pyrargyrite, the band positions in stephanite spectra are shifted to higher vibrational regions than those in pyrargyrite. This may be attributed to the complex structure of the stephanite and the effect of the surrounding elements.

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### **MS41 P06**

C and/or C<sub>2</sub> in Reduced Rare Earth Carbide Halides <u>Hansjürgen Mattausch</u>, Arndt Simon, *Max-Planck-Institut für Festkörperforschung*, *D*-70569 Stuttgart, Deutschland. E-mail: <u>hj.mattausch@fkf.mpg.de</u>

#### Keywords: Rare Earth, Cluster, Endohedrals

The variety of compounds of Rare Earth metal carbide halides REC<sub>v</sub>X<sub>z</sub> (X=Cl, Br, I) is unexpectedly large. As known from the structural chemistry of the metal-rich compounds of 4d and 5d elements frequently discrete or condensed metal clusters occur[1]. For many cluster topologies the  $M_6X_{12}$  with an octahedral core is dominating. For the electron-poor Rare Earth metals the clusters are nearly always stabilised by interstitial atoms [2]. In the case of carbon as endohedral (i) single C atoms, (ii) C<sub>2</sub> dimers are known as well as both C and C<sub>2</sub> entities simultaneously (iii). According to X-ray analysis the C atoms and the C<sub>2</sub> dumbbells are statistically disordered in the center of the RE octahedra for (iii). The  $C/C_2$  disorder is accompanied by an elongation/contraction of the Rare Earth metal clusters. The occurence of isolated C atoms or C2 units is determined firstly by the size of the surrounding RE cage and secondly by the electron count for the compound. A simple ionic treatment in the Zintl-Klemm concept in connection with the qualitative molecular orbital scheme for a  $C_2$  dimer can reasonably predict the expected length of the C-C-distance. In all known examples the maximum formal charge assigned to the  $C_2$  units is -6 corresponding to an ethanide ion  $C_2^{6-}$ . When the formal charge exceeds 6- the dimers are no longer stable with respect to dissociation into two C<sup>4-</sup> ions. On the other hand, when the surplus of electrons is consumed in metal metal bonds also C2 dimers are possible. When the formal charge on C<sub>2</sub> becomes less then 6-, shorter C-C distances result as in the ethenide ions  $C_2^{4-}$ . Our investigations on REC<sub>v</sub>X<sub>z</sub> compounds confirm these expectations.

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### **MS41 P07**

# Structural disorder in natural pearceite-T2ac: A combined TEM and SCXREF study

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Keywords: structural disorder, crystal structure, polytypism

Pearceite-T2ac is a member of the pearceite-polybasite group of minerals. These minerals - general formula  $[Ag_9CuS_4][(Ag_7Cu)_6M_2S_7]$  with M = Sb, As - have been recently structurally characterized [1,2,3]. On the whole, the structure of the polytype pearceite-T2ac can be described as a regular succession of two module layers stacked along the c axis: a first module layer (labeled A), with general composition  $[(Ag,Cu)_6(As,Sb)_2S_7]^2$ , and a second module layer (labeled *B*), with general composition  $[Ag_9CuS_4]^{2+}$ . In the structure, (As,Sb) forms isolated (As,Sb)S<sub>3</sub> pyramids typically occurring in sulfosalts, copper links two sulfur atoms in a linear coordination, and silver occupies sites with coordination ranging from quasi linear to almost tetrahedral. In the B layer the silver cations are found in various sites corresponding to the most pronounced probability density function locations of diffusion-like paths. The structure was solved and refined on a twinned crystal up to R = 4.34% in the space group P321. It was anticipated that correlated local ordering of the relative positioning of the heavily disordered Ag cations within the B module layers might give rise to structured diffuse scattering. An electron diffraction study searching for this was therefore carried out on the same natural sample used for the structural investigation (sample AB6829, Naturhistorisches Museum of Vienna). The discovery of a highly structured, essentially continuous diffuse intensity distribution (particularly in the vicinity of the [111] and [441] zone axis orientations) shows that the diffusion of neighbouring Ag ions must be highly correlated both within the *a-b* planes as well as from one such plane to the next. More detailed electron diffraction studies are underway to attempt to determine the detailed shape of the observed diffuse distribution and to model the real space Ag ion ordering presumed to be responsible.

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### MS41 P08

**Hybrid twinning in staurolite** <u>M. Nespolo<sup>a</sup></u>, G. Ferraris<sup>b</sup> <sup>a</sup>*LCM3B Université Henri Poincaré Nancy I, Nancy, France.* <sup>b</sup>*DSMP Università di Torino, Italy* E-mail: <u>Massimo.Nespolo@lcm3b.uhp-nancy.fr</u>

## Keywords: Effective twin index; Hybrid twinning; Staurolite

Staurolite gives two penetration twins, known as 90° or "Greek cross" twin 60° or "Saint Andrew" cross, with twin elements  $4_{[100]}$  or  $2_{[013]}$  for the former, and  $3_{[102]}$  or  $2_{[313]}$  for the latter [1,2]. The Greek cross twin has twin index 6, at the upper limit of Friedel's empirical limit for the occurrence of twinning, while the Saint Andrews twin has twin index 12, far too high to be more than an exceptional case. Despite this unusually high twin index, the Saint Andrews twin is the most frequent twin in staurolite and its occurrence frequency cannot be explained on the basis of the classical reticular theory of twinning.

The occurrence frequency of the Saint Andrews twin becomes less intriguing once it is explained as hybrid twin [3]. Hybrid twins are twins in which more than one concurrent sublattice exists, contributing to the overall lattice restoration, which is higher than what the classical twin index states. These concurrent sublattices occur when