

## HIGH RESOLUTION INFRARED SPECTROSCOPY OF NEOPENTANE

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Neopentane (2,2-dimethyl propane,  $C_5H_{12}$ ) is an unusual hydrocarbon with tetrahedral symmetry like methane. Neopentane may be formed by organic photochemistry chemistry in the atmosphere of Titan, the largest moon of Saturn, in which 9 hydrocarbons have already been discovered, including allene that was detected very recently by high resolution infrared emission spectroscopy.

High resolution infrared absorption spectra of neopentane have been recorded in the mid-infrared region at room temperature and 232 K. Neopentane is a spherical top with  $T_d$  symmetry. Four strong bands with characteristic rotational structure of  $t_2$  modes were observed at 1257.6, 1369.4, 1472.5 and 1489.0  $cm^{-1}$ , and a fifth very weak band was found near 924.2  $cm^{-1}$ . Quantum chemical calculations (B3LYP/6-311++(d,p)/VPT2 and harmonic CCSD(T)-pVTZ) were carried out in both normal and local mode representations to help with the vibrational assignments:  $\nu_{18}$  (924.2  $cm^{-1}$ ),  $\nu_{17}$  (1257.6  $cm^{-1}$ ),  $\nu_{16}$  (1369.4  $cm^{-1}$ ) and the 1472.5 and 1489.0  $cm^{-1}$  bands are a Fermi resonance pair between the  $\nu_{15}$  fundamental and the  $\nu_7 + \nu_{19}$  combination mode. A rotational analysis of the two Fermi resonance bands was successful. There is also a weaker Fermi resonance interaction between the  $\nu_{17}$  fundamental and the  $\nu_8 + \nu_{18}$  combination mode.