s2.m1.p23 **Electron Density Distribution in CaNi$_2$Si$_2$ using Synchrotron X-ray Diffraction and First Principles Calculations.** N.K. Hansen, G. Gavoille[+], *Lab. de Cristallographie et Modélisation de Matériaux Minéraux et Biologiques, UPRESA-CNRS-7036, Université Henri Poincaré – Nancy I, B.P. 239, 54506 Vandoeuvre-lès-Nancy CEDEX, France*, R. Welter, B. Malaman, *Lab. de Chimie du Solide Minéral, UMR-CNRS-7555, Université Université Henri Poincaré – Nancy I*, P. Herzig, *Institut f. Physikalische. Chemie, Universität Wien, Währinger Str. 42, 1090 Vienna, Austria* and H.-G. Krane, *HASYLAB* and *Mineralogisch-Petrologisches Institut, Universität Bonn, Poppelsdorfer Schloss, 53115 Bonn, Germany. e-mail: hansen@lcm3b.u-nancy.fr*
Keywords: electron density, synchrotron radiation, band structure.

CaNi$_2$Si$_2$ crystallises in the ThCr$_2$Si$_2$ type structure, one of the most frequently observed structures in ternary compounds with the formula RT$_2$X$_2$ (R alkaline earth or lanthanide element; T transition metal and X an element from group 13 to 16).

Concerning the silicides only the compounds containing manganese are magnetic, showing a great variety of behaviour ranging from ferromagnetism to antiferro-magnetism and canted magnetic structures.

This study is the first of a series in which we want analyse the electron density of a several compounds with ions having the *d*-band more or less completely filled. In the present report we compare with the results of a Full-Potential-Linearised-APW calculation of the band-structure and the valence electron density distribution.

The X-ray diffraction measurement was carried out at the four-circle diffractometer D3 at HASYLAB using a wavelength of 0.4 Å. This choice was made because of the high absorption of this dense compound and the small size of the sample. The analysis of the experimental data is also complicated by the high symmetry of the structure (I 4/mmm) with all atoms in highly symmetric special positions. The consequence is that certain classes of reflections are systematically weak and difficult to measure with a good accuracy.

Although the diffraction data are rather insensitive to diffuse components of the electron density, there is nevertheless a good agreement between theory and experiment.

A weak covalent Si-Si bond interaction is observed, but most pronounced is the preferred occupation of the nickel 3*d*-orbitals.

[+] G. Gavoille deceased in January 1999.

s2.m1.p24 **3D magnetic interactions in copper hydroxinitrate: contribution of accurate electron density study.** S. Pillet[a], M. Souhassou[a], C. Lecomte[a], P. Rabu[b] & C. Massobrio[b]. *[a] LCM3B, UHP Nancy I, BP 239, 54506 Vandoeuvre; [b] IPCMS, 67037 Strasbourg.*
Keywords: molecular magnetism, electron density, layered compound.

Copper hydroxinitrate (Cu$_2$(OH)$_3$NO$_3$) is the basic archetype of hybrid organic-inorganic layered materials exhibiting long range magnetic effects [1]. Their general structure can be described as 2D triangular arrays of transition metal atoms where the inter-plane connection is directly assisted by organic anions. In the particular case of Cu$_2$(OH)$_3$NO$_3$, the in-plane ferro and antiferromagnetic interactions between the two independent copper atoms are due to a super-exchange mechanism. The inter-plane coupling, and therefore the 3D magnetic ordering, are based on hydrogen bonds between the hydroxo and nitrate fragments.

In this context, we studied the distribution of electron density in this compound to investigate the different Cu-O-Cu interactions and hydrogen bonds. For this purpose, a high resolution X-ray diffraction measurement was performed using Kappa CCD detector. The electron density distribution allows to characterise and study all bonds which are of great interest to understand the origin and pathways of the magnetic interactions. Inspection of the 3d orbital populations obtained from the X-ray data does not allow to show any difference between the two copper atoms. However, a closer insight using topological analysis of the electron density permits to distinguish between the behaviours of the two copper atoms and to interpret these differences in term of magnetic interactions. The topological analysis of the electron density in the hydrogen bond regions enables also to characterise the dimensionality of these interactions.

The electron density distribution in this compound will also be compared to DFT calculations, which shows that the spin density differs from one plane to another [2].

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