

Resolving P-stereogenic enantiomers at nonambient-conditions

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The phosphorus (P)-stereogenic enantiomers are used in many fields of chemistry, for example in chiral catalysis, stereoselective transformation and optical resolution. They are in the forefront of interest in the last decade.

Several dialkyl-arylphosphine oxide compounds have been prepared by Péter Bagi and his co-workers [1]. The newly synthesized phosphorous derivatives are sensitive racemic compounds. Trying several resolving agents, resolution was performed and the enantiomers were separated with (R,R)- or (S,S)-spiro-TADDOL (-1,4-dioxaspiro[4.5]decane-2,3-diylbis(diphenylmethanol)) in gram scale. Some diastereomers of the series (i.e. methylphenylpropylphosphine oxide and ethylphenylpropylphosphine oxide) were crystallized in nitrogen atmosphere, and investigated by single crystal X-ray diffraction (Figure 1). The absolute configurations of the dialkyl-arylphosphine oxides were successfully determined [2]. We present the structures of a few diastereomers formed using TADDOL, where the SXRD results revealed the main interactions which contribute to the enantiomeric recognition. Hirshfeld surface analysis and DFT calculation were performed using the software Crystal Explorer in order to understand the secondary interaction network.

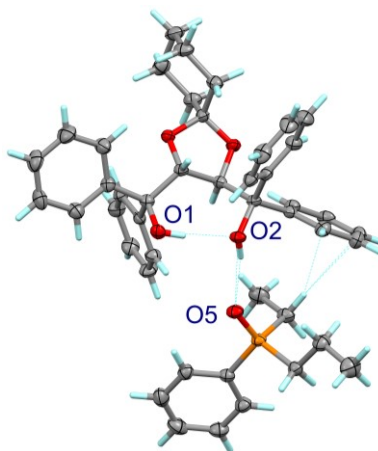


Figure 1. The asymmetric unit of (1,4-dioxaspiro[4.5]decane-2,3-diyl)bis(diphenylmethanol) and ethyl(phenyl)n-propylphosphine oxide crystal system

[1] Bagi, P. Ujj, V. Czugler, M. Fogassy, E. Keglevich, G. (2016). Dalton Trans., 45, 1823.

[2] Varga, B. Herbay, R. Székely, G. Holczbauer, T. Madarász, J. Mátravölgyi, B. Fogassy, E. Keglevich, G. Bagi, P. (2020). Eur. J. Org. Chem. 12, 1840.

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