Crystal Data


Données cristallographiques sur les composés Ni(C_{15}H_{11}N_{3})X_2.nH_2O, X = Cl^-, NO_2^-, NCO^-.* Par R. Cortes††, M. I. Arriortua§, J. L. Mesa†† et T. Rojo†. Departamentos de Química (Inorgánica) y Cristalografía, Facultad de Ciencias, Universidad del País Vasco, PO Box 644, Bilbao, Spain

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Abstract

Three members have been characterized of the family Ni(terpy)X_2.nH_2O, X = Cl^-, NO_2^-, NCO^-, prepared by reaction in solution. They have space groups P\textbar\textbar, P\textbar\textbar\textbar and P\textbar\textbar/n respectively. Powder patterns of Ni(terpy)Cl_2.3H_2O, Ni(terpy)(NO_2)_2.1H_2O and Ni(terpy)(NCO)_2.1H_2O have been indexed. For the chloride compound: a=6.970(5), b=9.670(2), c=13.658(8) Å, \( \alpha = 81.73(2) \), \( \beta = 78.99(4) \), \( \gamma = 75.51(2) \), \( V = 870.57(7) \text{ Å}^3 \), \( D_m = 1.60 \text{ Mg m}^{-3} \), \( Z = 2 \); for the nitrite compound: a=9.077(5), b=9.445(5), c=10.710(4) Å, \( \alpha = 76.69(2) \), \( \beta = 70.87(3) \), \( \gamma = 68.04(1) \), \( V = 798.44(4) \text{ Å}^3 \), \( D_m = 1.66(3) \), \( D_x = 1.68 \text{ Mg m}^{-3} \), \( Z = 2 \); and for the cyanate compound: a=9.435(4), b=13.593(4), c=13.704(6) Å, \( \beta = 107.51(2) \), \( V = 1676.3(8) \text{ Å}^3 \), \( D_m = 1.60(3) \), \( D_x = 1.58 \text{ Mg m}^{-3} \), \( Z = 4 \). The study of their spectroscopic and magnetic properties suggests an octahedral stereochemistry for Ni^II. The JCPDS Diffraction File Nos. are 36–1998 for Ni(terpy)Cl_2.3H_2O, 36–1997 for Ni(terpy)(NO_2)_2.1H_2O and 36–1996 for Ni(terpy)(NCO)_2.1H_2O.

New X-ray powder diffraction data for beryllium gallate, BeGa_2O_4. By Michihide Machida, Hideyo Tabata, Shoji Kawakami and Eiichi Ishii, Government Industrial Research Institute, Nagoya, Hirate-machi, Kita-ku, Nagoya 462, Japan

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Abstract

X-ray powder diffraction data for BeGa_2O_4 have been obtained from the synthesized compound. The space group was determined by using a hexagonal prismatic single crystal obtained from a lead pyrophosphate flux by slow cooling. The crystal of BeGa_2O_4 belongs to the hexagonal system, with unit-cell parameters \( a = 7.7525(3) \), \( c = 2.9817(2) \text{ Å} \), \( V = 155.19 \); space group P6_3 or P6_3/m, \( z = 2 \). The crystal lattice is isomorphous with \( \beta \)-Si_3N_4. BeGa_2O_4 melts at 2013 K and has fairly small thermal expansion coefficients: \( \alpha_{12} = 3.29 \times 10^{-6} \text{ K}^{-1} \), \( \alpha_{23} = 2.95 \times 10^{-6} \text{ K}^{-1} \) (298–1173 K average). \( D_e = 4.511 \text{ Mg m}^{-3} \) (323 K), \( D_x = 4.546 \text{ Mg m}^{-3} \) (298 K); Cu Kz, Cu Kx_2 radiation. The JCPDS Diffraction File No. for BeGa_2O_4 is 36–1493.