INTRAMOLECULAR-PROTON TRANSFER, EXPERIMENTAL AND THEORETICAL CHARACTERIZATION OF 3,3′-DIHYDROXY-4,4′-[4,4′-DIPHENYLMETHANEBIS (NITRILOMETHYLIDYNE)]-bis-PHENOL

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A newly synthesized Schiff base 3,3′-dihydroxy-4,4′-[4,4′-diphenylmethanebis(nitrilomethylidyne)]-bis-phenol is characterized experimentally. Also, the geometry optimization for the tautomers, tautomerism and assignment of the IR bands and NMR chemical shifts of the Schiff base were performed using the DFT method. Good consistency between the theoretical and experimental results confirms the validity of the optimized geometry. Geometries of four possible tautomers are fully optimized. None of them has a planar structure, but each of the benzene rings is in a separate plane. In the most stable tautomer **L1**, the phenolic protons are engaged in the intramolecular-hydrogen bond with the azomethine nitrogen atoms. Tautomerization of **L1** can occur in two different pathways which are computationally studied using DFT and the Atoms In Molecules (AIM) analysis. Both pathways have the same barrier energy.

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