MS23-P6 **Supramolecular structure of an unusual Nevirapine derivative.** Ferreira da Silva João,[1] Antunes Alexandra,[1] Sidarius Muna,[1] Novais David,[1] Harjivan Shrika,[1] Santos Pedro,[1] Beland Frederick,[1] Marques Matilde,[1] *[1]Centro de Química Estrutural, Instituto Superior Tecnico, Universidade Tecnica de Lisboa, Portugal, [2]Anational Center for Toxicological Research, Jefferson, AR 72079, USA*
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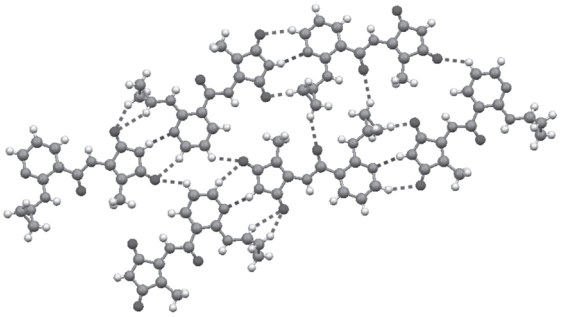
As part of a program aiming to evaluate the possible contribution of quinoid derivatives of Nevirapine (NVP) to the toxic responses elicited by the parent drug we have investigated the oxidation of 2-hydroxy-NVP with dipotassium nitroso-disulfonate, mimicking the one-electron oxidation involved in enzyme-mediated metabolic oxidations. The major product was a 1*H*-pyrrole-2,5-dione derivative, the result of an unusual pyridine ring contraction [1]. The supramolecular arrangement of this compound shows a primary pattern of chains formed by N-H···N and weaker C-H···O hydrogen bonds between adjacent molecules. These chains form 2D structures involving $C\text{-}H_{(piridine)}\cdots O_{(succinimide)}$ and $C\text{-}H_{(cyclopropyl)}\cdots O_{(carbonyl)}$ contacts. The final 3D supramolecular structure is obtained by - interactions between succinimide rings. Although the significance of this NVP derivative remains to be established, its availability is a valuable tool to assess its formation *in vivo*. Based upon structural considerations, its reaction with bionucleophiles is conceivable, and a potential role for this compound in the onset of toxic responses elicited by NVP cannot be excluded and will be clarified in further molecular toxicology studies.



[1] Antunes, A., Sidarius, M., Novais, D., Harjivan, S., Santos, P., Ferreira da Silva, J., Beland, F., Marques, M. (2012). *Molecules*, **17**, 2616-2627

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MS23-P7 **Study of pressure-induced structural transformations in bis(glycinium)oxalate.** A. Ivanova,[a] I. Makarova,[a] L. Dubrovinsky,[b] N. Dubrovinskaia,[c] R. Chitra,[d] *[a]A.V.Shubnikov Institute of Crystallography of RAS, Russia, [b]Bayerisches Geoinstitut, University of Bayreuth, Germany, [c]Physics Department, University of Bayreuth, Germany, [d] Solid State Physics Division, Bhabha AtomicResearch Center, India*
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Bis(glycinium) oxalate ($C_2H_6NO_2{\cdot}0.5C_2O_4$) is a complex of glycine, the simplest amino acid, and oxalic acid in 2:1 stochiometric ratio. High-pressure structural investigation of these crystals may provide a significant insight into the nature of weak intermolecular interactions and their dependence on molecular packing that can be helpful in crystal engineering of molecular crystals with desired properties. In this project we have carried out single crystal structure refinement of bis(glycinium) oxalate (a=4.917(1), b=9.957(1), c=10.873(1) Å, β=97.57(0)°, $P2_1/n$, R=0.04) and high-pressure investigation of this crystals by means of Raman spectroscopy. It was found that at pressure above 2GPa the structure transforms to a new phase which quite possible has a non-centrosymmetric space group that was confirmed by appearance of new Raman modes. Some of marked changes were not observed earlier in published powder investigations [1]. This transformation is realized by breaking weak N···HO hydrogen bonds and formation new ones between amino group of glycine molecules and oxalate ions. Above 7 GPa the structure becomes more disorder; some additional changes are observed at 19 GPa, then single-crystal sample breaks.

[1] Chitra, R., Choudhury, R.R. (2007). Acta Cryst. B63, 497–504.

Keywords: high-pressure; raman spectroscopy; glycinium oxalate