Crystal Data


Données cristallographiques sur les composés Ni(C₁₅H₁₁N₃)X₂.nH₂O, X = Cl⁻, NO₂⁻, 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)X₂.nH₂O, X = Cl⁻, NO₂⁻, NCO⁻, prepared by reaction in solution. They have space groups P1, P1 and P2₁/n respectively. Powder patterns of Ni(terpy)Cl₂.3H₂O, Ni(terpy)(NO₂)₂.1H₂O and Ni(terpy)(NCO)₂.1H₂O have been indexed. For the chloride compound: a=6.970(5), b=9.670(2), c=13.658(8) Å, α=81.73(2), β=78.99(4), γ=75.51(2), V=870.5(7) Å³, Dₘ=1.60 Mg m⁻³, Z=2; for the nitrite compound: a=9.077(5), b=9.445(5), c=10.710(4) Å, α=76.69(2), β=70.87(3), γ=68.04(1), V=798.4(4) Å³, Dₘ=1.68 Mg m⁻³, Z=2; and for the cyanate compound: a=9.435(4), b=13.704(6), c=13.593(4) Å, β=107.51(2), V=1676.3(8) Å³, Dₘ=1.68 Mg m⁻³, Z=4. The study of their spectroscopic and magnetic properties suggests an octahedral stereochemistry for Ni.

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New X-ray powder diffraction data for beryllium gallate, BeGa₂O₄. 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 BeGa₂O₄ 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 BeGa₂O₄ belongs to the hexagonal system, with unit-cell parameters a=7.7525(3), c=2.9817(2) Å, V=155.19; space group P6₃ or P6₃/m, Z=2. The crystal lattice is isomorphous with β-Si₃N₄. BeGa₂O₄ melts at 2013 K and has fairly small thermal expansion coefficients: α_α=3.29×10⁻⁶ K⁻¹, α_γ=2.95×10⁻⁶ K⁻¹ (298–1173 K average). Dₘ=4.511 Mg m⁻³ (323 K), Dₙ=4.546 Mg m⁻³ (298 K); Cu Kα, Cu Kα₁ radiation. The JCPDS Diffraction File No. for BeGa₂O₄ is 36–1493.

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