

**MS16 P14**

**Crystal structures of two rubrene derivatives** Götz Schuck<sup>a</sup>, Simon Haas<sup>b</sup>, Ulrich Berens<sup>c</sup> and Hans-Jörg Kirner<sup>c</sup>, <sup>a</sup>Laboratory for Neutron Scattering, ETH Zurich & Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, <sup>b</sup>Laboratory for Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland, <sup>c</sup>Ciba Specialty Chemistry Inc., 4002 Basel, Switzerland. E-mail: goetz.schuck@psi.ch

**Keywords: organic transistor material, polymorphism, electrical and optical properties**

The electronic properties of rubrene and rubrene derivatives are of great interest owing to fundamental questions on charge transport and associated applications [1].

One compound, with two polymorphs (A and B) is 5,11-bis-(4-tert-butyl-phenyl)-6,12-diphenyl-naphthacene, a derivate of rubrene where t-butyl sidegroups are added. The electric transport properties of the two polymorphs are completely different: in polymorph B the in-plane hole mobility of 12 cm<sup>2</sup>/Vs measured on single crystal FETs is just as high as in rubrene crystals, whereas polymorph A does not show any measurable field-effect [2]. The crystal structure of polymorph A is monoclinic, with space group P2<sub>1</sub>/c. The unit cell contains four molecules. The molecules form a layered structure, similar to linear acenes such as pentacene with the naphthacene backbone standing upright. The interplanar separation between two adjacent parallel molecules, along the  $\pi$ -stack, corresponds to 3.75 Å in unsubstituted rubrene [3]. Polymorph A has a structure drastically different from the packing of unsubstituted rubrene with enhanced backbone-backbone spacing between two molecules. Remarkably, the naphthacene backbone of the molecules is significantly twisted in polymorph A, with a twist angle of 43° between the two opposite C-C bonds at both ends of the backbone. The resulting backbone-backbone distances are not shorter than 6.5 Å, which is commonly expected to drastically reduce the  $\pi$  -  $\pi^*$  overlap. The structure of polymorph B could not be solved so far, as the material seems to exclusively grow as ultrathin platelets. From measurements of the d-spacing perpendicular to the extended crystal surface [2], a structure closely related to the one found for a constitutional isomer, 5,12-bis-(4-tert-butyl-phenyl)-6,11-diphenyl-naphthacene [4] was assumed for polymorph B.

The crystal structure of the second compound, 5,12-bis-(4-tert-butyl-phenyl)-6,11-diphenyl-naphthacene is orthorhombic, with space group Pnma. The unit cell contains four molecules. In the case of 5,12-bis-(4-tert-butyl-phenyl)-6,11-diphenyl-naphthacene, the in-plane arrangement of the molecules is very similar to that of rubrene [3], with even shorter distances between the naphthacene backbones (3.55 Å compared to 3.74 Å). However, the addition of the t-butyl groups increases the inter-layer spacing by 31%. Interestingly, it leaves the backbone almost perfectly planar.

[1] Sundar, V. C., Zaumseil, J., Podzorov, V., Menard, E., Willett, R. L., Someya, T., Gershenson, M. E. & Rogers, J. A. (2004). *Science*, 303, 1644-1646.

[2] Haas S., Stassen A. F., Schuck G., Pernstich K. P., Gundlach D. J., Batlogg B., Berens U. and Kirner. HJ., submitted to *Phys. Rev. B.*, (2007).

[3] Jurchescu, O. D., Meetsma A. & Palstra T. T. M. (2006), *Acta Cryst. B*62, 330-334.

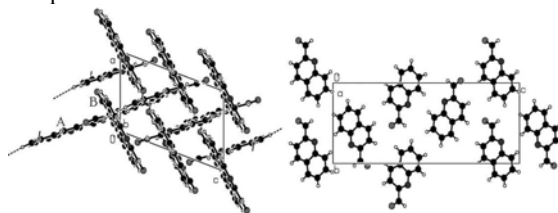
[4] Schuck, G., Haas, S., Stassen, A. F. & B. Batlogg (2007), to be published.

**MS16 P15****Two allotropic forms of 2-quinolinecarboxaldehyde**

M. Ramos Silva<sup>a</sup>, J. A. Silva<sup>b</sup>, C. Cardoso<sup>c</sup>, A. Matos Beja<sup>a</sup>, A. J. F. N. Sobral<sup>b</sup>, N.M.D. Martins<sup>a</sup> <sup>a</sup>CEMDRX, Physics Department, University of Coimbra, 3004-516 Coimbra, Portugal <sup>b</sup>Department of Chemistry, FCTUC, University of Coimbra 3004-535 Coimbra, Portugal <sup>c</sup>CFC, Physics Department, University of Coimbra, 3004-516 Coimbra, Portugal. E-mail: [manuela@pollux.fis.uc.pt](mailto:manuela@pollux.fis.uc.pt)

**Keywords; DFT calculations, allotropes, structure determination**

2,2'-Bipyridine has been used for over a century as the classical N,N'-bidentate ligand in coordination, organometallic and analytical chemistry. N,O-chelating ligands are somewhat less common but for instance 8-hydroxyquinoline and 8-methoxyquinoline has been used as versatile bidentate ligands [1-3]. We present here two distinct crystal structures of 2-quinolinecarboxaldehyde, a compound that we are starting to use as a ligand in metal complexation.



In crystal structure 1 (above figure, left) the molecules crystallize in the space group P2<sub>1</sub>/c with two independent molecules in the unit cell. Molecules A assemble in chains linked through C-H...O intermolecular interactions. These chains aggregate sideways the other symmetry independent molecules (B), again through C-H...O intermolecular interactions. Molecules A and B pack almost perpendicularly to each other forming a slightly distorted squared network. In crystal structure 2 (above figure, right), space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, only one independent molecule exists in the asymmetric unit and the molecules assemble in layers. No C-H...O intermolecular interactions are observed. The cell volume is half the volume of the unit cell of allotrope 1. We have also performed density functional theory calculations within the local density approximation using the code Abinit [4], that allows the calculation of the total energy for a system of molecules.

[1] Brinkmann, M., Gadret, G., Muccini, M., Taliani, C., Masciocchi, N., Sironi, A., *J. Am. Chem. Soc.*, 2000, 122, 5147.

[2] Deacon, G. B., Junk, P. C., Leary, S. G., *Zeit. Anorg. all. Chem.*, 2004, 630, 1541.

[3] Ouyang, J., Xu, Y., Khoo, L. E., *J. Organom. Chem.*, 1998, 561, 143.

[4] Gonze, X., Beuken, J.-M., Caracas, R., Detraux, F., Fuchs, M., Rignanese, G.-M., Sindic, L., Verstraete, M., Zerah, G., Jollet, F., Torrent, M., Roy, A., Mikami, M., Ghosez, Ph., Raty, J.-Y., Allan, D.C., *Computational Materials Science*, 2002, 25, 478.