Poster

Pressure- and temperature-driven polymorphism in PDI-C_6

P. Ratajczyk[1], S. Sobczak[1], M. Andrzejewski[2], M. Marchini[3], F. Marin[3], L. Maini[3], A. Katrusiak[1]

[1]Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland, [2]Paul Scherrer Institute, Forschungsstrasse 111, Villigen CH-5232, Switzerland, [3]Department of Chemistry "G. Ciamician", University of Bologna, via Selmi 2, 40126 Bologna, Italy

paulina.ratajczyk@amu.edu.pl

Organic semiconductors (OSCs) are receiving significant attention for their potential in photovoltaic applications, owing to their light weight, low-cost production, low-temperature processing, mechanical flexibility, and abundant availability. These materials, primarily consisting of π-bonded molecules or polymers made from carbon, nitrogen, oxygen, and hydrogen, can exist in multiple polymorphic forms. For successful commercialization in photovoltaic applications, precise control over these polymorphic forms is essential [1].

Recent advancements in high-pressure techniques have proven effective for modelling structural changes of OSCs, understanding the relationship between their structure and properties [2]. Our research focuses on perylene diimide derivatives (PDIs), which are polyaromatic π-conjugated molecules that belong to the *n*-type semiconducting family, known for their high photo- and thermal-stability, along with chemical inertness [3,4]. Here, we present the study on the pressure- and temperature-induced changes on structure of *N*,*N′*-Dihexyl-3,4,9,10-perylenedicarboximide (PDI-C_6, Fig.1).

Through a combination of differential scanning calorimetry (DSC), synchrotron and in-lab X-ray diffraction on PDI-C_6 single crystals, our investigation revealed the presence of its five distinct phases, including two high-temperature polymorphs (phase II forming at 470 K and phase III at 528 K) and two high-pressure polymorphs (phase IV at 1.05 GPa and phase V at 1.50 GPa). All five phases crystallize in the *P*-1 triclinic space group.

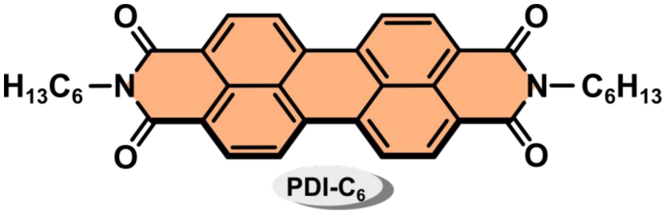

Figure 1. Molecular structure of *N*,*N′*-Dihexyl-3,4,9,10-perylenedicarboximide (PDI-C_6).

[1] Mas-Torrent, M. & Rovira, C. (2011). *Chem Rev*, **111**, 4833–4856.

[2] Coduri, M., Strobel, T. A., Szafrański, M., Katrusiak, A., Mahata, A., Cova, F. H., Bonomi, S., Mosconi, E., Angelis, F. & Malavasi, L. (2019). *J. Phys. Chem. Lett.*, **10**, 7398-7405.

[3] Liu, Z., Wu, Y., Zhang, Q. & Gao, X. (2016). *J. Mater. Chem. A.*, **4**, 17604-17622.

[4] Huang, C., Barlow, S. & Marder, S. R. (2011). *J. Org. Chem.*, **76**, 2386-2407.

P. R. is grateful to the Polish Ministry of Education and Science (Diamentowy Grant DI2019/0160/49) for their financial support).