PS-19-10 Poster Session

Nitroxide with diphenylphosphino moiety: synthesis, supramolecular structure, biology and catalysis

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The coupling of nitroxide and tertiary phosphane moieties offer unique opportunities in synthesis and catalysis as well as in biological effects. Surprisingly, no crystal structure report is found in CSD [1] for tertiary phosphane substituted pyrroline nitroxide. We first reported such structure [2] and synthesis of 3-(diphenylphosphino)-2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrol-1-yloxyl radical, I, Fig.1., left. Structural data clearly indicate the expected nitroxide radical. Analysis of supramolecular structure gave interesting results (Fig. 1., right). A simple derivative had shown better antiproliferative effect on MDA-MB-231 and MCF-7 human breast cancer lines than MITO-CP indicating the potential of the compound for use in cancer therapy [3]. Moreover, inclusion of phosphane and nitroxide moiety into the same ligand suggest versatile homogeneous catalytic activity by both metal center and ligand assisted mechanisms and they may serve as organocatalysts, too. Further studies to explore these potentials are under way in our laboratories.

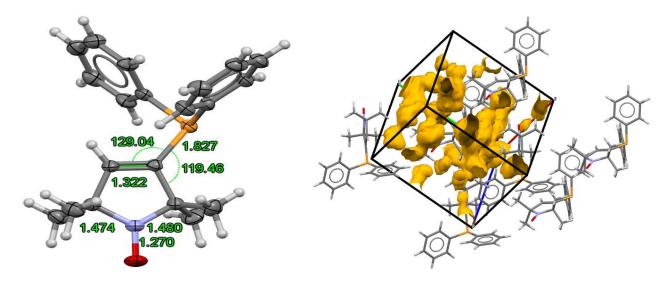


Figure 1. ORTEP view of *I* with selected bond length (Å) and angle (°) data (left) and packing diagram (right) showing voids with a small probe.

- [1] Groom, C.R., Bruno, I.J., Lightfoot, M.P., Ward, S.C. (2016), Acta Cryst. B72, 171-179. DOI: 10.1107/S2052520616003954
- [2] Isbera, M., Bognár, B. Gallyas, F., Bényei, A. Jekő, J. & Kálai, T. (2021). Molecules, in press.
- [3] Andreidesz, K., Szabó, A., Kovács, D., Kőszegi, B., Vantus, V.B., Isbera, M., Kálai, T., Bognár, Z., Kovács, K., Gallyas, F. (2021). International Journal of Molecular Sciences, submitted for publication

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