The pressure effect on crystal and magnetic structures of van der Waals material

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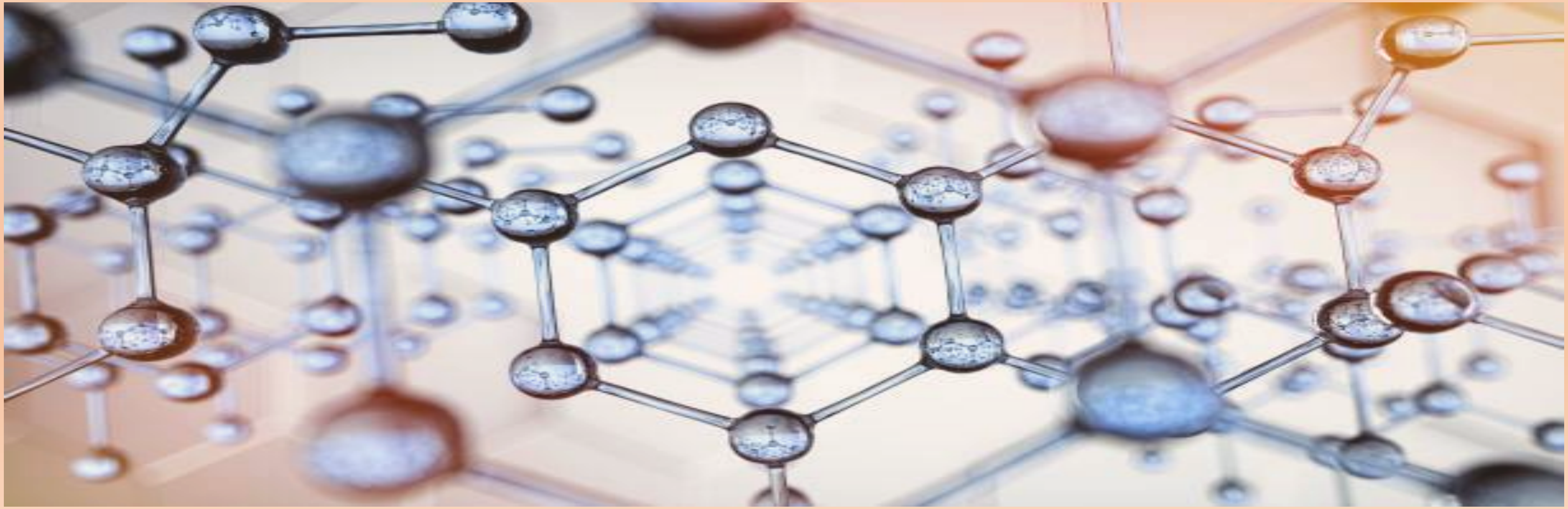
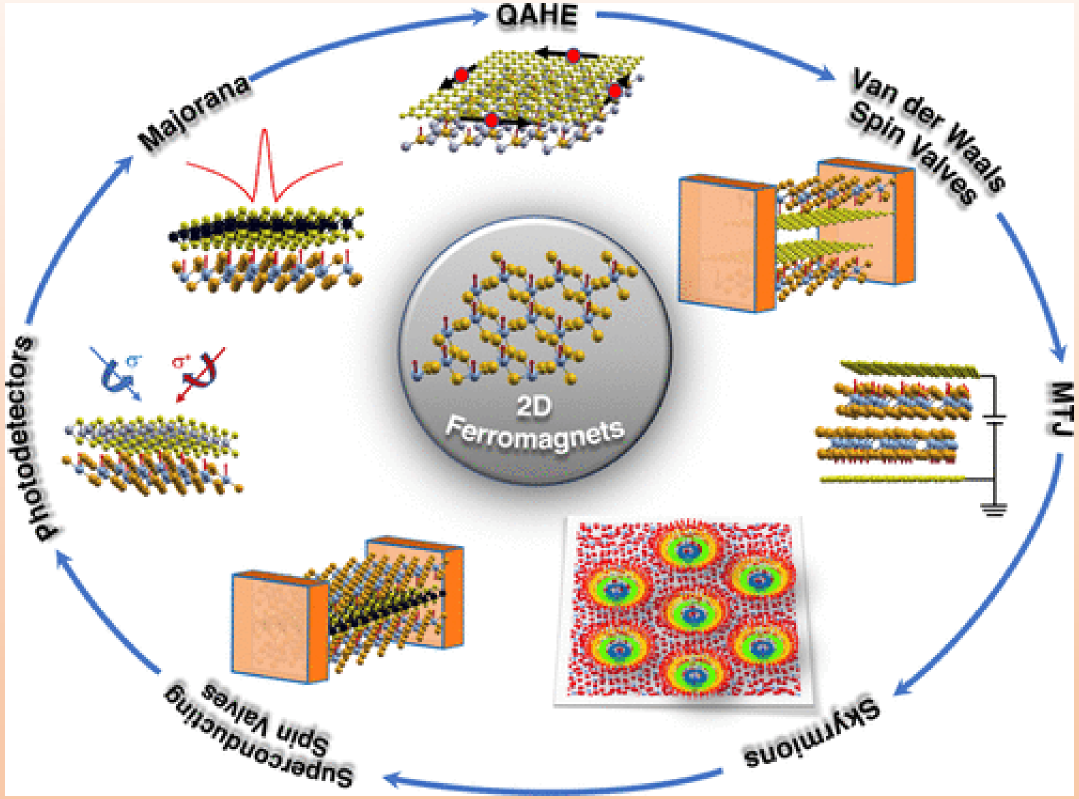
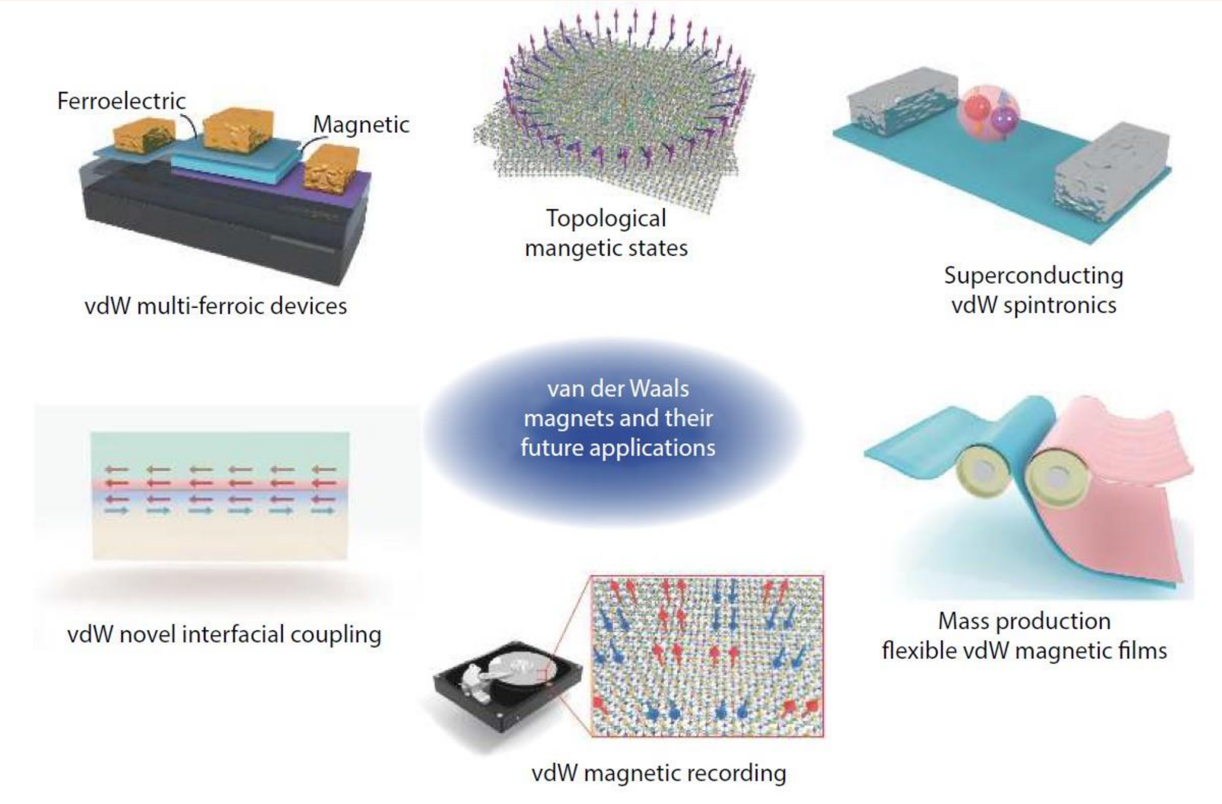


