
In the crystal structure of Pd4P3, space group R3 (No. 148), Z=3, (Andersson, Acta Chem. Scand. (1977) A31, 354) there are only tetrahedral interactions between the palladium atoms, corresponding to eleven 18-fold and two 6-fold positions. A neutron powder diffraction study of deuterated Pd4P3 (500 kPa D2 pressure, 196K) using Rietveld-type profile refinement techniques showed that deuterium partially occupied one of the 18-fold tetrahedral-type positions, corresponding to the formula Pd4P3D0.46.

The H/D atoms dissolved in the palladium phosphide structures preferentially occupy positions as far as possible from the phosphorus atoms, and the D-D (H-H) distances always exceed 2Å.

ZryPd which has the tetragonal MoSi2 structure, reacts readily with hydrogen at room temperature to form hydrides (Naeland, J. Less-Common Met. (1983), 89, 173-182). There are several potential interstitial sites for hydrogen in the MoSi2 structure. We have used neutron diffraction to establish which sites are occupied. Three compositions were studied ZryPd0.8, ZryPd1.71, and ZryPd4.8g. The structures were refined by the method of total profile analysis of the neutron diffraction powder patterns. The D atoms are located at the center of distorted tetrahedra of Zr atoms in all these samples. The results for ZryPd1.71 are representative. Space group I4/3mm, D=2, a=3.3208(2)Å, c=11.460(4)Å. The atomic coordinates are: Pd at (0,0,0) (2g) positions, Zr at (0,0,0) (4a) positions with Z=0.35632(2) and D at 0.5 0.5 0 (4d) positions. Temperature factors were 0.4 for Pd and Zr and 1.0 for D. Final R factors: R$_p$=9.53, R$_e$=7.11, R$_w$=9.06 and R$_F$=5.80.

Electron momentum distribution of the first stage lithium intercalated graphite (LiC$_6$) is measured by X-ray inelastic scattering and compared to the graphite one. The Compton profiles difference is consistent with a transfer of the lithium conduction electron to a 5-like band as expected in a rigid band model. But this model is clearly insufficient to explain all the measured profile difference features which actually reflect the total variation of outer (both valence and conduction) electrons density. Two facts are to be taken into account:

a. introduction of an excess outer electron.

b. modification of the graphite charge distribution due to the presence of the partially or totally ionized lithium that can be illustrated in particular by the stacking change in intercalation.

The excellent agreement between this measured difference and the computed one (by Cohen group) from the Bolivar wave functions points out in particular, the importance of the valence distortion due to the lithium ion. (G. Loupjas, J. Chomilier and B. Guerard, J. Physique Letters, April 1st 1984).