

# Structural and vibrational properties of the $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}$ francisite at high-pressure

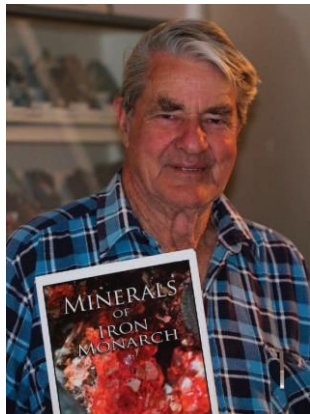
A.V. Rutkauskas<sup>1</sup>, B. Abdurakhimov<sup>2</sup>, G.S. Rimski<sup>2</sup>, D. P. Kozlenko<sup>1</sup>,  
S.E. Kichanov<sup>1</sup> and B.N. Savenko<sup>2</sup>

<sup>1</sup> *Joint Institute for Nuclear Research, Dubna, Russia*

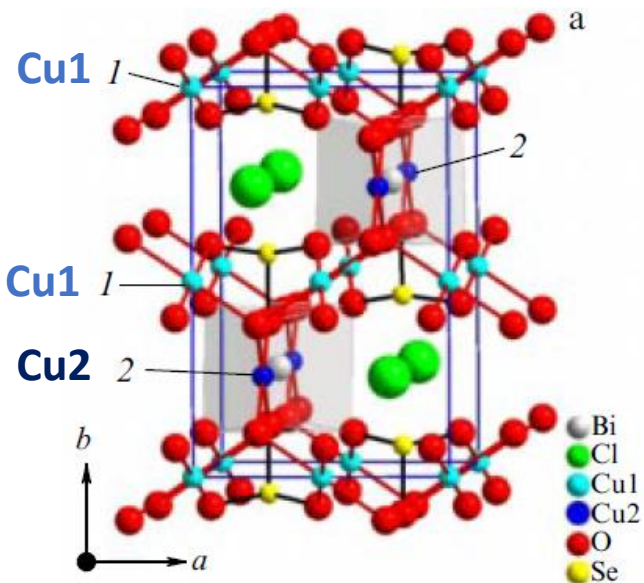
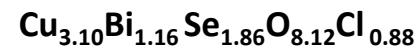
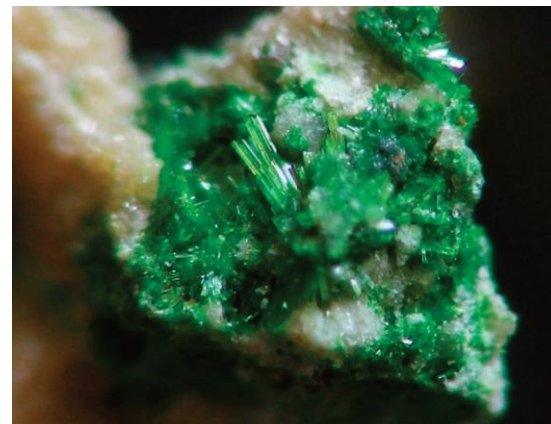
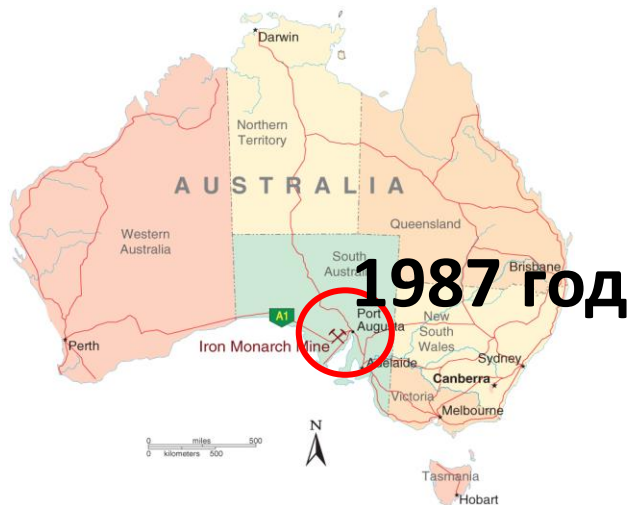
<sup>2</sup> *SSPA «Scientific-Practical Materials Research Centre of NAS of Belarus», Minsk, Belarus*



