

Preparation and X-Ray Structure of 3,5-Dimethyl-1,4-dichloro-1,2,6-thiadiazine-1-oxide

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Crystal Structure, 1,2,6-Thiadiazines, Sulfanuric Chloride

The title compound was obtained by the reaction of 3,5-dimethyl-2*H*-1,2,6-thiadiazine-1,1-dioxide with PCl_5 in chloroform. It crystallizes in the monoclinic system, space group $P2_1/c$, $a = 7.521(7) \text{ \AA}$, $b = 8.400(4) \text{ \AA}$, $c = 13.908(4) \text{ \AA}$, $\beta = 100.35(4)^\circ$, $V = 864.4(8) \text{ \AA}^3$, and $Z = 4$. The S(VI) atom lies 0.43 \AA out of the plane of the π -delocalized NCCCN unit. The mean S-N bond distance is $1.569(3) \text{ \AA}$.

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