THE ROTATIONAL SPECTRA OF DIMETHYLDISELENIDE

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Rotational spectra of dimethyldiselenide, $CH_3SeSeCH_3$, were obtained with a pulsed-beam Fourier-transform microwave spectrometer. Selenium has six naturally occurring isotopomers and the presence of two selenium atoms in dimethyldiselenide gives rise to a large number of different isotopic lines for each rotational transition. In addition each isotopic line of dimethyldiselenide is further split by the internal rotation of the two equivalent methyl tops. The μ_b-type transitions of the A_1A_1 internal rotor state of the $^{80}Se^{80}Se$, $^{78}Se^{80}Se$, and $^{78}Se^{82}Se$ isotopomers of dimethyldiselenide have been assigned and least squares fit to a semi rigid Watson Hamiltonian. Rotational constants of the $^{80}Se^{80}Se$ isotopomer obtained from the fit of the A_1A_1 state are A = 5156.3163(9) MHz, B = 1481.1874(4) MHz and C = 1420.1673(3) MHz. The absence of μ_a- and μ_c-type transitions and the large inertial defects (Δ= -83.35143 u·Å for the $^{80}Se^{80}Se$ isotopomer) show dimethyldiselenide has C_2 symmetry. Substitution coordinates obtained from the $^{78}Se^{80}Se$ and $^{80}Se^{80}Se$ isotopic moments of inertia give a Se-Se bond distance of 2.332(3) Å which is in good agreement with the value of 2.326(4) Å reported in an electron diffraction study of dimethyldiselenide[a]. A comparison of the rotational constants calculated using the electron diffraction structural parameters with the experimental rotational constants obtained for the three isotopomers described above support the skew conformation with a CSeSeC dihedral angle of 87.5° as found by electron diffraction[a]. Work is currently underway to assign the internal rotor splitting and obtain the barrier to internal rotation of the two equivalent methyl tops.