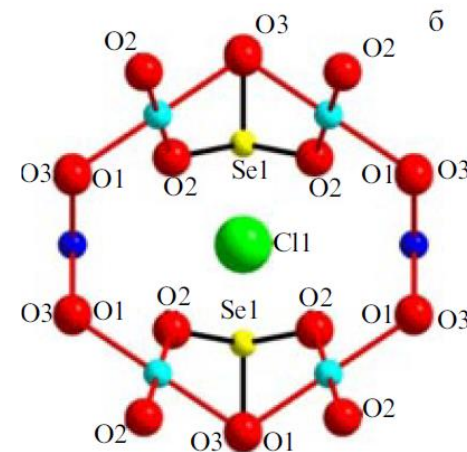
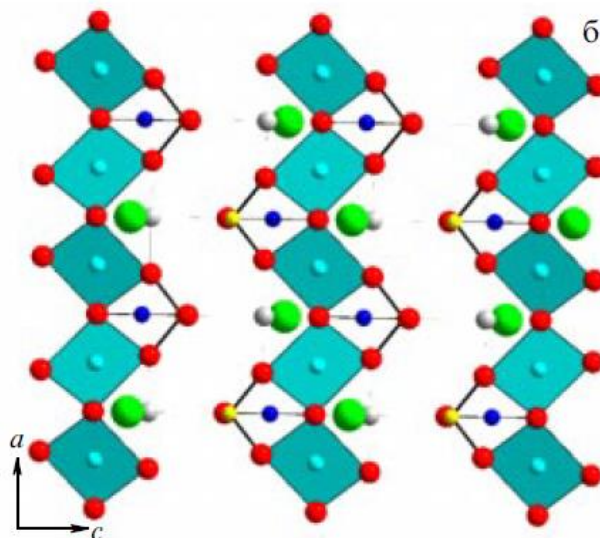
# Crystal structure of $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}$ compound



Glyn L. Francis



The orthorhombic structure  $Pmmn$



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# Isostructural compounds based on the Francisite

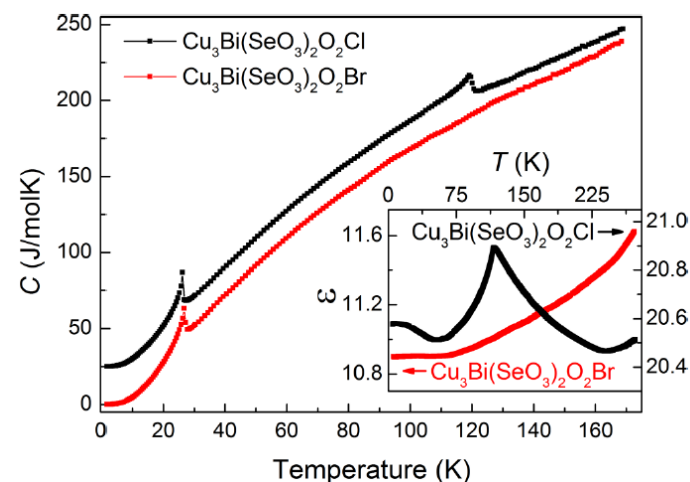
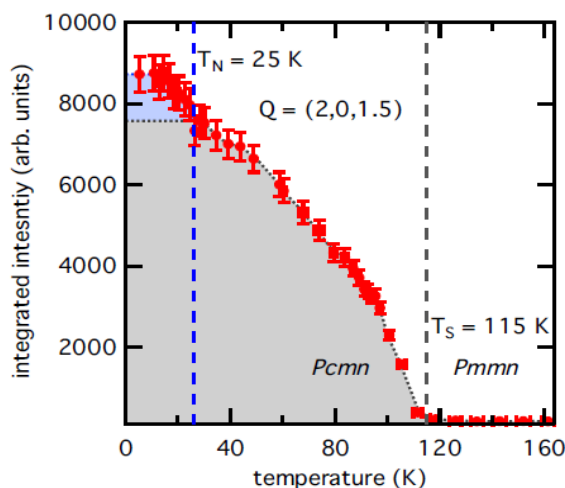
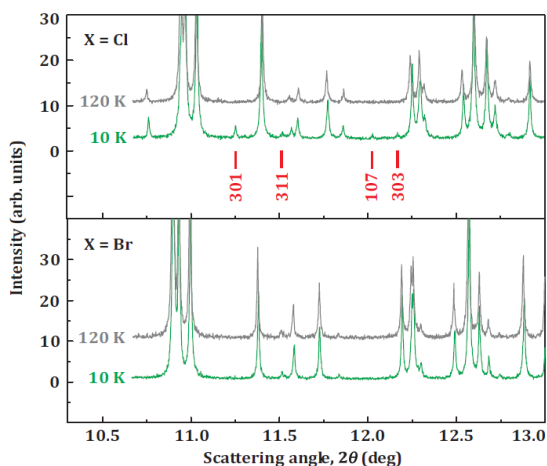
## $\text{Cu}_3\text{R}(\text{Se}_{1-x}\text{Te}_x\text{O}_3)_2\text{O}_2\text{X}$ compounds

R – rare earth elements, X – Cl, Br, I

1	$\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	10	$\text{Cu}_3\text{Dy}(\text{SeO}_3)_2\text{O}_2\text{Cl}$
2	$\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Br}$	11	$\text{Cu}_3\text{Ho}(\text{SeO}_3)_2\text{O}_2\text{Cl}$
3	$\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{I}$	12	$\text{Cu}_3\text{Er}(\text{SeO}_3)_2\text{O}_2\text{Cl}$
4	$\text{Cu}_3\text{Y}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	13	$\text{Cu}_3\text{Yb}(\text{SeO}_3)_2\text{O}_2\text{Cl}$
5	$\text{Cu}_3\text{La}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	14	$\text{Cu}_3\text{Lu}(\text{SeO}_3)_2\text{O}_2\text{Cl}$
6	$\text{Cu}_3\text{Nd}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	15	$\text{Cu}_3\text{La}(\text{SeO}_3)_2\text{O}_2\text{Br}$
7	$\text{Cu}_3\text{Sm}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	16	$\text{Cu}_3\text{Nd}(\text{SeO}_3)_2\text{O}_2\text{Br}$
8	$\text{Cu}_3\text{Eu}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	17	$\text{Cu}_3\text{Sm}(\text{SeO}_3)_2\text{O}_2\text{Br}$
9	$\text{Cu}_3\text{Gd}(\text{SeO}_3)_2\text{O}_2\text{Cl}$	18	$\text{Cu}_3\text{Gd}(\text{SeO}_3)_2\text{O}_2\text{Br}$

