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Editorial

Non-Covalent Interactions in Coordination Chemistry

Alexey S. Kubasov and Varvara V. Avdeeva *

Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Leninskii pr. 31, Moscow 119991, Russia; fobosax@mail.ru
* Correspondence: avdeeva.varvara@mail.ru

Non-covalent interactions [1] play a crucial role in the final design of supramolecular and biological systems, encompassing drug production, catalysis, synthesis, crystal engineering, etc. Among the weak interactions, hydrogen [2,3], chalcogen [4,5], dihydrogen [6,7] and halogen [8–11] bonds, π–π stacking [12–14], semi-coordination [15,16], and π-hole interactions [17] are worthy of mention. These directed interactions are capable of linking individual components, including crystallizing molecules, into various associates, clusters, and supramolecular systems, ultimately forming new functional materials [18].

Recently, interest in this area of chemistry has only increased. Special volumes and article collections are being created that are dedicated to this type of chemical binding in compounds (see, for example, references [19–25]).

This Special Issue covers a diverse range of 'composition–structure' relations identified using X-ray diffraction and supported by quantum–chemical calculations. Five articles were submitted and published.

The authors of reference [26] explore a recently described type of non-covalent interaction between elements of group 12 (Hg) and Lewis bases (S), known as the spodium bond [27–30]. This bond was detected in the structures of homoleptic complexes $Hg(S_2CNR_2)_2$ (R = ethyl, isobutyl, and cyclohexyl); the features of the complexes, depending on the type of alkyl substituent, are discussed.

In reference [31], the authors considered the impact of halogen atoms (Cl, Br, and I) on the interconversion of kinetically (a) and thermodynamically (b) controlled regioisomers, leading to equilibrium mixtures of the isomers. The study reveals that thermodynamic favorability for the formation of thermodynamically controlled regioisomers increases in the order Cl < Br ≈ I and correlates well with the energy difference between S···N and S···X (where X = Cl, Br, or I) chalcogen bonds in kinetically and thermodynamically controlled products.

In reference [32], the interaction between trinuclear silver(I) pyrazolate $[AgPz]_3$ and pyridine-substituted chalcones was studied and the role of E-Z isomerization on the formation of final complexes was established. The authors found that chalcones in the E form adopt planar structures via multiple π–π/M–π interactions, with carbonyl and pyridine fragments participating in coordination with $[AgPz]_3$. In contrast, chalcones in the Z form coordinate the silver (I) macrocycle via chelating metal ions using O and N atoms.

In reference [33], lead (II) complexes with *closo*-decaborate anions, containing monohydroxy-derivatives $[B_{10}H_9OH]^{2-}$, $[B_{10}H_9O(CH_2)_2O(CH_2)_2O(CH_2)_2OH]]^{2-}$, and $[B_{10}H_9O(CH_2)_5O(CH_2)_2OH]]^{2-}$, were prepared in the presence of bipy. In the final lead (II) complexes, a combined coordination of the boron cluster via the 3c2e PbHB bonds and O atoms of the substituents was observed; N atoms of bipy molecules complete the coordination sphere of lead (II). An extensive network of weak intra- and intermolecular non-covalent interactions were found, including π–π stacking, Pb···B, Pb···H, and CH···HB interactions.

In reference [34], the authors studied Sn and Pb dichlorine-containing supramolecular compounds $(Me_3NH)_2\{[MCl_6]Cl_2\}$ using X-ray diffraction and Raman spectroscopy; Cl···Cl

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interactions were revealed in both compounds. The authors showed the crucial role of multiple cation···anion hydrogen bonds in the overall stabilization of the compounds of the type $(R_3NH)_2\{[MCl_6]Cl_2\}$ (M = Sn, Pb).

Thus, the articles collected in this Special Issue present the versatile nature of non-covalent interactions found in coordination compounds, as previously detected by single-crystal X-ray diffraction and supported by spectroscopic data, including IR, UV-vis, NMR, and Raman spectroscopy, as well as DFT calculations.

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