

THE PRESSURE EFFECT ON THE CRYSTAL AND MAGNETIC STRUCTURE PROPERTIES OF VAN DER WAALS MATERIAL CrBr₃

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Two-dimensional (2D) magnetic materials have attracted immense attention for their possible use in a variety of spin-based applications, ranging from spin-tronics, magnetic memories to topologically protected magnons. In layered magnetic materials, the strength of interlayer and

the intralayer magnetic interaction remains significantly different, opening the possibility to control their interlayer interaction electrically. Chromium tribromide, which crystal structure is comprising two-dimensional sheets of composition CrBr₃ van der Waals bonded to one another, is of particular interest due to its extraordinary electronic and magnetic properties. The Curie temperature for CrBr₃ is reported to be about 37 K, crystallizing in the rhombohedral BiI₃ structure of R $\bar{3}$ symmetry and retains this structure at low temperatures [1]. The recent discoveries of magnetism in the monolayer limit have also opened up new possibilities for the study of two-dimensional materials [2]. Although the knowledge of CrX₃ in general is still limited, these compounds, especially CrBr₃, are perfect model systems to search for possible spin-lattice coupling phenomena in CrX₃ family due to absence of structural phase transitions at low temperatures and similarity of magnetic order in bulk and few-layer forms.

The present work focuses on the investigations of crystal and magnetic structures of chromium tribromide in wide temperature and pressure ranges. The detailed studies of the crystal structure of CrBr₃ were carried out using neutron diffraction on a DN-6 diffractometer of a pulsed high-flux IBR-2 reactor (FLNP, JINR, Dubna, Russia) in temperature range of 6-300 K and at pressure up to 5 GPa. Neutron diffraction investigations of CrBr₃ revealed to observe the formation of the long-range ferromagnetic order which leads to the negative thermal volume expansion and anomalous thermal variation of interatomic distances and angles, caused by the spin-lattice coupling. Related effects were found in vibrational spectra of this compound. Noticeable anomalies near the Curie point are observed on the temperature dependences of Raman peak frequencies as well as on their full-width at half-maximum which indicates the strong spin-phonon coupling in CrBr₃. The high pressure effect made it possible to identify unusual changes in the diffraction spectra and changes of Raman modes, which may be associated with some crystal changes in CrBr₃. However, X-ray diffraction shows that the structure with initial symmetry remains up to high pressures. It was also obtained the evolution of the unit cell parameters, bond lengths under high pressure.

[1] E. J. Samuelsen, R. Silberglitt, G. Shirane, and J. P. Remeika (1971). Spin Waves in Ferromagnetic CrBr₃ Studied by Inelastic Neutron Scattering. *Phys. Rev. B.* 3. 157

[2] H.H. Kim, Bowen Yang, Siwen Li, et al. (2019). Evolution of interlayer and intralayer magnetism in three atomically thin chromium trihalides. *Proc. Natl Acad. Sci. USA* 116, 11131–11136