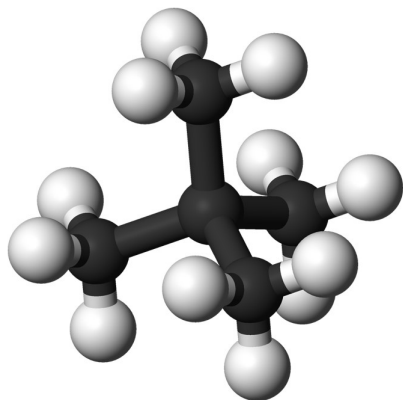


HIGH RESOLUTION INFRARED SPECTRA OF NEOPENTANE: ROVIBRATIONAL ANALYSIS OF BANDS AT 8.3-6.4 μm

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1472.5 and 1489 cm^{-1} .

New high resolution (0.0014 cm^{-1}) infrared spectra of neopentane (2,2-dimethylpropane) have been recorded at 203 K by use of synchrotron radiation (Canadian Light Source). Spectra were recorded in the IR (8.3-6.4 μm) with 8 m of optical path. Neopentane is a spherical top molecule with T_d (tetrahedral) symmetry. A low temperature is favorable for a detailed rotational analysis of its fundamental bands. This study focuses on the analysis of 3 band systems of neopentane. The first system is a dyad consisting of a ν_{15} fundamental band and a $\nu_7 + \nu_{19}$ combination band located at 1472.5 and 1489 cm^{-1} , respectively. The second system is a ν_{16} fundamental band located at 1369.4 cm^{-1} with uncertain band origin. The third band system is a dyad of a ν_{17} fundamental and a $\nu_8 + \nu_{18}$ combination band. Only the ν_{17} fundamental band was analyzed in this last system due to the weaker structure of the combination band. For all spectral simulations and calculations the 'XTDS' program based on the tensorial formalism by V. Boudon was used. A subprogram 'SPVIEW', paired with XTDS, was used for spectral assignment.

A special emphasis will be given to the first dyad located at