CRYSTALLOGRAPHIC STUDIES OF TEMPO RADICAL AND ITS NOVEL DERIVATIVES

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2,2,6,6-Tetramethylpiperidine-1-oxyl radical (TEMPO) and its derivatives have gained significant interest due to their functionality in organic synthesis as catalysts [1]. It was reported that they exhibit both ferromagnetism and antiferromagnetism at low temperatures [2]. Furthermore, the TEMPO-related radicals might be also interesting object of crystallographic research.

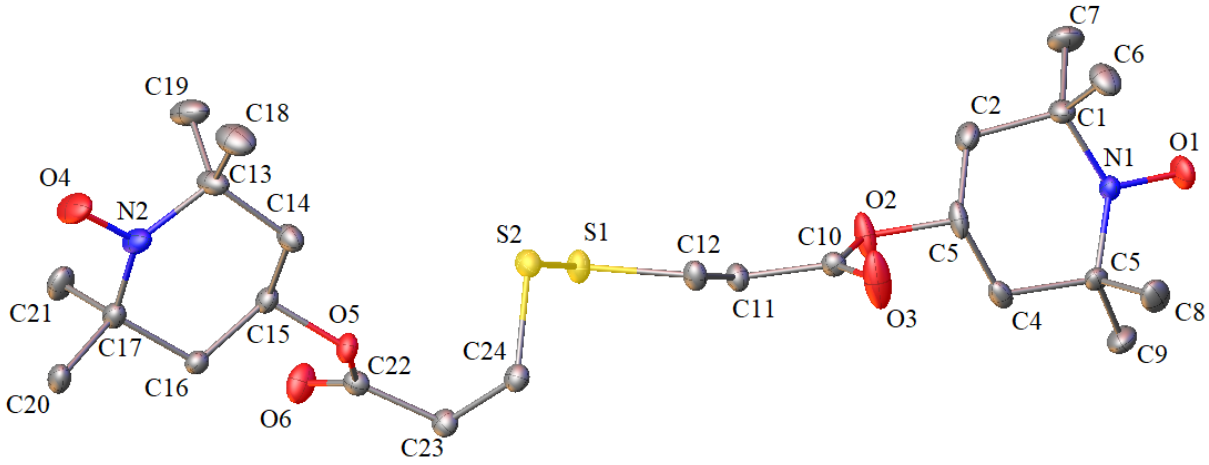

Fig.1. The asymmetric unit of the crystal lattice of DISSPK showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The H-atoms were omitted for clarity.

In this work we focused on TEMPO radical and its novel derivative DISSPK. Both of the compounds' crystals were measured using Agilent Technologies SuperNova Dual Source diffractometer. Diffractometric measurements were performed with CuKα radiation at 100 K.

Although the crystal structure of TEMPO radical is known since 1974 the DISSPK compound have not been characterized yet. In case of both investigated systems the piperidine rings adopt chair conformation with two methyl substituents on each side. Crystallographic analysis revealed that their supramolecular architecture in crystal exhibit different structural features. In this presentation those differences will be discussed in details along with characterization of the significant intermolecular interactions (e.g. hydrogen bonds) occurring in their crystal networks.

„This research was carried out at the Biological and Chemical Research Centre, University of Warsaw, established within the project co-financed by European Union from the European Regional Development Fund under the Operational Programme Innovative Economy, 2007 – 2013. The data collection was accomplished at the Core Facility for Crystallographic and Biophysical research to support the development of medicinal products sponsored by the Foundation for Polish Science (FNP)."

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