Conformations and Structures of N,N’-Bis(2-methoxybenzylidene)-
1,3-diamino-propanol and N,N’-Bis(3-methoxybenzylidene)-1,3-
diamino-propanol

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N,N’-bis(2-methoxybenzylidene)-1,3-diamino-propanol (C\textsubscript{19}H\textsubscript{22}N\textsubscript{2}O\textsubscript{4}) \textsuperscript{1} and N,N’-bis(3-methoxybenzylidene)-1,3-diamino-propanol (C\textsubscript{19}H\textsubscript{22}N\textsubscript{2}O\textsubscript{4}) \textsuperscript{2} have been investigated by X-ray analysis and AM1 semi-empirical quantum mechanical method. \textsuperscript{1} is in the monoclinic space group C2/c with \(a = 33.694(6), b = 6.735(1), c = 17.681(3) \, \text{Å}, \beta = 114.72(2)^\circ, V = 3645(1) \, \text{Å}^3, Z = 8, D_c = 1.248 \, \text{mg} \, \text{cm}^{-3}\) and \(\mu(\text{Mo-K}\alpha) = 0.088 \, \text{mm}^{-1}\). \textsuperscript{2} is in the monoclinic space group C2/c with \(a = 19.173(4), b = 7.626(2), c = 11.788(2) \, \text{Å}, \beta = 91.72(2)^\circ, V = 1722.8(6) \, \text{Å}^3, Z = 4, D_c = 1.320 \, \text{mg} \, \text{cm}^{-3}\) and \(\mu(\text{Mo-K}\alpha) = 0.093 \, \text{mm}^{-1}\). The crystal structures of \textsuperscript{1} and \textsuperscript{2} were solved by direct methods and refined to \(R = 0.053\) for \textsuperscript{1} and \(R = 0.041\) for \textsuperscript{2}. Both molecules are not planar and \textsuperscript{2} has twofold axes on C9 atom. Intramolecular hydrogen bonds occur between O1 and N1 [2.541(3) \, \text{Å}] and between O3 and N2 [2.573(4) \, \text{Å}] atoms for \textsuperscript{1} and between O1 and N1 [2.631(2) \, \text{Å}] atoms for \textsuperscript{2}. The optimized geometries of the crystal structures of \textsuperscript{1} and \textsuperscript{2} corresponding to non-planar conformation are the most stable conformation in all calculations. The results strongly indicate that the minimum energy conformation is primarily determined by non-bonded hydrogen-hydrogen and hydrogen-carbon repulsions.

\textit{Key words:} X-Ray, Schiff Base, AM1, Photochromism, Thermochromism