Quantitative Tools for Noncovalent Bonds in Crystals

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The recent progress in synthesis of chalcogenazoles has spurred widespread research in the area of potential applications of these compounds in materials science. The understanding of the nature of noncovalent bonds in molecular crystals provides our influence on the properties of novel materials. Thione-iodonium three-center four-electron halogen bonds [S-I$^+$-S] and the other electrostatically driven noncovalent interactions in dithiazolium salts with polyiodide motifs are in the focus of our study.

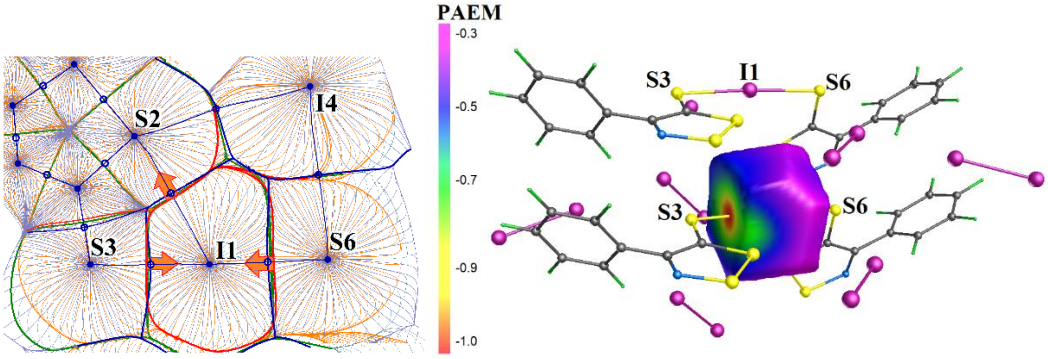

Figure 1 a) Superposition of gradient fields for PAEM, electrostatic potential and electron density with nuclei and bond critical points; b) PAEM (a.u.) mapped on the surface of iodonium atomic basin for three-center halogen bond [S-I$^+$-S] in 1,2,3-dithiazole-5-thione polyiodide crystal[1].

As a powerful tool for identifying and quantitative characterization of bond properties in molecular crystals, we suggested using the potential acting on an electron in a molecule (PAEM). Superposition of the boundaries of atomic basins in PAEM, electron density and electrostatic potential allows us to understand the features of strong and weak halogen or chalcogen bonds, and their synergistic effects in organic crystals. Calculations have been performed in WinXPRO 3.4.11 and 3DPlot programs[2].

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