Crystal structure of the Heavy Fermion compound $YbFe_2Zn_{20}$ doped with Cd.

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The Heavy Fermion compound $YbFe_2Zn_{20}$ was doped with Cd atoms. This compound adopts the complex cubic $CeCr_2Al_{20}$ - type structure with space group $Fd\bar{3}m$. In this structure Yb an 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 $YbFe_2Zn_{20}$ and $YbFe_2Zn_{18.6}Cd_{1.4}$ 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 $YbFe_2Zn_{18.6}Cd_{1.4}$ and an increase of this factor for the other atoms with respect to the pure compoud. 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 $YbFe_2Zn_{20}$, $YbFe_2Zn_{19}Cd$, $YbFe_2Zn_{18.7}Cd_{1.3}$ and $YbFe_2Zn_{18.6}Cd_{1.4}$. These measurements indicate that the Yb valence is very close to Yb^{3+} for the pure and doped materials.

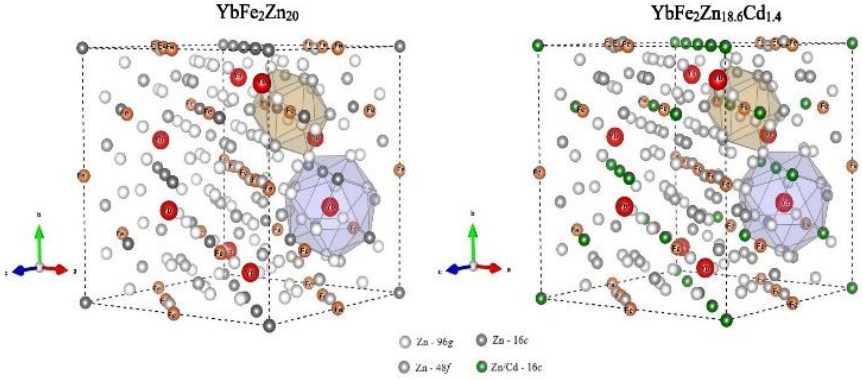

Figure 1: Crystal structure of $YbFe_2Zn_{20}$ and $YbFe_2Zn_{18.6}Cd_{1.4}$. The Cd atoms introduced in this compound substitute the Zn atoms at the 16c crystallographic site

[1] Cabrera-Baez, M. , Ribeiro, R. A. and Avila, M. A. , *Journal of Physics: Condensed Matter*, **28**, 375601 (2016).

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