

Guanylurea(1+) Hydrogenphosphite – A New Material for Non-Linear Optics

M. Fridrichová¹, I. Němec¹, P. Němec²

¹Charles University in Prague, Faculty of Science, Department of Inorganic Chemistry, Hlavova 2030,
128 40 Prague 2, Czech Republic

²Charles University in Prague, Faculty of Mathematics and Physics, Department of Chemical Physics
and Optics, Ke Karlovu 3, 121 16 Prague 2, Czech Republic

Guanylurea(1+) hydrogenphosphite belongs to the family of salts of nitrogen-containing organic compounds with delocalized π - electrons. This group of compounds has potential to have interesting non-linear optical properties, especially high efficiency of the second harmonic generation (SHG).

In this contribution we are reporting on preparation, crystal structure determination, spectroscopic and optical characterisation of guanylurea(1+) hydrogenphosphite. This salt can be prepared by acid hydrolysis of cyanoguanidine water solutions. It crystallizes as single crystals or more usually as aggregates in good yield from solutions with stoichiometric concentration or even a little excess of phosphorous acid. Its crystals are transparent, relatively hard, non-hygroscopic and resistant. The non-centrosymmetric lay-out of guanylurea(1+) hydrogenphosphite and its laminated structure, assembled by numerous hydrogen bonds (see Fig.1), are essential for optical properties of the compound.

FTIR and FT Raman spectra were recorded and interpreted according to computations based on B3LYP 6-31+G(d,p) (ultrafine grid) method. SHG efficiency of powdered guanylurea(1+) hydrogenphosphite was determined at 800 nm.

Guanylurea(1+) hydrogenphosphite is due to its easy preparation and advantageous physical and optical properties a very promising material for applications in non-linear optics.

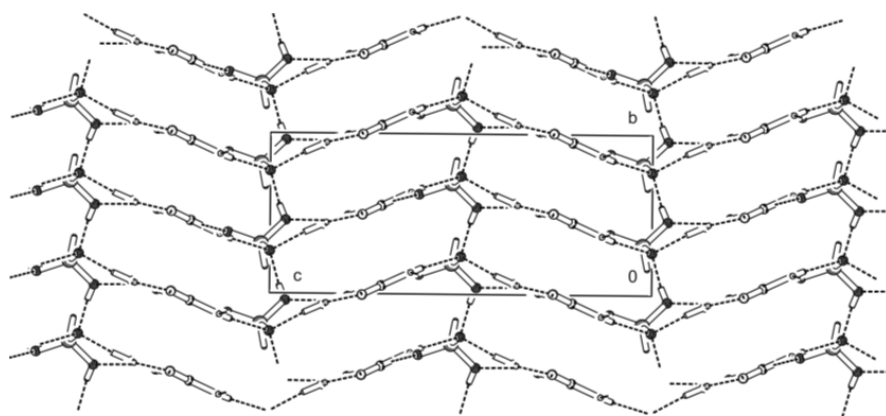


Fig. 1: Guanylurea (1+) hydrogenphosphite structure assembly
(view in crystallographic direction 100)