

LiCu₂[BP₂O₈(OH)₂]: A Lithium Copper Borophosphate with Chains of distorted CuO₅ Square Pyramids

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Cu(II) compounds with complex oxo-anions of non-metals attract large attention due to their diverse structural chemistry and the related variety of quantum spin properties [1–5]. As the first example containing copper coordinated in square pyramidal chains, LiCu₂[BP₂O₈(OH)₂] was prepared under hydrothermal conditions from concentrated acidic solutions of CuCl₂, H₃BO₃ and LiH₂PO₄ at 443 K in a closed system. The crystal structure (*C2/c*, *a* = 15.1082(15) Å, *b* = 4.7639(7) Å, *c* = 9.6666(9) Å, *β* = 91.01(1)°, *Z* = 4) comprises distorted CuO₅ square pyramids and the borophosphate trimers [BP₂O₈(OH)₂]²⁻ (Fig. 1, *left*). Distorted CuO₅ square pyramids are connected to each other by sharing common O-corners to form infinite *zigzag* chains running along [010] (Fig. 1, *right*). Borophosphate trimers, placed within the voids between the square pyramidal chains, interconnect these chains to form a 3D open-framework structure with alternating 6-membered ring and 4-membered ring channels running along [010]. Li⁺ ions reside in the small 4-membered ring channels. The magnetic susceptibility obeys a Curie-Weiss law for *T* > 20 K with *θ* = +5.0 K and an effective magnetic moment *μ*_{eff} of 1.89 *μ*_B which is a typical value for square pyramidal Cu²⁺-compounds. Interestingly, ferromagnetic ordering is observed at 3.6(2) K.

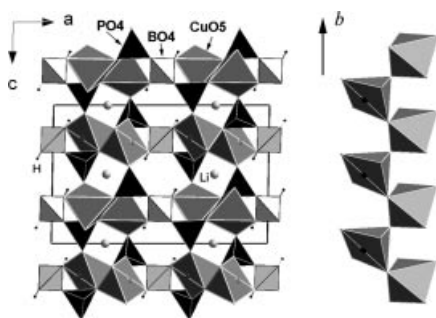


Fig. 1 Crystal structure of LiCu₂[BP₂O₈(OH)₂] viewed along [010] (left) and the one-dimensional copper(II)-square pyramidal chain (right) (BO₄ tetrahedra: grey, PO₄ tetrahedra: black, CuO₅ square pyramids: grey, Li atoms: white spheres, H atoms: small black spheres).

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