THEORETICAL ANALYSIS OF THE $A^3\Pi$-$X^3\Sigma^-$ BANDS OF NH/D-Ne

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Rotationally resolved bands of NH/D-Ne have been observed in association with the $A^3\Pi$-$X^3\Sigma^-$ 1-0 and 0-0 transitions of NH/D. To guide the analysis of the spectra for the complex we have used high-level theoretical methods to calculate potential energy surfaces for the X and A states. The ground state surface has a well depth of 40 cm^{-1} and a linear NH-Ne equilibrium structure. The bending potential is predicted to be very shallow, so the zero-point level of the complex is expected to exhibit a large amplitude bending motion. The potential surface for the A state is more deeply bound (D_e=90 cm^{-1}) and anisotropic. The global minimum is for linear NH-Ne, but there is a secondary minimum for linear Ne-NH with a well depth of 45 cm^{-1}. Ro-vibronic levels of NH/D(A)-Ne were calculated from the potentials by numerical solution of the close-coupled equations. The results were in reasonably good agreement with the observed energy level structure. With one exception the bands that exhibited sharp rotational structure could be assigned to levels that correlate with the NH/D($A^3\Pi_2$)-Ne spin-orbit component. A single sharp feature was assigned to NH/D($A^3\Pi_1$)-Ne. Details of the calculations and a discussion of the assignments for the observed levels will be presented.