

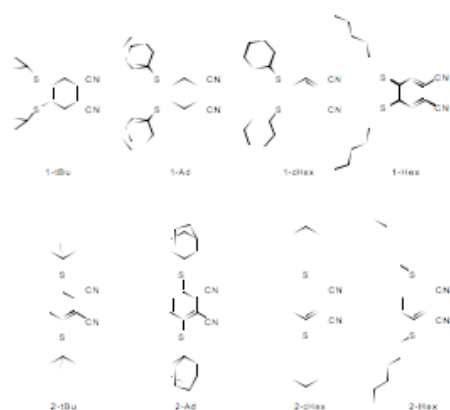
# Poster Presentations

[MS10-P03] **Comparative X-ray structure analyses of 4,5- and 3,6-dialkylsulfanylphthalonitriles of different bulkiness** *Yunus Zorlu, Ümit İşçi, Ufuk Kumru, Fabienne Dumoulin, Vefa Ahsen*

*Department of Chemistry, Gebze Institute of Technology, P.O. Box 141, 41400 Gebze-Kocaeli, Turkey*  
E-mail: yzorlu@gyte.edu.tr

Phthalonitriles are synthetic precursors of phthalocyanines which are used as high-tech materials in important application areas such as photodynamic therapy (PDT), catalysis, liquid crystal, chemical sensors, non-linear optics (NLO) [1]. We have recently established the X-ray crystal structures of phthalonitriles and phthalocyanines of interest in our researches [2,3].

In this study, we comparatively studied the set of eight phthalonitriles shown in Fig. 1, constitute two groups of molecules: 4,5- peripherally substituted phthalonitriles, and corresponding 3,6- non peripherally substituted phthalonitriles. Crystallographic data regarding the tert- butyl derivatives are compared to those of the adamantyl, cyclohexyl and hexylthio derivatives in terms of the influence of the position of the substituents on structural parameters [4].



**Fig. 1** The set of phthalonitriles investigated in this study.

- [1] Photosensitizers in Medicine, Environment, and Security; Nyokong, T.; Ahsen, V. Eds; (2012), Springer.
- [2] U. Kumru, F. Dumoulin, E. Jeanneau, F. Yuksel, Y. Cabezas, Y. Zorlu & V. Ahsen, (2012), *Struct. Chem.* **23**, 175-183.
- [3] Y. Zorlu, U. Kumru, Ü. İşçi, E. Jeanneau, F. Dumoulin & V. Ahsen, *unpublished works*.
- [4] Y. Zorlu, Ü. İşçi, İ. Ün, U. Kumru, F. Dumoulin & V. Ahsen, *Struct. Chem.* DOI 10.1007/s11224-012-0126-8.

**Keywords:** phthalonitriles; X-ray crystallography; comparative structural studies