QUANTUM CHEMICAL AND MICROWAVE SPECTROSCOPIC ANALYSIS OF 1-CYANOPROPENE AND 1-CHLOROPROPENE

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The 1-cyanopropene and 1-chloropropene molecules are methylated derivatives of propene which contain a nitrogen and a chlorine atom, respectively. They belong to a group of important substances playing a major role in astrophysics[1] and atmospheric chemistry. The aim of this work is to study their gas phase structures using a combination of pulsed molecular jet Fourier transform microwave spectroscopy and quantum chemical calculations. The microwave spectra were measured in the frequency range from 2 to 40 GHz. Quantum chemical calculations were performed at the B3LYP-D3BJ/6-311++G(d,p), MP2/6-311++G(d,p), and MP2/6-31G(d,p) levels of theory to obtain the optimized molecular geometries. Due to internal rotation of the methyl group, all rotational transitions split into an A and an E torsional species. In addition, each of these two torsional species contains further hyperfine splittings arising from the quadrupole coupling of the nitrogen as well as the chlorine nucleus. The complex spectral splittings were analyzed and modeled using the *XIAM*[2] and the *BELGI*[3,4] programs to obtain experimental molecular parameters and validate the quantum chemical results.

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