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## ABSTRACT BOOK

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# Synthesis, characterization and crystal structure of *N*-((3-methoxyphenyl)carbamothioyl)cyclohexanecarboxamide

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*N*-((3-Methoxyphenyl)carbamothioyl)cyclohexanecarboxamide was synthesized in excellent yield following the method described by Douglass and Dains [1]. The obtained compound was characterized by elemental analyses, IR spectroscopy and $^1$H NMR spectroscopy. Title compound was also characterized by a single crystal X-ray diffraction study. Molecule formula of this compound, $C_{15}H_{20}N_2O_2S$: monoclinic, space group C2/c (no. 15), $a$ = 16.454(3) Å, $b$ = 6.6034(13) Å, $c$ = 28.559(6) Å, $\beta$ = 106.51(3)°, $V$ = 2975.0(10) Å$^3$, $Z$ = 8, μ(MoKα) = 0.221 mm$^{-1}$, *Dcalc* = 1.306 g/mm$^3$, 8979 reflections measured (5.96 ≤ 2Θ ≤ 50.3), 2643 unique ($R_{int}$ = 0.0318) which were used in all calculations. The final $R_1$ was 0.0328 (>2sigma(I)) and $wR_2$ was 0.0683 (all data). The bond lengths and angles in the thiourea moiety are typical for thiourea derivatives; the C8-S1 and C9-O1 bonds both show a typical double-bond character with 1.672(2) and 1.228(2) Å, respectively. The intramolecular hydrogen bond N1-H1···O1 (1.882(1) Å) forms a 6-membered ring with C8, N2 and C9 [2].

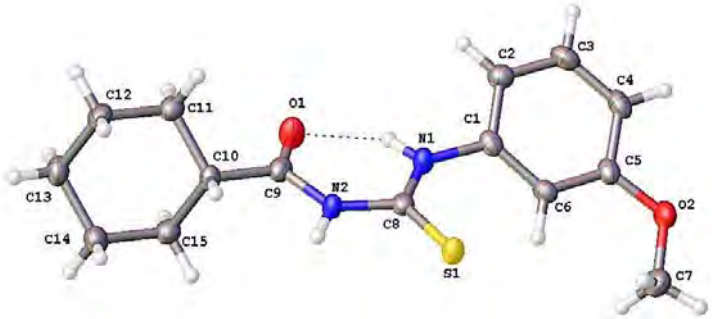


Figure 1. Molecular structure of title compound.

***Keywords*:** Thiourea, Cyclohexanecarboxamide, X-ray single crystal diffraction, Synthesis, Thiourea derivatives.

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