## MS38-P3 Crystal structure of hydrated fluorides $MF_2.4H_2O$ (M= Zn, Ni, Co): a combined approach

K. Forsberg[1], G. Nénert[2], T. Tao[3], P. S. Halasyamani[3]

1. School of Chemical Science and Engineering, KTH Royal Institute of Technology, Teknikringen 42, 100 44 Stockholm, Sweden
2. PANalytical B.V., Lelyweg 1, 7602 EA, Almelo, The Netherlands
3. Department of Chemistry, University of Houston, Houston, Texas 77204-5003, USA

email: kerstino@kth.se

Inorganic metal fluorides and oxide-fluorides have significant importance in the development of many new technologies within for example energy production and storage, microelectronics and photonics, catalysis and the automotive industry. There is a need for better knowledge of the relationships between the structure of these compounds and some pertinent physicals properties [1].

Based on single crystal X-ray work, $ZnF_2.4H_2O$ has been suggested to crystallize in the polar space group $Pca2_1$ [2]. The possibility for non-linear optical properties of this compound and related phases motivated us to investigate this family further. Very little is known about the crystallography of the $MF_2.4H_2O$ family. Compositions such as $MF_2.4H_2O$ (M: Co, Ni, Fe) have been reported but not characterised structurally [3]. The crystal structure determination of such materials is particularly complicated as oxygen and fluorine atoms exhibit very similar scattering cross sections irrespective of the source (X-ray or neutron).

Using a combined approach of X-ray, neutron and second harmonic generation, we show that actually the crystal structure of these materials is centrosymmetric, in contradiction with previous reports. We discuss the crystal structure of these materials ($MF_2.4H_2O$, M= Zn, Co, Ni) using combined refinements using neutron and X-ray diffraction data. The use of complementary techniques was a key to determine the correct structure of these materials.

[1] Leblanc M., Maisonneuve, Tressaud A., *Chem. Rev.*, **115(2)**, pp 1191- 1254 (2015).

[2] Bukvetskii B.V., Polishchuk S.A., Simonov V.I., *Sov. Phys. Crystallogr.*, **18(5)**, pp 600-602 (1974).

[3] Lange B.A., Haendler H.M., *J. Inorg. Nucl. Chem.*, **35**, pp 3129- 3133 (1973); Swanepoel J., Heyns A.M., *Spectrochimica Acta*, 47A(2), pp 243-253 (1991).

**Keywords:** fluorides; crystal structure; X-ray diffraction; second harmonic generation

## MS38-P4 Investigation of the ultra-fast structural changes in metal-organic complexes: comparison spectroscopy and time-resolved XRD

Dirk Raiser[1], Darina Storozhuk [2], Sreevidya Thekku Veedu[2], Simone Techert[1,2,3]

1. Structural Dynamics of (Bio)chemical Systems, Max-Planck-Institute for biophysical chemistry, Am Faßberg 11, 37077 Göttingen, Germany
2. Structural Dynamics in Chemical Systems, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany
3. Institute for X-Ray Physics, Faculty of Physics of the Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

email: dirk.raiser@mpibpc.mpg.de

Our aim is a detailed understanding of the ultrafast structural dynamics and the underlying basic mechanisms of molecular switches under optical excitation, which are still not fully understood in its variety. In order to monitor the occurring structural changes in molecules and alloys we are taking advantage of time-resolved x-ray diffraction measurements. But since the important electronic changes due to optical excitation take place on very short ps- and sub-ps timescales it gives rise to the necessity of faster time-resolved measurements than those which are currently possible at third generation synchrotrons. Besides new attempts of directly monitoring the structural changes with shorter x-ray pulses by femtosecond FEL- and XPS-pump-probe experiments, we are currently gaining more insight in the structural dynamics by indirect measurements using our fs-time-resolved transient absorption spectroscopy. Therefore we will present our recent spectroscopic data of a metal-organic complex which will be related to certain structural changes, while the near future aim is to prove these by further x-ray experiments.

**Keywords:** ultra-fast structural changes, metal-organic complex, transient absorption spectroscopy, time-resolved XRD