Introduction

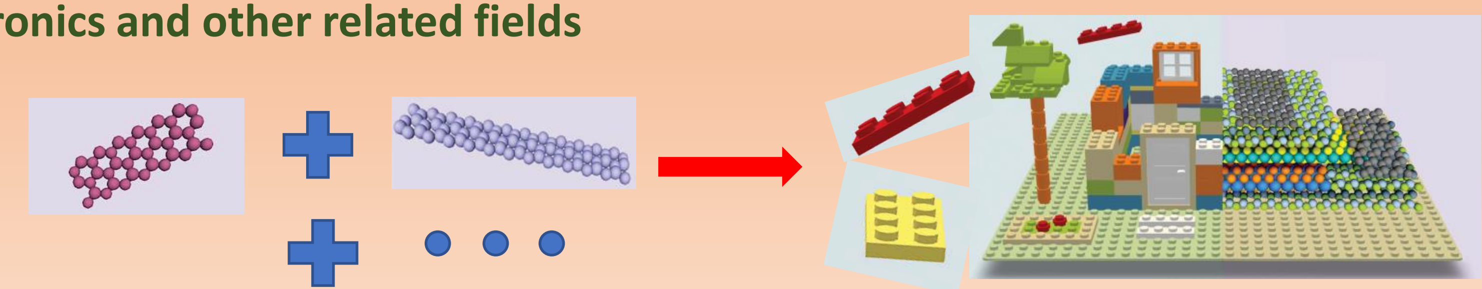


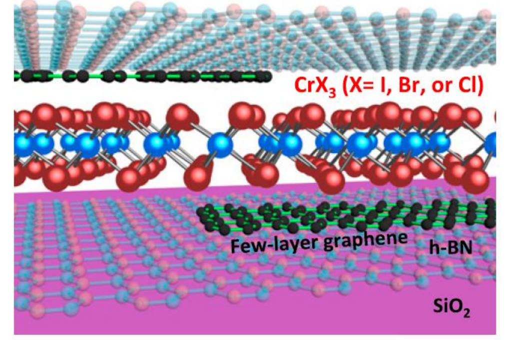


Applications of 2D ferromagnets in van der Waals heterostructures and twisted lattices

! Recent studies of two-dimensional forms of van der Waals magnets have shown that the magnetic ordering in them can be maintained at sufficiently high temperatures up to the limit of the atomic monolayer.

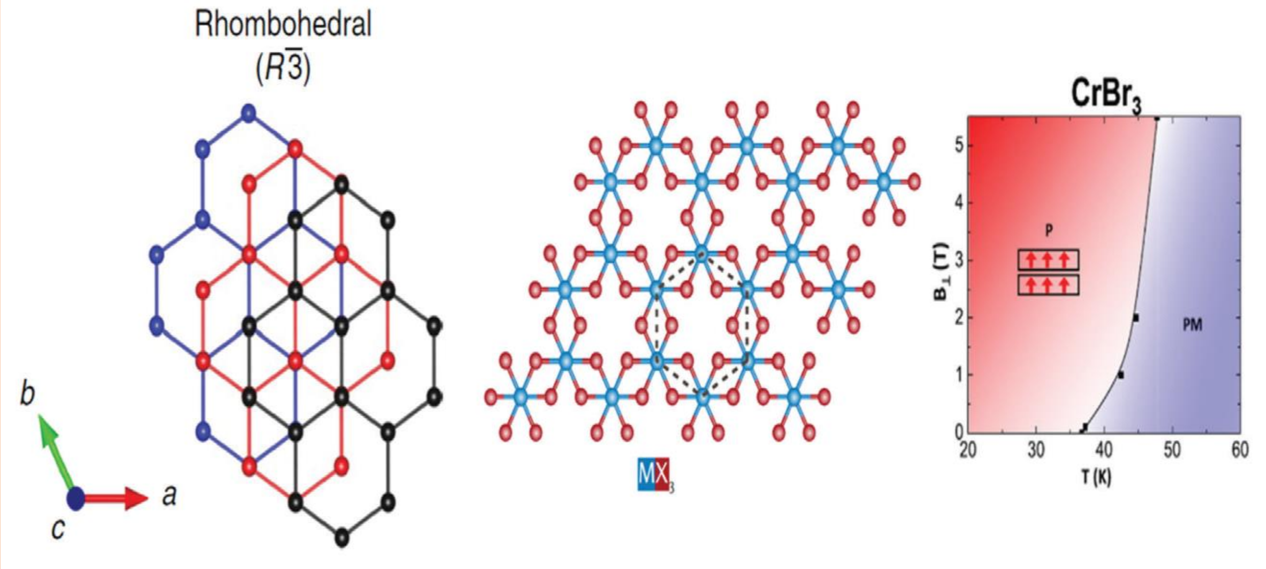
Future – the search and creation of various heterostructures with potential use in spintronics and other related fields





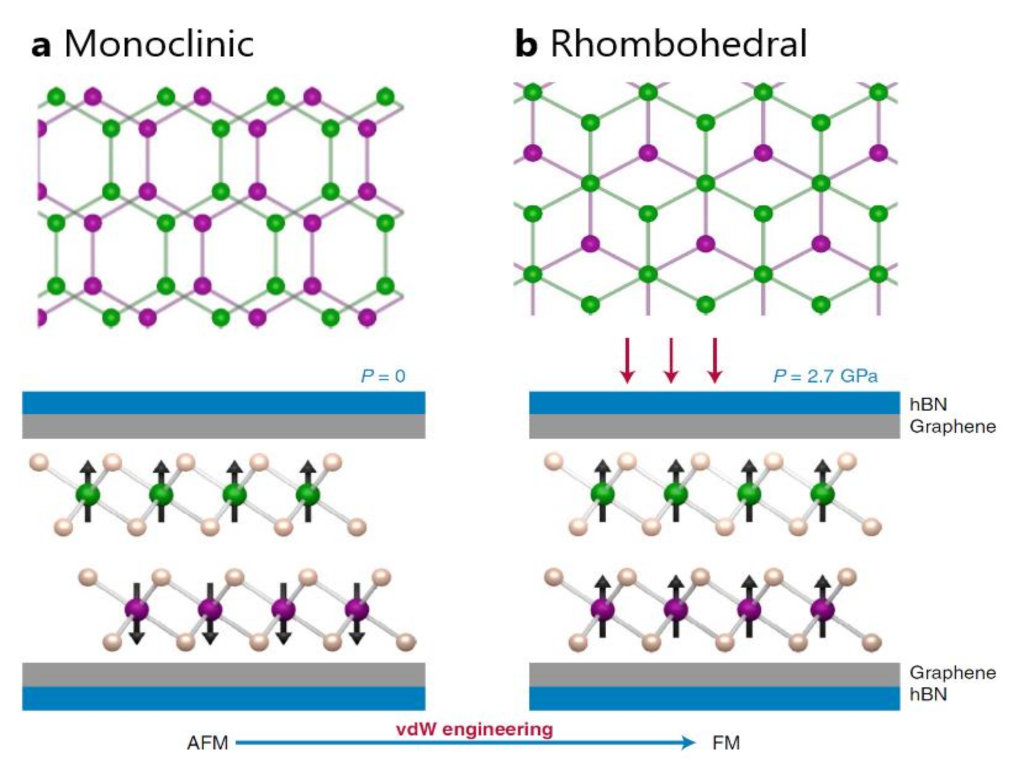
Introduction

The general atomic structure of CrX_3, where the Cr atoms, are arranged in a honeycomb plane, are surrounded by six halide atoms in an octahedral geometry. In general, CrX_3 possess relatively strong in-plane exchange coupling but weak interlayer coupling, thus allowing their magnetism to be stabilized in the monolayer regime.



The crystallographic structure of monolayer of $CrBr_3$ and the phase diagram vs temperature and magnetic field.