1	$\text{Cu}_3\text{Bi}(\text{TeO}_3)_2\text{O}_2\text{Cl}$
2	$\text{Cu}_3\text{Bi}(\text{Se}_{0,8}\text{Te}_{0,2}\text{O}_3)_2\text{O}_2\text{Cl}$
3	$\text{Cu}_3\text{Bi}(\text{Se}_{0,6}\text{Te}_{0,4}\text{O}_3)_2\text{O}_2\text{Cl}$
4	$\text{Cu}_3\text{Bi}(\text{Se}_{0,4}\text{Te}_{0,6}\text{O}_3)_2\text{O}_2\text{Cl}$
5	$\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}_{0,5}\text{Br}_{0,5}$

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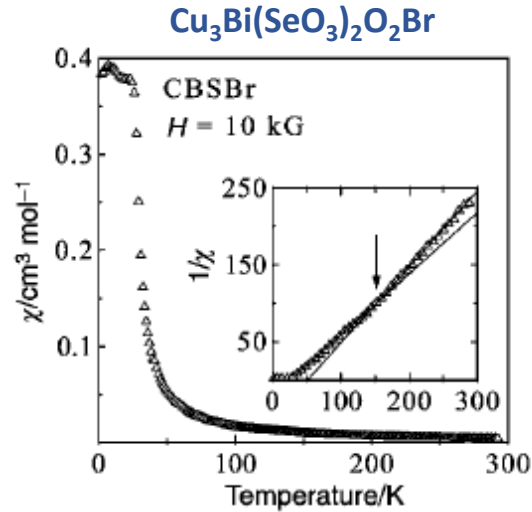
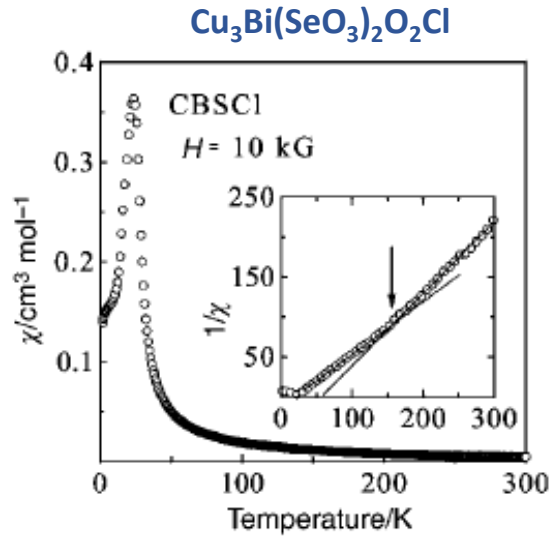


PHYSICAL REVIEW B **95**, 064102 (2017)

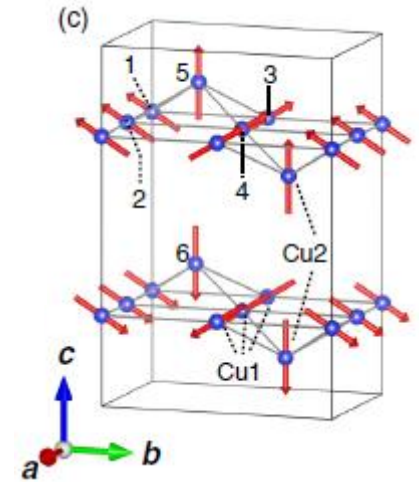
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PHYSICAL REVIEW B **96**, 115144 (2017)

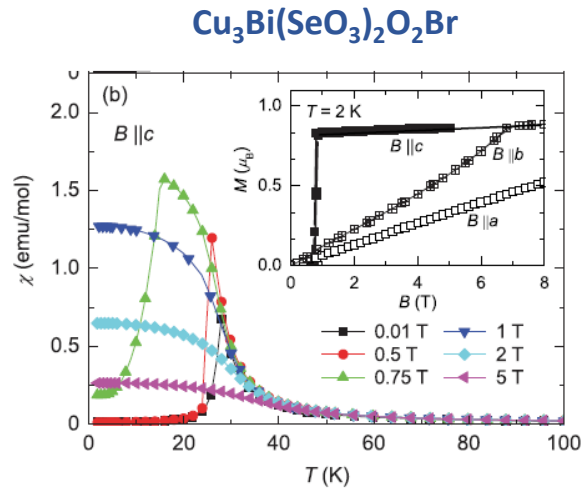
# Magnetic properties of $\text{Cu}_3\text{R}(\text{Se}_{1-x}\text{Te}_x\text{O}_3)_2\text{O}_2\text{X}$ compounds



