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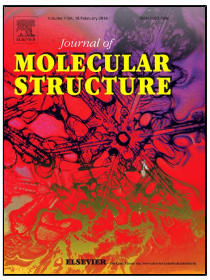

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Synthesis, characterization, single crystal X-ray and DFT analysis of disubstituted phosphorodithioates

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Abstract:

Disubstituted phosphorodithioates of the type [{(2,5-CH_3)$_2$$C_6H_3O$}$_2$$PS_2HNEt_3$] (**1**) and [{(3,5-$CH_3$)$_2$$C_6H_3O$)$_2$($PS_2$)}$_2$] (**2**) were synthesised and characterized by IR and NMR (^{1}H,^{13}C and ^{31}P) spectroscopic studies and as single crystal X-ray analysis. The compound **1** crystallizes in monoclinic space group $P2_1/c$ whereas compound **2** crystallizes in triclinic space group $P\bar{1}$. The X-ray analysis reveals that in compound **1** phosphorus atom is coordinated to the two S and two O atoms to form tetrahedral geometry. The structure is stabilized by cation–anion N–H···S hydrogen bonded interactions. In compound **2,** the two phosphorus atoms have a distorted tetrahedral geometry coordinated to two (3,5-CH_3)$_2$$C_6H_3O$ groups. The molecule possesses a crystallographic center of symmetry and consists of *zig-zag* array of S=P–S–S–P=S linkages with two diphenyldithiophosphate moieties in the *trans* configuration. Molecular geometries,

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