BROADBAND ROTATIONAL SPECTRA OF THE SOMAN-RELATED COMPOUNDS: PINACOLYL ALCOHOL AND PINACOLONE

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The related pair of compounds, pinacolyl alcohol and pinacolone, are reaction precursors/degradation products related to the nerve gas, Soman. Here, the rotational spectra of pinacolyl alcohol $(CH_3)_3CC(OH)CH_3$ and pinacolone $(CH_3)_3CC(=O)CH_3$ have been recorded on the University of Virginia CP-FTMW instrument and the cavity mini-FTMW spectrometers at NIST and the University of Virginia. The rotational constants of the alcohol are: A = 3085 MHz, B = 2226 MHz, C = 1859 MHz. No internal rotor splittings from the lone methyl top are observed for the alcohol. For pinacolone, the rotational constants for the A-state are A = 3192 MHz, B = 2293 MHz, C = 1928 MHz. For pinacolone, in addition to the A-state transitions, a number of transitions have been observed that are believed to arise from splittings caused by internal rotation of the lone methyl top in the molecule. The barrier to internal rotation is calculated to be 93 $cm^{-1}$ at the MP2/6-311++G(d,p) level. Rotational assignments of the E-state transitions are pending.