THE MOLECULAR STRUCTURES OF 1,2-DISELENIN AND 2-SELENATHIIN

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The rotational spectra of the 1,2-dichalcogenins, 1,2-diselenin and 2-selenathiin, were obtained with a pulsed-beam Fourier-transform microwave spectrometer. The least squares fit of the observed μ_b-type transitions of the $^{80}Se^{80}Se$ isotopomer of 1,2-diselenin to a semi rigid Watson Hamiltonian gave rotational constants of A = 2081.4262(9) MHz, B = 1659.1768(9) MHz and C = 1003.0117(4) MHz. Nuclear spin statistical weights, the presence of only μ_b-type transitions, and a large inertial defect of Δ = -43.5389 u·Å^2 show 1,2-diselenin has C_2 symmetry. The six-member ring, CH=CH–CH=CH–Se–Se, is twisted about the Se-Se bond and 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 2.325(3) Å. An analogous fit of the observed μ_a- and μ_b-type transitions of the $^{80}Se^{32}S$ isotopomer of 2-selenathiin gave rotational constants of A = 2983.8426(6) MHz, B = 2056.7288(6) MHz and C = 1325.1405(2) MHz. The large inertial defect Δ = -33.7140 u·Å^2 shows the ring of 2-selenathiin, CH=CH–CH=CH–Se–S, is not planar. An r_s Se-S bond distance of 2.205(16) Å is calculated from substitution coordinates obtained from the $^{80}Se^{32}S$, $^{78}Se^{32}S$, and $^{80}Se^{34}S$ isotopic moments of inertia. The structural parameters derived from the spectroscopic data will be compared to ab initio geometries of the 1,2-dichalcogenins.