Preparation and Characterization of $NiCl(NO)(PPh_3)_2$

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Previous work [1] on the title compound reports an intractable disorder problem; the complex was prepared again following the method of Feltham [2], and purple crystals were prepared by vapour diffusion of hexane into a benzene solution. The compound crystallizes in a *C*-centered monoclinic space group, with a cell of dimensions: a = 17.399(3), b = 13.136(3), c = 16.954(3) Å, β = 104.74(1)°, Z = 4 and T = 296 K.

FTIR spectral absorptions attributed to aromatic ν(C−H) at 3050 cm^{-1}, ν(N−O) at 1716 cm^{-1}, aromatic ν(C−C) at 1434 cm^{-1}, and bands for CH in- and out-of-plane bending at 1095 cm^{-1} and 693 cm^{-1}, respectively. The supramolecular structure contains the expected [3] six-fold phenyl embrace, 6PE, chains linking nickel bis(phosphine) moieties into one-dimensional zigzag chains. However, the lattice also contains a benzene solvate. The benzene molecule is able to form considerably more C−H···π interactions than a phenyl ring and becomes the major link, interconnecting three of the 6PE chains via ten C−H···π interactions centered about the benzene of crystallization. Additional weak noncovalent interactions supplement these major interactions to form an extensive three-dimensional crystal structure.

[1] Haller K.J., Enemark J.H., *Inorg. Chem.*, 1978, **17(12)**, 3552. [2] Feltham R.D., *Inorg. Chem.*, 1964, **3(1)**, 116. [3] Dance I., Scudder M., *J. Chem. Soc., Chem. Comm*., 1995, **10**, 1039.

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