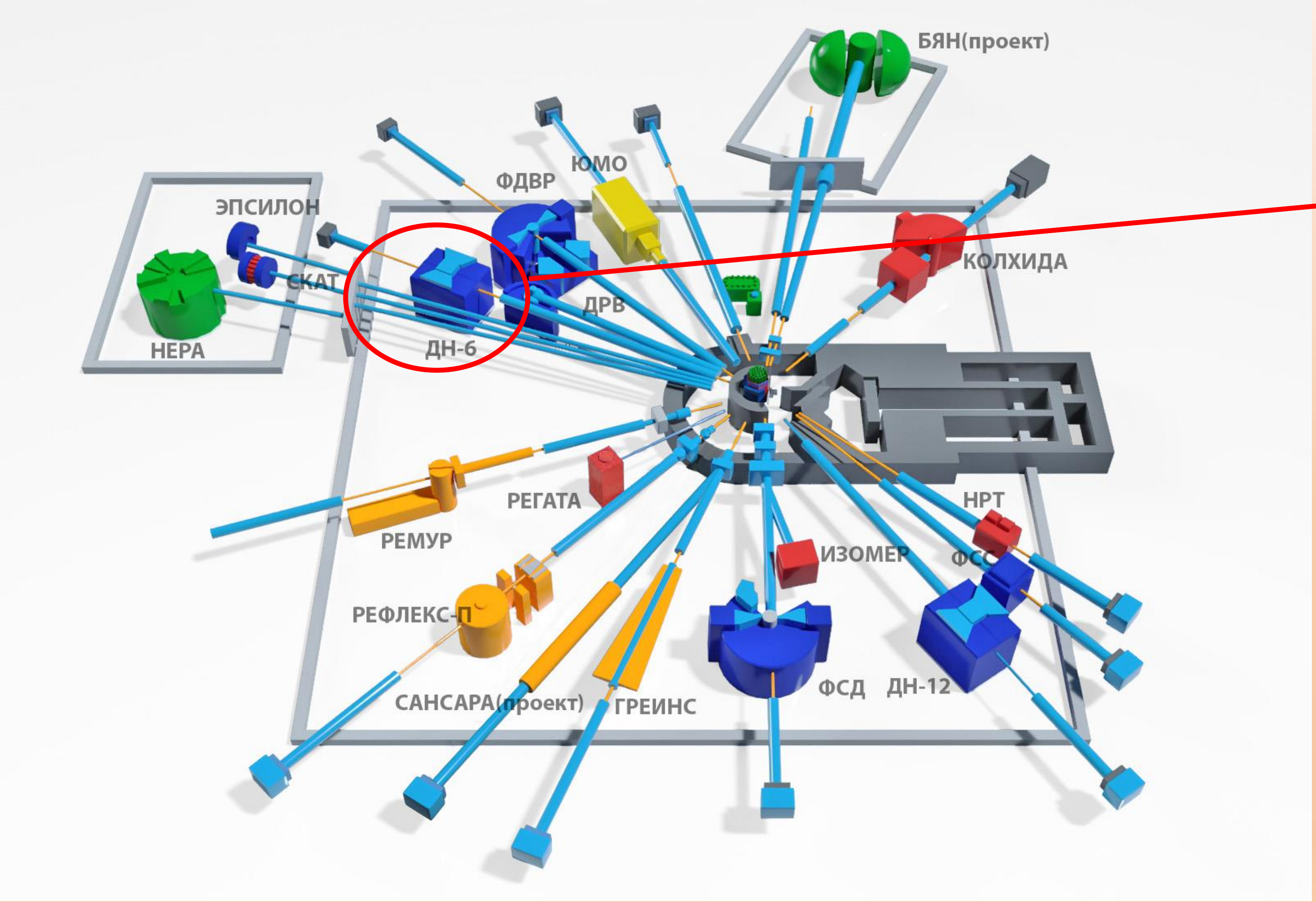
VdW CrI_3



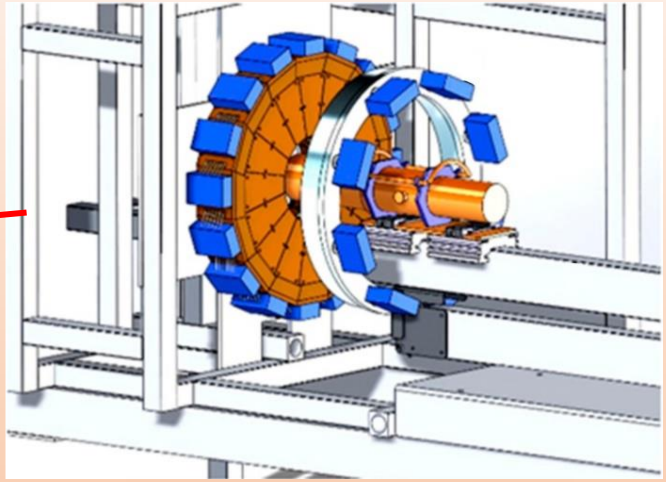
Pressure-induced changes in the layer stacking order is found to result in new magnetic ground states in two-dimensional insulating CrI_3.

!!! A significant advantage of 2D materials is that their physical properties are highly tunable by means of external control parameters that include temperature, electrostatic doping, pressure, strain

Experimental methods: Neutron diffractometer DN-6



Experimental hall of the IBR-2 reactor with 14 neutron output channels and the layout of the DN-6 diffractometer



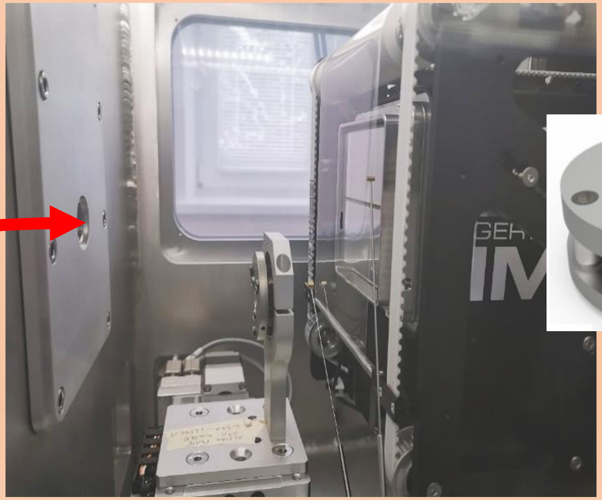
High-pressure cell with sapphire anvils

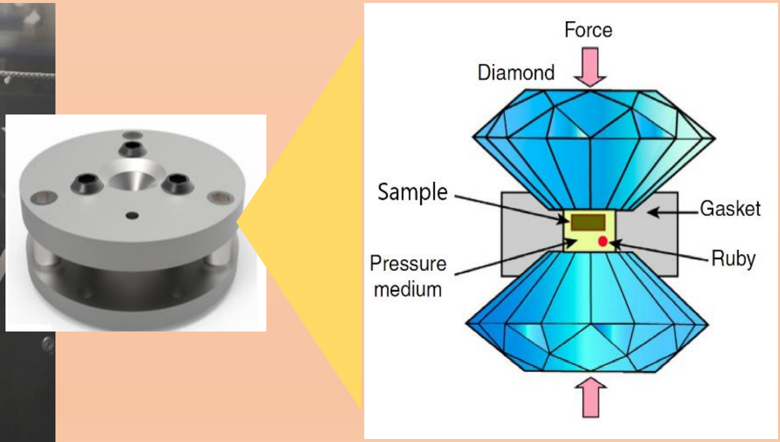
Experimental methods : X-ray и Raman

LabRAM HR Evolution spectrometer with a wavelength excitation of 632.8 nm emitted from He–Ne laser, 1800 grating. The low-temperature Raman measurements were carried out using low vibration helium refrigerator in temperature range 19–300 K.

Xeuss 3.0

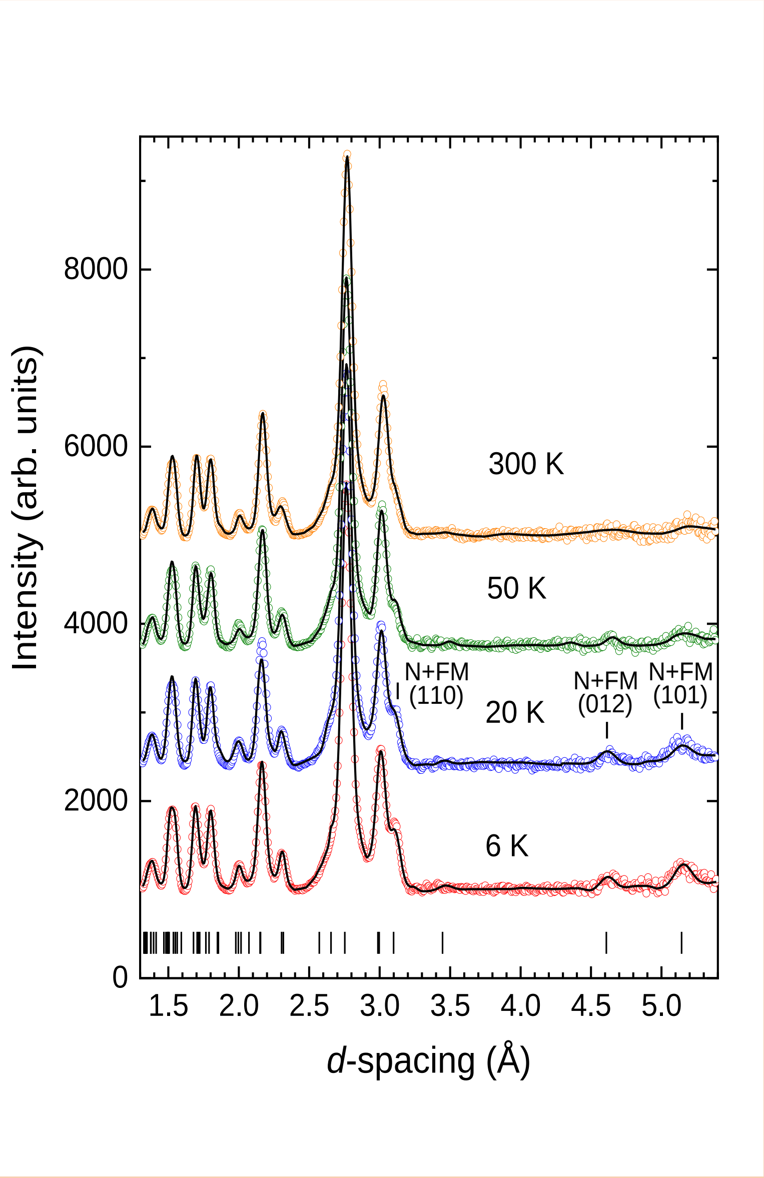
Cu radiation
(λ = 1.54184 Å)
Mo radiation
(λ = 0.71078 Å)

