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Towards an unified chemical model of secondary bonding.

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Streszczenie

The concept of secondary bond covers a wide range of non-covalent interactions involving an acceptor (or electrophilic) molecule and an electron donor (or nucleophilic) one. It involves triel, tetrel, pnictogen, chalcogen, halogen, and aerogen bonds as well as hydrogen bonds. Such interactions yield complexes in which the internuclear distance of the electrophilic and nucleophilic centers is intermediate between the sums of the covalent and van der Waals radii of these atoms. These complexes can be considered as precursors of hypothetical nucleophilic substitution or addition reactions. As a consequence of the least motion principle, in the complex, the arrangement of the ligands around the electrophilic center should look like that of the hypothetical transition state or addition product. In a same fashion, the geometry around the nucleophilic center is determined by the location of the lone pair or of the bond involved in the interaction. In this picture of secondary bonding, the structure of the valence shell of the electrophilic atoms determines the geometry of the complex rather than the group to which belongs the elemental atom. The reorganization of the complexes in terms of the arrangement of the bonding and non-bonding electronic domains around the electrophilic center enables to rationalize the geometries in a systematic fashion. A set of VSEPR inspired rules enabling the building up of secondary bonded isomers are proposed and checked by quantum chemical calculations performed on representative test systems of the $AX_{4-n}E_n$ type.

Słowa kluczowe

Non-covalent interactions, Secondary bonds

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