Pressure-induced phase transitions in vdW magnets

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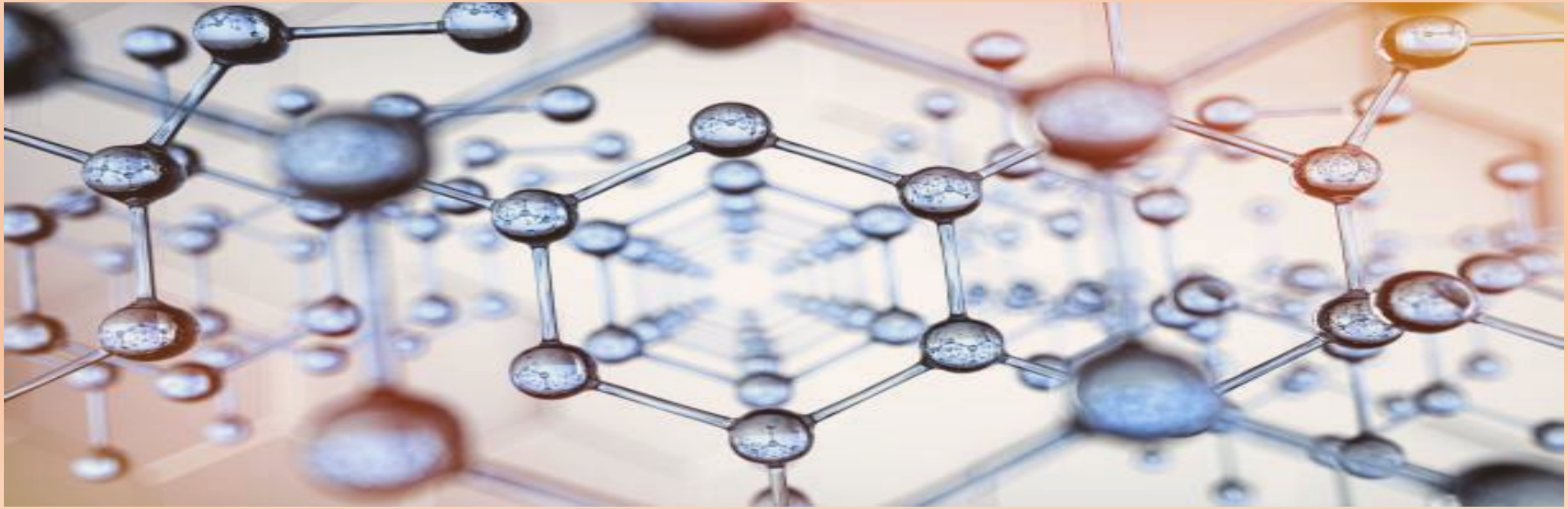
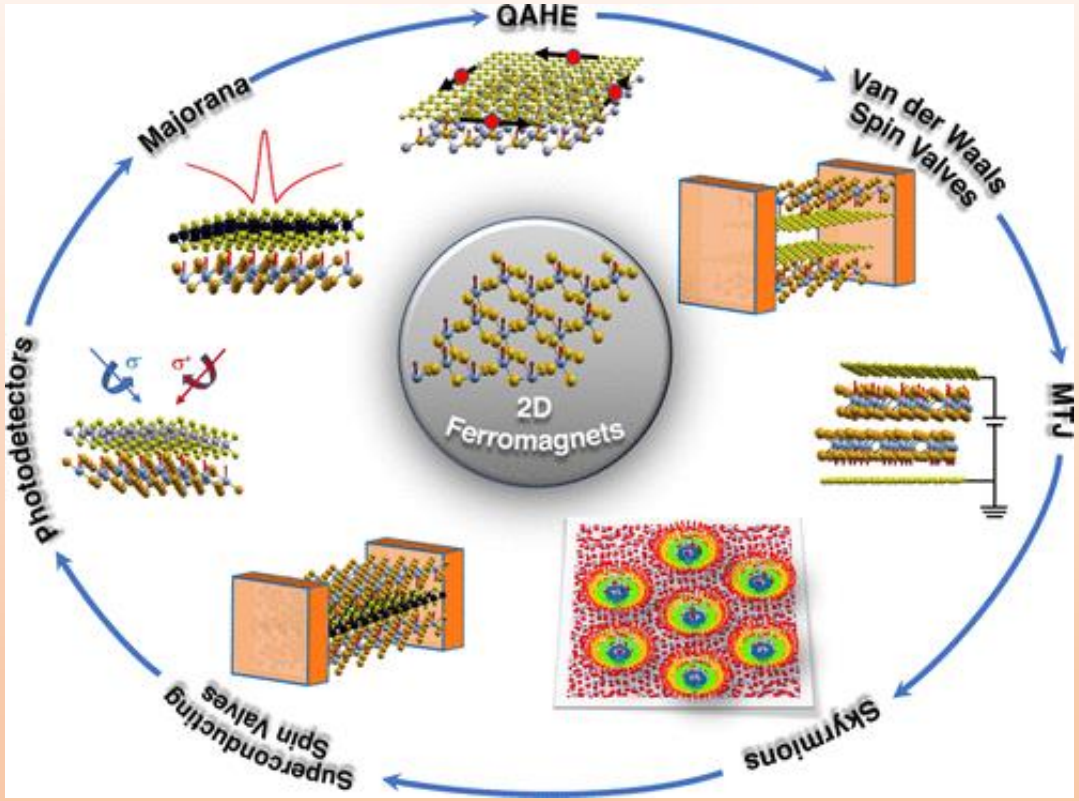
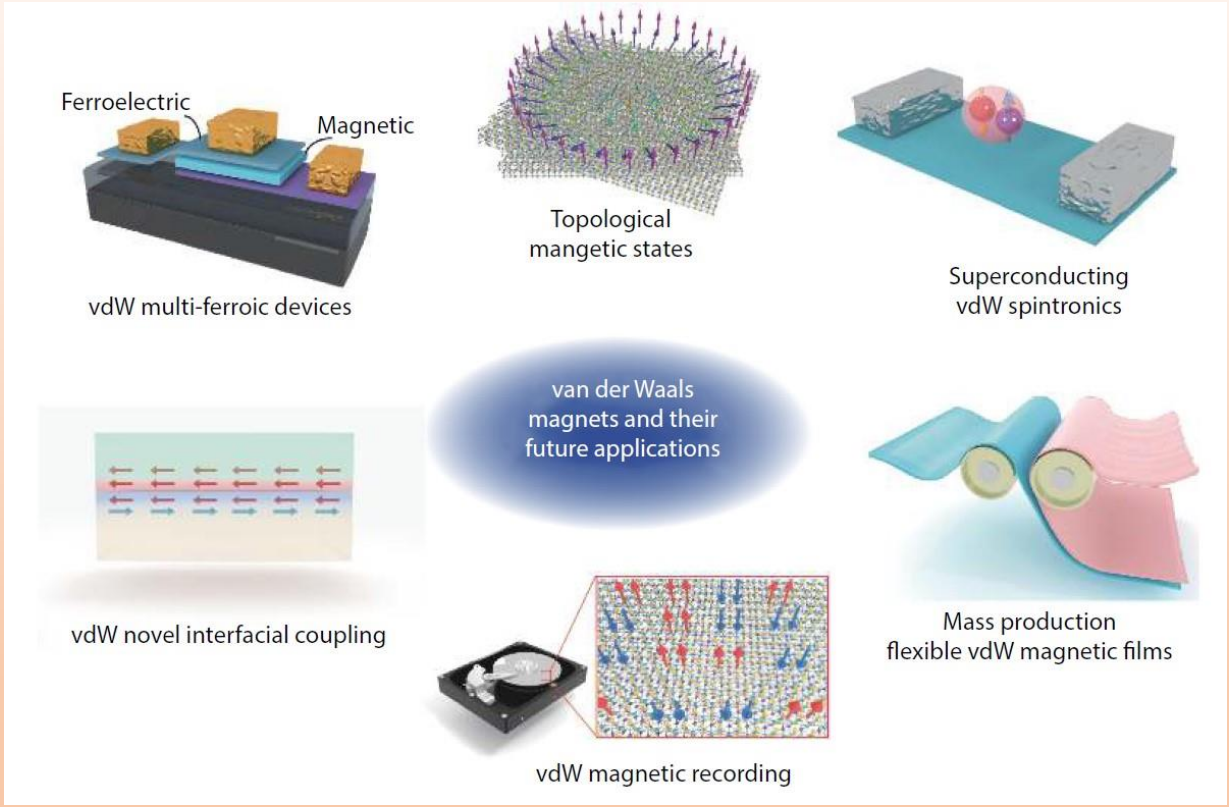


Introduction

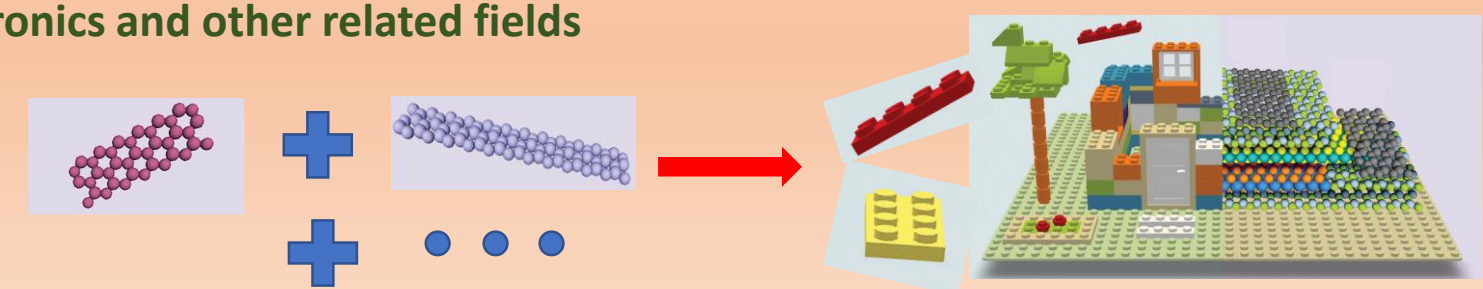


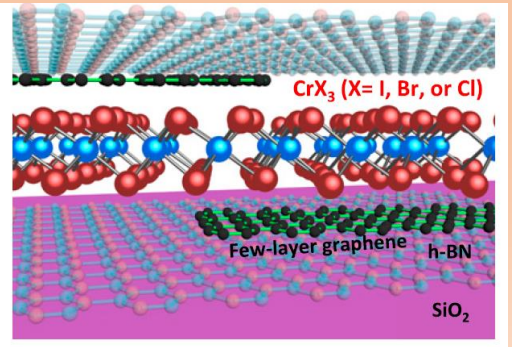
Applications of 2D ferromagnets in van der Waals heterostructures and twisted lattices



! 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.

