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Theoretical study of 3-(4-chlorophenyl)-2,1-benzisoxazole-5-carbonyl chloride structure

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Abstract

Optimized molecular geometry, bond order, charges on each atom of 3-(4-chlorophenyl)-2,1-benzisoxazole-5-carbonyl chloride were modeled by different quantum chemistry methods. Results of modeling by semi-empirical quantum chemistry methods PM3 and PM6, *ab initio* HF and MP2 methods were compared with X-Ray Structural Analysis data. Mulliken atom charge analysis was done. Intermolecular interactions were detected.