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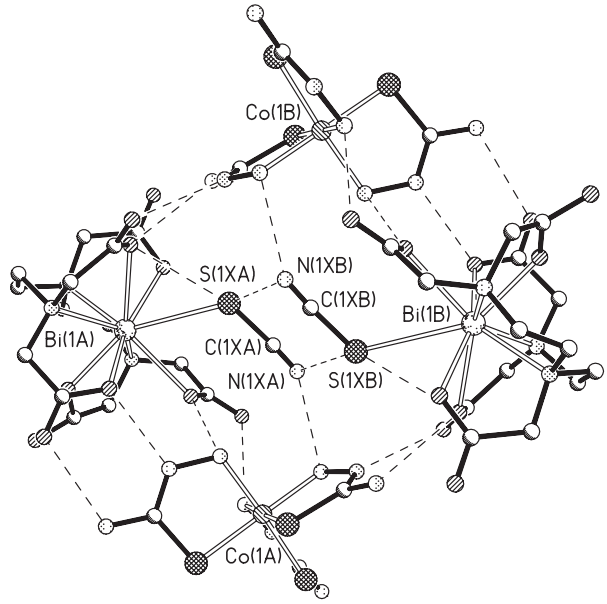
CRYSTAL STRUCTURE OF $[Co(thios)_3]_2[Bidtpa]_2(NCS)(OH)\cdot 8H_2O$

P.Petrenko[1], I.Bulimestru[2], Yu.Simonov[1], M.Gdaniec[3], A.Gulea[2]

[1]Institute of Applied Physics, Academy of Sciences of Moldova,5 Academiei str.,Chisinau, Moldova
Tel. 738154, Fax. 725887, E-mail: Peter.Petrenko@phys.asm.md
[2]State University of Moldova, Chisinau, Moldova
[3]A. Mickiewicz University, Faculty of Chemistry, Poznań, Poland

Bismuth-based mixed-oxides have been studied extensively for a number of potentially useful physical properties like oxygen ion conductivity, ferroelectricity, superconductivity and catalysts in different oxidation processes. The use of bismuth complexes as precursors for new heterometallic oxide systems turned out to be a more effective route compared to traditional ceramic synthesis. Thus, controlled pyrolysis of alkoxide, carboxylate or polyaminopolycarboxylate precursors has frequently been used to synthesize highly dispersed bismuth containing mixed-oxides and solid solutions.



Diethylenetriaminepentaacetic acid (H_5Dtpa) gives numerous stable complexes with *d*, *f*, and *p* elements, including Bi. Most frequently, complexes with H_5Dtpa are more stable than those with its analogues. Recently, we have characterized two heterometallic coordination compounds, $[Co(thios)_3]_2[Bi(Dtpa)]_2SO_4\cdot 6H_2O$ (**I**) and $[Co(thios)_3]_4[BiDtpa]_4\cdot(SO_4)_2\cdot 20H_2O$ (**II**) containing complex cations and anions (*thios*=thiosemicarbazide). In this work we present synthesis and crystal structure of a new heterometallic compound $[Co(thios)_3]_2[BiDtpa]_2\cdot(NCS)(OH)\cdot 8H_2O$ (**III**) (see fig.). The crystal structure of **III** is built of complex cations $[Co(thios)_3]^{3+}$, three types of anions $[Bi(Dtpa)]^{2-}$, $[NCS]^{2-}$, $(OH)^-$ and water molecules. The Bi atom coordination polyhedron is a nanohedron and its coordination number is nine. The coordination of *Dtpa* residues to the bismuth atom gives rise to five glycine and two ethylenediamine metallocycles which are essentially non-planar. The complex cation $[Co(thios)_3]^{3+}$ is a typical Co(III) tristhiosemicarbazide *fac*-isomer.