

FTIR Conformational Studies of Triclosan in an Argon Matrix

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The preferred conformations of triclosan, a commonly used antibacterial and antifungal agent, and their vibrational spectra were studied by matrix-isolation Fourier transform infrared spectroscopy in argon matrix ($T = 13$ K), and interpreted on the basis of DFT(B3LYP)/6-311++G(d,p) calculations. The calculated ground-state potential energy surface of triclosan exhibits two low-energy minima (Figure 1), differing by orientation of the C1-C6-O7-C8 (β_1) and C6-O7-C8-C9 (β_2) dihedral angles. The most stable conformer I ($\beta_1 = 160.3^\circ$, $\beta_2 = 123.8^\circ$) was found to be lower in energy at 0 K, by *ca.* 1.4 kJ mol⁻¹, than conformer II ($\beta_1 = -93.1^\circ$, $\beta_2 = 177.7^\circ$). At room temperature, due to the higher entropy of conformer I, the order of conformational stability is reverse and is *ca.* 0.73 kJ mol⁻¹ in favour of form II. Therefore, I and II are expected to constitute *ca.* 43% and 57% of the total population in gas phase, at room temperature. The barrier for conversion between forms I and II was calculated to be *ca.* 15 kJ mol⁻¹. The IR spectrum of the compound isolated in solid argon was obtained and interpreted. Preliminary photochemical experiments on the matrix-isolated triclosan were also undertaken. The compound was found to react upon UV irradiation ($\lambda > 200$ nm) giving rise to a ketene, which is identifiable by observation of the ketene antisymmetric stretching characteristic intense IR band around 2140 cm⁻¹.

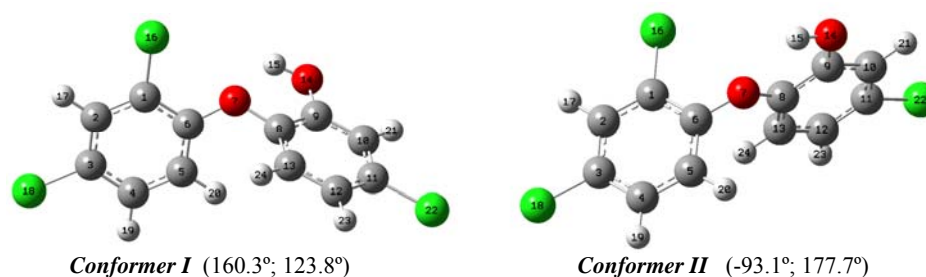


Figure 1 - Calculated conformers of triclosan. Values in parenthesis are C1-C6-O7-C8 and C6-O7-C8-C9 dihedrals.