Poster

Solid-to-solid phase transitions in two isostructural Bi(III) complexes and their solid solution.

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Two isostructural at room temperature complexes of Bi(III) with halogens and, 1-phenylethyl-N-ethylthiosemicarbazide have been investigated in order to scrutinize the solid-to-solid phase transitions induced by temperature in analogous structures.



Figure 1. (left) Perspective views of the complex 1 at 100K. The ellipsoids are drawn at the 50% probability level, hydrogen atoms are shown as fixed-size spheres and (right) superposition of complex 1(green), 2 (orange) and solid solution(yellow)

The experiments allowed establishing the structures of chloride (1, Fig. 1) and bromide (2) complexes of general formula (μ_2 -X) (BiX₂L₂)₂ where X is Cl or Br, as well as of the solid solution of 1 and 2 with predominance of the latter. With the help of different methods of examination of the new phase (single crystal XRD, variable-temperature powder XRD, and DSC studies) we were able to establish several phases of 1 and 2 characterised and compared with each other as well as with the solid solution. As some of the structural changes were very subtle, it was crucial to use different, complementary techniques to establish and describe new phases. Besides many similarities, some differences can be pointed out, like additional phase in complex 1, the shift of the corresponding transitions to higher temperatures and more continuous character of these transitions in 1. Moreover, for complex 2 it was found that the phase type in the given temperature depends on the thermal path to this temperature (on heating or on cooling), while in complex 1 similar phenomenon was not observed.