3-BUTENESELENOL: MICROWAVE SPECTRUM AND AB INITIO CALCULATIONS

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3-Buteneselenol H_2C=CHCH_2CH_2SeH was investigated by microwave Fourier transform (5-20 GHz) and microwave Stark (24-62 GHz) spectroscopies. The spectra look rather complex due to the large number of possible conformers (15) and the number of isotopic species for selenium (6). Moreover in the Stark spectra the low-lying excited states are also detected. Quantum mechanical calculations (G2 method at the MP2 and B3LYP levels of theory) were carried to precise the relative energies of all these conformers. Their geometrical structures, centrifugal distortion constants and dipole moments were also calculated, leading to the identification of the three more stable conformers. The most stable conformer exhibits an intramolecular hydrogen bond involving the selenium atom.