INTERNAL ROTATION ANALYSIS OF THE FT-MW SPECTRUM OF EIGHT ISOTOPOMERS OF DIMETHYL DISELENIDE

PETER GRONER, *Department of Chemistry, University of Missouri - Kansas City, Kansas City, MO 64110*; CHARLES W. GILLIES, *Department of Chemistry, Rensselaer Polytechnic Institute, Troy, NY*; JENNIFER Z. GILLIES, *Department of Chemistry, Siena College, Loudonville, NY*.

The rotational spectra of eight isotopomers of dimethyl diselenide, $CH_3SeSeCH_3$, were recorded between 6 and 18 GHz with a pulsed-beam Fourier-transform microwave spectrometer. All rotational transitions of the symmetric isotopomers with C_2 symmetry, $CH_3{}^{78}Se^{78}SeCH_3$ and $CH_3{}^{80}Se^{80}SeCH_3$, are split into four components because of the interaction with the internal rotation of the methyl groups. The rotational transitions of the asymmetric isotopomers $CH_3{}^{76}Se^{80}SeCH_3$, $CH_3{}^{77}Se^{80}SeCH_3$, $CH_3{}^{78}Se^{80}SeCH_3$, $CH_3{}^{78}Se^{82}SeCH_3$, and $CH_3{}^{80}Se^{82}SeCH_3$ are split into five components. The spectra for these isotopomers (100 to 125 frequencies each) were fit with experimental precision (1.5 kHz) to the effective rotational Hamiltonian for molecules with two periodic internal motions [a]. The fits required eight rotational and quartic centrifugal distortion constants and five or nine internal rotation and tunneling parameters for the symmetric or asymmetric isotopomers, respectively. For $CH_3{}^{80}Se^{80}SeCH_3$, the principal results were: A = 5156.15730(41) MHz, B = 1481.13557(56) MHz, C = 1420.13993(60) MHz, ρ = 0.013930(49), β = 36.554(52)°, α = 39.093(14)°, resulting in I_τ = 3.0816(80) u$\AA^2$. A similar fit was performed for $^{13}CH_3Se^{80}Se^{80}CH_3$ where fewer lines were measured due to the low intensity of the spectrum recorded in natural abundance. Substitution parameters were calculated in the $CH_3{}^{80}Se^{80}SeCH_3$ isotopic frame using the $CH_3{}^{78}Se^{80}SeCH_3$ and $^{13}CH_3{}^{80}Se^{80}SeCH_3$ moments of inertia to give r_s(Se-Se) = 2.332 $\AA$, r_s(Se-C) = 1.957 $\AA$, θ(CSeSe) = 99.41° and ϕ(CSeSeC) = 85.25°.

[a] P. Groner, J. Chem. Phys. 107, 4483 (1997)