Abstract Submitted
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H_2N: Part 1. Hyperfine energies ARTHUR S. BRILL, Univ. of Virginia — H_2N, (from frozen, irradiated ammonia), is the smallest of the large group of π (or p)-electron free radicals. With ^{1}H, ^{2}H, ^{14}N and ^{15}N there are 4 H_2N isotopes, with corresponding sets of hyperfine interactions, available for measurements. In a simple model of H_2N, 1.0 electron spin is in a Slater N2p-wave perpendicular to the molecular plane and -0.033 electron spin density in 1s waves on each H; the small effects of 0.066 electron spin (in other waves) required for net unit electron spin can be added. In a more complex model, the electronic structure is expressed with the 19 function 6-31G* basis. Nuclear spin-state mixing arises from linear combinations of dipolar off-diagonal matrix elements, e.g. $M_{xx} \equiv \sigma\kappa < \Psi|\Sigma(S_{kz}x_{kn}^2/r_{kn}^5 + S_{k'z}x_{k'n}^2/r_{k'n}^5)|\Psi >$ (Airne and Brill, Phys. Rev.A **63** 052511). The M's are calculated in a molecular coordinate system with formulas applicable to any basis. Euler angles transform from molecular to lab spherical polar angles giving **B** with respect to the principle hyperfine axes at each nucleus. It is now shown that the principle hyperfine A-values can be expressed in terms of the M's, e.g. $A_{zz} = A_{Fermi} - (4/3\sigma)(M_{xx} + M_{yy} - 2\,M_{zz})$, thereby simplifying the energy matrices.

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