FOURIER TRANSFORM MICROWAVE SPECTROSCOPY OF 1,1- DIMETHYLSILACYCLOBUTANE. INTERPLAY OF TWO TYPES OF LARGE-AMPLITUDE MOTIONS: TWO-TOP INTERNAL ROTATION AND RING PUCKERING

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The rotational spectra of 1,1-dimethylsilacyclobutane (CH3)2SiCH2CH2CH2 were observed to consist of eight components due to the four internal- rotation states AA, AE, EA and EE, each further split into the symmetric and antisymmetric states of puckering, and were analyzed by two formulations: one being a combination of a standard two-top internal rotation and ring puckering theory and the other a theory of large- amplitude motions developed by Hougen and coworkers, to yield two sets of molecular parameters, which were in good agreement with each other. Using spectra of Si and C isotopic species, molecular structure parameters were derived, including the puckering angle: 28.64 or 30.26 (two possible sets, I and II). The splitting between the two lowest puckering states was determined to be 11.90(22) MHz, which, combined with the equilibrium puckering angle, led to the puckering potential barrier of 395.3 and 347.0 cm-1 for the two sets I and II, respectively. The first-order (or linear) internal rotation terms were analyzed to give the potential barrier to CH3 internal rotation to be 567.8 and 505. 1 cm-1, respectively, for the AE (two CH3 groups rotating in the same direction, as viewed from Si) and EA (two CH3 rotating in the opposite direction) states.