ROTATIONAL SPECTRA OF THE N_2O-*para*D_2 COMPLEX

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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 $^{14}N^{14}NO$-*p*D_2, $^{15}N^{14}NO$-*p*D_2, $^{14}N^{15}NO$-*p*D_2 and $^{15}N^{15}NO$-*p*D_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 *p*D_2 (I_{tot}=1) were detected and analyzed. Three potential energy surfaces with different orientations of the *p*D_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.