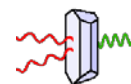


MATERIALS FOR NONLINEAR OPTICS



Head of research group:

prof. RNDr. Ivan Němec, Ph.D.



✓ Professor

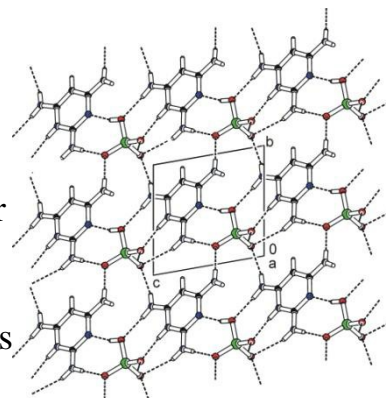
✓ **M.Sc.** (1990), **Ph.D.** (1998), **Doc.** (2009) and **Prof** (2017) Faculty of Science, Charles University

✓ Contact: Department of Inorganic Chemistry, Faculty of Science, Charles University, Hlavova 8, 128 40 Prague 2, Czech Republic
phone: +420 221 951 247, fax: +420 221 951 253

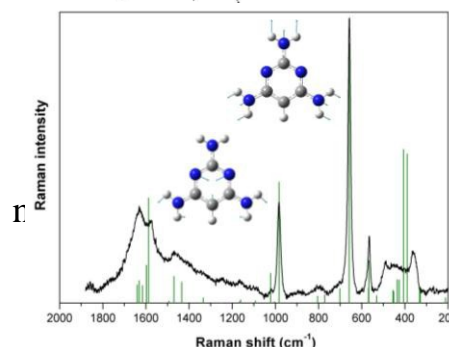
e-mail: ivan.nemec@natur.cuni.cz

Research topics

☞ Preparation and characterization of novel materials for nonlinear optics (**NLO**), especially for second harmonic generation (**SHG**), based on hydrogen-bonded compounds (i.e. salts or cocrystals) of organic nitrogen-containing bases



☞ Characterization of the prepared materials by the combination of diffraction (X-ray structural analysis) and spectroscopic methods (FTIR and Raman macro- and micro-spectroscopy, NMR, UV-VIS-NIR, MS). Utilization of quantum chemical computations (Gaussian and CRYSTAL software).



☞ Application of vibrational spectroscopy in the solids – i.e. solid state and material chemistry, mineralogy, artworks, exobiology etc.



☞ Cooperating departments:

Department of Chemical Physics and Optics (Faculty of Mathematics and Physics, Charles University), Department of Dielectrics and Department of Structure Analysis (Institute of Physics, Academy of Sciences of the Czech Republic, v.v.i.), Section Crystallography (Institute of Geology and Mineralogy, University of Cologne, Germany), Institute of Geochemistry, Mineralogy and Mineral Resources (Faculty of Science, Charles University), Department of Crystal Chemistry and Crystal Physics (Faculty of Chemistry, Jagiellonian University in Kraków), Department of Plant and Environmental Sciences (The Alexander Silberman Institute of Life Sciences, The Hebrew University of Jerusalem), etc.

☞ prof. RNDr. Ivan Němec, Ph.D. **ORCID:** [0000-0001-9630-3169](https://orcid.org/0000-0001-9630-3169),
ResearchID: [S-1734-2016](https://pubs.rsc.org/author/S-1734-2016), **Scopus Author ID:** [7004626064](https://orcid.org/7004626064)

☞ Current group members:

RNDr. Irena Matulková, Ph.D. – assistant professor

Mgr. Martin Zábanský, Ph.D. – assistant professor

Mgr. Soňa Kohúteková – PhD student

Bc. Miriam Basová – MSc student

☞ List of selected papers:

Galáš, P; Popelář, T; Khun, J; Matulková, I; Němec, I; Newell, KD; Michalcová, A; Scholtz, V; Kůsová, K, The red and blue luminescence in silicon nanocrystals with an oxidized, nitrogen-containing shell, **FARADAY DISCUSSIONS** 222(2020)240, DOI: 10.1039/c9fd00092e