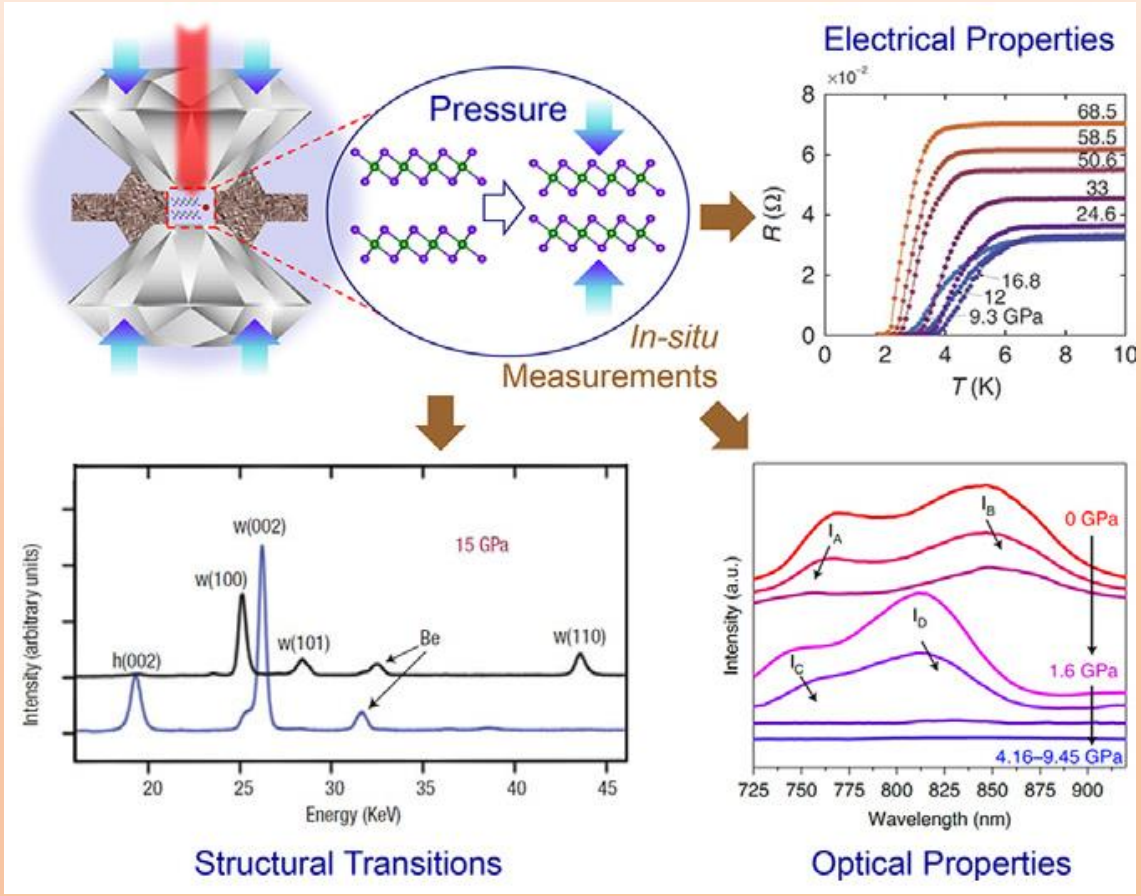
Future – the search and creation of various heterostructures with potential use in spintronics and other related fields



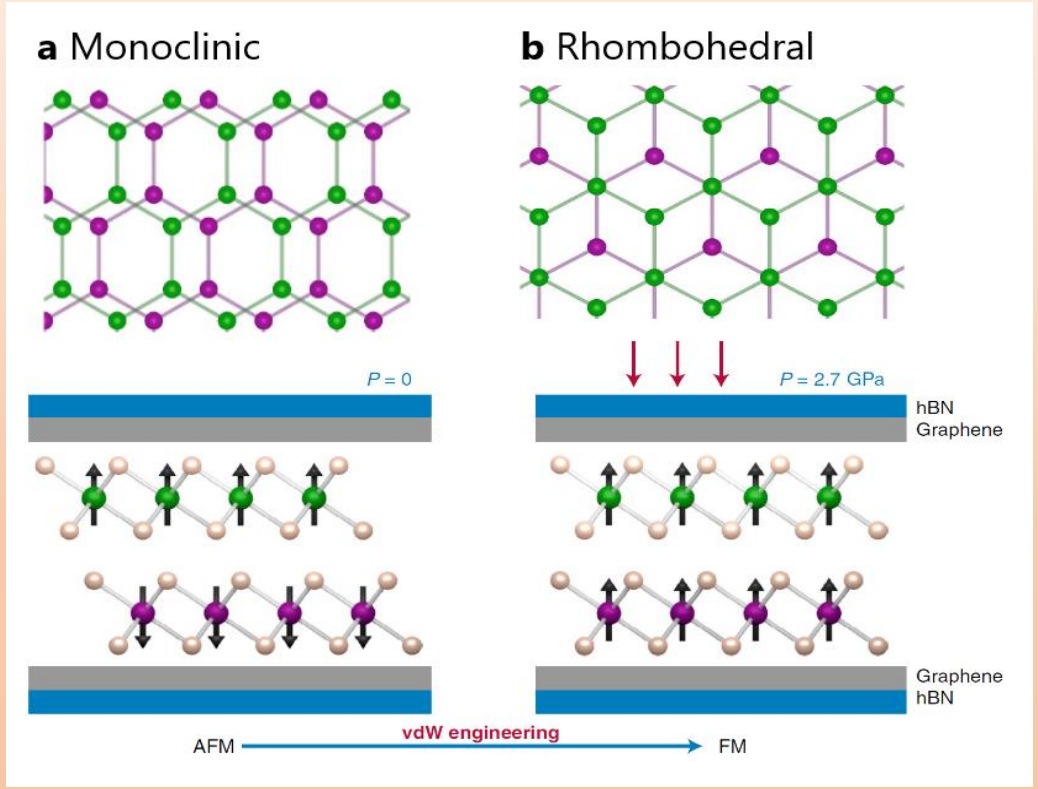


Introduction

The effect of high pressure on the electrical, optical and structural properties of van der Waals compounds



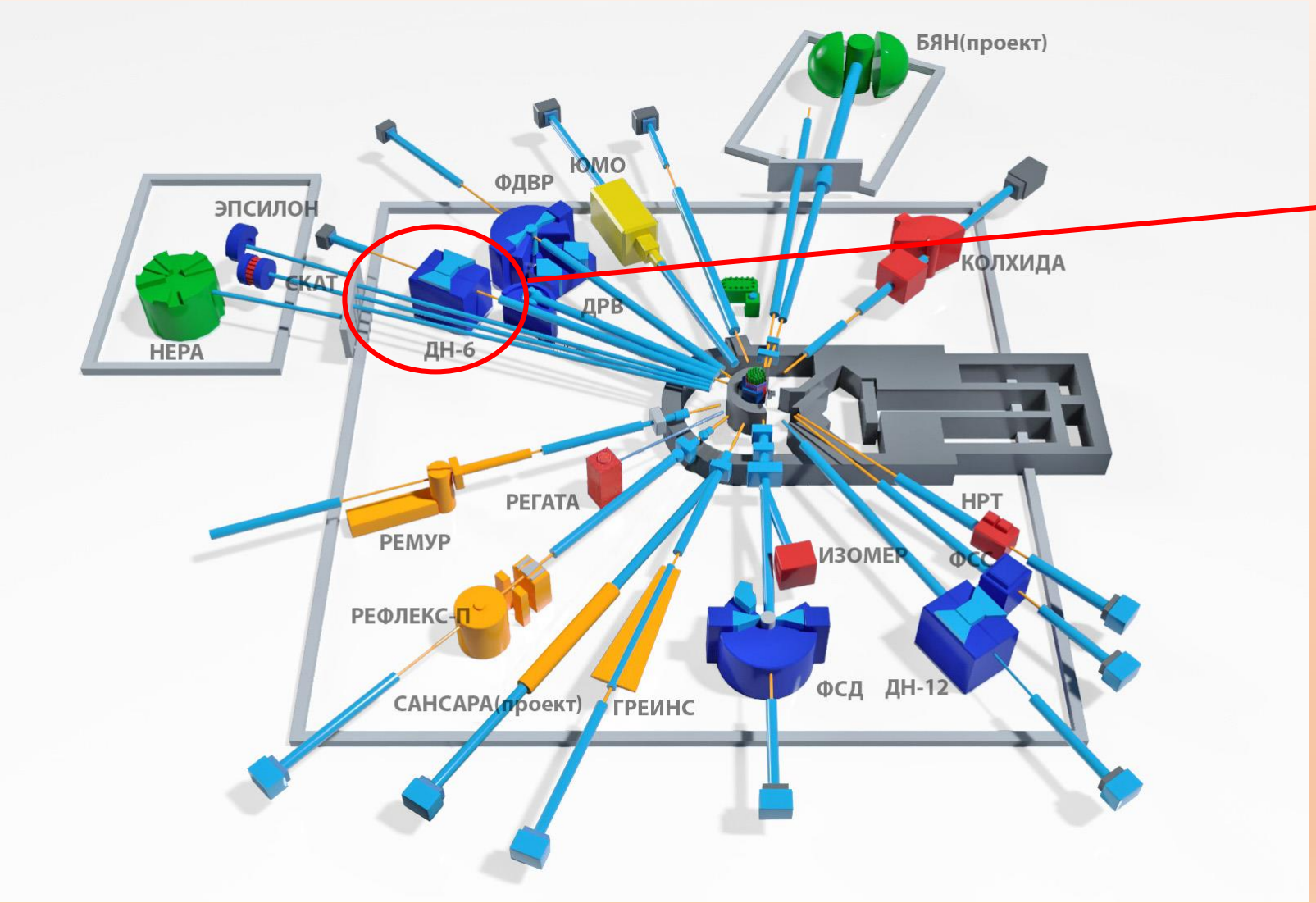
VdW CrI_3

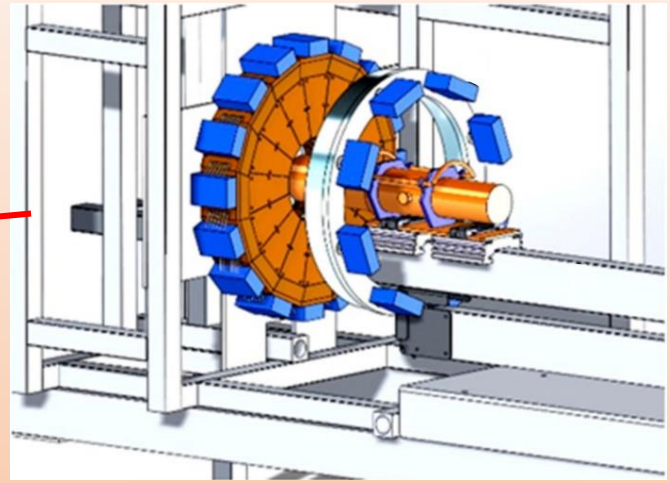


Pressure-induced changes in the layer stacking order is found to result in new magnetic ground states in two-dimensional insulating CrI_3.

!!! 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

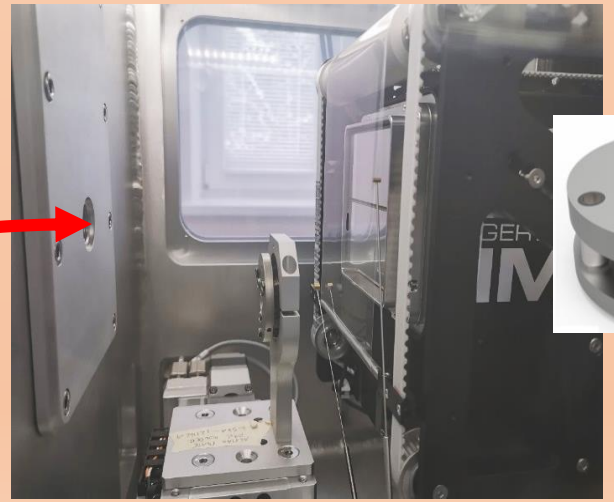
Experimental methods : X-ray и Raman

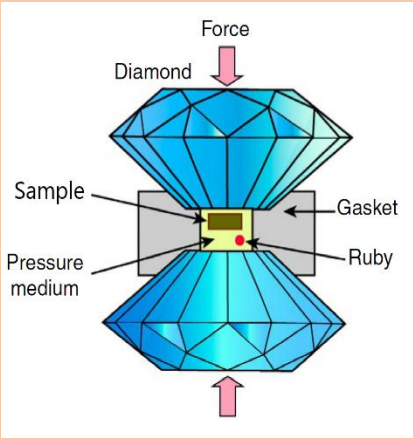
P = 1 GPa ~ 10 000 atm.