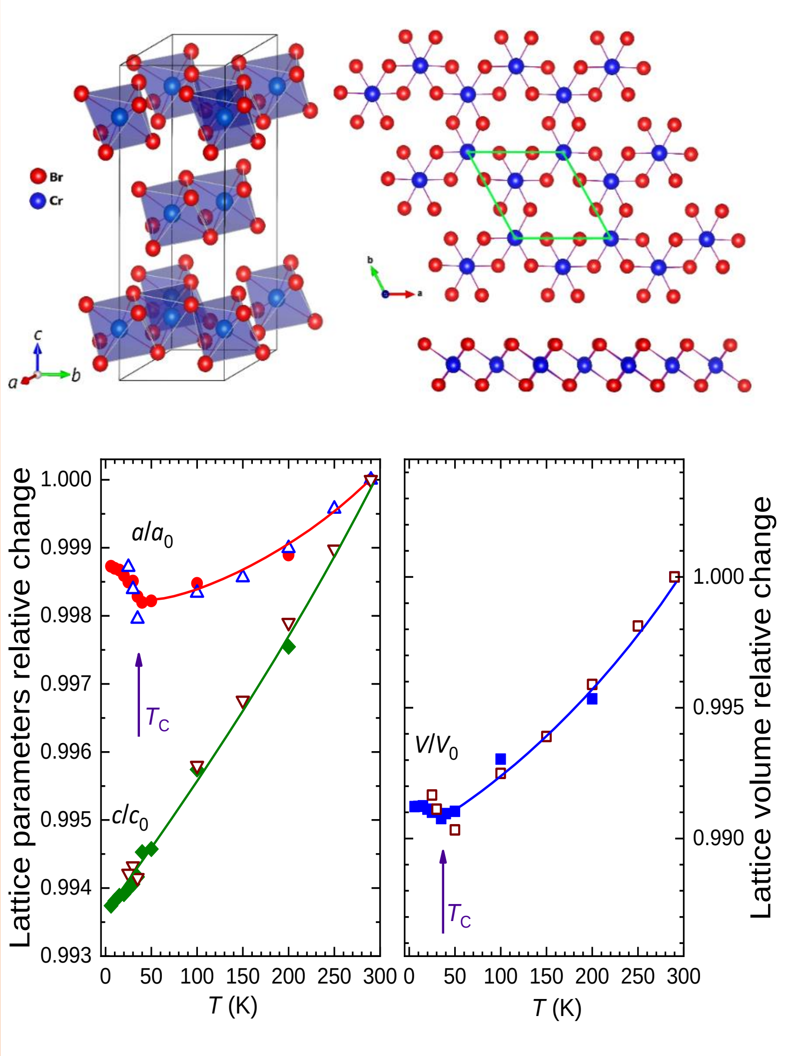


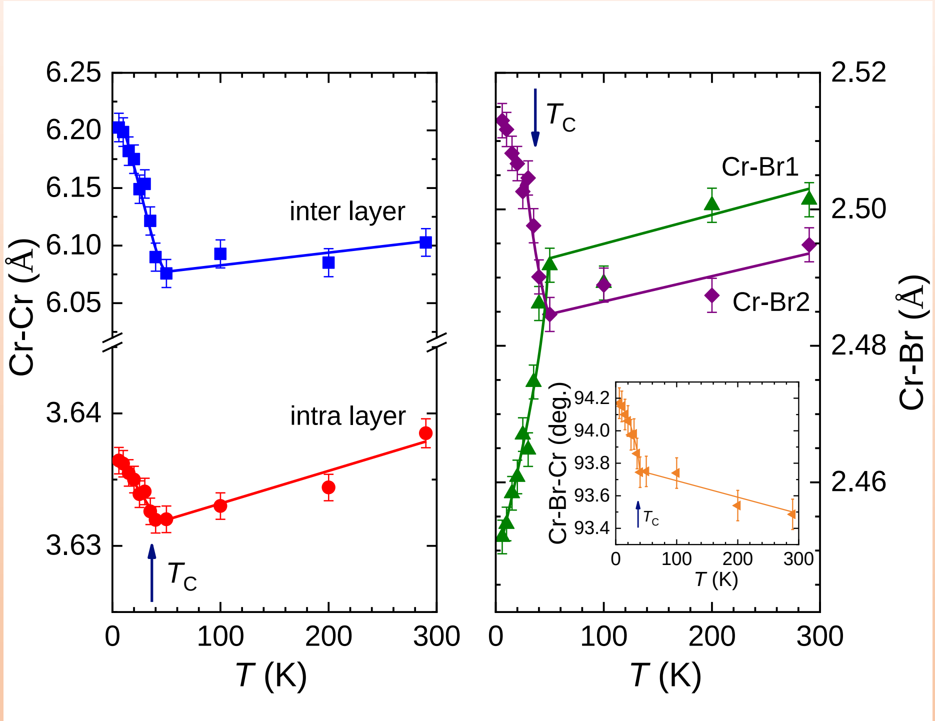


High-pressure cell with diamond anvils

Neutron diffraction at low temperature







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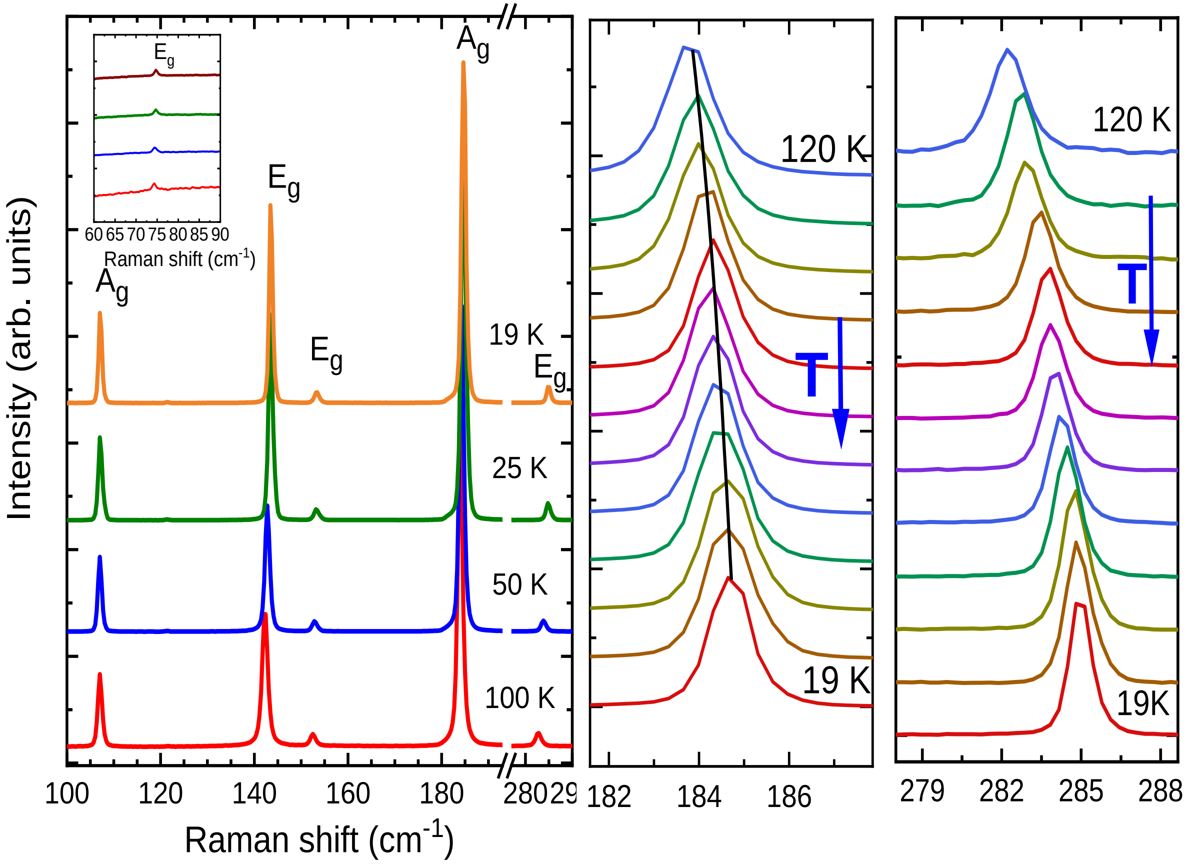
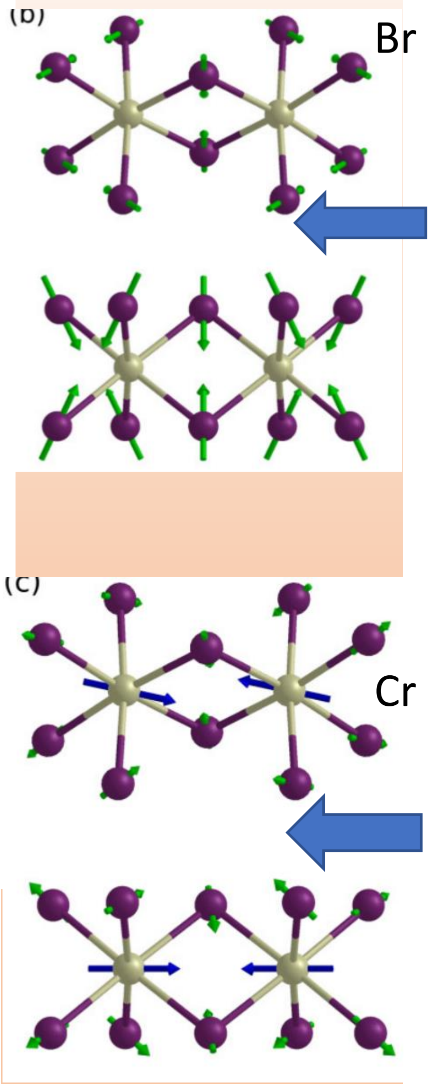
The temperature dependences of the lattice parameters and volume obtained from neutron and X-ray diffraction measurements

