

Poster Presentation

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Two types of adjacent dimer layers in the low-temperature phase of BaCuSi₂O₆

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The low-temperature crystal structure of BaCuSi₂O₆ has been investigated with high-resolution synchrotron x-ray and neutron powder diffraction techniques and has been found to be on average (ignoring the incommensurate modulation) orthorhombic, with the most probable space group Ibam. The Cu-Cu dimers in this material are forming two types of layers with distinctly different interatomic distances. Subtle changes also modify the partially frustrated interlayer Cu-Cu exchange paths. The present results corroborate the interpretation of low-temperature nuclear magnetic resonance and inelastic neutron scattering data in terms of distinct dimer layers. The experimentally determined low-temperature crystal structure of BaCuSi₂O₆ is discussed in terms of its relation to the newer findings of theory and of the complementary experiments.

[1] D.V. Sheptyakov, V.Yu. Pomjakushin, R. Stern, I. Heinmaa, H. Nakamura and T. Kimura, *Phys. Rev. B* (2012) 86, 014433.

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