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

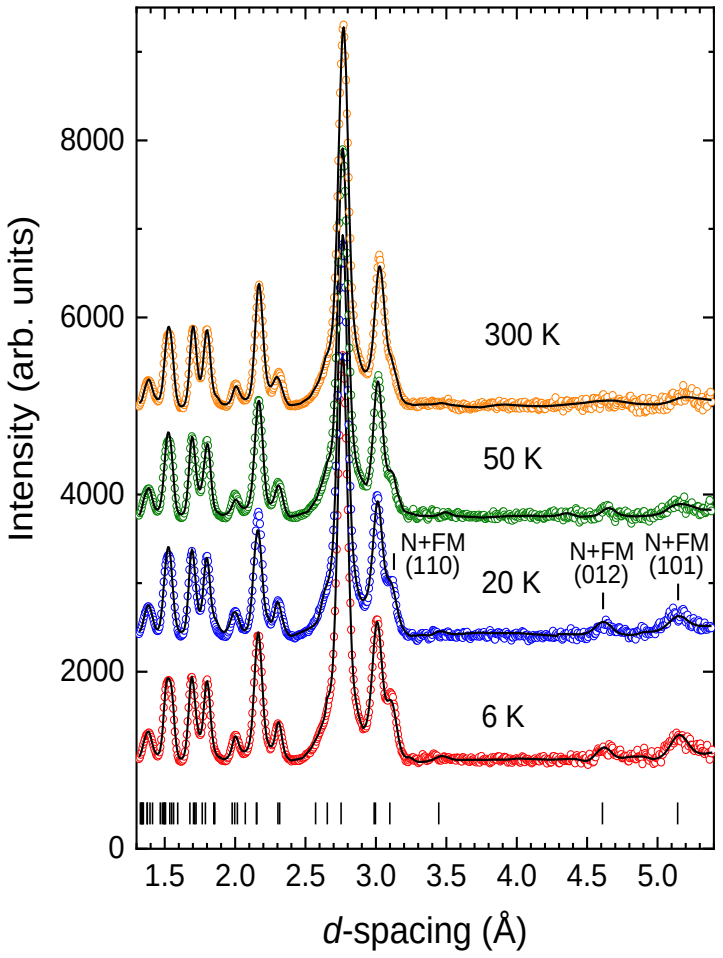
Cu radiation
(λ = 1.54184 Å)
Mo radiation
(λ = 0.71078 Å)

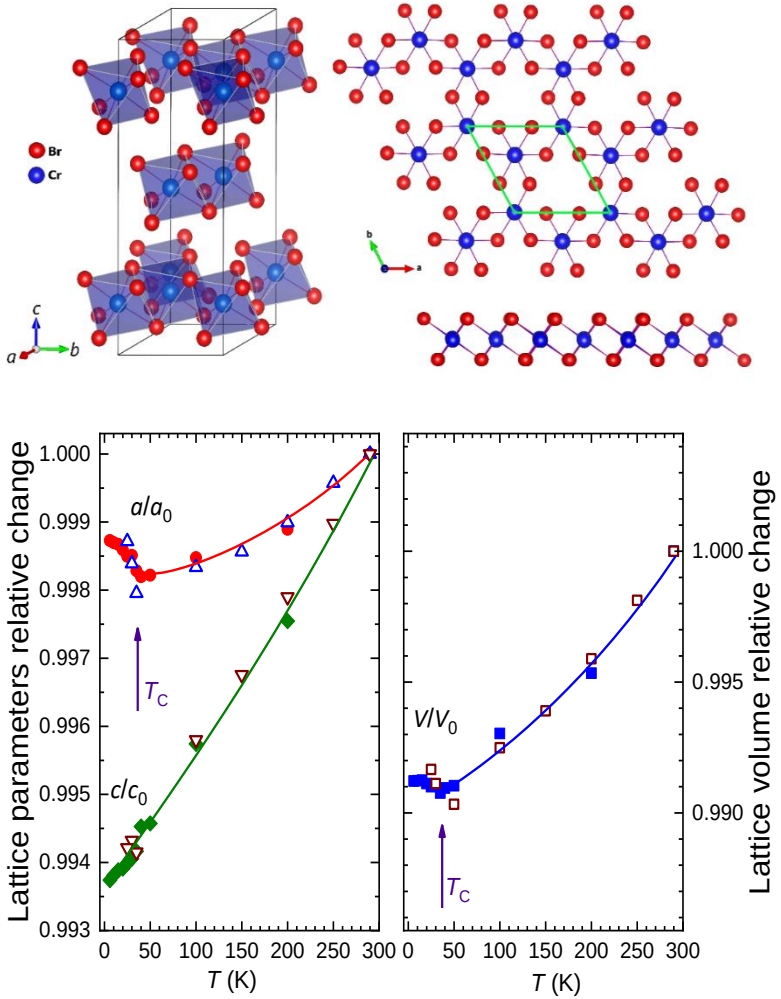


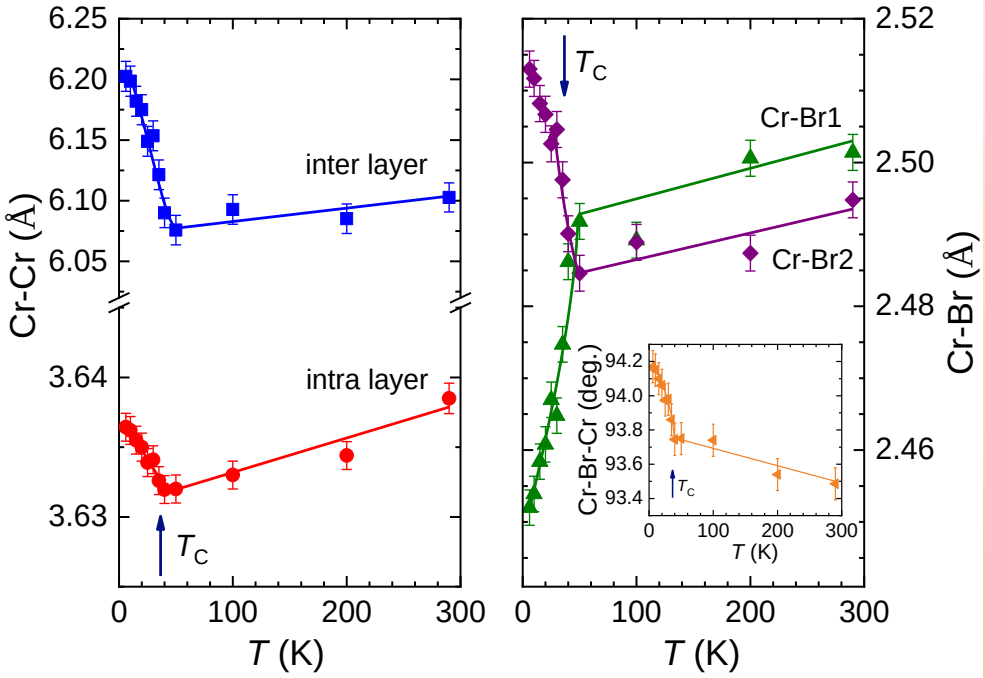


High-pressure cell with diamond anvils

Neutron diffraction at low temperature







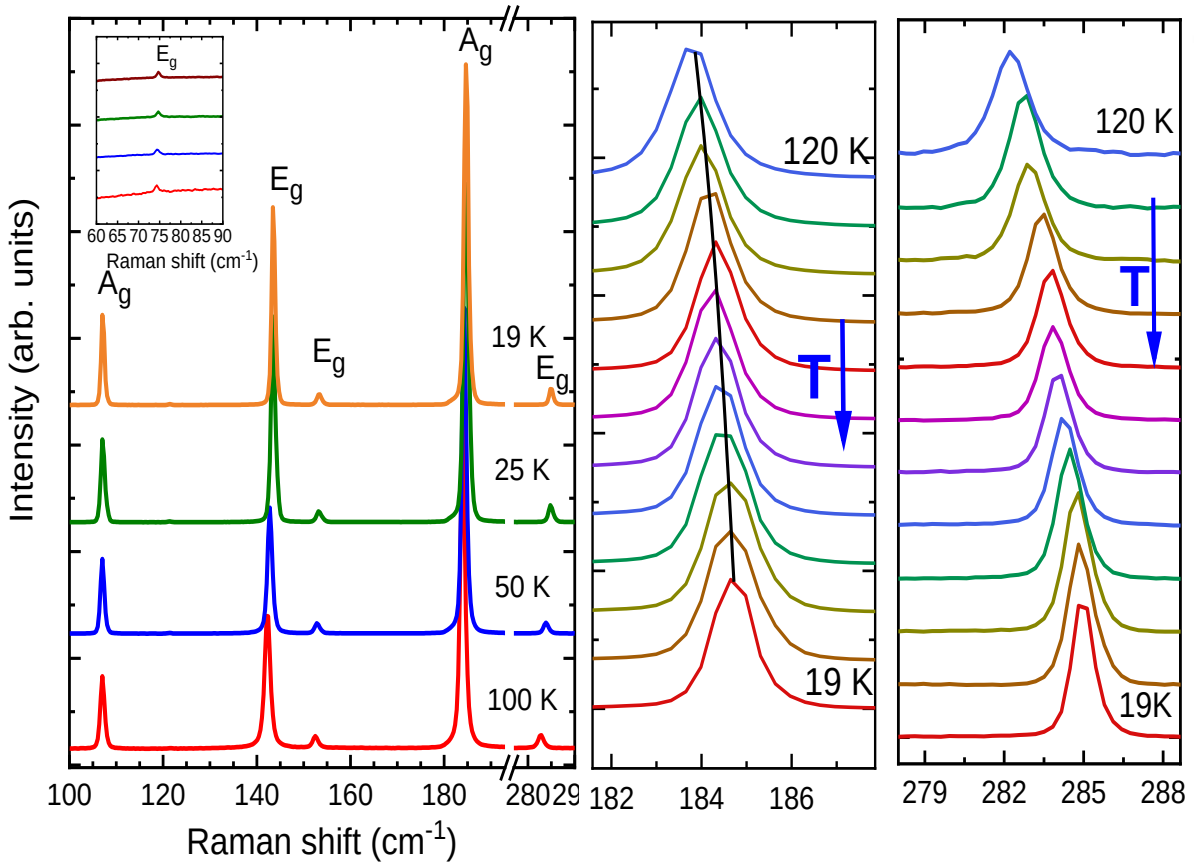
a) The thermal expansion of $CrBr_3$ lattice is strongly anisotropic with the pronounced variation of the c lattice parameter.

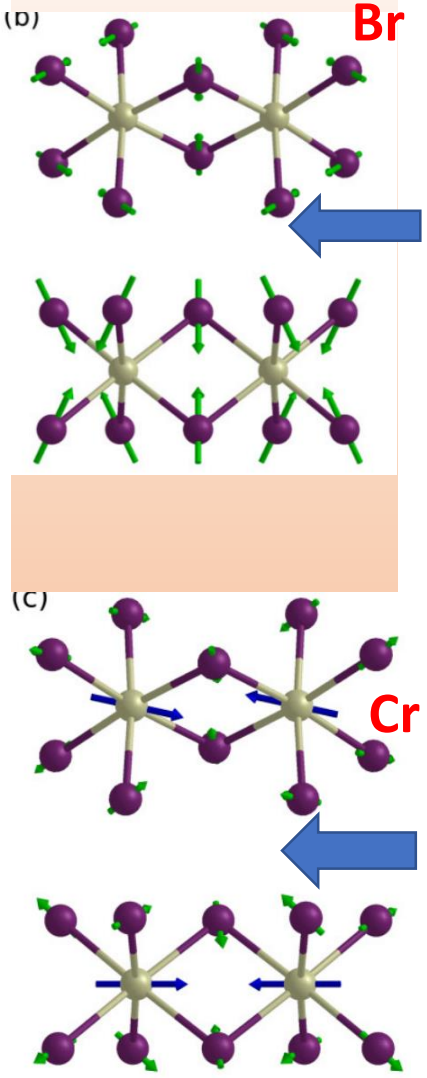
b) The interatomic intralayer and interlayer Cr–Cr distances decrease slightly on cooling in the temperature range above T_C and they also demonstrate opposite increasing trend for $T < T_C$

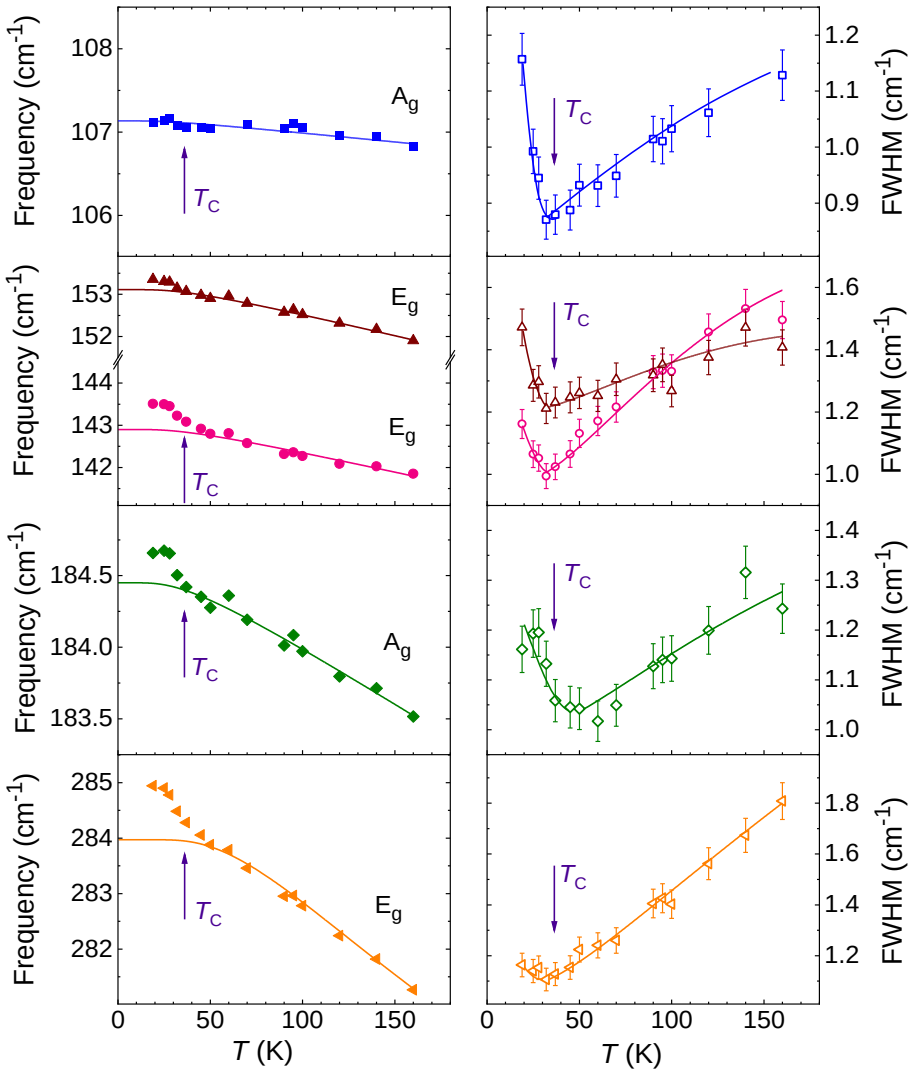
The temperature dependences of the lattice parameters and volume obtained from neutron and X-ray diffraction measurements