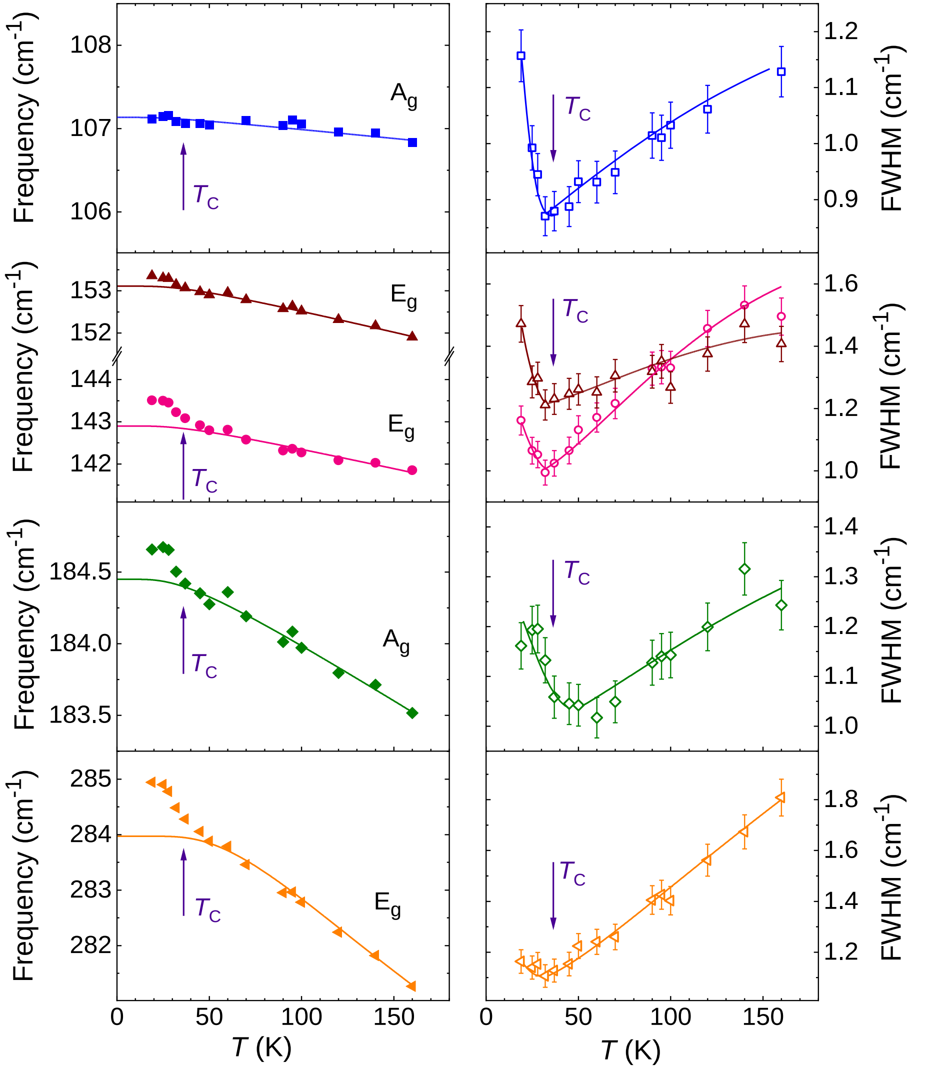
a) The thermal expansion of $CrBr_3$ lattice is strongly anisotropic with the pronounced variation of the c lattice parameter.

b) The interatomic intralayer and interlayer Cr–Cr distances decrease slightly on cooling in the temperature range above T_C and they also demonstrate opposite increasing trend for $T < T_C$

