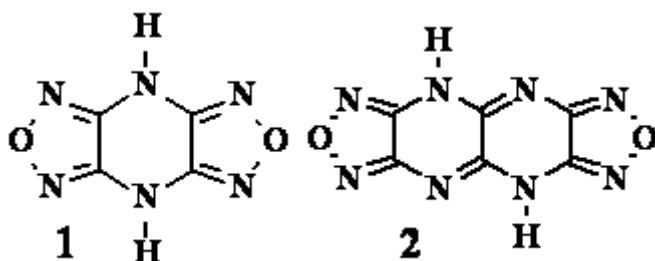


Experimental Investigation of Stacking Interaction in Furazan Derivatives. Boris Averkiev¹, Konstantin Lyssenko, Mikhail Antipin^{1,2}, Aleksey Sheremetev³, and Tatiana Timofeeva¹, ¹Dept. of Natural Sciences, New Mexico Highlands Univ., Las Vegas, New Mexico, USA, ²Inst. of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia, ³N.D. Zelinsky Inst. of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia.

The crystal structures of furazan derivatives **1** and **2** have been studied by X-ray analysis. These structures possess interesting features: the densities of structures (2.032 (**1**) and 1.882 (**2**) g cm⁻³) are very high for organic compounds. Also there are rather short interplanar distances between overlapping molecules (3.086 (**1**) and 2 3.118 (**2**) Å). Such shorten interplanar contacts suggest the presence of stacking interaction



between molecules. To visualize the presence of such interaction we carried out high-resolution low-temperature X-ray diffraction experiments. Obtained electron density distribution was analyzed in the framework of Bader's theory of "Atoms in Molecules" (AIM). This analysis showed the presence of critical points (3, -1) in the area

between overlapping molecules. In AIM theory (3, -1) points correspond to chemical bonding. The analysis of properties of the critical points showed that this is a weak interaction, analogues to other specific interactions, such as O...O, N...H, which were also observed in these crystals.