Kozlenko, D.P., Lis, O.N., Kichanov, S.E. et al. npj Quantum Mater. 6, 19 (2021)

Raman spectroscopy at low temperature





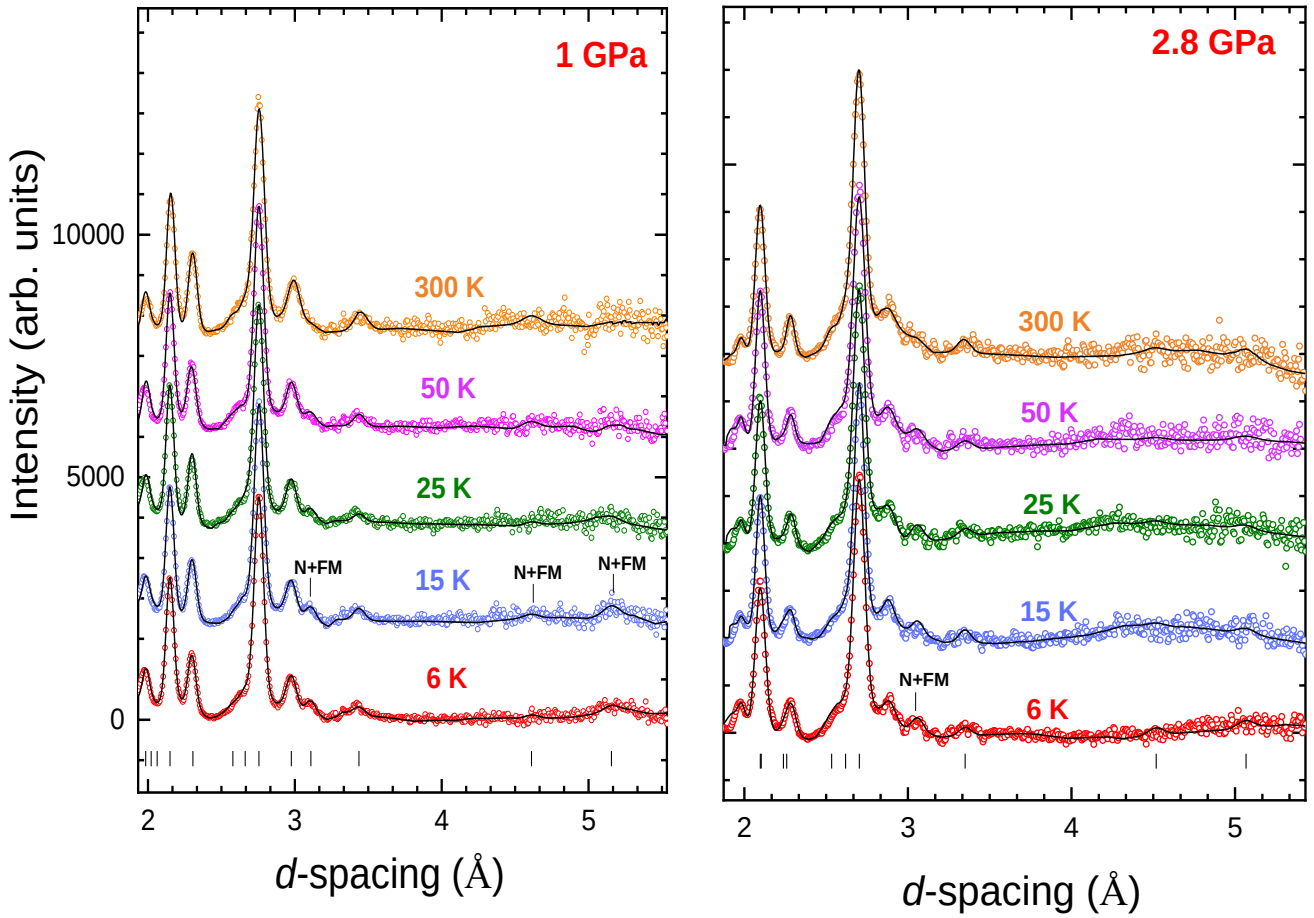


The FWHM of all the observed phonon modes reach minimum in the vicinity of T_C and demonstrate anomalous reversal broadening in the $T < T_C$ range. Both effects reveal a presence of the strong spin–phonon coupling in $CrBr_3$. The spin–phonon coupling is associated with the modification of the magnetic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

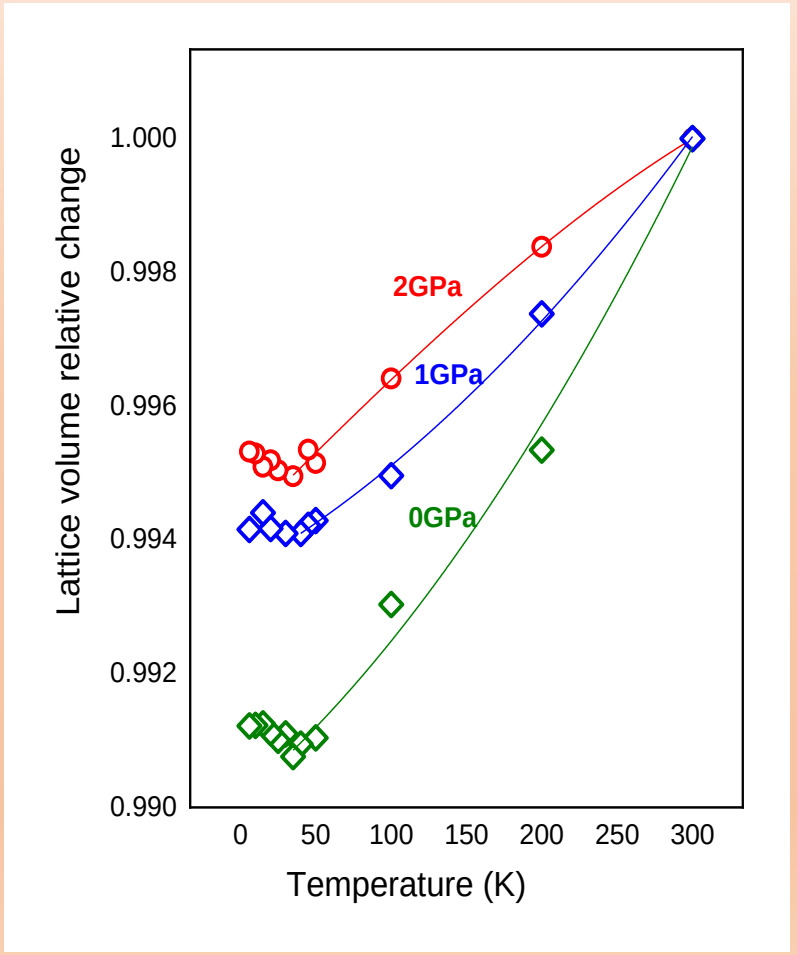
Neutron diffraction at high pressure and low temperature

P = 1 GPa ~ 10 000 atm.

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

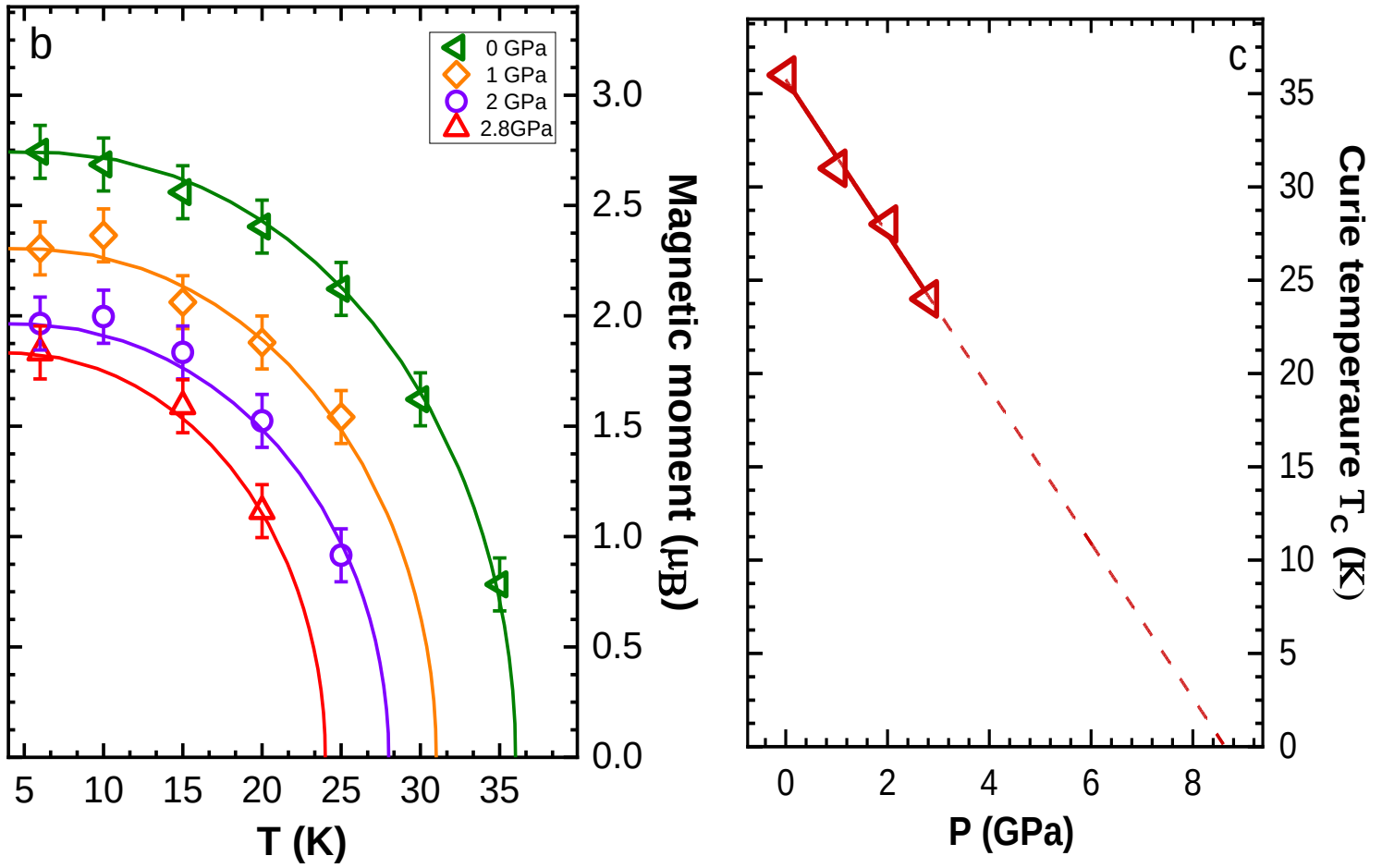


The negative volume thermal expansion in $CrBr_3$ persists even with the application of high pressure



O.N. Lis, D.P. Kozlenko, S.E. Kichanov, E.V. Lukin, et al. Materials – 2023. – 16(1). – 454