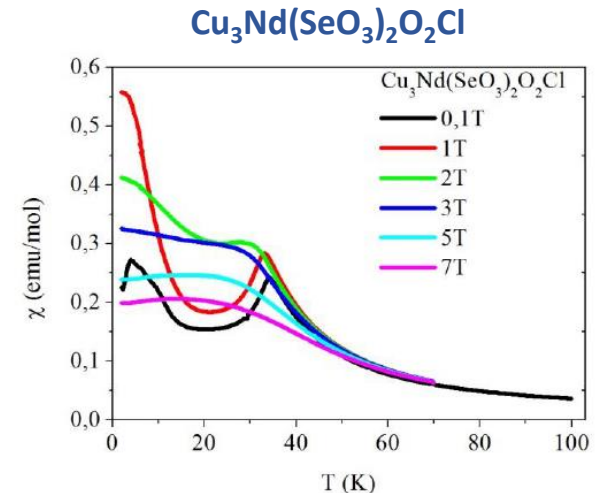
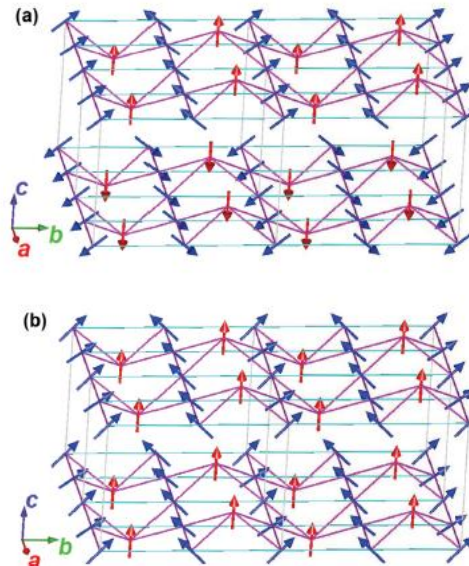
*J. Mater. Chem.*, 2001, 11, 1152–1157



PHYSICAL REVIEW B 96, 014413 (2017)



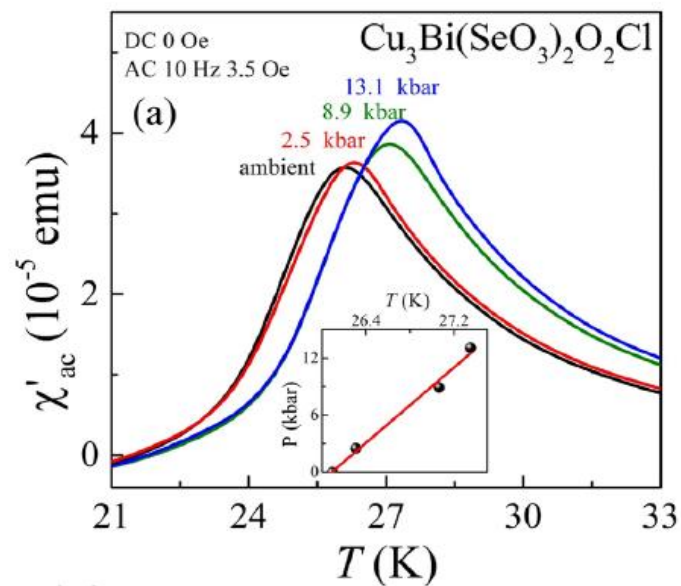
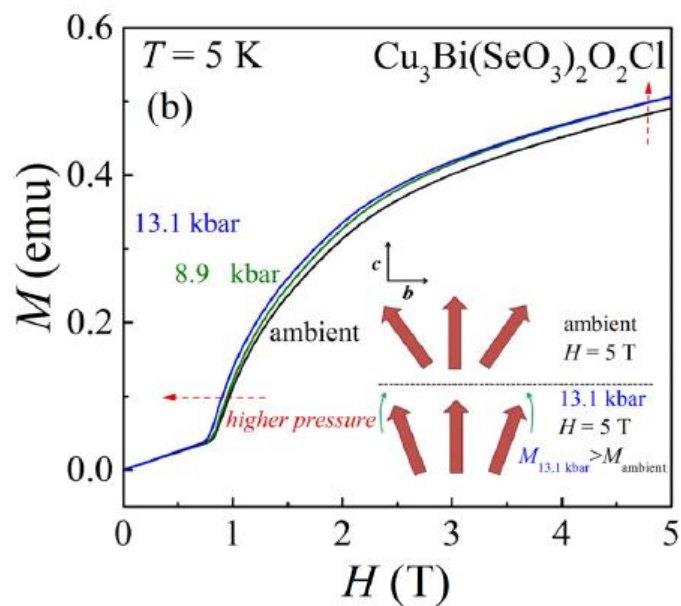
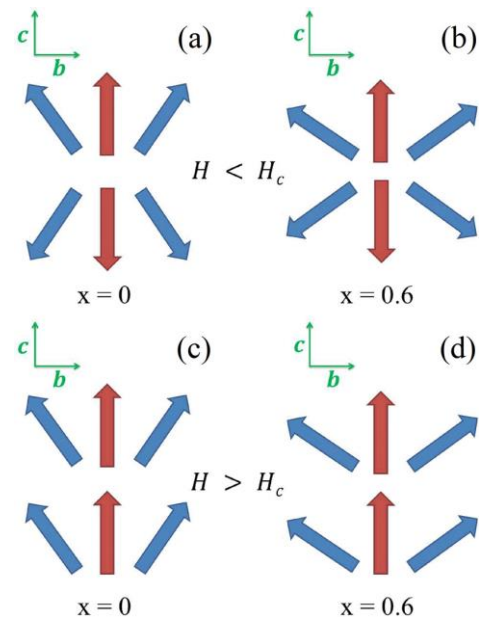
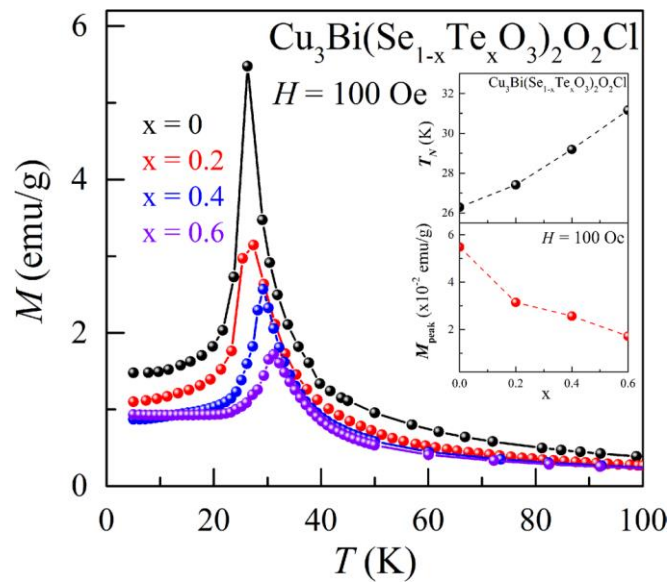
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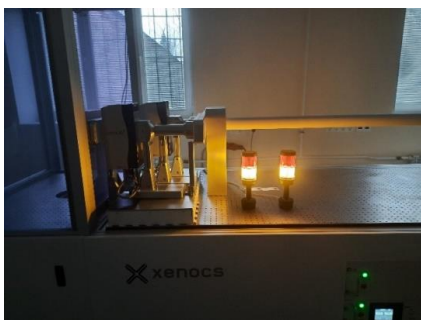
Markina M M et al. *J. Magn. Magn. Mater.*

