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Salts of guanylurea – novel materials promising for optical applications. Michaela Fridrichová[a], Ivan Němec[a], Ivana Císařová[a], Petr Němec[b] and Jan Kroupa[c]
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Searching for novel compounds with a potential for applications in optics is an actual task of materials research. Particular attention is focused on materials exhibiting desirable nonlinear optical properties. Polarizable organic compounds with delocalized π-electrons often exhibit such properties as second harmonic generation with high efficiency. Preparation of non-centrosymmetric salt materials containing cations of such molecules, interconnected by the system of hydrogen bonds with anions of inorganic or also organic acids, can lead to materials with interesting combination of optical, chemical and physical properties. Guanylurea(1+) is a cation combining structure motives of urea and guanidine and posessing a high first order molecular hyperpolarizability β [1]. Some of its salts are well known and do not exhibit any interesting optical properties [2, 3], but recently a very promising material, guanylurea(1+) hydrogen phosphite, was prepared [1]. Another interesting material is guanylurea(1+) tartrate [4]. Study of various novel guanylurea(1+) salts has been carried out as an effort to tune the properties by means of crystal engineering through the choice of the counterion. This contribution tries to provide a deeper insight into the structure assembly of guanylurea(1+) salts and its relation to materials properties. Grant Agency of Charles University in Prague (Grant No. 58608), Czech Science Foundation (Grant No. 203/09/0878) and the long term Research Plans of the Ministry of Education of the Czech Republic (No. MSM0021620857 and MSM0021620834) are acknowledged for financial support.

[1] Fridrichová M., Němec I., Císařová I., Němec P., *CrystEngComm* 2010, DOI: 10.1039/B924973G. [2] Lotsch B. V., Schnick W., *Z. Anorg. Allg. Chem.*, 2005, 631, 2967. [3] Scoponi M., Polo E., Bertolasi V., Carassiti V., Bertelli G., *J.Chem.Soc.,Perkin Trans.*, .1991, 2, 1619. [4] Fridrichová M., Němec I., Císařová I., Němec P., *MOLMAT 2010*, Montpellier, France.

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