Raman spectroscopy at low temperature



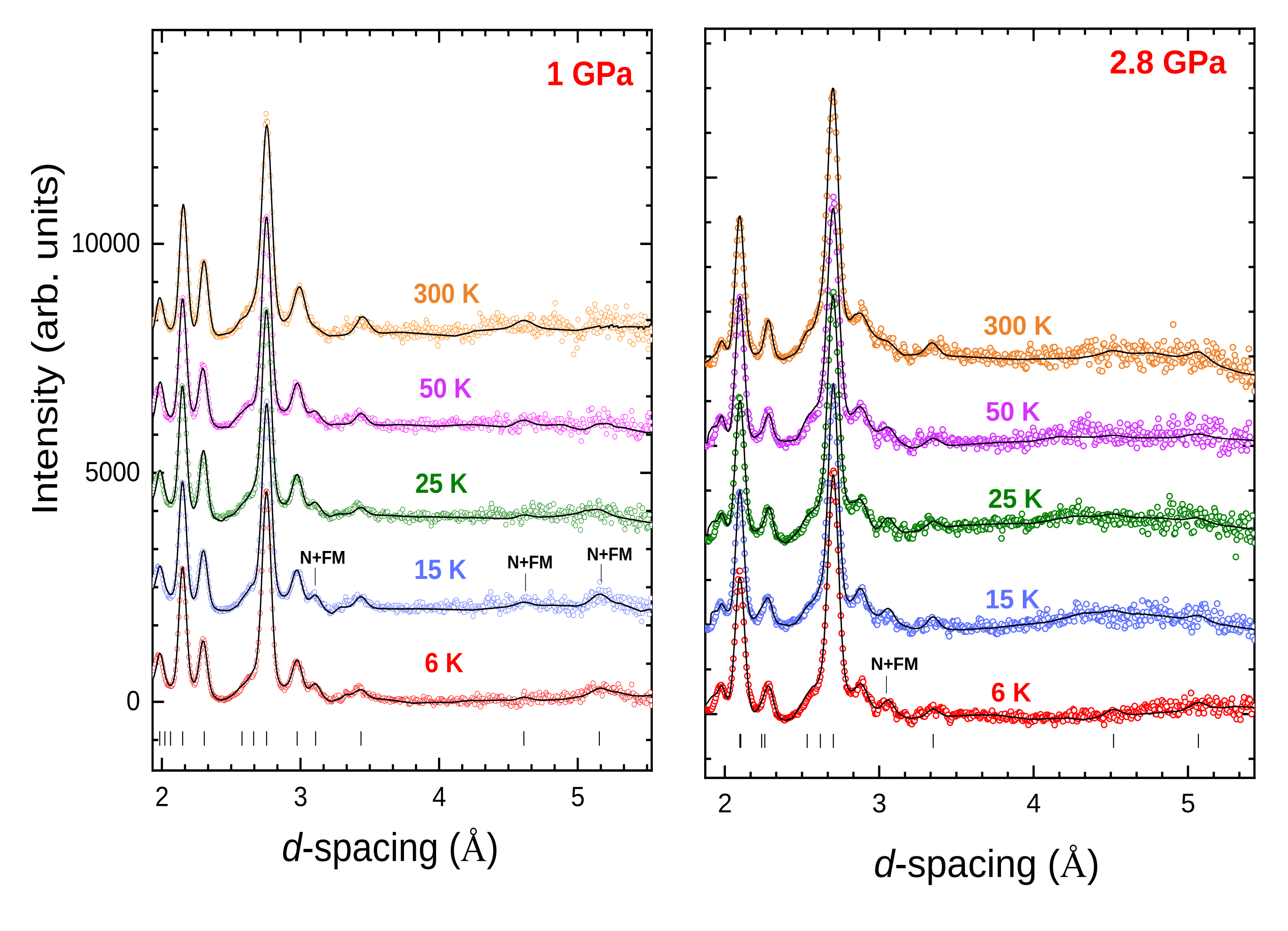




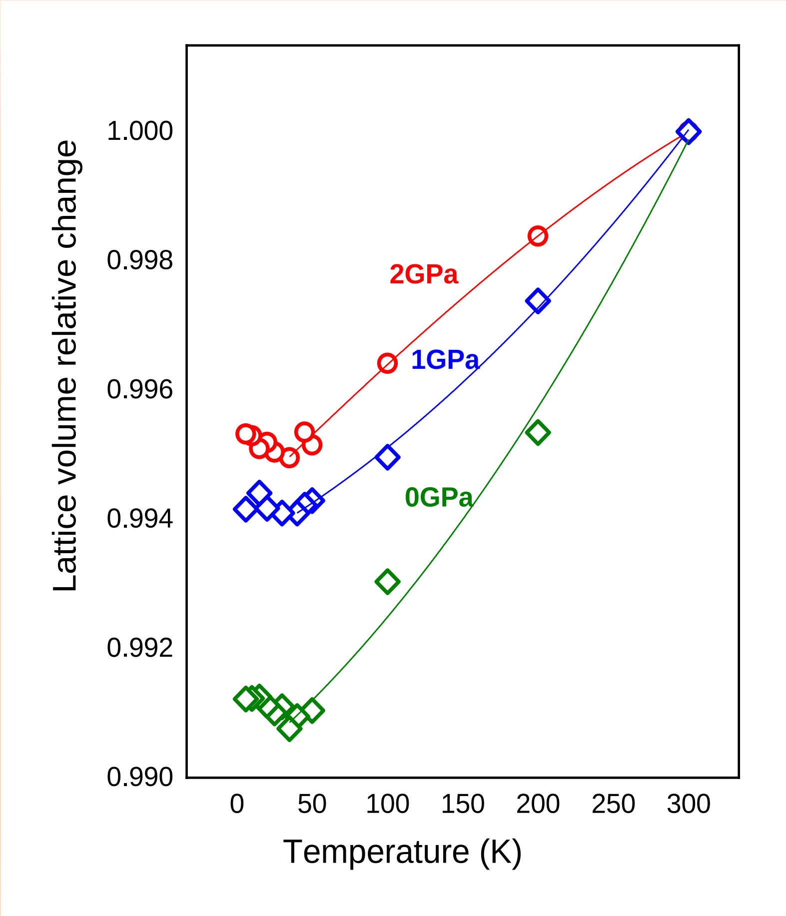
The FWHM of all the observed phonon modes reach minimum in the vicinity of T_C and demonstrate anomalous reversal broadening in the $T < T_C$ range. Both effects reveal a presence of the strong spin–phonon coupling in $CrBr_3$. The spin–phonon coupling is associated with the modification of the magnetic exchange interactions caused by the ionic motions

Neutron diffraction at high pressure and low temperature

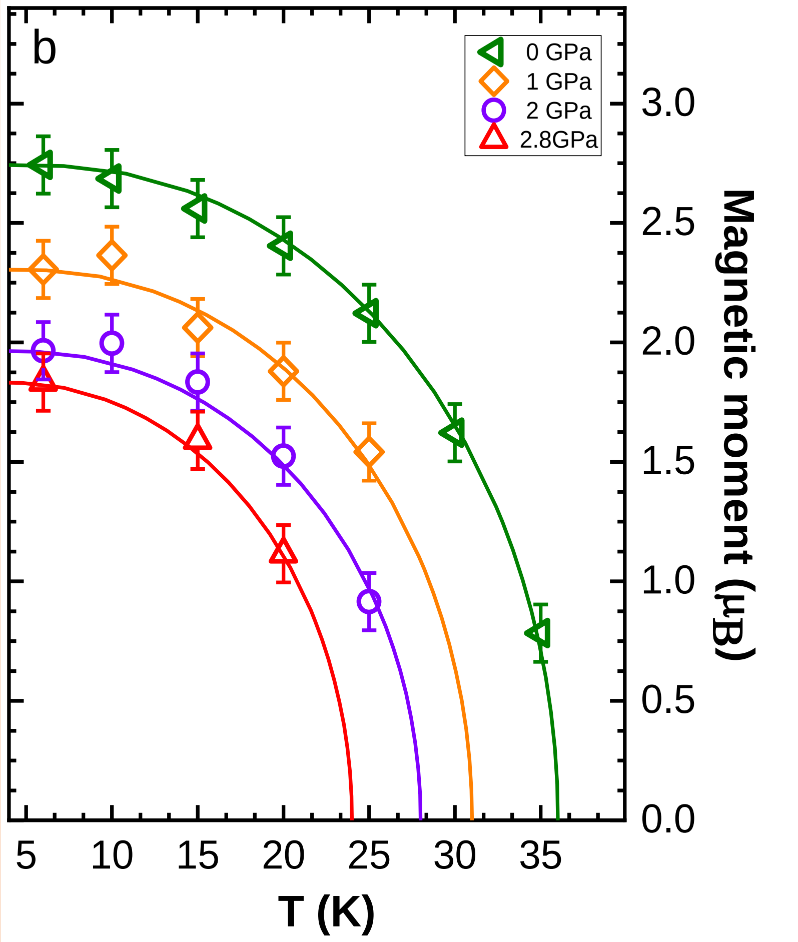
Neutron diffraction patterns of $CrBr_3$ measured at selected pressures, room and low temperatures.



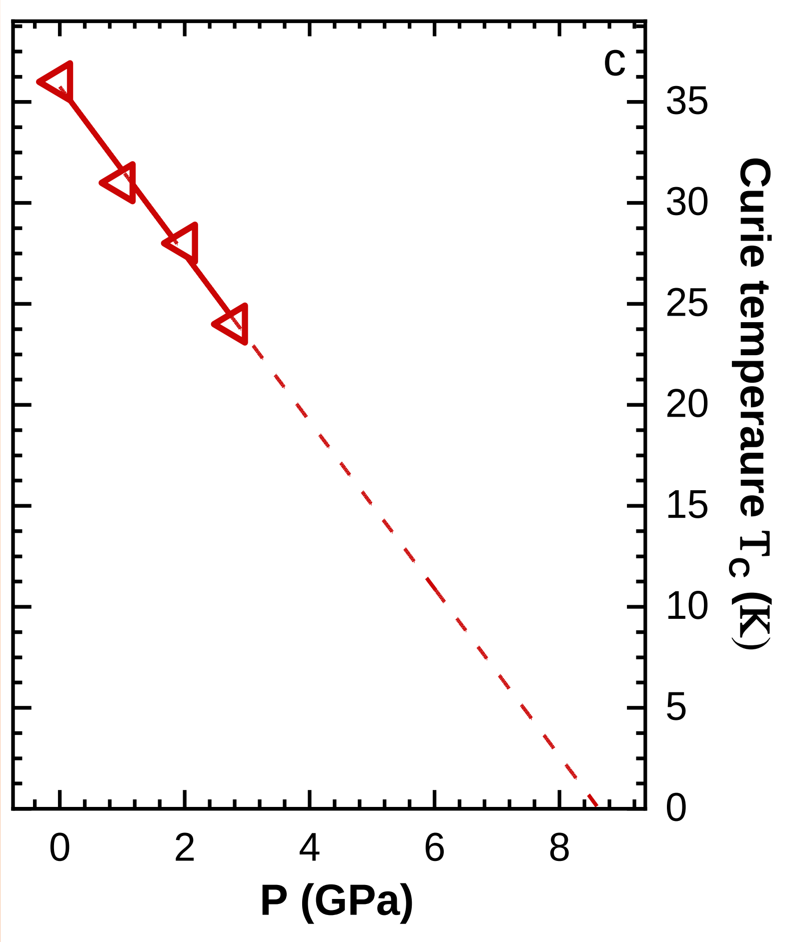
The negative volume thermal expansion in $CrBr_3$ persists even with the application of high pressure



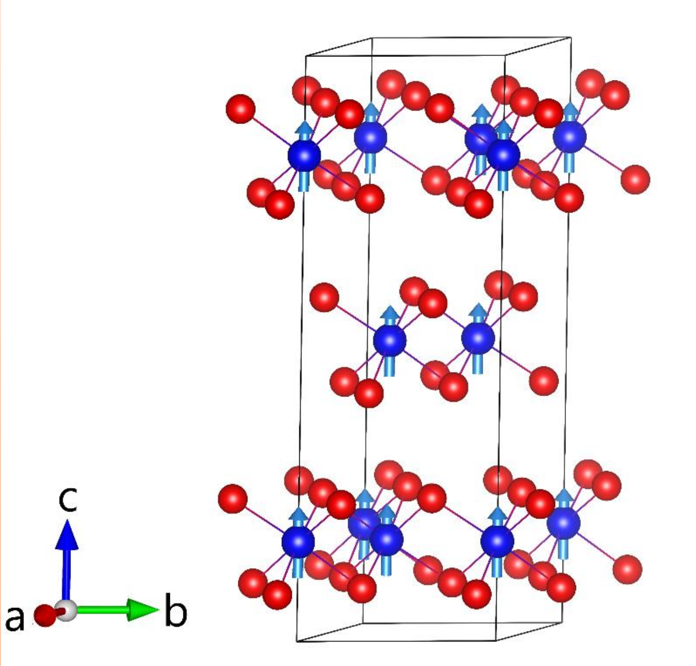
Neutron diffraction at high pressure and low temperature