492 165721 (2019)

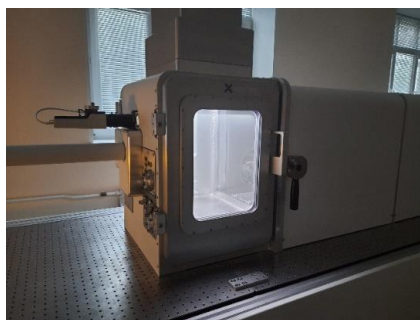
# Cu<sub>3</sub>Bi(Se<sub>1-x</sub>Te<sub>x</sub>O<sub>3</sub>)<sub>2</sub>O<sub>2</sub>Cl compounds under high pressure



# X – ray diffractometers Xeuss , FLNP JINR (Dubna, Russia)



Maximum pressure ~ 35 GPa



Temperature is 300 K



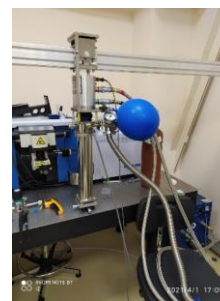
# LabRAM spectrometer Horiba, FLNP JINR (Dubna, Russia)



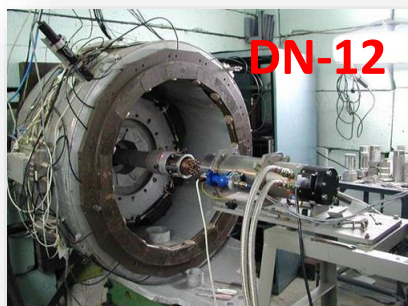
Maximum pressure ~ 35 GPa



Temperature range: 15 -300 K



# Neutron diffractometers at IBR-2 reactor: DN-12 и DN-6

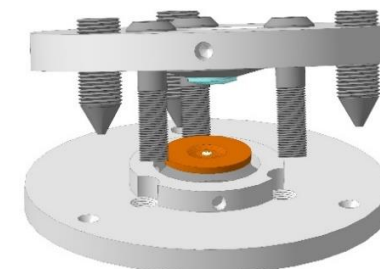


Maximum pressure ~ 8 GPa =80 000 atm.

