Investigation of Electronic Structure and Properties of Solid EuC_2 and YbC_2

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EuC_2 crystallizes in a different space group (C 2/c) in comparison to all other rare earth carbides (I 4/mmm) [1] that have been synthesized.
In addition the unit cell volumes of solid EuC_2 and YbC_2 do not fit in the lanthanide row. It has been proposed that this effect might be caused by a difference in the valence of the lanthanide atoms (Ln^{2+} vs. Ln^{3+}). Generally rare earth atoms prefer a valence of 3+ in molecules and crystals. It is possible that the rare earth atoms in EuC_2 and YbC_2 may better be described as a Ln^{2+} than a Ln^{3+} since a half and fully occupied 4f-shell (Eu^{2+}: $4f^7$, Yb^{2+}: $4f^{14}$) is favoured.
In our work we focussed on the structures of EuC_2 and YbC_2. The calculations were carried out with the CRYSTAL06 program [2]. Geometries of both carbide compounds have been fully optimized. Band structures were derived and frequencies were analyzed. Our results agree with experimental presumtions. We could show that Eu is more likely to show a 2+ valence in the carbide compound and Yb a 3+ valence, respectively.

Literature:

[1] D. Wandner, U. Ruschewitz, M. Abd Elmeguid, M. A. Ahmida and O. Heyer, *Z. Anorg. Allg. Chem.*, **632**, 2099 (2006).

[2] R. Dovesi, V. R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N. M. Harrison, I. J. Bush, P. D'Arco, M. Llunell **CRYSTAL06**, University of Torino, Torino, Italy (2006).