

Conformation of Dioxaphosphopin Ring – Structures of 6-Substituted Benzo and Dibenzo [d,f] [1,3,2] Dioxaphosphopin 6-oxide (I) and Sulphide (II)

Musali Krishnaiah¹, J. Radha Krishna¹, Vedavathi G., Purank²,

¹*Department of Physics, Sri Venkateswara University, Tirupati-517502.* ²*Center of Material Characterization, National Chemical Laboratory, Pune – 411 008, INDIA.* E-mail: mkphysvu@yahoo.co.in

The hetro cyclic form of organophosphorous compounds containing phosphoryl unit with suitable substitution exhibits significant physiological activity and they have unique multifaceted applications. Structural studies of organophosphorous compounds have gained considerable importance recently because of their use as insecticides, anti-cancer agents, lubricating oil additives and polymer stabilizers. As part of our continuing investigations on this molecules, we have investigated the structures of 6-substituted benzo and dibenzo [d,f] [1,3,2] dioxaphosphopin 6-oxide and sulphide to know the dependence of substituents on the conformation and geometrical parameters of dioxaphosphin hetro ring. compound (I): C₁₅ H₁₅ O₄ P, colourless crystals grown from methanol are Monoclinic P₂₁/c with a = 9.441(1) ; b = 15.202(2) and c = 9.746(1)Å ; β = 95.8(2)°; V = 1391.5(3) Å³; Z = 4; F(000) = 608; ρ_c = 1.385 g cm⁻³; μ(Mo Kα) = 2.08 cm⁻¹; R=4.96 and R_w = 0.1157 for 2457 unique reflections. compound (II): C₁₈ H₁₁ O₃ Cl₂ P S, colourless crystals obtained from 2-propanol, Monoclinic P₂₁/n with a = 10.816(6) ; b = 13.615(8) and c = 12.321(7)Å ; β = 99.6(9)°; V = 1789.5(2) Å³; ρ_c = 1.519 g cm⁻³; Z = 4; F(000) = 832; λ(Mo Kα) = 0.71073 Å ; R=0.048 and R_w = 0.130 for 2410 unique reflections. based on intensity data collected on Bruker Smart Apex diffractometer using Monochromated MoKα radiation, structures were solved by the direct methods and refined by full-matrix least squares methods. The seven membered dioxaphosphin ring exhibits a pseudo- chair form for the former where as a distorted boat like conformation for the later. This is evident for the structural changes with different substituents fused to the hetro ring and also attached to the phosphorous.

Keywords: organophosphorous compounds, conformation of dioxaphosphopin ring, seven membered hetro ring