Temperature range: 10 -320 K

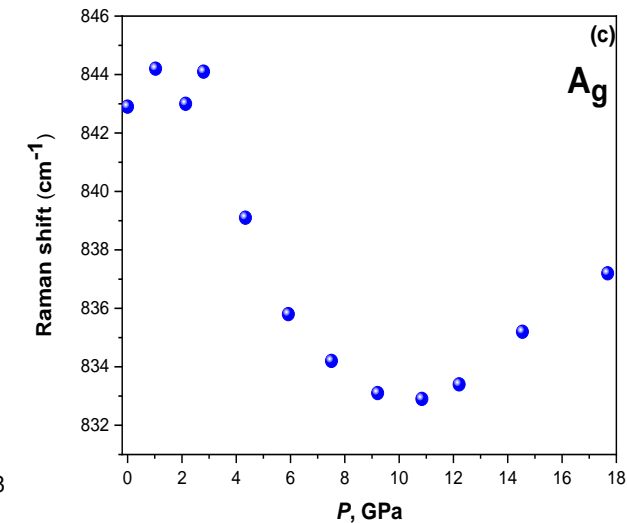
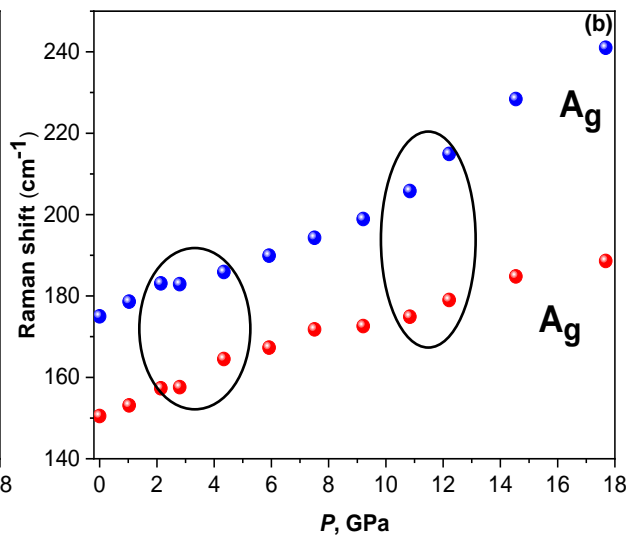
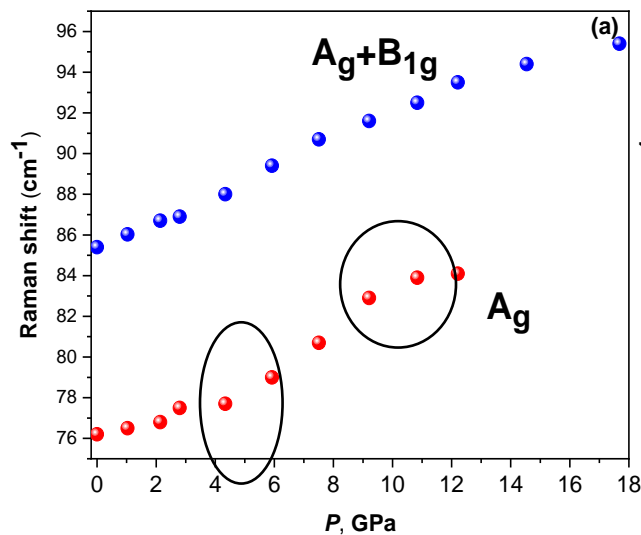
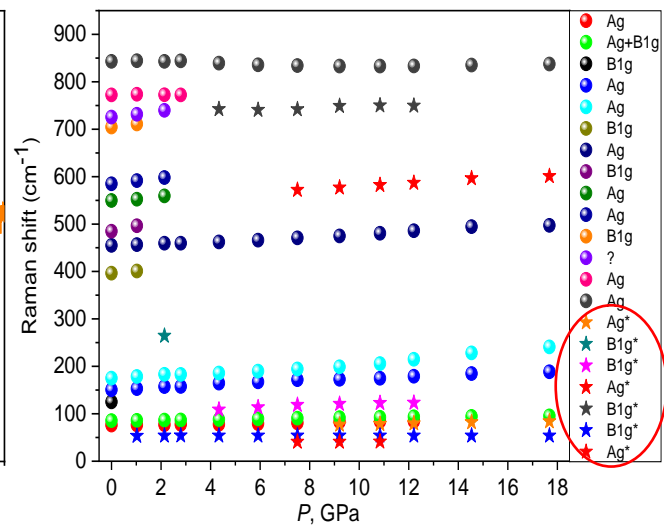
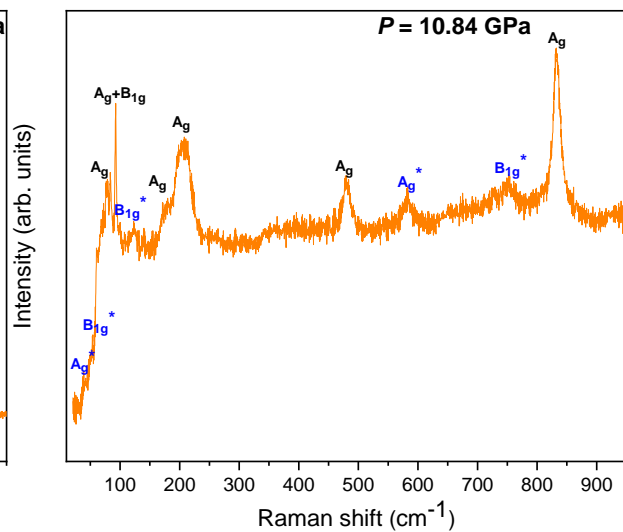
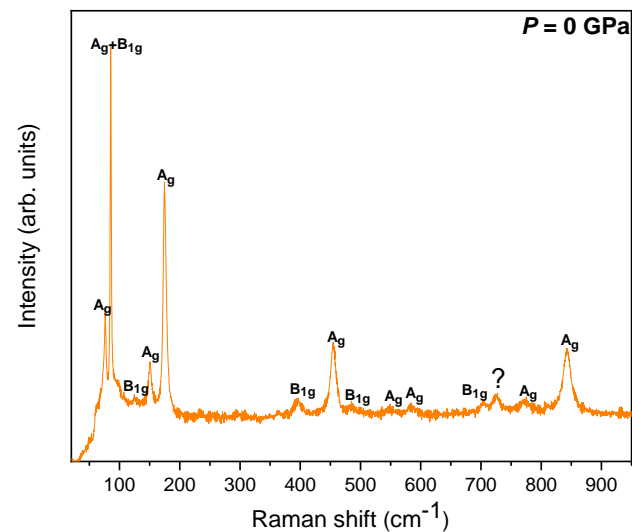


