MS36-01 Borates under extreme conditions. Hubert Huppertz Institute of General, Inorganic and Theoretical Chemistry, University of Innsbruck, Innrain 80-82, A-6020 Innsbruck, Austria E-mail: Hubert.Huppertz@uibk.ac.at

High-pressure investigations in borate chemistry are rare and have been mainly performed from a geological point of view. In the last decade, systematic high-pressure experiments up to maximum pressures of 16 GPa have been carried out in our group focusing on high-pressure solid state chemistry of borates using the multianvil technique [1]. In the context of these investigations into new rare-earth and transition metal oxoborates, several new high-pressure polymorphs of known compositions, *e.g.* β -MB₄O₇ (M = Ca, Zn, Hg), χ -*RE*BO₃ (*RE* = Dy, Er), ν -DyBO₃, γ -*RE*(BO₂)₃ $(RE = La-Nd), \delta - RE(BO_2)_3$ $(RE = La, Ce), and \delta - BiB_3O_6$ [2], were discovered. These investigations led to fundamental insights into the structural behaviour of oxoborates under high-pressure conditions. Especially the coordination of the boron and rare-earth atoms were of special interest in our investigations. Next to the synthesis of new modifications, new compositions were realized in our group. For example, all attempts to produce rare-earth metal(III) oxoborates with the ratio RE_2O_3 : $B_2O_3 = 2:3$, 1:2, and 3:5 failed under normal-pressure conditions. In contrast, the corresponding high-pressure experiments led in most cases to phase pure rare-earth metal(III) oxoborates $RE_4B_6O_{15}$ (RE = Dy, Ho) and $a-RE_2B_4O_9$ (RE = Sm-Ho), exhibiting the new structural unit of edge-sharing tetrahedra. Our latest experiments yielded in a third compound, exhibiting edge-sharing tetrahedra. The special feature of the compound HP-NiB2O4 is that in contrast to the first two compounds all tetrahedra are linked to each other via one common edge and two common corners [3]. Recently, we were able to synthesize a new alkali metal borate with the composition HP-KB₃O₅, exhibiting all three possible conjunctions simultaneously: corner-sharing BO₃ groups, corner-sharing BO₄ units, as well as edge-sharing BO₄ tetrahedra [4].

The talk will introduce into several examples including the synthesis of new fluoride borates, which impressively underline the importance of the parameter pressure for the synthesis of new materials in solid state and materials chemistry.

- [1] Huppertz, H. (2011) Chem. Commun. 47, 131-140.
- [2] Knyrim, J. S., Becker, P., Johrendt D. & Huppertz H. (2006) Angew. Chem. Int. Ed. Engl. 45, 8239-8241.
 [3] Knyrim, J. S., Roeßner, F., Jakob, S., Johrendt, D., Kinski, I.,
- [3] Knyrim, J. S., Roeßner, F., Jakob, S., Johrendt, D., Kinski, I., Glaum, R., Huppertz, H. (2007) *Angew. Chem. Int. Ed. Engl.* 46, 9097-9100.
- [4] Neumair, S. C., Vanicek, S., Kaindl, R., Többens, D. M., Martineau, C., Taulelle, F., Senker, J. & Huppertz, H. (2011) *Eur. J. Inorg. Chem.* 4147-4152.

Keywords: Borates; High-pressure; Multianvil

MS36-02 Inelastic x-ray scattering: phonon spectroscopy under extreme conditions. <u>Alexei Bosak</u>, Michael Krisch. *European Synchrotron Radiation Facility, Grenoble, France* E-mail: <u>bossak@esrf.fr</u>

The dynamical properties of condensed matter are responsible for a wealth of physical properties, such as thermal and electrical conductivity, melting, elastic properties, phase stability and transformation, and many others. Lattice dynamics studies are predominantly conducted using inelastic neutron scattering (INS) and inelastic x-ray scattering (IXS) [1]. IXS has matured into a valuable scattering technique, especially in cases where INS techniques are difficult to apply. In the context of high pressure the crucial parameter is the necessary sample volume. While INS experiments require typical sample volumes of several mm³, IXS measurements can be performed utilising volumes several orders of magnitude smaller $(10^{-5} - 10^{-4} \text{ mm}^3)$. This opens up possibilities to study materials only available in very small quantities and/or to perform their investigation in extreme thermodynamic conditions, most notably at very high pressures using diamond anvil cell techniques [2, 3]. Our presentation gives an overview of the work performed on crystalline materials.

- Krisch, M. and Sette, F. (2007) Light Scattering in Solids IX, Novel Materials and Techniques, eds. Cardona, M. and Merlin, R., Chapter "Inelastic X-ray Scattering from Phonons," (Springer Verlag Berlin Heidelberg), pp. 313-370.
- [2] Fiquet, G., Badro, J., Guyot, F., Bellin, Ch., Krisch, M., Antonangeli, D., Mermet, A., Requardt, H., Farber, D. and Zhang, J. (2004). Physics of the Earth and Planetary interiors 143-144, 5-18 (2004).
- [3] Giordano, V.M., Krisch, M. and Monaco, G. J. Synchr. Radiation 16, 707-713 (2009).

Keywords: phonons; inelastic scattering; extreme conditions