

ZrzPd which has the tetragonal Mo₅S₃ structure, reacts readily with hydrogen at room temperature to form hydrides (Maeland, J. Less-Common Met. (1983), 89, 173-182). There are several potential interstitial sites for hydrogen in the Mo₅S₃ structure. We have used neutron diffraction to establish which sites are occupied. Three compositions were studied ZrzPd₀, ZrzPd₀.71, and ZrzPd₁.₉₉. 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 ZrzPd₀.₇₁ are representative. Space group I₄/mmm, Z=2, a=3.3208(2)Å, c=11.606(1)Å. The atomic coordinates are: Pd at 000 (2a) positions, D at 00z (4(a) positions) with z=0.3653(2) and D at 0 z2/1 0 (4(d) positions). Temperature factors were 0.4 for Pd and 2.5 and 1.0 for D. Final R factors: R_p=9.53, R_p=7.11, R_p=9.06 and R_p=5.80.

07.6-3 NEUTRON-DIFFRACTION STUDY OF B-CaNi₅Bₓ. By L.S. Calvert*, B.M. Powell* and J.J. Murray*, *National Research Council of Canada and **Atomic Energy of Canada Ltd.

A neutron diffraction powder pattern of B-CaNi₅B₁.₇₇ showed it to be orthorhombic, Pmnh, a=5.6033(12) b=5.0810(9) c=7.8557(13) A contrary to earlier reports giving Pna₂. (Gainsford et al Adv. X-Ray Analysis (1983) 26 163) and Tam (Y.K. Cho et al J. Less-Common Metals (1982) 88 125). Rietveld profile analysis based on the metal atom positions proposed by Gainsford et. al gave integrated intensities which were used to obtain possible deuterium positions from Fourier and difference syntheses calculated using the NRC PDPS structure package. This model was refined successfully by a Rietveld profile refinement. Deuterium atoms occupy two octahedral sites equivalent to 3(f) positions in the parent P₆₃/mmm Ca₅B₆ type structure. These "octahedra" are formed by 4 Ni atoms in the equatorial plane with 2 Ca atoms at the apices. The D atoms are displaced from the central position towards one Ca apex. Distances are D-M₁ = 1.50 - 1.92 Å and D-Ca = 2.30 - 3.51 Å.


Electron momentum distribution of the first stage lithium intercalated graphite (LiC₆) 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 IT-like band as expected in a rigid band model. But this model is clearly insufficient to explain all the measured profile differences 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 Bolzarth wave functions points out, in particular, the importance of the valence distortion due to the lithium ion. (G. Loupias, J. Chomilier and B. Guérard, J. Physique Letters, April 1st 1984).