MICROWAVE SPECTRA OF THE Xe-N_2 VAN DER WAALS COMPLEX: A COMPARISON OF EXPERIMENT AND THEORY

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Rotational transitions of the Xe-N_2 complex were measured in the 4-18 GHz frequency region using a pulsed-nozzle Fourier-transform microwave spectrometer. Twelve (four) a-type transitions were recorded for the ^{132}Xe-^{14}N$_2$ and ^{129}Xe-^{14}N$_2$ (^{131}Xe-^{15}N$_2$) isotopomers. In addition, the nuclear quadrupole hyperfine structures due to the presence of the ^{14}N (I=1) and ^{131}Xe (I=3/2) nuclei were detected and analyzed. A high level *ab initio* potential energy surface was calculated at the CCSD(T) level of theory. Well-Tempered Basis Set (WTBS) with additional polarization functions was used for the Xe atom and aug-cc-pVTZ basis set for the N atoms. The basis sets were supplemented with midbond functions. This surface has a global minimum at a T-shaped geometry with a well depth of -122.6 cm^{-1}. Bound state energies supported by the potential energy surface were determined using the JACOBI computer code of X. Song and P. N. Roy. The quality of the *ab initio* potential energy surface is evaluated by comparison of the experimental transition frequencies and rotational and centrifugal distortion constants with those derived from the bound state energies. A scaled potential energy surface was obtained which has excellent agreement with the experimental data.