Crystal Data


Crystal data for \( \rho \)-bromochlorobenzene/\( \rho \)-dibromobenzene mixed crystals at 293 K.* By T. CALVET, M. A. CUEVAS, E. TAULER and M. LABRADOR, Departament de Cristallografia, Universitat de Barcelona, Gran Via 585, 08007 Barcelona, Spain, Y. HAGET, Laboratoire de Cristallographie et de Physique Cristalline LA 144, Université de Bordeaux I, 351 Cours de la Libération, 33405 Talence CEDEX, France and E. ESTOP, Departament de Cristallografia, Universitat Autònoma de Barcelona, Bellaterra, Spain

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Abstract

The powder data for \( \rho \)-bromochlorobenzene/\( \rho \)-dibromobenzene mixed crystals \( [\rho \text{BCB}]_x[\rho \text{DBB}]_{1-x} \) at 293 K are reported; their thermal stability at 293 K is given. Vertical diffractometer, graphite monochromator, Cu K\( \alpha \), \( \lambda = 1.54056 \) Å. They are all isomorphous, monoclinic, P2\( _1 \)/a with \( Z = 2 \). \( a = 15.176(6), b = 5.847(3), c = 4.078(2) \) Å, \( \beta = 112.57(3) ^\circ \), \( V = 334.2 \) Å\(^3\), \( D_\text{x} = 1.947 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.90}[\rho \text{DBB}]_{0.10} \); JCPDS No. 36-1975. \( a = 15.222(7), b = 5.847(3), c = 4.083(2) \) Å, \( \beta = 112.60(3) ^\circ \), \( V = 335.5 \) Å\(^3\), \( D_\text{x} = 2.024 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.80}[\rho \text{DBB}]_{0.20} \); JCPDS No. 36-1974. \( a = 15.260(5), b = 5.839(2), c = 4.084(2) \) Å, \( \beta = 112.57(1) ^\circ \), \( V = 336.1 \) Å\(^3\), \( D_\text{x} = 2.064 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.70}[\rho \text{DBB}]_{0.30} \); JCPDS No. 36-1973. \( a = 15.298(4), b = 5.845(3), c = 4.091(2) \) Å, \( \beta = 112.60(2) ^\circ \), \( V = 337.7 \) Å\(^3\), \( D_\text{x} = 2.096 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.60}[\rho \text{DBB}]_{0.40} \); JCPDS No. 36-1972. \( a = 15.340(4), b = 5.844(2), c = 4.097(2) \) Å, \( \beta = 112.62(2) ^\circ \), \( V = 339.6 \) Å\(^3\), \( D_\text{x} = 2.134 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.50}[\rho \text{DBB}]_{0.50} \); JCPDS No. 36-1971. \( a = 15.370(5), b = 5.843(2), c = 4.097(2) \) Å, \( \beta = 112.66(2) ^\circ \), \( V = 341.4 \) Å\(^3\), \( D_\text{x} = 2.209 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.40}[\rho \text{DBB}]_{0.60} \); JCPDS No. 36-1970. \( a = 15.404(6), b = 5.842(2), c = 4.104(2) \) Å, \( \beta = 112.67(2) ^\circ \), \( V = 340.4 \) Å\(^3\), \( D_\text{x} = 2.172 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.30}[\rho \text{DBB}]_{0.70} \); JCPDS No. 36-1969. \( a = 15.437(5), b = 5.842(2), c = 4.103(2) \) Å, \( \beta = 112.60(2) ^\circ \), \( V = 341.9 \) Å\(^3\), \( D_\text{x} = 2.237 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.20}[\rho \text{DBB}]_{0.80} \); JCPDS No. 36-1968. \( a = 15.468(4), b = 5.838(2), c = 4.104(2) \) Å, \( \beta = 112.70(2) ^\circ \), \( V = 341.9 \) Å\(^3\), \( D_\text{x} = 2.249 \) Mg m\(^{-3}\) for \( [\rho \text{BCB}]_{0.10}[\rho \text{DBB}]_{0.90} \); JCPDS No. 36-1967.

*The full text and the powder data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42669 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.


Crystal data for an adduct of orthotelluric acid and urea, Te(OH)\(_6\).2CO(NH\(_2\))\(_2\),* By J. LOUB and M. DUŠEK, Department of Inorganic Chemistry, Charles University, Hlavova 8/2030, 128 40 Praha 2, Czechoslovakia

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Abstract

The crystal data of the title compound have been determined from single-crystal data [Loub, Haase & Mergehenn (1979). Acta Cryst. B35, 3039–3041]: C\(_2\)/c, \( a = 14.828(8), b = 8.891(6), c = 10.023(7) \) Å, \( \beta = 129.13(3) ^\circ \), \( V = 1025.09(9) \) Å\(^3\), \( Z = 4 \). \( D_\text{c} = 2.31(3), D_\text{x} = 2.27 \) Mg m\(^{-3}\) Power data obtained with powder diffractometer, \( \theta-2\theta \) scan, \( T = 295 \) K, Cu K\( \alpha \) radiation are presented. Infrared and Raman spectra are given. Thermal decomposition is reported [Fábry, Loub & Feltl (1982). J. Therm. Anal. 24, 95–100]. The JCPDS Diffraction File No. for C\(_2\)H\(_4\)N\(_4\)O\(_7\)Te(OH)\(_6\) is 36–1470.

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