Synthesis, crystal structure and theoretical calculations of *N*-benzyl-1-(5-(3-chlorophenyl)-1,3,4-oxadiazol-2-yl)cyclopentanamine.

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Streszczenie

N-benzyl-1-(5-(3-chlorophenyl)-1,3,4-oxadiazol-2-yl)cyclopentanamine was syn- thesized via one-pot reaction of appropriate benzylamine, cyclopentanone, (N-isocyanimino)tri-phenylphosphorane and m-chlorobenzoic acid. The quantum theoretical calculations for crystal structure were performed by density functional theory (DFT/B3LYP/6-311+G*). From the optimized structure, geometric parameters were obtained and experimental measurements were compared with the calculated data. Frontier molecular orbitals (FMOs), total density of states (DOS), molecular electrostatic potential (MEP), molecular properties, natural charges, NMR parameters and NBO analysis for the product were investigated by theoretical calculations.

Słowa kluczowe

N-isocyaniminotriphenylphosphorane, cyclopentanone, m-chlorobenzoic acid, 1,3,4-oxadiazole, aza-Wittig reaction, DFT, NBO analysis

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