VAN DER WAALS COMPLEXES OF ORGANOMETTALIC MOLECULES: THE ROTATIONAL SPECTRUM OF DIMETHYLSILANE···ARGON

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We have investigated the rotational spectrum of this adduct both with a free-jet millimeter wave absorption spectrometer (59-78 GHz) and with a molecular beam fourier transform microwave spectrometer (6-18 GHz). By using their complementary information we could determine very precise rotational constants, all quartic, sextic and some octic centrifugal distortion constants. We also found the barrier to the internal rotation of the two methyl groups and the energy splitting between the two levels of the inversion motion of the Ar above and below the C-Si-C plane. We studied in detail the pathway and energetics of this latter motion by using the simple distributed polarizability model implemented in Kisiel's RGDMIN program and performing ab initio MP2/6-311++G** calculations.