CO2), strong alkaline aqueous solutions, silica and alkaline-earth cations (Ba and Sr, Ca) at room temperature. Under these alkaline conditions, the precipitation of alkaline-earth carbonates (witherite, strontianite or calcite/aragonite) coupled with silica precipitation entering an autocatalytic mechanism that explains their bizarre morphological behaviour, hierarchy and self-organization [3]. In this communication, rather than on morphology I will focus on the description and explanation of the crystalline texture of silica biomorphs and their relevance to the understanding of the formation of biomineral structures.

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Keywords: crystallization; self-assembled textures; biomorphs

FA2-MS02-O4

Electronic and Magnetic Structure of Pyroxenes I: Hedenbergite, $CaFeSi_2O_6$. Michael Grodzicki[a], Günther Redhammer[a], Michael Reissner[b], Walter Steiner[b], Georg Amthauer[a]. [a]*Department of Materials Engineering and Physics, Salzburg University, Austria.* [b]*TU Vienna, Austria.*
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The electronic and magnetic structure of the chain silicate hedenbergite ($CaFe^{2+}Si_2O_6$) has been investigated by a number of experimental methods (neutron diffraction, Mössbauer spectroscopy, low temperature magnetic measurements), as well as by electronic structure calculations for clusters of different size in the local spin density approximation. The calculated size-converged spectroscopic data (*d-d* excitation energies, hyperfine parameters) are in quantitative agreement with the respective experimental values. The calculated magnetic coupling constants are about +25 cm^{-1} and -4 cm^{-1} for intra-chain and inter-chain coupling, respectively. The latter value shows that weak superexchange via edges of silicon tetrahedra is well reproduced by the calculations, and it is in qualitative agreement with an observed metamagnetic transition at 4.2 K in an external magnetic field with an onset around 4 T but saturation is not achieved in fields up to 14.5 T. The large ferromagnetic intra-chain coupling is attributed to a nearly degenerate ground state. The ratio between the two magnetic coupling constants agrees with earlier estimates on similar compounds. Finally, it is demonstrated how the detailed discussion of the various exchange pathways contributes to an improved understanding of the connection between magnetic properties and the geometrical structure.

Keywords: hedenbergite; mössbauer spectroscopy; magnetic measurements

FA2-MS02-O5

Structural Characterization of Maya Blue Analogous Hybrid Pigments. Catherine Dejoie[a], Pauline Martinetto[a], Eric Dooryhée[a], Devendro Bhange[a], Christophe Lepoittevin[a], Michel Anne[a]. [a]*Institut NEEL CNRS & Université Joseph Fourier, 25 rue des Martyrs, 38042 Grenoble, France.*
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The search for stable dyes, resisting heat and moisture in particular, places several organic-inorganic hybrids as particularly appropriate and environmentally friendly solutions: the colour can be durably fixed by trapping or encapsulating the organic dye on a mineral or in a clay matrix [1]. In the present work, we examine the diffusion and the fixing process of the indigo molecules inside the cages and channels of appropriate alumino-silicates such as zeolites. We succeed in producing a stable composite, whose colour and stability resemble those of the historical Maya Blue pigment [2]. Part of our project is to revisit the structural and spectroscopic features of Maya Blue using the indigo-zeolite complex as a model case. Our new zeolitic analogues are characterized by optical and vibrational spectroscopies, quasi-elastic neutron scattering, and synchrotron X-ray powder diffraction. Formation of the hybrid is followed by in situ X-ray diffraction. Insertion of the indigo molecules inside the matrix causes a monoclinic-to-orthorombic structural change of the zeolite crystal. Fourier difference syntheses reveal extra electronic density inside the zeolitic channels due to the presence of the organic dye. The global organic molecule position in the channel network of the zeolite is obtained by simulated annealing. Further structure refinements complete the structural determination of this new organic-inorganic hybrid.

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Keywords: rietveld refinement; zeolite; structure solution