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Supporting information for article:

Synthesis, crystal structure and magnetic properties of diaquabis(2,6-diamino-7*H*-purin-1-ium-κN^9)bis-(4,4′-oxydibenzoato-κ*O*)cobalt(II) dihydrate

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AIM Analysis

AIM (an acronym for the "Atoms In Molecules" theory, Bader, 1990) interprets chemical bonding in terms of shared (covalent bonds) or closed-shell (H-bonding, ionic bonding, van der Waals, etc.) interactions. The relevant parameters used to characterize the attractive bonding character of short contacts are the electron density ($\rho(r)$), its gradient vector ($\nabla\rho(r)$), its Laplacian ($\nabla^2\rho(r)$), the kinetic, potential and total energy densities in the region of the BCP (G(r), V(r), E(r)).

In some seminal papers on the subject (Bader, 1990, 2009) the author discloses two fundamental concepts on which the theory is based:, viz., the "Bonding Path" (BP), a line linking atomic nuclei along which the charge density has a maximum with respect to any lateral shift and the "Bond Critical Point" (BCP), an eventual minimum along these lines which provide an indicator of interatomic interaction. In addition, the sign and magnitude of $\rho(r)$,$\nabla^2\rho(r)$ at the BCP characterizes the interaction type. The interactions are considered as "shared" when $\nabla^2\rho(r) < 0$ (viz., electronic charge concentrated at the BCP) or of the "closed-shell" type when $\nabla^2\rho(r) > 0$ (viz., electronic charge drifted away from the interatomic surface, towards the nuclei). In this latter case, $\rho(r)$ is relatively low in value, and the fact that $\nabla^2\rho(r) > 0$, a result of the (positive) curvature of $\rho(r)$ along the interaction line or bond path (BP) due to the exclusion principle forcing a relative depletion of charge in the atomic surface. AIM has been a matter of debate on theoretical grounds (viz., Haaland *et al.*, 2004; Poater *et al.*, 2006; Krapp & Frenking, 2007 vs. Bader, 2009) and still goes on being a controversial issue (Dunitz, 2015 vs. Thakur *et al.*, 2015; Lecomte *et al.*, 2015). Even if now accepted as an extremely valuable tool, some critical viewpoints concerning the application of the method when "absolute" AIM values are analyzed have been raised (Spackman, 2015); nevertheless, its use for "relative" comparisons (as in the present approach) is steadily gaining generalized acceptability (Wang *et al.*, 2016, etc.)

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