Synthesis, crystal structure and ESR study of some new phosphoylated spin traps

Yang Liu[1], Ying-kai Xu[1], Jian Sun[2], Zhong-wei Chen[1] and Ke Liu[1]

[1]Institute of Chemistry, The Chinese Academy of Sciences, Beijing 100080, China

[2]Dept of Biochemistry, Dartmouth Medical School, Hanover, New Hampshire 03756

Synthesis of new a-phosphorus-containing spin traps, such as 2-(Diethoxyphosphoryl)-2-phenethyl-3,4-dihydro-2H-pyrrole 1-Oxide(DEPPEPO) and 2-(Diethoxyphosphoryl)-2, 5–dimethyl-3,4-dihydro-2H-pyrrole 1-Oxide (DEPDMPO), characterization of their molecular structures and the evaluation of their ability to trap oxygen radicals have been described in this report. Single crystal X-ray structure analysis of DEPPEPO reveals that there exists a pair of enantiomers in the solid state. The phenethyl in DEPPEPO locates out of the nitronyl plane and also far away from the diethoxyphosphoryl group. One side of the nitronyl face is probably hindered by phosphoryl oxygen, which might be responsible for the stereo-selection of the free radical additions on the nitronyl moiety. Comparing with DEPMPO, DEPPEPO is more lipophilic(partition coefficient in 1-octanol/water is 7.6) that contributed by the 2-phenethyl substitutions. The ESR spectral simplification on the corresponding spin adducts can be performed by DEPDMPO, a 5-methyl substituted analogue of DEPMPO. Finally, the stability of the superoxide spin adducts formed with DEPMPO, DEPPEPO, DEPDMPO, DMPO and M3PO were comparatively evaluated according to their molecular structures.

[1]. Y. K. Xu, J. Sun, K. Liu, Z. W. Chen, Y. Liu, *Chem. J. Chin. Uni.*, **22,** 1732-34, 2001