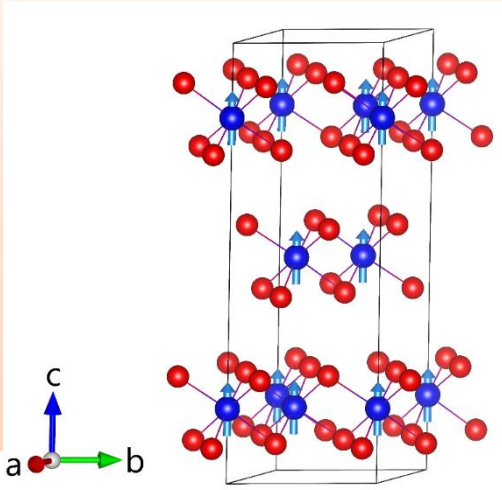
Neutron diffraction at high pressure and low temperature

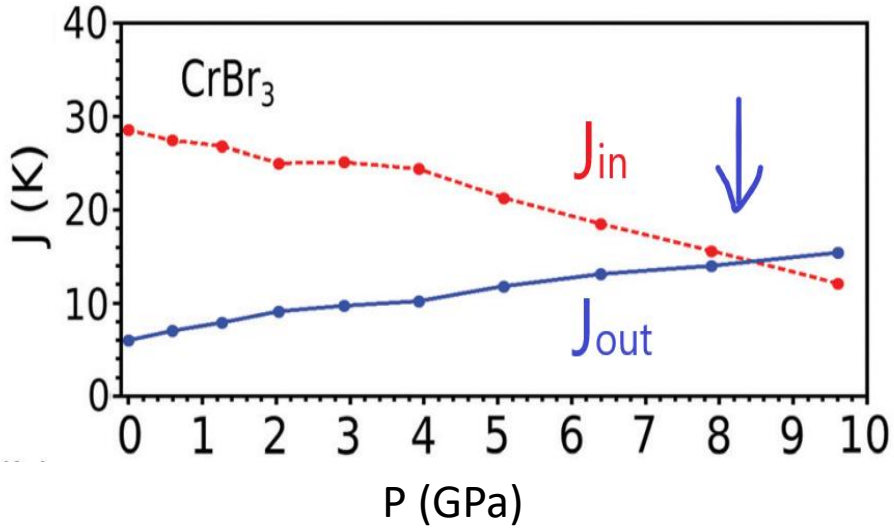


The obtained temperature dependences of the Cr magnetic moment of ferromagnetic FM phase at different pressures

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

P_{Tr} ~ 8.4 GPa

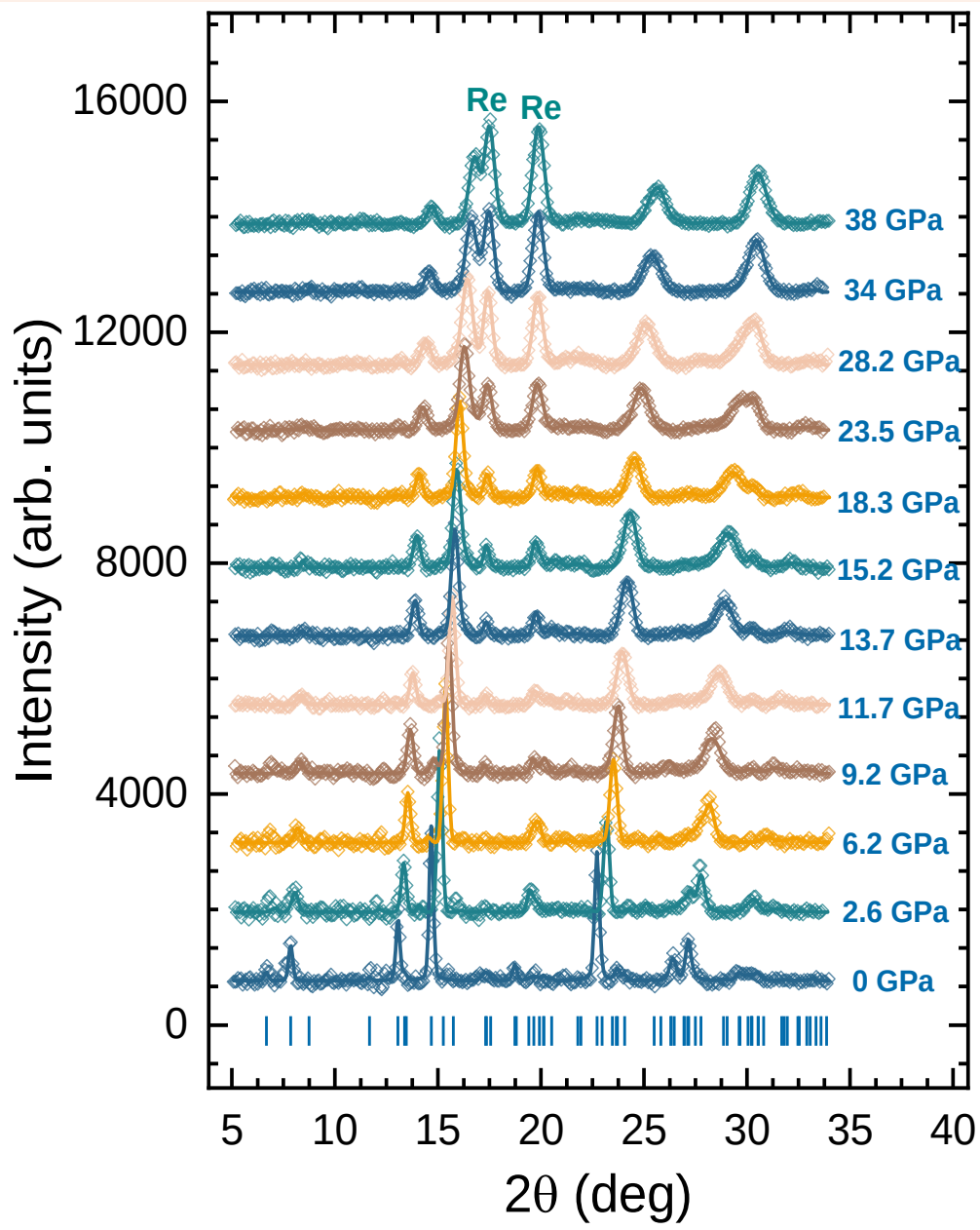


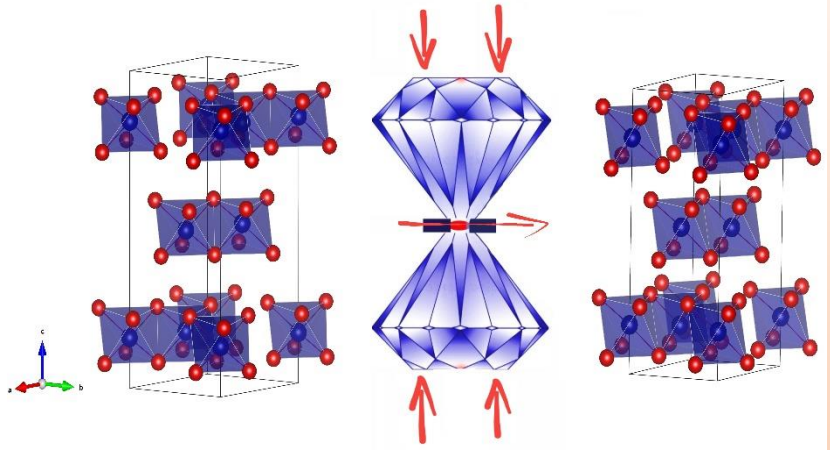


Values of the exchange constants for $CrBr_3$. Jout in blue, Jin in red. The out-of-plane coupling becomes larger as pressure is applied

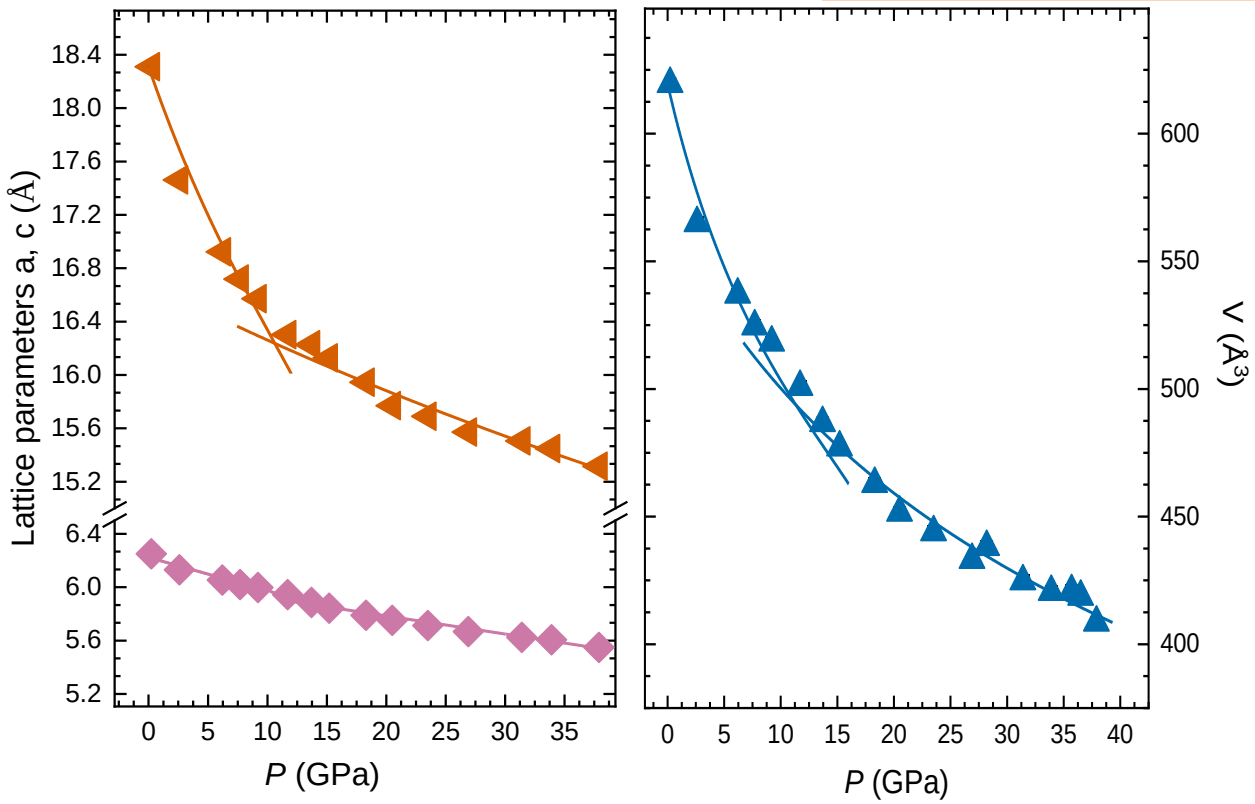
A. O. Fumega, et.al. J. Mater. Chem. C, 2020,8, 13582-13589

XRD patterns measured at selected pressures and the baric dependences of the unit cell parameters of $CrBr_3$



