Crystal Data


Crystal data for 1,4-epoxy-4-[(4-nitrophenyl)methyl]-1-phenyl-1H-2,3-benzodioxepin-5(4H)-one (C_{22}H_{15}NO_{6}) and 1,4-epoxy-4-[(4-bromophenyl)methyl]-1-phenyl-1H-2,3-benzodioxepin-5(4H)-one (C_{22}H_{15}BrO_{4}).* By D. F. MULLICA, J. S. BELEW and E. L. SAPPENFIELD, Chemistry Department, Baylor University, Waco, Texas 76798, USA

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Abstract

The indexed X-ray diffraction powder data of 1,4-epoxy-4-[(4-nitrophenyl)methyl]-1-phenyl-1H-2,3-benzodioxepin-5(4H)-one (OZONO, C_{22}H_{15}NO_{6}) and 1,4-epoxy-4-[(4-bromophenyl)methyl]-1-phenyl-1H-2,3-benzodioxepin-5(4H)-one (OZOBR, C_{22}H_{15}BrO_{4}) are reported. OZONO and OZOBR crystallize in the monoclinic space groups \( P2_1/c \) and \( P2_1/a \), respectively. The cell constants are \( a = 8.200(4) \), \( b = 14.574(6) \), \( c = 15.908(7) \), \( V = 1870.5 \), \( D_m = 1.36(1) \), \( D_x = 1.38 \) \( \text{Mg m}^{-3} \) for OZONO and \( a = 12.217(5) \), \( b = 8.945(2) \), \( c = 17.062(5) \), \( \beta = 96.85(2) \), \( V = 1851.2 \), \( D_m = 1.49(1) \), \( D_x = 1.52 \) \( \text{Mg m}^{-3} \) for OZOBR. The quantitative figures of merit \( F_2 \) are \( F_2^2 = 62(0.007, 48) \) and \( F_2^2 = 28(0.016, 58) \), respectively. The JCPDS Diffraction File No. for OZONO is 36-1988 and for OZOBR 36-1989.

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Crystal data for di-\( \mu \)-chloro-bis[2-(di-tert-butylphosphino)-2-methylpropyl]dipalladium(II) (C_{24}H_{52}Cl_{2}P_{2}Pd_{2}, DIPAL) and [2-(di-tert-butylphosphino)-2-methylpropyl]triphenylarsinopalladium(II) chloride (C_{30}H_{41}AsClIPPd).* By D. F. MULLICA and E. L. SAPPENFIELD, Chemistry and Physics Departments, Baylor University, Waco, Texas 76798, USA

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Abstract

The indexed X-ray diffraction powder data of di-\( \mu \)-chloro-bis[2-(di-tert-butylphosphino)-2-methylpropyl]dipalladium (C_{24}H_{52}Cl_{2}P_{2}Pd_{2}, DIPAL) and [2-(di-tert-butylphosphino)-2-methylpropyl]triphenylarsinopalladium(II) chloride (C_{30}H_{41}AsClIPPd, ARPAL) are reported. DIPAL and ARPAL crystallize in the monoclinic space groups \( P2_1/c \) and \( P2_1/m \), respectively. The refined cell parameters were determined by employing a Siemens Debye-Scherrer camera (Fe K\( \alpha \) radiation, \( \lambda_{\text{meas}} = 1.93736 \) \( \text{Å} \)). The cell constants are \( a = 7.707(1) \), \( b = 15.186(3) \), \( c = 13.389(2) \), \( \beta = 105.79(1) \), \( V = 1507.9 \), \( D_m = 1.47(1) \), \( D_x = 1.511 \) \( \text{Mg m}^{-3} \) for DIPAL; and \( a = 9.626(2) \), \( b = 14.347(3) \), \( c = 11.966(3) \), \( \beta = 112.01(1) \), \( V = 1532.1 \), \( Z = 2 \), \( D_x = 1.407 \) \( \text{Mg m}^{-3} \) for ARPAL. The quantitative figures of merit \( F_2 \) are \( F_2^2 = 20(0.108, 108) \) and \( F_2^2 = 38(0.009, 64) \), respectively. The JCPDS Diffraction File No. for DIPAL is 36-1982 and for ARPAL 36-1980.

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