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Crystal structure analysis of Methyl-1-methyl-8-nitro-3-phenyl-1,2,3,9b-tetrahydrothiochromeno[4,3-b]pyrrole-3a(4H)-carboxylate

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Abstract : The title compound, $C_{20}H_{20}N_2O_4S$, has been synthesized and characterized by X-ray crystallography. The structure is solved in monoclinic with space group $C2/c$ with $a = 22.368(3)\text{\AA}$, $b = 8.1187(10)\text{\AA}$, $c = 20.185(3)\text{\AA}$, $\beta = 94.472(6)^\circ$, $V = 3654.4(9)\text{\AA}^3$, $Z = 8$. The pyrrole ring adopts an envelope conformation with C9 atom at the flap, deviating from the mean plane defined by the plane of the other ring atoms by 0.708\AA . Crystal data were collected using BRUKER SMART APEX II CCD X-ray diffractometer. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares procedures to the final R_1 of 0.040 using SHELXL programs.

Key Words : Pyyrole, thiochromene and crystal structure.

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