Maximum pressure ~ 35 GPa

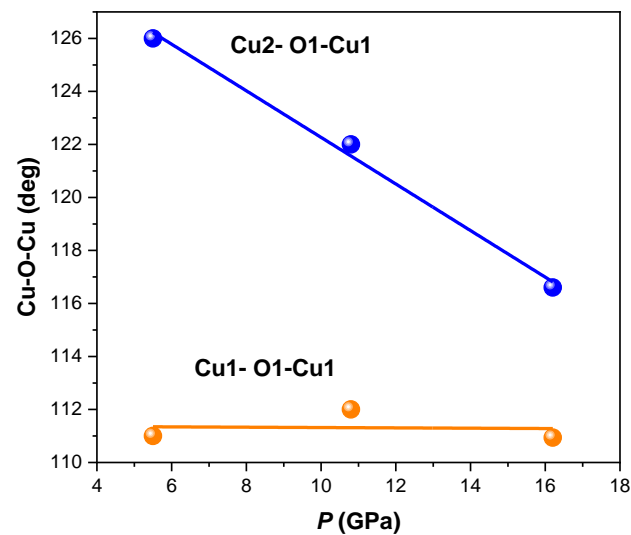
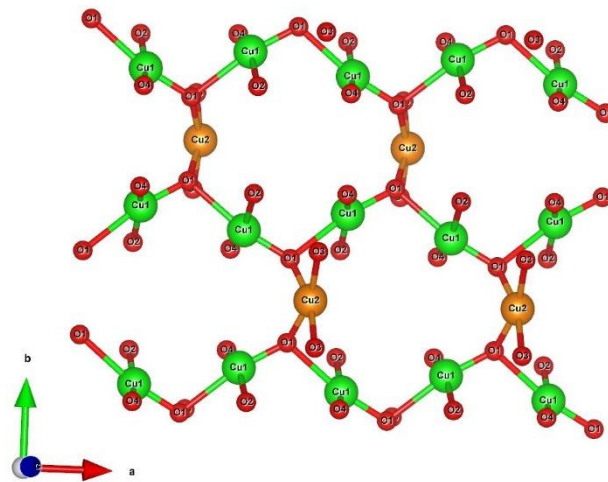
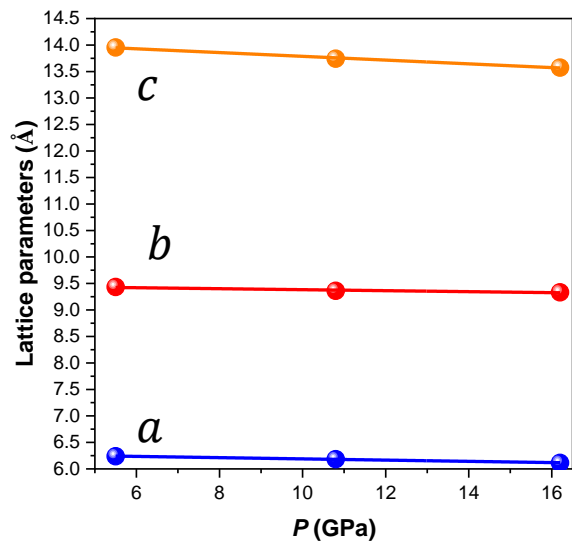
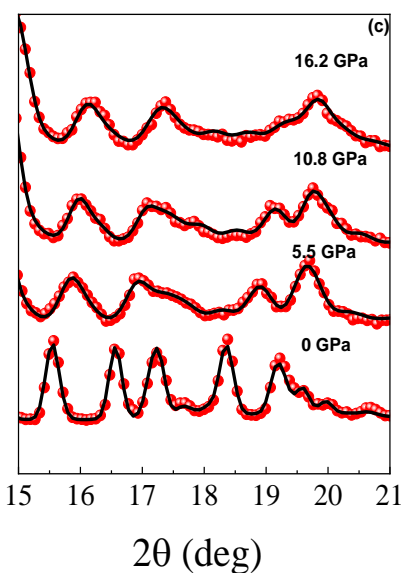
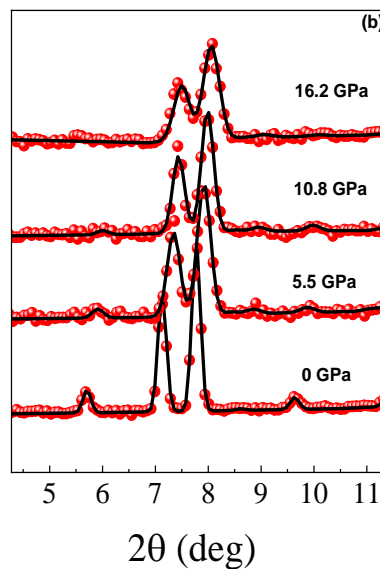
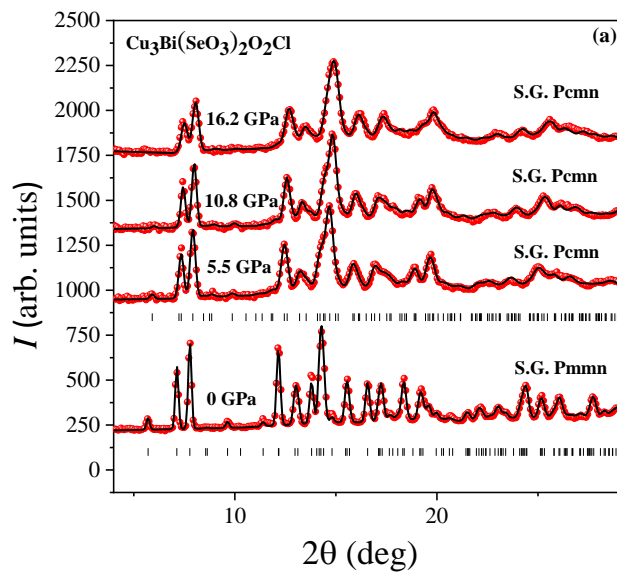


