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**Structure deformation and spectroscopic properties of blue halite from Klodawa.** Sylwia Zelek<sup>a</sup>, Katarzyna Stadnicka<sup>a</sup>. <sup>a</sup>*Faculty of Chemistry, Jagiellonian University, Poland.*

E-mail: [zelek@chemia.uj.edu.pl](mailto:zelek@chemia.uj.edu.pl)

X-ray structure analysis was used to investigate single crystals of navy-blue, pale blue, purple and colourless halite from Klodawa Salt Mine, Poland (Zechstein evaporite basin). All the samples were characterised by UV-VIS spectroscopy in the range 200-900 nm [1]. For navy-blue samples two main absorption bands were observed at 630 and 385 nm, whereas for pale blue and purple samples the dominant bands appeared to be those at 610 nm and 580 nm, respectively. X-ray diffraction study performed for the single crystals of blue halite indicated that their crystal structures are deformed at atomic level [2]. As a measure of the structure-deformation degree, the deviation from cubic symmetry (typical for NaCl) was considered: the single crystals from navy-blue fragments were found to be mainly monoclinic (rarely tetragonal), those from pale blue fragments were either rhombohedral or orthorhombic, those from purple fragments appeared to be cubic or triclinic, whereas the single crystals from natural colourless samples and those from the recrystallized samples belonged to cubic space group Fm-3m. In the cases of symmetry lower than cubic, it was usually possible to force a transformation to Fm-3m. The decreasing of symmetry was confirmed by the observation of birefringence under polarizing microscope. The deformation degree of the blue halite structure, from that characteristic for the pure cubic NaCl, could be correlated with a particular hue of the blue colour. Therefore one can assume that in certain thermodynamic conditions dispersed F-centres might possibly aggregate (in the studied samples there were no bands characteristic for F-centres, i.e. at 465 nm [3]). The various types of colour centre aggregates are stabilized by different sort of already existing lattice defects. The size of colour centre aggregates and the type of structure deformation would have an effect on the energy of the whole system and thus could be regarded as responsible for the observed variety of absorption bands and for relatively stable blue or purple hue of the halite from Klodawa Salt Mine. Thus an attempt was made to estimate the size of colour centres aggregates by means of X-ray diffuse scattering approach.

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**Inelastic x-ray scattering from phonons.** Elena Borissenko, Björn Wehinger, Andrew Walters, Alexey Bossak, Michael Krisch. *European Synchrotron Radiation Facility, France.*

E-mail: [elena.borissenko@esrf.fr](mailto:elena.borissenko@esrf.fr)

The vibrational properties of matter provide important information on their elastic and thermodynamic properties. Techniques such as Brillouin and Raman light scattering, as well as infrared spectroscopy, are limited to momentum transfers close to zero and consequently probe the dynamics over macroscopic length scales. Access to the mesoscopic and microscopic region is primarily provided by inelastic neutron scattering (INS) or inelastic x-ray scattering (IXS).

The uniqueness of the IXS technique employed using synchrotron radiation is primarily due to two main points: i) there is no fundamental restriction on the energy-momentum transfer region to be explored, and ii) crystalline materials in very small quantities and at very high pressures can be studied.

Since pioneering work in the late 1980s, IXS has evolved into a mature technique and has contributed to the advancement of knowledge in different scientific disciplines ranging from fundamental solid-state physics to planetary science [1, 2]. The key characteristics of IXS shall be summarised and the present state-of-the-art be illustrated by a few representative examples. These comprise high-pressure studies using diamond anvil cell techniques, strongly correlated electron systems, as well as bulk and surface-sensitive studies of liquids.

The lattice dynamics of iron and iron-bearing minerals at high pressure up to 100 GPa allowed the determination of sound velocities and provides precious insight into the elastic properties and the composition of Earth's core. [2,3].

The comparison of the phonon dispersion curves of SmFeAsO and superconducting SmFeAsO<sub>0.6</sub>F<sub>0.35</sub> crystals underlined the fluorine doping dependence of two optical modes that vary strongly with the momentum transfer. This study supports the importance of spin-phonon coupling in superconducting iron pnictides [4].

The inelastic x-ray scattering experiment on liquid indium in grazing angle incidence geometry illustrates the unique possibility to study surface and bulk properties in a single experimental set-up.[5].

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