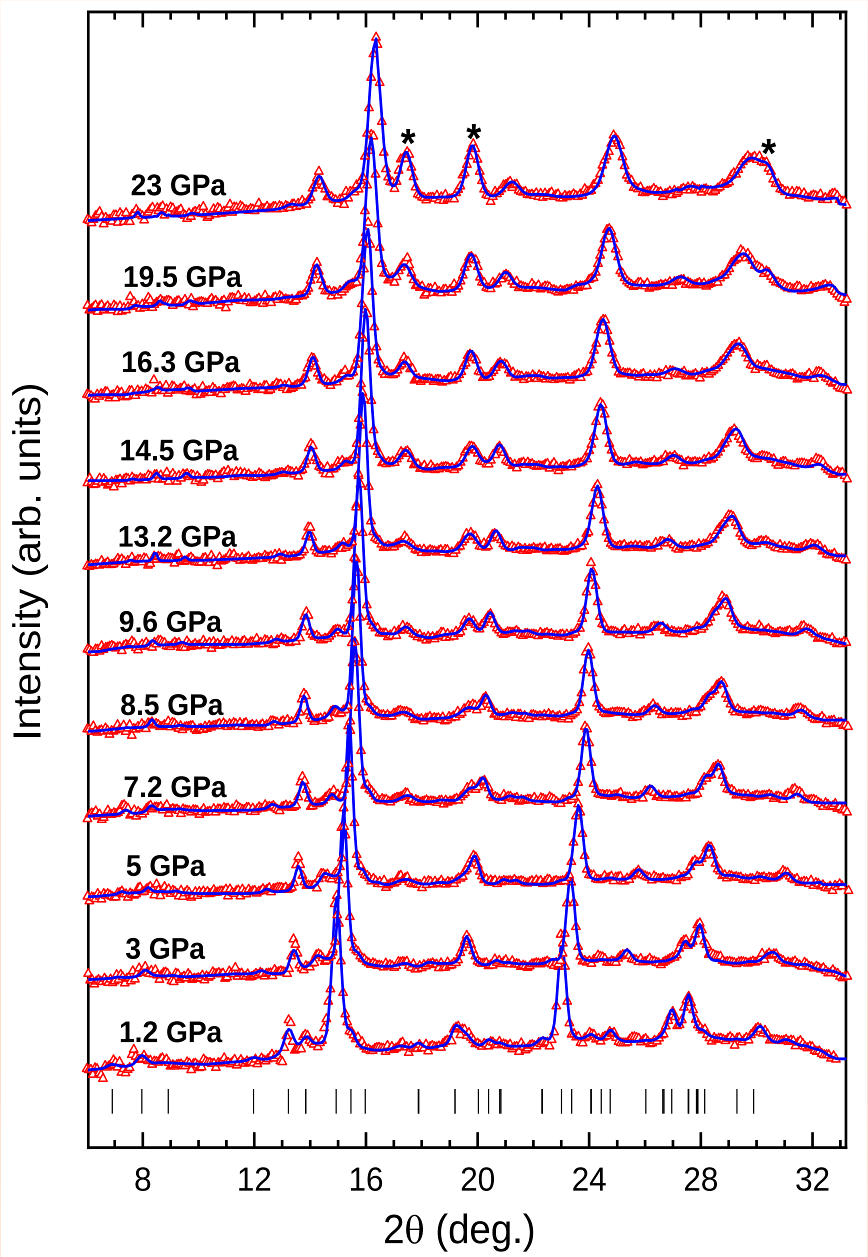
The obtained temperature dependences of the Cr magnetic moment of ferromagnetic FM phase at different pressures

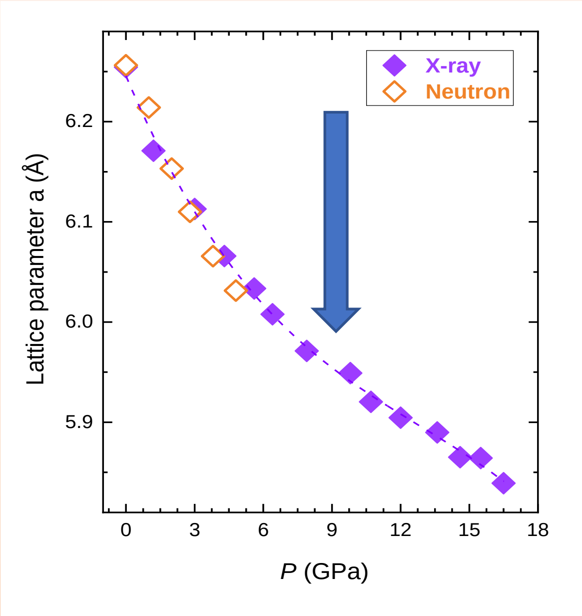


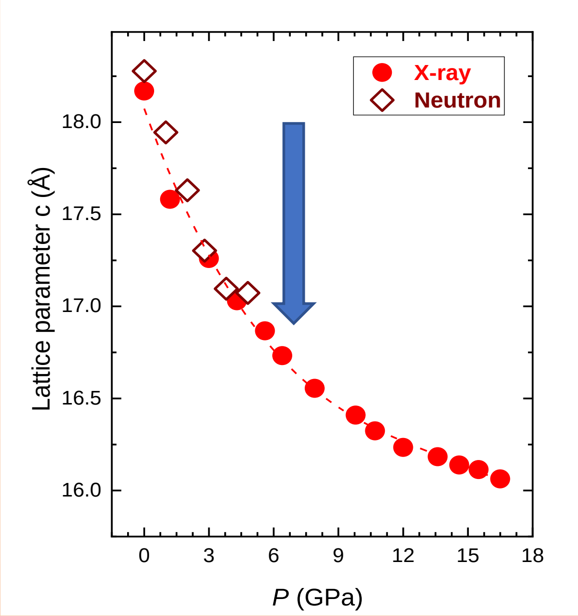
The Curie temperatures of the $CrBr_3$ as a function of the pressure



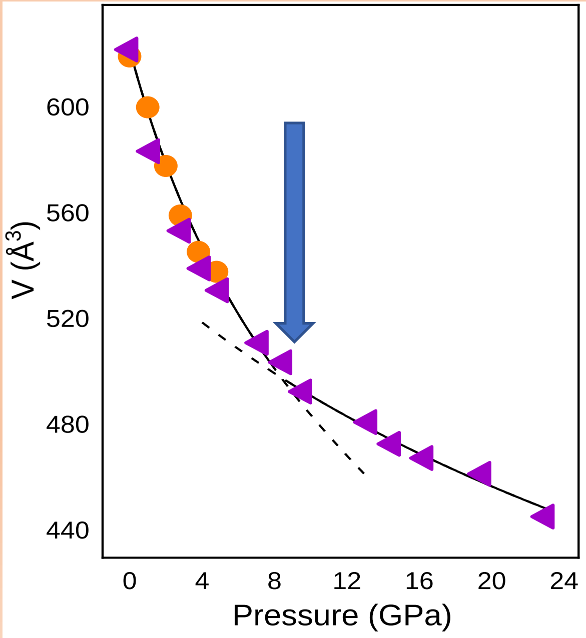
X-ray diffraction of $CrBr_3$
The baric dependences of the unit cell parameters

