

MS24-P5 **Low-temperature & high-pressure polymorphism in a room-temperature ionic liquid.** Sofiane Saouane,^a Sarah E. Norman,^b Tristan G. A. Youngs,^b Christopher Hardacre,^b Francesca P. A. Fabbiani,^a ^a*GZG, Abteilung Kristallographie, Georg-August-Universität Göttingen, Göttingen, Germany,* ^b*School of Chemistry & Chemical Engineering, Queen's University Belfast, Belfast, United Kingdom*
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Due to their tunable physical and chemical properties, Room Temperature Ionic liquids (RTILs) have found numerous applications as solvents in industry and the life sciences. The number of reported crystal structures of RTILs has been steadily increasing; however, the phenomenon of polymorphism has been less widely investigated. Up to three crystalline phases of 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF₆]) under non-ambient conditions were previously characterized by DSC [1,2], Raman [1,3,4], and solid-state NMR spectroscopy [5] as well as powder X-ray diffraction [2]; in contrast, only one crystal structure was reported [6,7]. We here present the single-crystal structures of all three polymorphs of this compound obtained under low-temperature and high-pressure crystallisation conditions. These polymorphs and their interconversion were also investigated by Raman spectroscopy and optical microscopy. By elucidating the conformations adopted by the cation and anion in the three structures, we clarify the polymorphic behaviour and previous phase diagrams of this compound.

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MS24-P6 **Experimental and theoretical studies of the NLO properties of a chiral crystal.** Pedro S. Pereira Silva,^a Hasnaa El Ouazzani,^b Manuela Ramos Silva,^a José António Paixão,^a Bouchta Sahraoui,^b ^a*CEMDRX, Physics Department, University of Coimbra, Coimbra, Portugal,* ^b*Institut des Sciences et Technologies Moléculaires d'Angers, MOLTECH ANJOU, CNRS UMR 6200, Université d'Angers, Angers, France*
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There is on-going research interest to develop organic materials with large second-order nonlinear optical (NLO) properties for possible application in the optical and optoelectronic devices. Nonlinear optical effects can be used for the generation of new optical frequencies, not available with existing lasers, in particular compact blue coherent light sources. One of the most important effects is optical frequency doubling [1].

The classical molecular requirements for second-order (NLO) effects have led to the development of strongly elongated and conjugated molecules, asymmetricized by interacting donor and acceptor groups. Such compounds are (highly) anisotropic dipolar structures like p-nitroaniline derivatives, substituted stilbenes, and push-pull polyenes. Although they often exhibit extremely large hyperpolarizabilities, some major drawbacks are associated with their dipolar character, e.g. a high tendency towards unfavourable aggregation, difficult non-centrosymmetric crystallization, and small off-diagonal tensor components [2]. It was recognized that octupolar molecules can circumvent the aforementioned disadvantages, since these nonpolar molecules combine excellent (second-order) NLO characteristics with a strict cancellation of all vectorial properties [3]. Hence, much effort is currently put on the search for new octupolar molecules and materials where the drawbacks of dipolar materials are absent.

The molecular hyperpolarizabilities of several octupolar molecules were calculated using Time Dependent Density Functional Theory, Hartree-Fock and Semi-empirical methods.

The experimental second and third order nonlinear optical properties of these compounds will be presented and compared with the theoretical values.

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