

# Synthesis, Crystal Structures and Properties of New Barium Thiocyanato Coordination Polymers with *trans*-1,2-Bis(4-pyridyl)ethylene as Ligand

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Reactions of barium thiocyanate with *trans*-1,2-bis(4-pyridyl)ethylene (bpe) in acetonitrile/water using different molar ratios always lead to the formation of a new barium coordination polymer of composition  $\{[[\text{Ba}(\text{NCS})(\text{H}_2\text{O})_5]_2(\text{bpe})\}(\text{NCS})_2(\text{bpe})_3(\text{H}_2\text{O})_2$  (**1**). During the preparation of single crystals of compound **1**, three additional new compounds were obtained (**2–4**), of which one crystallizes in two different polymorphic modifications (**4I** and **4II**). In compound **1** the Ba cations are coordinated by six water molecules, two *N*-bonding thiocyanato anions and one N atom of a bpe ligand within an irregular polyhedron. Two Ba cations are linked by two water molecules and two  $\mu$ -1,1-*N*-bridging thiocyanato anions into centrosymmetric dimers that are further connected by the bpe ligands into chains. The coordination topology in the crystal structure of compound **2** is very similar to that in **1** in that two coordinating water molecules are exchanged by two terminal bpe ligands. As in **1**, Ba dimers are observed that are connected by the bpe ligands into chains. In  $[[\text{Ba}(\text{NCS})_2]_2(\text{bpe})_3$  (**3**) the barium cations are linked by two  $\mu$ -1,3-bridging anions and one side-on-bridging thiocyanato anion into chains that are further linked by the bpe ligands into layers. In the first polymorphic modification of composition  $[\text{Ba}(\text{NCS})_2(\text{bpe})(\text{H}_2\text{O})(\text{CH}_3\text{CN})]\text{CH}_3\text{CN}$  (**4I**) each Ba cation is coordinated by one terminal *N*-bonding and two  $\mu$ -1,1,3(*N,N',S*)-bridging thiocyanato anions, two bridging water molecules, one acetonitrile molecule and one bpe ligand within an irregular polyhedron. The Ba cations are connected into chains that are further linked *via* O-H $\cdots$ N hydrogen bonding. The crystal structure of the second form **4II** is very similar to that of form **4I**, and significant differences are found predominantly in the packing of the complexes. Investigations using simultaneous differential thermoanalysis and thermogravimetry on compound **1** have shown that this compound decomposes in three steps with the formation of compound **3** in the second TG step.

*Key words:* Coordination Chemistry, Barium(II) Thiocyanates, Crystal Structures, Thermal Properties