ROTATIONAL SPECTRA OF THE N_2O-$para D_2$ COMPLEX

JEN NICOLE LANDRY AND WOLFGANG JÄGER, *Department of Chemistry, University Of Alberta, Edmonton, AB T6G 2G2, Canada*.

Using a pulsed-nozzle Fourier-transform microwave spectrometer, rotational transitions of the N_2O-$para D_2$ complex were measured in the 5 - 21 GHz frequency region. For each of the $^{14}N^{14}NO$-pD_2, $^{15}N^{14}NO$-pD_2, $^{14}N^{15}NO$-pD_2 and $^{15}N^{15}NO$-pD_2 isotopmers, 4 transitions were recorded. In addition, the nuclear quadrupole hyperfine structure due to the presence of two ^{14}N (I=1) nuclei and pD_2 (I_{tot}=1) were detected and analyzed. Three potential energy surfaces with different orientations of the pD_2 unit relative to N_2O were calculated at the CCSD(T) level of theory. The aug-cc-pVTZ basis set was used for all atoms in the complex. Midbond functions were used to complement the basis set. The strategy is to construct a hybrid surface that can reproduce the observed transition frequencies.