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The low-dimensional magnetic van der Waals compound FeOCl at extreme conditions: pressure and temperature induced phase transitions and structural evolution

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FeOCl features a simple structure built from Fe-O double layers stacked along the c-axis and separated through bi-layers of chlorine; the latter are bonded through weak van der Waals forces. On cooling, an orthorhombic-to-monoclinic lattice distortion occurs at T_N = 81 K [1] which removes the geometric frustration of magnetic order of Fe^{3+} moments, as it exists on the orthorhombic lattice [1,2]. This allows antiferromagnetic order to develop [1,2]. The quasi-two-dimensional magnetic character of FeOCl stems from the unpaired 3d electrons (Fe^{3+} with $3d^5$ electronic state), which results in strong intra- and interchain exchange interactions in the ab-plane of the structure [2,3]. (Quasi-)hydrostatic pressure, applied within a diamond anvil cell (DAC) up to ≈ 38 GPa, provides a way of modifying the interlayer van der Waals gap and more importantly, through geometrical modifications of the $FeCl_2O_4$ octahedra, a way to modify and tune the magnetic exchange interactions. These experiments have been carried out above and below the Néel temperature, which allows us to investigate the interplay of magnetic order and pressure-induced structural changes in FeOCl. Here we present one of the essential steps in this project: a detailed analysis of the pressure and temperature dependent structural evolution of FeOCl, as investigated by high-pressure low-temperature single crystal X-ray diffraction at beamline P02.2/PETRA III (Hamburg, Germany). This includes the phase transitions and an in-depth analysis of bond lengths and -angles, which sheds light on the magneto-elastic interplay in this compound. This may further contribute to the understanding of the mechanisms in exotic strongly correlated systems in general and low dimensional magnetic compounds in particular.
[1] Zhang et al., Phys. Rev. B 86, 134428 (2012).
[2] Angelkort et al., Phys. Rev. B 80, 144416 (2009).
[3] Glawion et al., Phys. Rev. B 80, 155119 (2009).

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