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Solid State Structure of 1,2,3-selenadiazole Derivatives. Nigam P. Rath^a, A. Marx^b, V. Manivannan^b, S. Saravanan^c, S. Muthusubramanian^c, ^aDept. of Chemistry and Biochemistry, Univ. of Missouri- St. Louis, ^bDept. of Physics, Presidency College, Chennai-600005, India, ^cDept. of Organic Chemistry, Madurai Kamaraj Univ., Madurai-625021, India.

Heterocyclic compounds containing selenium are of interest due to their biological and synthetic applications. 1,2,3-selenadiazoles have attracted much attention as versatile intermediates in organic synthesis and for their biological properties. For example, some of the 1,2,3-selenadiazole derivatives exhibit antifungal, antibacterial, antimicrobial and insecticidal activities. As naturally occurring nitro compounds exhibit broad antibiotic activity and certain alkyl nitro compounds exhibit antitumor activity we decided to synthesize and structurally characterize a set of 1,2,3-selenadiazoles with nitro group in the side chain. Geometrically, the conformation around the CH-CH in the side chain and the possible hydrogen bonding of nitro group with other substituents in the ring in the solid state and in solution may be of interest in these compounds. In order to better understand the structural properties of these compounds we have determined the solid state structure of several 1,2,3-selenadiazoles using single crystal x-ray diffraction studies. The results of these studies will be presented in this poster.