Wojnarska, J; Gryl, M; Seidler, T; Rydz, A; Oszajca, M; Stadnicka, KM; Marzec, M; Matulková, I; Němec, I; Němec, P, Crystal structure and (non)linear optical properties of a cyanuric acid isoniazid <1/1> co-crystal: shortcomings of phase matching determination from powdered samples, **CRYSTAL GROWTH & DESIGN** 19(2019)6831, DOI: 10.1021/acs.cgd.9b01023

Bohatý, L; Matulková, I; Cisařová, I; Němec, I; Schneeberger, H; Kaminskii, AA; Becker, P, Crystal growth, thermal expansion, pyroelectricity and vibrational spectroscopy of barium antimony tartrate, Ba[Sb-2((+)C4H2O6)(2)]center dot 3H(2)O, **OPTICAL MATERIALS** 91(2019)70, DOI: 10.1016/j.optmat.2019.02.051

Matulková, I; Kovaříček, P; Šlouf, M; Němec, I; Kalbáč, M, Surface enhanced infrared absorption spectroscopy for graphene functionalization on copper, **CARBON** 124(2017)250, DOI: 10.1016/j.carbon.2017.08.045

Němec, I; Matulková, I; Held, P; Kroupa, J; Němec, P; Li, DX; Bohatý, L; Becker, P, Crystal growth, crystal structure, vibrational spectroscopy, linear and nonlinear optical properties of guanidinium phosphates, **OPTICAL MATERIALS** 69(2017)420, DOI: 10.1016/j.optmat.2017.04.012

Němec, P; Pasztor, F; Brajer, M; Němec, I, Spectrally- and polarization-resolved hyper-Rayleigh scattering measurements with polarization-insensitive detection, **OPTICS COMMUNICATIONS** 388(2017)21, DOI: 10.1016/j.optcom.2016.10.072

Matulková, I; Cisařová, I; Vaněk, P; Němec, P; Němec, I, Novel organic NLO material bis(N-phenylbiguanidium(1+)) oxalate - a combined X-ray diffraction, DSC and vibrational spectroscopic study of its unique polymorphism, **SPECTROCHIMICA ACTA PART A** 170(2017)256, DOI: 10.1016/j.saa.2016.07.023

Jehlička, J; Němec, I; Varnali, T; Culka, A; Svatoš, A; Frank, O; Oren, A; Edwards, HGM, The pink pigment prodigiosin: vibrational spectroscopy and DFT calculations, **DYES AND PIGMENTS** 134(2016)234, DOI: 10.1016/j.dyepig. 2016.07.018

Košařová, V; Hradil, D; Hradilová, J; Čermaková, Z; Němec, I; Schreiner, M, The efficiency of micro-Raman spectroscopy in the analysis of complicated mixtures in modern paints: Munch's and Kupka's paintings under study, **SPECTROCHIMICA ACTA PART A** 156(2016)36, DOI: 10.1016/j.saa.2015.11.027

Jehlička, J; Edwards, HGM; Osterrothova, K; Novotna, J; Nedbalova, L; Kopecky, J; Nemecek, I; Oren, A, Potential and limits of Raman spectroscopy for carotenoid detection in microorganisms: implications for astrobiology, **PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A - MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES** 372 (2014), DOI: 10.1098/rsta.2014.0199

Matulková, I; Cihelka, J; Pojarová, M; Fejfarová, K; Dušek, M; Císařová, I; Vaněk, P; Kroupa, J; Němec, P; Tesařová, N; Němec, I, Molecular crystals of 2-amino-1,3,4-thiadiazole with inorganic oxyacids - crystal engineering, phase transformations and NLO properties, **CRYSTENGCOMM** 16(2014)1763, DOI: 10.1039/c3ce42306a.

Kaminskii, AA; Becker, P; Rhee, H; Lux, O; Kaltenbach, A; Eichler, HJ; Shirakawa, A; Yoneda, H; Němec, I; Fridrichová, M; Bohatý, L, Stimulated Raman scattering in monoclinic non-centrosymmetric guanylurea(1+) hydrogen phosphite (GUHP), **PHYSICA STATUS SOLIDI B - BASIC SOLID STATE PHYSICS** 250(2013)137, DOI: 10.1002/pssb.201349201