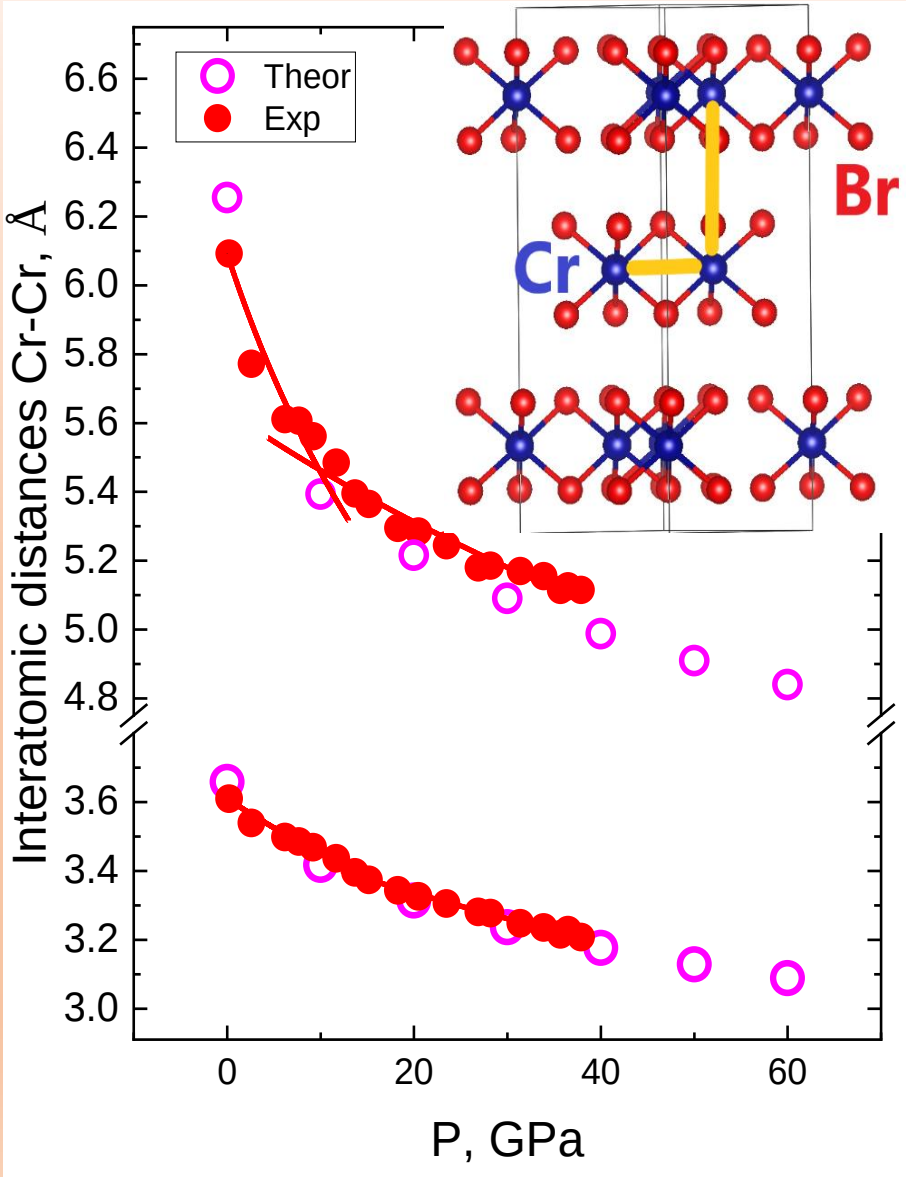


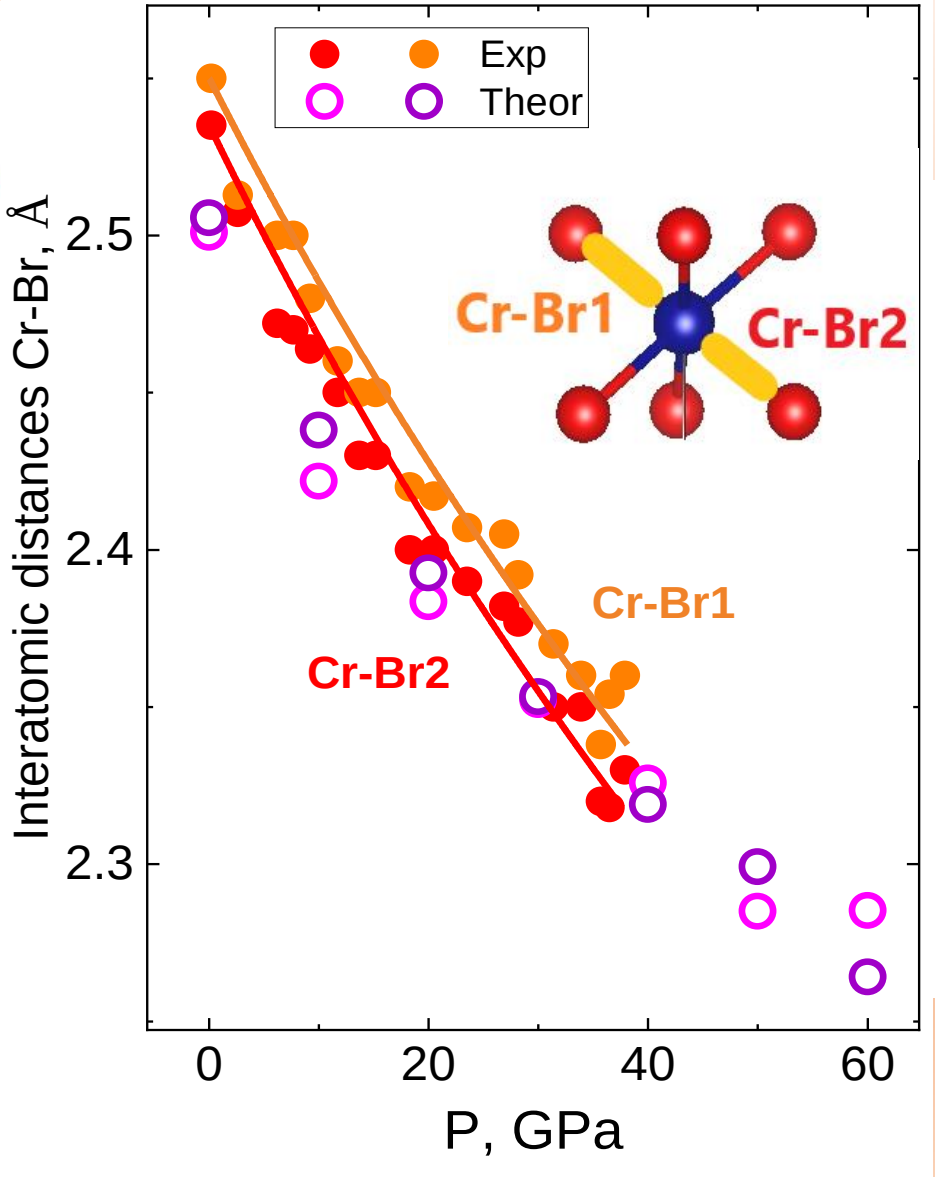
B_0 - bulk modulus
$CrBr_3$
LP phase: B_0=31 GPa
HP phase: B_0=62 GPa

