A Novel Inorganic-Organic Hybrid Material: Synthesis and X-Ray Structure Studies of 1,3-Dimethyl-1,2,3-benzotriazolium Silver-Thiocyanate Complex

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Abstract

A novel 1,3-dimethyl-1,2,3-benzotriazolium silver-thiocyanate complex $[(CH_3)_2Bz]$ [Ag(SCN)₂] has been synthesized and structurally characterized by single-crystal X-ray diffraction. This hybrid material is expected to take the advantage of organic, inorganic and polymeric materials. It is crystallized in the monoclinic unit cell and space group P2₁/n. The structure is consisting of discrete 1,3-dimethyl-1,2,3-benzotriazolium cation and negative charge infinite dithiocyanato-argentat. Each silver atom in the coordination polymer anion is surrounded by four thiocyanate groups. Silver coordinates two different thiocyanate N-atoms and two further different thiocyanate S-atoms. These lead to a distorted tetrahedrally coordination geometry and are linking into two dimensional layers. The adjacent layers are parallel to each other, whereas 1,3-dimethyl-1,2,3-benzotriazolium cations fill in between layers.

Keywords: Benzotriazolium, Thiocyanate; Silver Complex; Crystal Structure