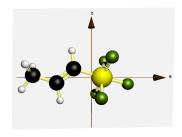
FURTHER STUDIES OF A FOUR-FOLD BARRIER TO INTERNAL ROTATION: THE ROTATIONAL SPECTRA OF PROPEN-1-YLSULFUR PENTAFLUORIDE AND BUTEN-1-YLSULFUR PENTAFLUORIDE

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The rotational spectra of the two title molecules and several isotopologues have been recorded in the frequency region of 6 GHz to 20 GHz using Fourier transform microwave spectroscopy.

For propen-1-ylsulfur pentafluoride, triplets of rotational transitions were observed appropriate for the A, B, and doubly degenerate E torsional substates arising from the four-fold barrier to internal rotation of the $-SF_5$ group against the propen-1-yl frame. However, the observed splittings, which are on the order of tens of kHz, were considerably smaller in magnitude than those analogous splittings observed in the spectra of the vinylsulfur pentafluoride, which were on the order of thousands of kHz. For the buten-1-ylsulfur pentafluoride, for which two conformers have been observed, at the resolution of the chirped pulse FTMW spectrometer used, splittings were not observable and the observed spectrum could be fit using the Hamiltonian of a semi-rigid rotor. Further experiments using a cavity FTMW spectrometer are underway. Constants from the spectral



analyses, together with the results of quantum chemical calculations have allowed for the alkene- SF_5 barrier to internal rotation to be examined as a function of alkene chain length and the results will be presented.