
High resolution x-ray powder diffraction data were collected for a series of CdS and CdSe intercalates in a host zeolite-Y framework. The measurements were made on beam line X13a at the National Synchrotron Light Source, Brookhaven National Laboratory. Each diffractogram was analysed using the profile fitting technique originally devised by Rietveld (H.M. Rietveld, J. Appl. Cryst., 1969, 2, 65), and the extra-framework material was located using standard Fourier methods. Four samples, with different concentrations of Cd, S and Se, were investigated and an example of the excellent agreement between observed (solid line) and calculated (dotted line) profiles for CdSe in zeolite-Y is given in Fig. 1. Also shown is the difference between these two curves.

In all cases Cd prefers to occupy a site within the sodalite unit, capping the double-6-ring, coordinated to framework oxygens. Also associated with this particular Cd is an oxygen of a hydroxyl group or water molecule which results from inadequate dehydration and gives an occluded arrangement around the cation. As the concentration of Cd is increased occupation of the 12-ring occurs. These results provide a possible explanation for the interesting results found from U.V. spectroscopy, which show that above a critical loading the intercalate acts like a semiconductor. Within the sodalite unit of zeolite-Y there exist cubes of cadmium and sulphur. These are discrete entities at low semiconductor loadings. However, as the concentration is increased a network is set up which is modulated by the host framework.

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