Poster Presentation

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Halogen bonding in iron(II) and cobalt(II) tris(dichloroglyoximates)

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The understanding of the interplay between intermolecular strong and weak interactions requires approaches that are able to identify and quantify all of them, and are applicable to as large number of objects as possible. The QTAIM approach [1] nicely meets the first criteria. Less rigorous approaches, such as the Stockholder [2] and the Voronoi [3] partitioning have the second advantage. The latter can also give qualitative, quantitative and visual representation of intermolecular interactions. We compared how all these approaches would perform for two polymorphs of Fe(Cl2Gm)3(BCH3)2 (monoclinic C (1a), and less stable monoclinic P (1b)) and Co(Cl2Gm)3(BCH3)2 (2) isostructural with 1b (Cl2Gm = dichloroglyoximate). The Voronoi and Stockholder partitionings showed that three fourths of molecular surfaces were attributed to Cl...X (X = Cl, O, N) and C-H...Cl bonds. According to the QTAIM theory, each chlorine atom takes part in at least four intermolecular contacts. The Voronoi tessellation was found to be valid for determinating of the graph of intermolecular bonding. Indeed, in the isostructural 1b and 2 the sets of weak interactions do not coincide due to various conformations of iron- and cobalt-containing clathrochelate cages. Nevertheless, the resulting graph of intermolecular bonding (the gpu-x net) is the same. Qualitative (for all three approaches) and quantitative (for two partitionings) correlation for various methods was demonstrated. This study was supported by the Council of the President of the Russian Federation (MK-5181.2013.3 and MD-3589.2014.3).

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