High-pressure effect on crystal, magnetic structure and vibrational spectra of van der Waals $CrBr_3$

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Van der Waals (vdW) compounds are currently one of the most interesting objects of research in the field of condensed matter physics due to the recently discovered magnetic properties in their two-dimensional forms. The structure features lead to a significant sensitivity of the physical properties in these compounds to external influences, which can cause many unusual phenomena. High pressure investigation is a direct method of controlled change in magnetic interactions due to variations in interatomic distances and angles. Investigations at high pressures provides a unique opportunity to study the relationship between changes in structural parameters and magnetic structure, which is necessary to understand the nature and mechanisms of physical phenomena observed in the objects under study. This work is devoted to the study of the crystal, magnetic structure and vibrational properties of vdW $CrBr_3$ in wide temperature and pressure ranges using neutron diffraction at DN-6 diffractometer of the IBR-2 reactor (JINR), also using x-ray powder diffraction and Raman spectroscopy. A negative thermal volume expansion in $CrBr_3$ below $T_C = 37$ K was observed, associated with spin-lattice coupling. The effect of high pressure leads to the suppression of magnetic ordering, and the transition from the initial ferromagnet state is expected at 8.4 GPa to antiferromagnet or paramagnet state. Our results also demonstrate an isostructural phase transition in a $CrBr_3$ ferromagnet (2.5–7 GPa). With a further increase in pressure up to 38 GPa, significant changes are observed in the behavior of the frequencies of the vibrational modes, which is associated with the transition to a metallic state above 26 GPa.