

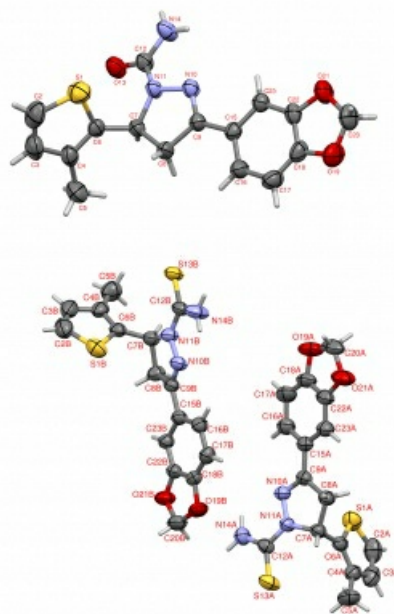
*Crystal structure and hirshfeld surface analysis of novel pyrazole derivatives*Karthik Kumara¹, Naveen S², Lokanath N K¹¹DoS In Physics, University Of Mysore, Mysuru, India, ²Institution of Excellence, Vijnana Bhavana, University of Mysore, Mysuru, India

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New pyrozole derivatives, 3-(benzo[d][1,3]dioxol-5-yl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide (I) and 3-(benzo[d][1,3]dioxol-5-yl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carbothioamide (II) are synthesized. These compounds were characterized using elemental analyses, ¹H NMR, ¹³C NMR and mass spectral studies. Finally the molecular structures were confirmed by single crystal X-ray diffraction method. Both compounds (I) and (II) crystallizes in the triclinic crystal system, P $\bar{1}$ space group. The crystal structures revealed that the five membered pyrazole ring adopts E-form conformation. The crystal structures are stabilized by inter molecular hydrogen bonds, C—H...O and C—H...S chains build up two dimensional arrays, which are extended to 3D network. The bridging of molecules through N—H...O hydrogen bond interactions between amidogen and oxygen atom (compound I), and N—H...S, between amidogen and sulphur atom (compound II) form R²₂ (8) ring motif. The cooperative mode of these hydrogen bonding linkages forms supramolecular self-assembly. Further, Hirshfeld surface analysis was carried out to quantify the intermolecular contacts, which are involved in the formation of supramolecular architecture.

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