

INFLUENCE OF AROMATIC SUBSTITUENTS ON THE SYNTHESIS OF SCHIFF BASES DERIVED FROM TRANS-(*R,R*)-DIAMINOCYCLOHEXANE: A SPECTROPHOTOMETRIC AND DFT B3LYP STUDY

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Abstract. In this work, the synthesis of Schiff bases derived from trans-(*R,R*)-diaminocyclohexane by microwave irradiation (MW) is presented. The reaction yields varied between 31% and 69%, being influenced by the electronic nature of the substituents (H, Cl, Br, NO₂, MeO, *t*-BuO, BnO, and 4-(4-Me)PhO) and the reaction temperature. The spectrophotometric properties of the products were investigated by UV-Vis spectrophotometry, revealing bathochromic and hypsochromic effects attributable to the different substituent groups. These effects were interpreted by DFT calculations with the B3LYP functional using the 6-311G(d,p) basis set. The results suggest that the electronic properties of the substituents in the *para* position have a significant impact on the spectroscopic characteristics of the Schiff bases. The synthesized Schiff bases exhibit great potential for applications in areas such as optical sensors and functional materials, as the substituents can precisely modulate their spectrophotometric properties. This opens up new opportunities for designing compounds with tunable properties for various technological and scientific applications.

Keywords: Schiff base, MW irradiation, substituent effect, spectrophotometric property, DFT calculation.

Received: 15 September 2025/Revised final: 28 November 2025/Accepted: 1 December 2025
