MOLECULAR STRUCTURE OF 2-METHOXY-4-PYRROLIDINYL-6-TRINITROMETHYL-1,3,5-TRIAZINE

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An X-ray diffraction study of 2-methoxy-4-pyrrolidinyl-6-trinitromethyl-1,3,5-triazine was carried out. The crystals are triclinic; $C_9H_{11}N_7O_7$; $M = 329.25$; $a = 8.536(1)$ Å, $b = 9.378(2)$ Å, $c = 9.7401(8)$ Å; $\alpha = 79.13(1)°$, $\beta = 73.974(8)°$; $\gamma = 72.76(1)°$; $V = 710.8(2)$ Å^3, $d_c = 1.54$ g/cm^3, $Z = 2$, space group $P\bar{1}$. The molecule on the whole is planar, except the pyrrolidine ring, which has a *twist* conformation. No significant π–π interactions and hydrogen bonds of C–H···N or C–H···O type were found in the crystal, and the molecule packing is stabilized only due to van der Waals interactions.

Keywords: organic chemistry, crystal structure, 2-methoxy-4-pyrrolidinyl-6-trinitromethyl-1,3,5-triazine.