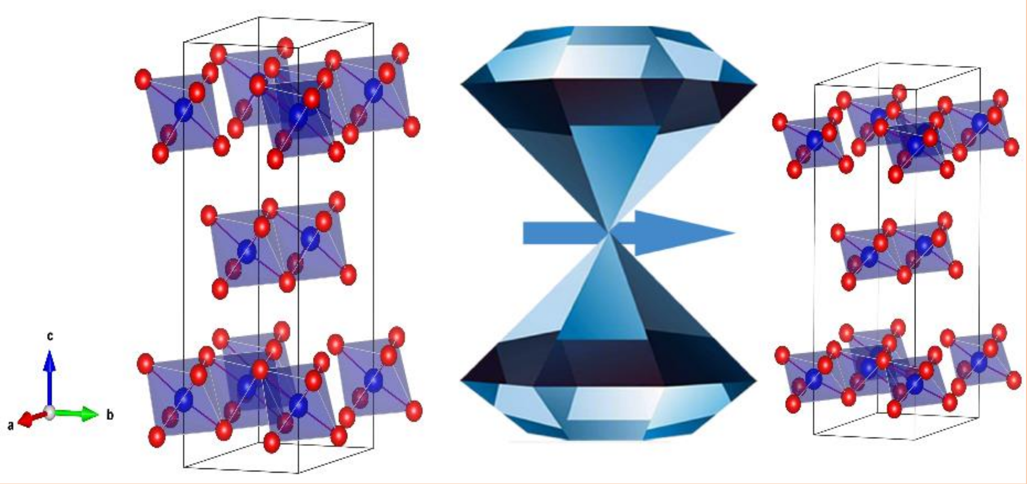




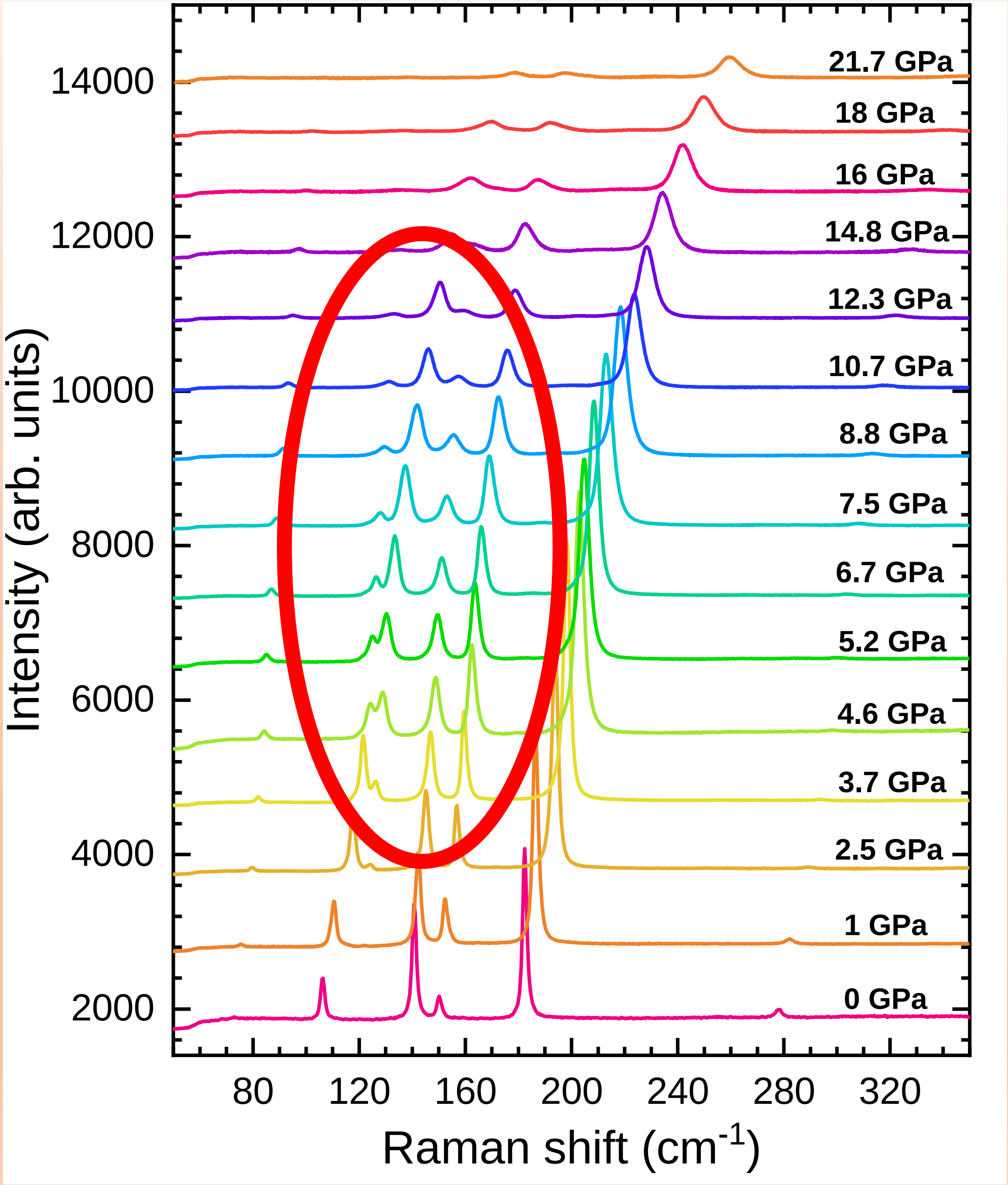


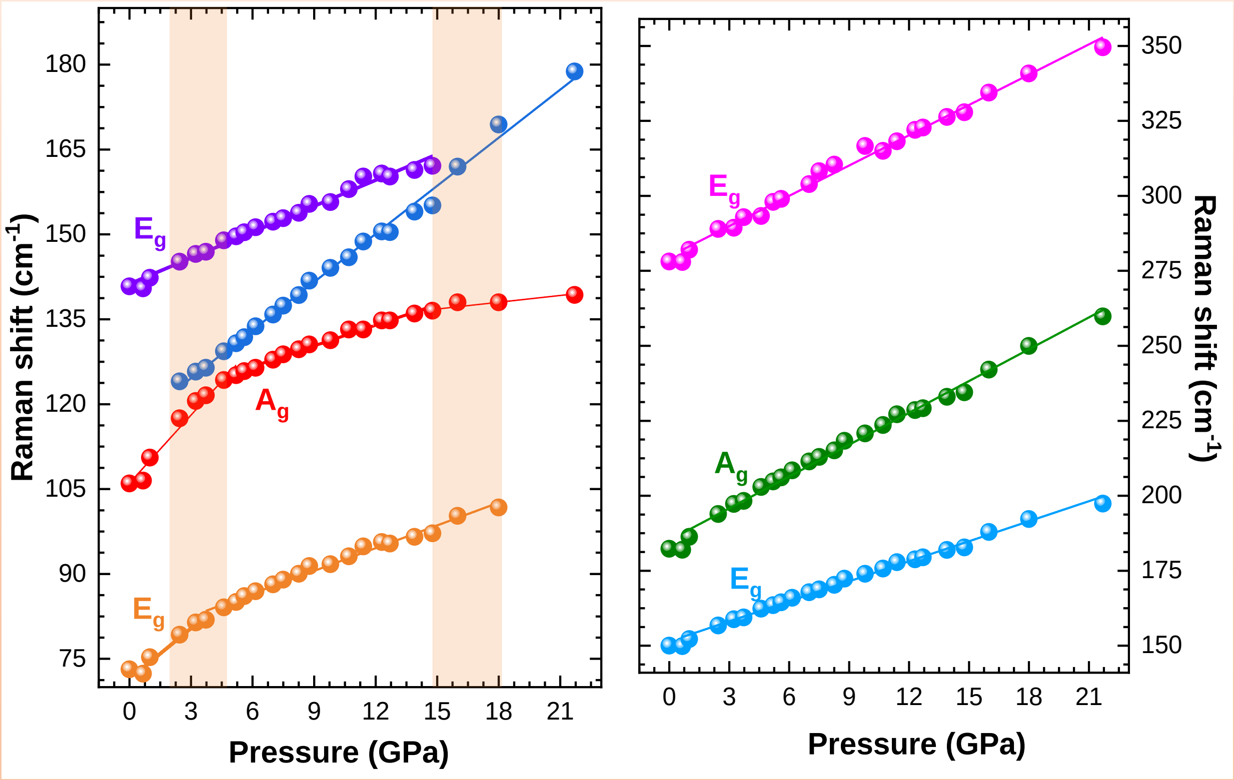
B_0 - bulk modulus
$CrBr_3$
LP phase: B_0=27 GPa
HP phase: B_0=98 GPa





Raman spectroscopy of $CrBr_3$ at high pressure





Transition associated with the motions of Br ions (polyhedral reorientation or new HP phase) or the change in electronic structure – ???

Conclusions

- The negative volume thermal expansion was observed below the Curie temperature in $CrBr_3$, as well as obvious anomalies in the interatomic distances, Raman shifts and corresponding full-width at half-maximum (FWHM) dependences, which is due to a complex interplay between spin and lattice degree of freedom. The same effect have been revealed also at high pressure (up to 2.8 GPa).

- Our results demonstrate that the pressure induced isostructural phase transition evolves gradually in vdW ferromagnet $CrBr_3$ over pressure range **2.5 - 7 GPa**. This transition emerges in Raman spectra around ***P*** **~ 2.5 GPa** by appearance of extra Raman mode and manifests finally by anomalies in pressure behavior of lattice parameters, unit cell volume, and A_g^1 and E_g^1 vibrational mode frequencies at ***P*** **~ 6-7 GPa**, when a volume of the pressure-induced phase becomes sufficiently dominant. The Curie temperature of $CrBr_3$ is reduced rapidly, implying instability of the initial FM order. A full suppression of the FM state and a magnetic transition to either AFM state or into a magnetically disordered one is expected at ***P*** **~ 8.4 GPa**. Additional anomalies in pressure behavior of Raman mode frequencies, detected at ***P*** **~ 15 GPa**, point to another phase transformation, presumably associated with the metallization process.

Thank you for your attention!