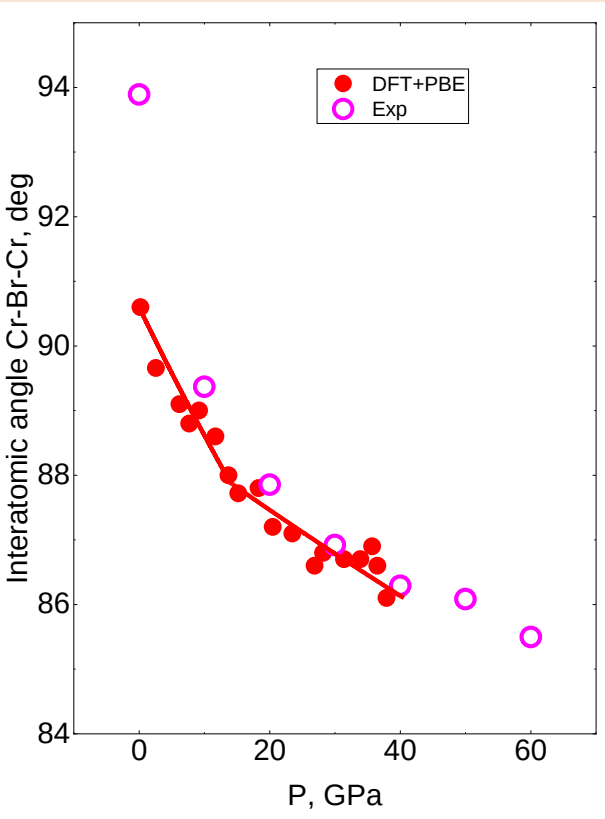


XRD of $CrBr_3$

The baric dependences of the interatomic distances and angles

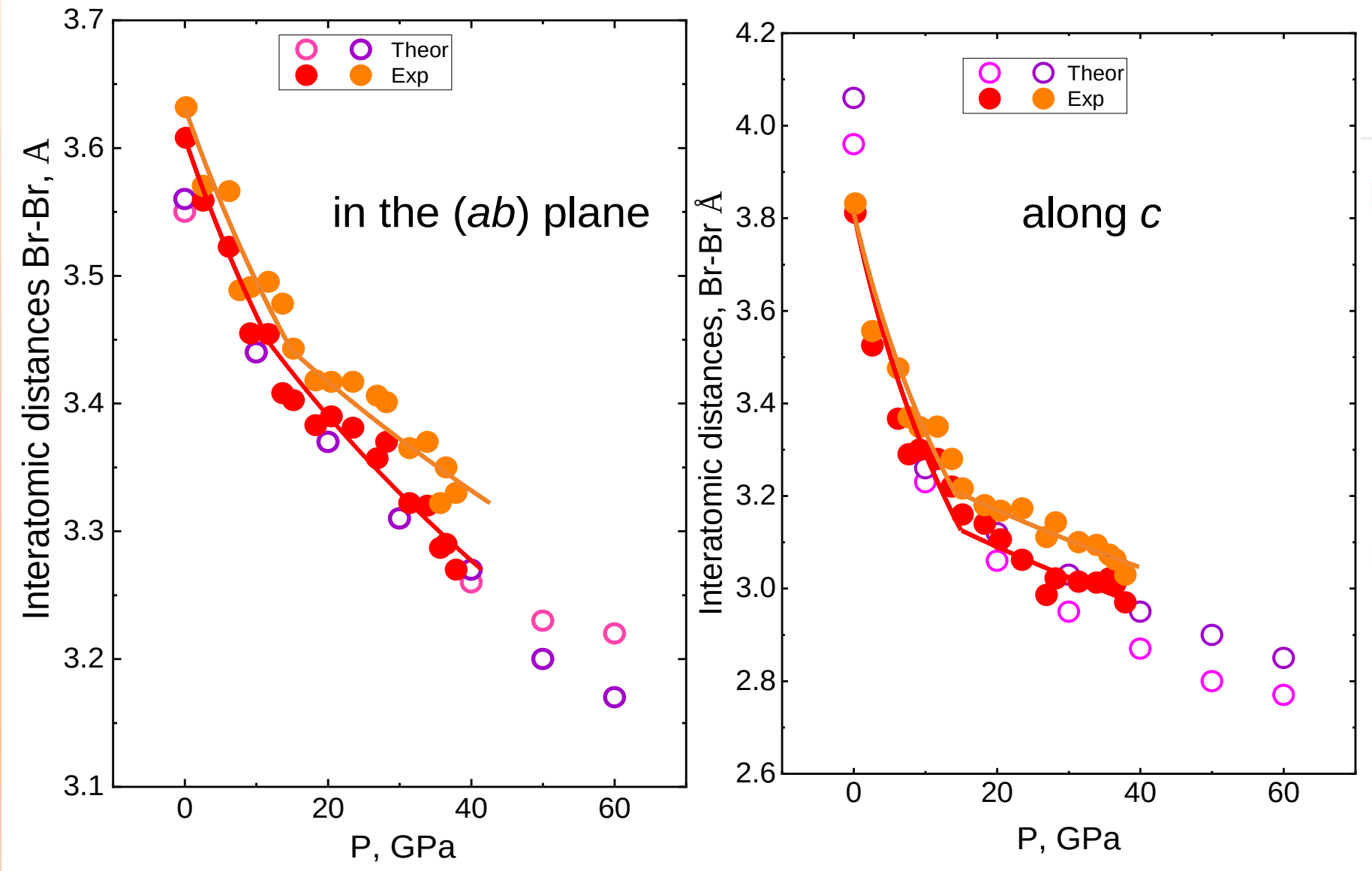


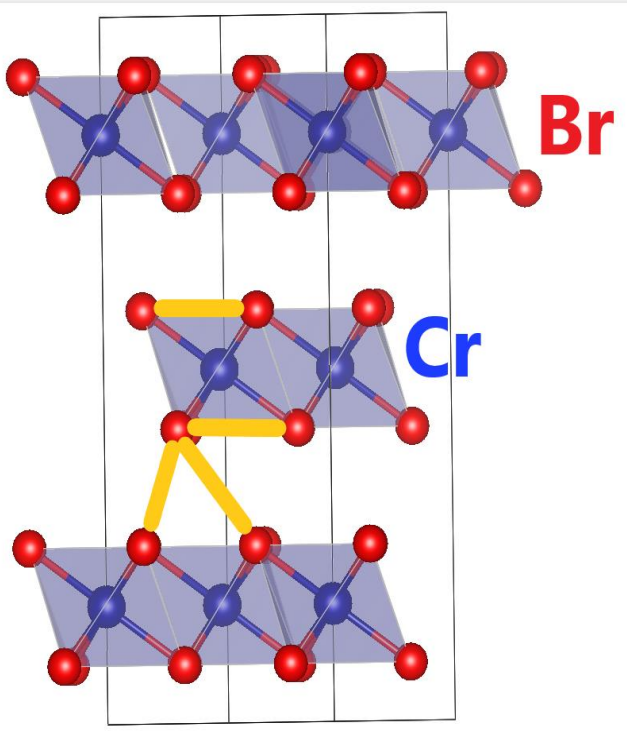




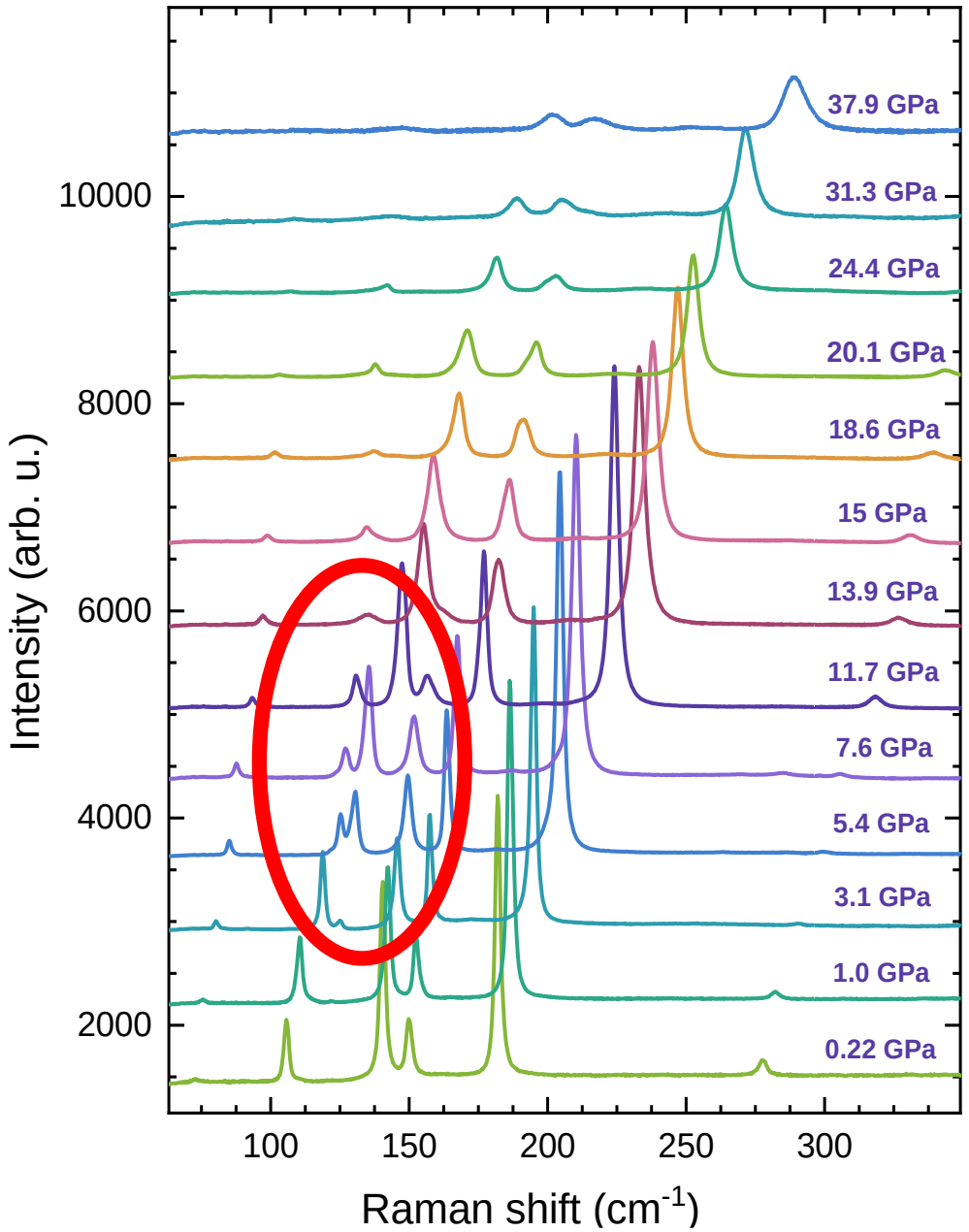
XRD of $CrBr_3$

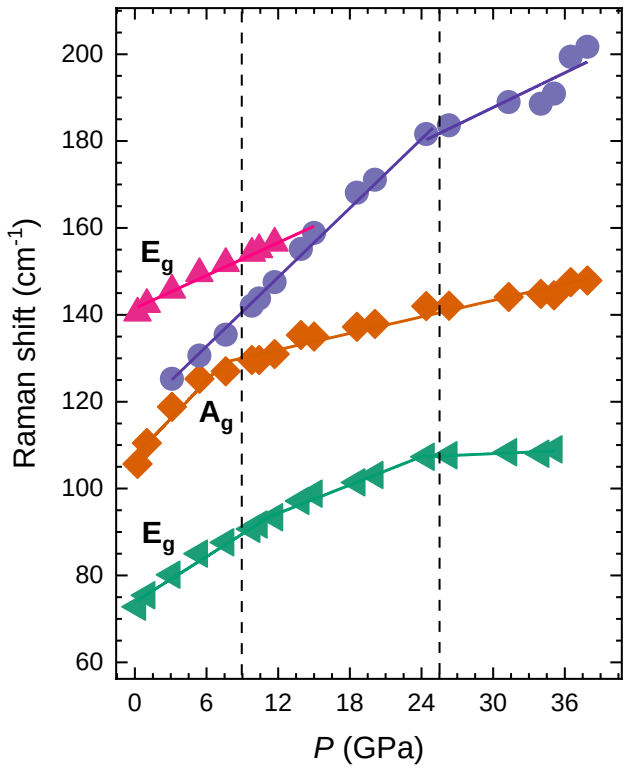
The baric dependences of the interatomic distances and angles

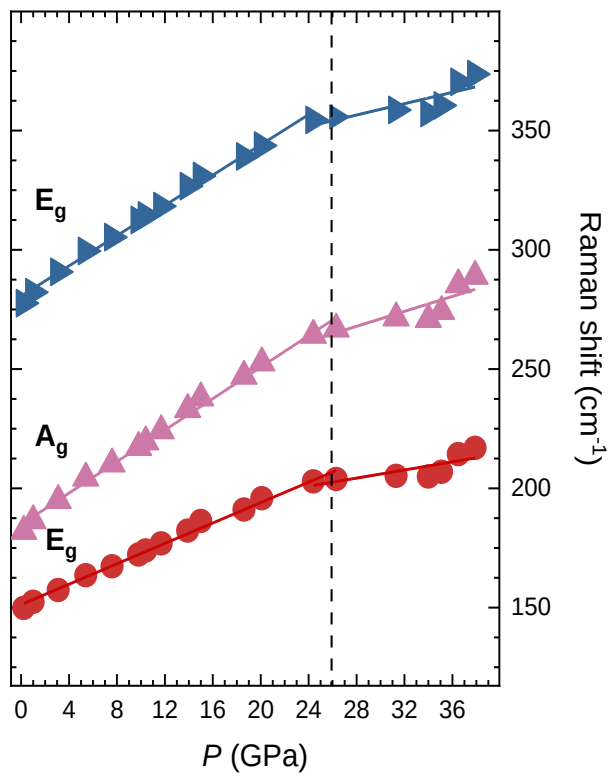




Raman spectroscopy of $CrBr_3$ at high pressure

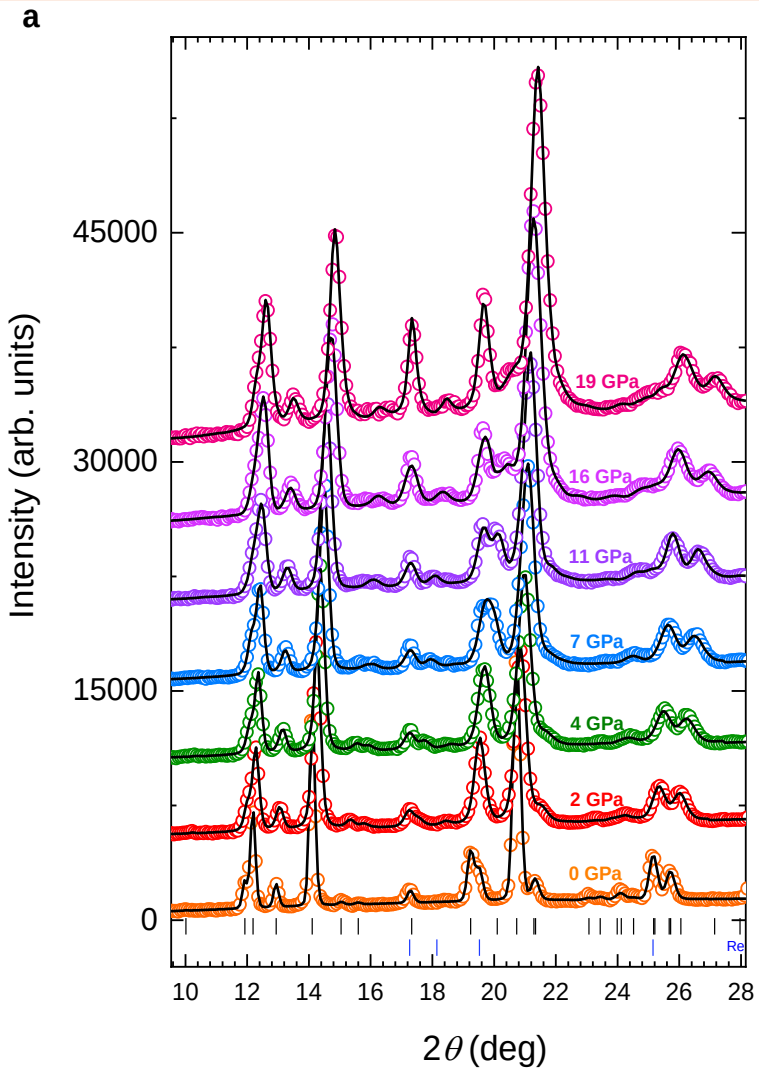


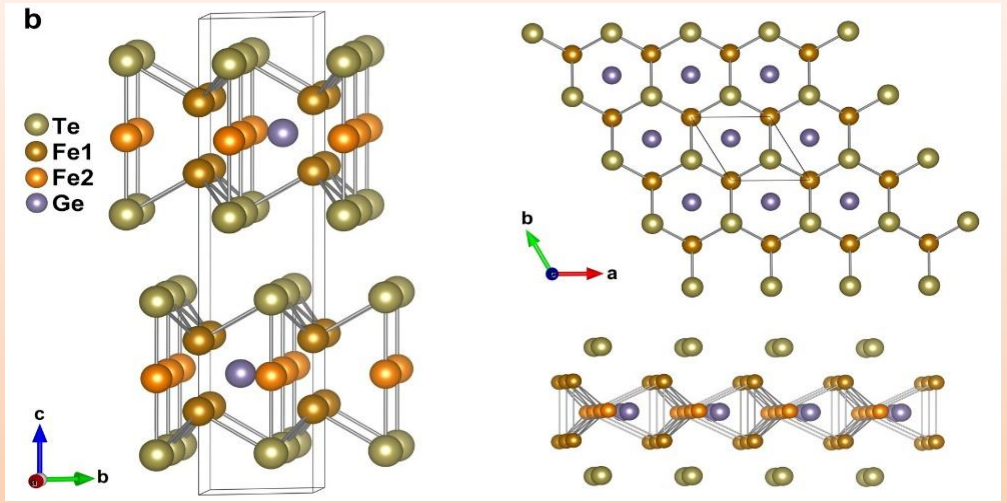




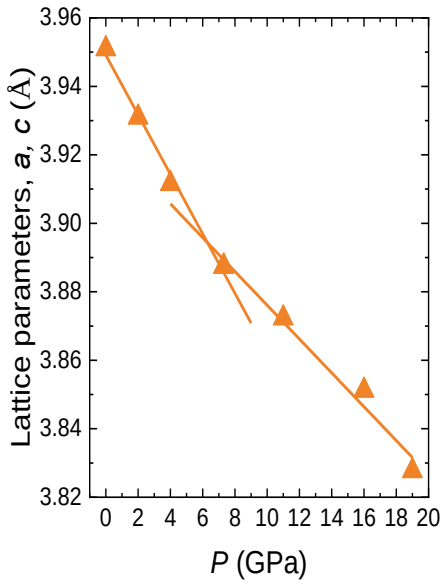
1. Isostructural phase transition in pressure range 2.5 - 10 GPa
2. Transition to metallic state at 26 GPa

