Synthesis, Crystal Structure and Vibrational Spectrum of Cobalt(II)orotate Trihydrate, $[Co(C_5N_2O_4H_2) \cdot 3\,H_2O$

Wolfgang Brockner, Robert Branscheid, Mimoza Gjikaj, and Arnold Adam

Institute of Inorganic and Analytical Chemistry, Clausthal University of Technology, Paul-Ernst-Straße 4, D-38678 Clausthal-Zellerfeld, Germany

Reprint requests to Prof. Dr. A. Adam. Fax + 49 (0)5323 / 72-2995.
E-mail: arnold.adam@tu-clausthal.de

Z. Naturforsch. **60b,** 175 – 179 (2005); received September 20, 2004

Cobalt orotate trihydrate, $[Co(C_5N_2O_4H_2)]\cdot 3H_2O$, has been synthesized and its crystal structure determined. The title compound crystallizes in the orthorhombic space group $P2_12_12_1$ (no. 19) with $a = 771.5(2)$, $b = 788.9(7)$, $c = 1470.4(2)$ pm, and $Z = 4$. Bridging orotate anions coordinate in a mono- and bidentate manner to the Co atom resulting in infinite chains of alternating Co(II) cations and orotate (OrH^{2-}) anions parallel to the *c* axis. The distorted octahedral Co coordination geometry is completed by three H_2O molecules. The FT-Raman and FT-IR spectra of the crystalline compound have been recorded and an assignment of the vibrational modes is proposed. The thermal behavior (TG) was investigated.

Key words: Cobalt(II)orotate Trihydrate, Crystal Structure, Vibrational Spectrum, Thermal Behavior