3.5.5	Specific Intermolecular Interaction in Liquid 1,3-Dioxolanes	110
3.5.6	Energies of H-bonds and Specific Intermolecular Interaction in Liquid Cyclic Methoxy and Dimethoxy Compounds	117
3.5.7	The Energies of Specific Intermolecular Interaction in Phenol Ethers	122
	References	130
4	Specific Intermolecular Interactions of Ketones	131
4.1	Specific Interactions in Saturated Ketones and Their Isostructural Analogous	131
4.2	Energies of Specific Interactions in Liquid Unsymmetrical and Symmetric Ketones	141
4.3	Unsaturated Ketones and Diketones	149
4.4	Energies of Specific Interactions in Liquid Cyclic Ketones	152
4.5	Energies of Specific Interactions in Solid Ketones	158
4.6	Energies of Specific Interactions and H-bonds in Solid Diketones and Oxyketones	163
4.7	The Thermodynamics and Energies of Specific Interactions in Saturated and Unsaturated Ketones C ₁₃ , C ₁₈	172
	References	179
5	Types and Energies of Hydrogen Bonds and Specific Intermolecular Interactions in Alcohols	181
5.1	Specific Interactions in Saturated Monohydric Alcohols	181
5.2	The Thermodynamics of Saturated Monohydric Alcohols with Branched Structure	192

5.3	Role of Isostructural Functional Groups in Saturated Alcohols and Specific Interactions	205
5.4	Energies of Specific Interactions of Liquid Polyhydric Alcohols ...	225
5.5	Energies of Hydrogen Bonds and Specific Interactions in Cyclic Alcohols	235
5.6	Energies of Hydrogen Bonds and Specific Interactions in Solid Alcohols	244
5.7	Energies of Hydrogen Bonds and Specific Interactions in Unsaturated Alcohols	255
5.8	Thermodynamics of Vaporization of Acetylene Alcohols and Isophitol. Energies of Specific Interactions	260
5.9	Extrastabilizing Effect of Isostructural Methyl Groups	269
	References	274
6	Specific Intermolecular Interactions and H-bonds in Aldehydes and Esters	277
6.1	Specific Interactions and H-bonds in Aldehydes	277
6.1.1	Saturated Aldehydes	277
6.1.2	Unsaturated Aldehydes	284
6.2	Energies of Specific Interactions and H-bonds in Esters	290
6.2.1	Esters of Formic, Acetic, and Propionic Acids	290
6.2.2	Methyl, Ethyl, Propyl, and Butyl Esters	301
6.2.3	Esters of Dicarboxylic Acids	303
6.2.4	Esters with Isostructural Methyl Group	307
6.2.5	Solid Esters	310
6.2.6	Unsaturated Esters	311
6.2.7	Cyclic Esters	314
	References	323
7	Types and Energies of Specific Intermolecular Interactions in Carboxylic Acids	325
7.1	Specific Interactions in Saturated Monocarboxylic Acids	325
7.2	Energies of Specific Interactions in Monocarboxylic Acids	332
7.3	Saturated Monocarboxylic Acids with Isostructural Methyl Group	336
7.4	Energies of Hydrogen Bonds in Hydroxycarboxylic Acids	341
7.5	Energies of Specific Interactions in Methoxy- and Ethoxycarboxylic Acids	344
7.6	Energies (kJ mol) of Specific Interactions in Peroxycarboxylic Acids	345
7.7	Hydrogen Bonds in Unsaturated Monocarboxylic Acids	352
7.8	Energies of Hydrogen Bonds in Dicarboxylic Acids	355
7.9	Energies of Hydrogen Bonds and Specific Interactions in Cyclic Carboxylic Acids	362

7.9.1 Saturated Cyclic Carboxylic Acids and Benzoic Acids	362
7.9.2 Methylbenzoic Acids	373
7.9.3 Hydroxybenzoic Acids	382
7.9.4 Methoxybenzoic Acids	385
References	390
8 Specific Intermolecular Interactions of Hydrocarbons	393
8.1 Specific Interactions in Hydrocarbons with Tetrahedral Structure of Molecules	393
8.2 Energies of Specific Interactions in Saturated Hydrocarbons	395
8.3 Energies of Specific Interactions in Saturated Cyclic Hydrocarbons	403
8.4 Energies of Specific Interactions in Branched Saturated Hydrocarbons	405
8.5 Energies of Specific Interactions in Alkenes	409
8.6 Energies of Specific Interactions in Alkynes	419
8.7 Energies of Specific Interactions in Branched Unsaturated Hydrocarbons	424
References	429
Index	431

Specific Intermolecular Interactions of Organic
Compounds

Baev, A.K.

2012, XVIII, 434 p., Hardcover

ISBN: 978-3-642-21621-3