Crystal structure of the Heavy Fermion compound YbFe$_2$Zn$_{20}$ doped with Cd.

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The Heavy Fermion compound YbFe$_2$Zn$_{20}$ was doped with Cd atoms. This compound adopts the complex cubic CeCu$_2$Al$_2$ - type structure with space group $Fd\bar{3}m$. In this structure Yb and Fe atoms occupy the Wyckoff positions 8a and 16d, respectively, while the Zn atoms occupy three different crystallographic sites (16c, 48f and 96g). The introduction of Cd disturbs the system and an increase of the lattice parameter is observed. A refinement of crystalline structure of YbFe$_2$Zn$_{20}$ and YbFe$_2$Zn$_{18.6}$Cd$_{1.4}$ using single crystal x-ray diffraction data was performed to determine which crystallographic site the Cd atoms occupy. The results of the refinements show that Cd substitutes only those Zn atoms that occupy specifically the 16c crystallographic site. Our results also show a decrease of the Debye-Waller factor for the crystallographic site 16c that are occupied by Cd and Zn atoms in the compound YbFe$_2$Zn$_{18.6}$Cd$_{1.4}$ and an increase of this factor for the other atoms with respect to the pure compound. In order to study the possible valence shift of Yb atoms in this compound due to Cd doping, we performed x-ray absorption near the edge spectroscopy (XANES) measurements for YbFe$_2$Zn$_{20}$, YbFe$_2$Zn$_{19}$Cd, YbFe$_2$Zn$_{18.7}$Cd$_{1.3}$ and YbFe$_2$Zn$_{18.6}$Cd$_{1.4}$. These measurements indicate that the Yb valence is very close to Yb$^{3+}$ for the pure and doped materials.

Figure 1: Crystal structure of YbFe$_2$Zn$_{20}$ and YbFe$_2$Zn$_{18.6}$Cd$_{1.4}$. The Cd atoms introduced in this compound substitute the Zn atoms at the 16c crystallographic site.


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