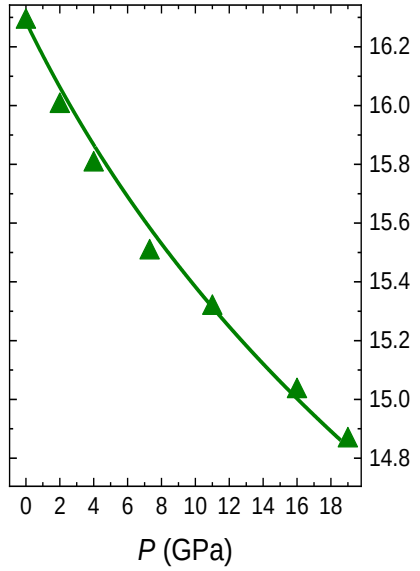
X-ray diffraction of Fe_3GeTe_2
The baric dependences of the unit cell parameters

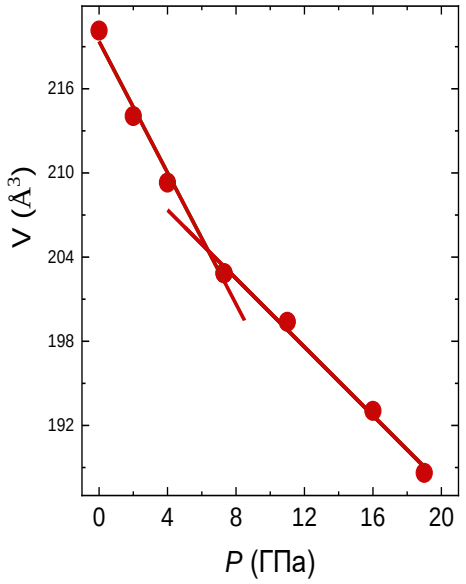




Sp. gr. $P6_3/mmc$	
T = 300 K, P = 0 GPa	
a, Å	3,950(1)
c, Å	16,285(2)
V, Å^3	220,159(3)
R_p,% R_{wp},%	6,51 6,75
B_0 at $P < 7$ GPa B_0 at $P > 7$ GPa	71,6 GPa 93,9 GPa





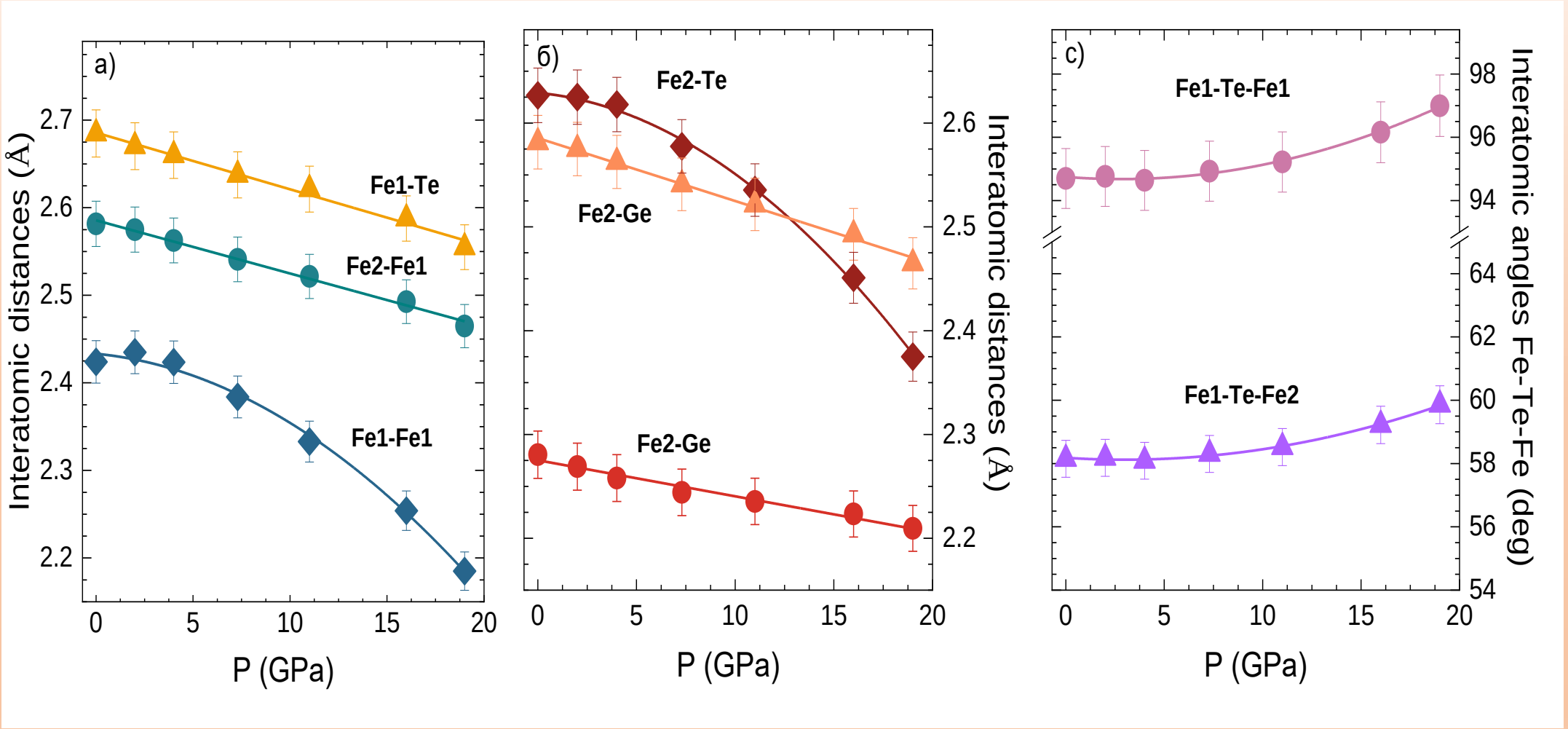


An isostructural phase transition is observed in Fe_3GeTe_2 at pressure P ~7 GPa.

N.-T. Dang, D. P. Kozlenko, O. N. Lis, S. E. Kichanov, Y. V. Lukin, N. O. Golosova, B. N. Savenko, D.-L. Duong, T.-L. Phan, T.-A. Tran, M.-H. Phan, *Adv. Sci.* 2023, 10, 2206842.

X-ray diffraction of Fe_3GeTe_2

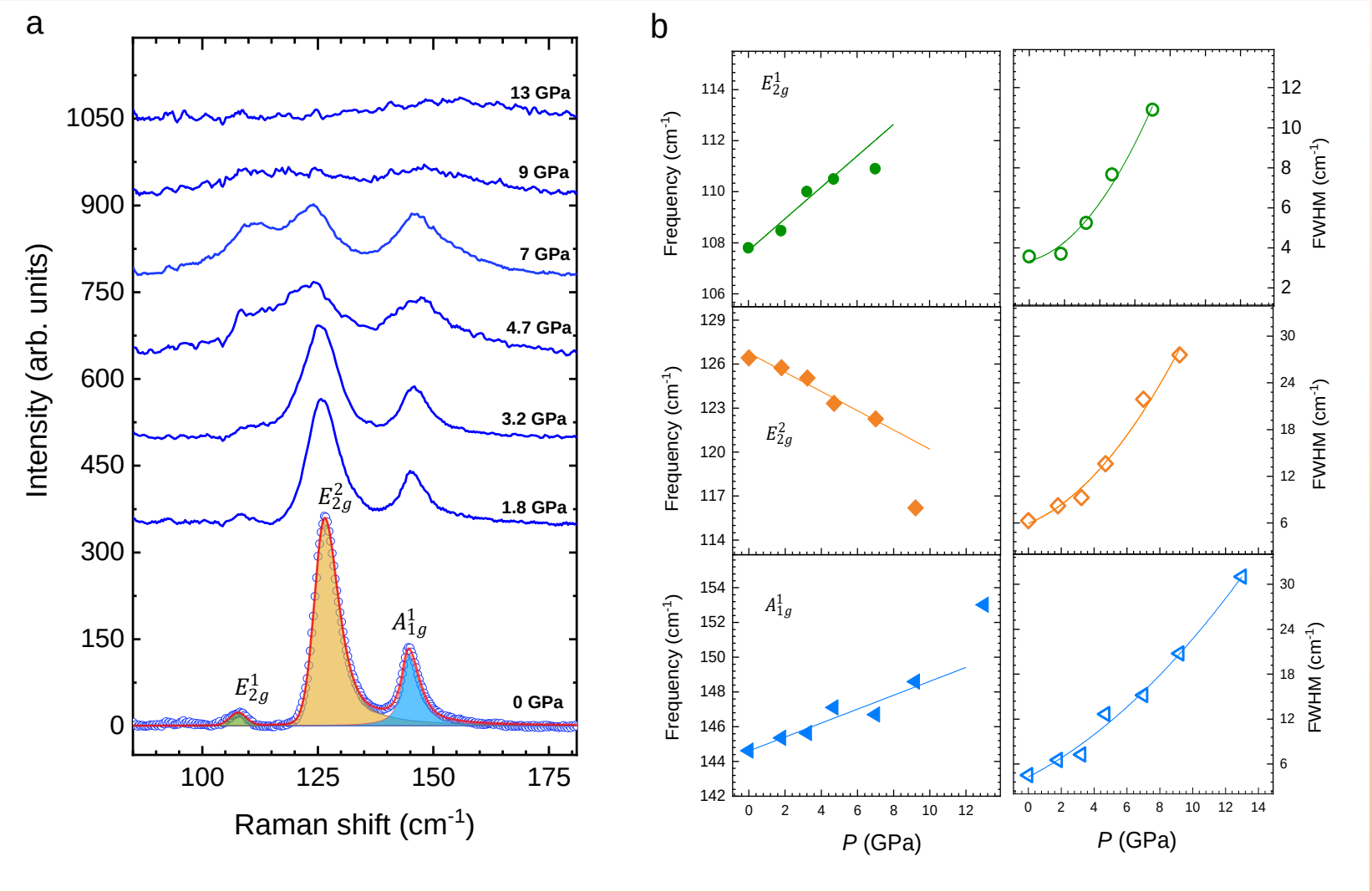
The baric dependences of the interatomic distances and angles

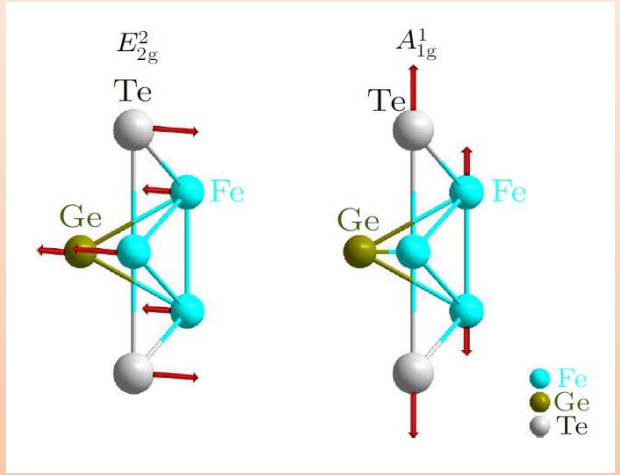


N.-T. Dang, D. P. Kozlenko, O. N. Lis, S. E. Kichanov, Y. V. Lukin, N. O. Golosova, B. N. Savenko, D.-L. Duong, T.-L. Phan, T.-A. Tran, M.-H. Phan, *Adv. Sci.* 2023, 10, 2206842.

Experimental results

Raman spectroscopy of Fe_3GeTe_2





Raman spectra obtained at different pressures at 15 K and the baric dependences of the frequencies of the vibrational modes and their FWHM. Abnormal behavior of frequencies and FWHM of Fe_3GeTe_2 vibrational modes in the vicinity of a structural transition associated with anomalous behavior of the Fe2-Te interatomic distance and Fe1-Ge-Fe1 angles(2).

N.-T. Dang, D. P. Kozlenko, O. N. Lis, S. E. Kichanov, Y. V. Lukin, N. O. Golosova, B. N. Savenko, D.-L. Duong, T.-L. Phan, T.-A. Tran, M.-H. Phan, *Adv. Sci.* 2023, 10, 2206842.

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 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 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* ~ 26 GPa**, point to another phase transformation, associated with the metallization process.
- An isostructural phase transition is observed in Fe_3GeTe_2 at ***P* ~ 7 GPa.** It manifests itself in the form of abnormal behavior of some parameters of the crystal structure, interatomic distances and angles, vibrational modes, and is associated with the competing nature of intraplane and interplane interactions in this compound.

Thank you for your attention!