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Molecular structure of novel photoacylotropic (2*Z*)-2-(*N*-acyl-*N*-arylaminomethene)benzo[*b*]thiophene-3(2*H*)-ona with migrating chiral group

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Abstract

X-ray diffraction analyses of novel photoacylotropic (2*Z*)-2-(*N*-acyl–*N*-arylaminomethene)benzo[b]thiophene-3(2*H*)-ona with migrating chiral group has been carried out and characteristics of its molecular structure have been discussed.

Non-empirical calculations (B3LYP/LANL2DZ approximation) of this compound have been performed with full optimization of geometry. It has been shown that fragments – phthalimidic, anisolic and benzo[b]thiophenic are structurally hard elements of this connection and the influence of crystalline environment on their geometric structure is reduced to their insignificant mutual turn.