Synthesis, crystal structure and magnetic properties of diaquabis(2,6-diamino-7H-purin-1-ium-kappa N-9)bis(4,4 '-oxydibenzoato-kappa O)cobalt(II) dihydrate

Por: Atria, AM (Maria Atria, Ana)[1]; Parada, J (Parada, Jose)[1]; Moreno, Y (Moreno, Yanko)[2]; Suarez, S(Suarez, Sebastian)[3]; Baggio, R (Baggio, Ricardo)[4]; Pena, O (Pena, Octavio)[5]

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Resumen

The title mononuclear Co-II complex, [Co(C5H7N6)(2)(C14H8O5)(2)(H2O)(2)]center dot 2H(2)O, has been synthesized and its crystal structure determined by X-ray diffraction. The complex crystallizes in the triclinic space group P (1) over bar, with one formula unit per cell (Z = 1 and Z' = 1/2). It consists of a mononuclear unit with the Co-II ion on an inversion centre coordinated by two 2,6-diamino-7H-purin-1-ium cations, two 4,4'-oxydibenzoate anions (in a nonbridging kappa O-monodentate coordination mode, which is less common for the anion in its Co-II complexes) and two water molecules, defining an octahedral environment around the metal atom. There is a rich assortment of nonbonding interactions, among which a strong N+-H center dot center dot center dot O- bridge, with a short N center dot center dot center dot O distance of 2.5272 (18) angstrom, stands out, with the H atom ostensibly displaced away from its expected position at the donor side, towards the acceptor. The complex molecules assemble into a three-dimensional hydrogen-bonded network. Avariable-temperature magnetic study between 2 and 300 K reveals an orbital contribution to the magnetic moment and a weak antiferromagnetic interaction between Co-II centres as the temperature decreases. The model leads to the following values: A (crystal field strength) = 1.81, lambda (spin-orbit coupling) = -59.9 cm(-1), g (Lande factor) = 2.58 and zJ (exchange coupling) = -0.5 cm(-1).

Palabras clave

Palabras clave de autor:cobalt complex; magnetism; anti-ferromagnetic interaction; crystal structure; AIM; computational chemistry; temperature dependence
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Información del autor

Dirección para petición de copias: Atria, AM (autor para petición de copias)

+ Univ Chile, Fac Ciencias Quim & Farmaceut, Santiago, Chile.

Direcciones:

+ [1] Univ Chile, Fac Ciencias Quim & Farmaceut, Santiago, Chile
+ [2] Univ Andres Bello, Dept Ciencias Quim, Fac Ciencias Exactas, CP2520000, Vina Del Mar, Chile
+ [3] Univ Buenos Aires, Dept Quim Inorgan Analit & Quim, Fis INQUIMAE, CONICET,Fac Ciencias Exactas & Nat, Buenos Aires, DF, Argentina
+ [4] Comis Nacl Energia Atom, Gerencia Invest & Aplicac, Ctr Atom Constituyentes, Buenos Aires, DF, Argentina
+ [5] Univ Rennes 1, Inst Sci Chim Rennes, Rennes, France

Direcciones de correo electrónico:aatria@ciq.uchile.cl

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