Temperature range: 4 -320 K

# Raman spectroscopy of $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}$ under high pressure



# Crystal structure of $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Cl}$ under high pressure



$$k_a = 1.9(1) \times 10^{-3} \text{ GPa}^{-1}$$

$$k_b = 1.0(2) \times 10^{-3} \text{ GPa}^{-1}$$

$$k_c = 2.0(2) \times 10^{-3} \text{ GPa}^{-1}$$

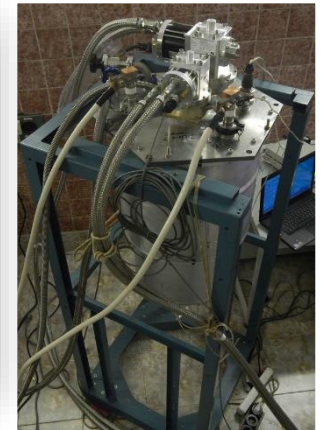
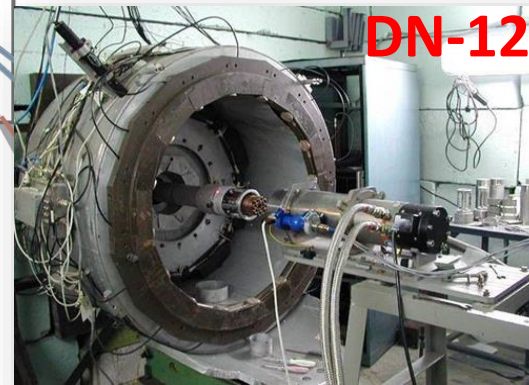
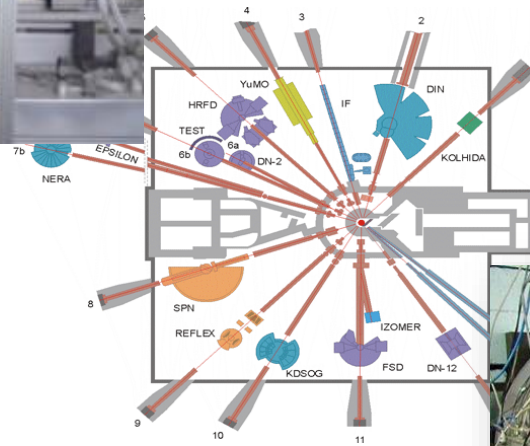


# Conclusion

## Plans for the future:



Neutron diffraction experiments under high pressure up to 30 GPa and at low temperature up to 5 K



Neutron diffraction experiments in the magnetic field up to 3 T under high pressure up to 5 Gpa and at low temperature up to 10 K

IOP Conf. Series: Journal of Physics: Conf. Series **1021** (2018) 012048

doi:10.1088/1742-6596/1021/1/012048

Development of the sample environment system for the DN-12 diffractometer on the IBR-2M pulsed reactor (pressure – temperature – magnetic field). Project status.

**Thank you for your attention!**