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Synthesis and crystallographic study of laflammeite (Pd3Pb2S2) and thalhammerite (Pd9Ag2Bi2S4)

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Mineral laflammeite ($Pd_3Pb_2S_2$) was firstly described by Barkov et al. (2002) from the Kirakkajuppura platinum-deposit, Penikat layered complex, Finland. Barkov et al. (2002) provided chemical and physical characterisation of this mineral, however its detailed crystal structural analysis has been lacking. Thalhammerite ($Pd_9Ag_2Bi_2S_4$) was discovered in millerite-pyrite-chalcopyrite vein-disseminated ore from the Komsomolsky mine in the Talnakh deposit, Russia (Sluzhenikin and Mokhov, 2015). Crystal structures of both minerals and relevant crystal-chemical implications will be presented.

Laflammeite occurs as subhedral platelets up to 150 μm, however the crystals are finely twinned and consequently unsuitable for a direct crystal structure study (Barkov et al. 2002). Thalhammerite occurs as tiny inclusions (from few μm up to about 40-50 μm) in sulphide ore where it forms intergrowns with other Pd-bearing minerals. Therefore, both minerals were synthetized by silica glass tube technique by heating at 400 ºC from stoichiometric mixture of elements. The prepared synthetic analogues of laflammeite and thalhammerite were used for a crystal structure study. The structural identity between natural and synthetic materials was subsequently confirmed by an electron-backscattered diffraction.

Laflammeite, $Pd_3Pb_2S_2$, crystalizes in *Pmmn* space group (a = 5.78, b = 8.18, c = 5.96 Å) and Z = 2. Its crystal structure show many similarities with structures of shandite ($Ni_3Pb_2S_2$, $R\bar{3}m$), parkerite ($Ni_3Bi_2S_2$, $C2/m$) and vymazálovaite (Pd$_3Bi_2S_2$, $I2_13$). All these minerals show a common structure motive: a pseudocubic subcell of the CsCl-type composed of Bi(Pb) and S atoms. A half of available octahedral voids is occupied by Ni(Pd) atoms. The distribution of Ni(Pd) atoms (i.e. the ordering scheme) determines the structure type (Weihrich et al. 2007). Laflammeite can be considered as antiperovskites superstructures.

Thalhammerite, $Pd_9Ag_2Bi_2S_4$ shows *I4/mmm* symmetry (a = 8.02, c = 9.15 Å) and Z = 2. Its unique crystal structure is based on a three-dimensional framework which consists of two types of blocks of polyhedra that interpenetrate and support each other. The first type consists of corner-sharing [PdS_4] and [$PdBi_2S_2$] squares. The second is formed by flattened tetrahedra [$PdBi_2S_2$]. Silver atoms occupy channels running along the *c* direction. Thalhammerite crystal structure merges metallic building blocks with structure motives typical for polar sulphides.

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Carbon molecules in space: a thermal equation of state study of solid hexamethylentetramine

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Equations of State (EoSs) show how the thermodynamic variables of temperature (T), pressure (P) and volume (V) are inter-related. The ideal gas law, $PV = nRT$, is an example of an EoS which is used as a simple but effective model to explain the properties of gases. EoSs can also be applied to solids, where they can be used to show how energy changes when the solid experiences dramatic changes in its environment. Such information is relevant to understand the fate of carbon in the context of planetary settings, from comets to gas giants. Despite the large heterogeneity of galactic and interstellar regions, the organic chemistry of the universe seems to follow common pathways. Molecules of high astrobiological relevance such as N-heterocycles and amino acids have been identified in trace quantities in meteorites but they can be considered fragile species easily destroyed by raditions, shocks and thermal processes through the Solar System.

Alhough it is quite common to model thermal expansion at ambient pressure with a VT equation of state (EoS), and compression using a PV EoS, determinations of PVT EoSs are much less common, particularly for molecular materials. The paucity of data reflects the difficulty in varying pressure and temperature simultaneously in crystallographic experiments, especially at reduces temperatures. These difficulties are addressed by the variable temperature insert for the Paris-Edinburgh cell available on the PEARL instrument at the ISIS Neutron Spallation Source.

A PVT EoS provides access to a rich array of thermodynamic properties which revel the changes in different contributions to the thermodynamic properties such as internal energy, enthalpy and entropy occur in response to compression. The same quantities can be modelled using computational methods such as the PIXEL method and Density Function Theory, making EoS measurements sensitive tests of theory. This poster will describe a PVT EoS determination for hexamethylentetramine-d_{12} a high-symmetry crytalline solid which remains in the same phase from 130 to 480 K and between ambient pressure and 5 GPa.

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