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H_2N: Part 2. Mixed spin-states and magnetic resonance transition probabilities ARTHUR S. BRILL, Univ. of Virginia — In the absence of nuclear spin-state mixing (i.e. each state pure m_I) there are, e.g. 10 epr transitions in $D_2^{15}N$ and 15 in $D_2^{14}N$, all $\Delta m_I = 0$ fully allowed. In the presence of mixing there are 243 in $D_2^{15}N$ and 729 in $D_2^{14}N$, with large differences in probability among transitions, many 0 or small. Because of numerous, at least partially allowed, overlapping transitions, useful information can be obscured in EPR spectra; Part 3 deals with experimental conditions to aid in extracting this information. In the literature there is quantitative disagreement among measured hyperfine splittings in H_2N, and spectral features have the appearance of little nuclear spin-state mixing (L. G. DeMarco, A. S. Brill and D. G. Crabb, J. Chem. Phys. **108** 1423 (1998) and references cited therein). With substantial spin-state mixing present, the latter behavior can be simulated over small ranges of a few parameters. Among these parameters is the HNH bond angle which affects both the M matrix elements discussed in Part 1 and how the contributions from the two H superpose. This bond angle is 104.4^o in the 6-31G* model, but is probably along a soft scissors mode.

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