AN *AB INITIO* STUDY OF THE $\tilde{A}\ ^2\Pi$ STATE AND THE $\tilde{A}\ ^2\Pi \leftarrow \tilde{X}\ ^2\Sigma^+$ ELECTRONIC TRANSITION OF MgNC

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We have used the RENNER program system[b] to make a detailed calculation of the rovibronic energies in the first excited electronic state, $\tilde{A}\ ^2\Pi$, of the MgNC radical. This calculation was based on recent *ab initio* surfaces (MR-SDCI(+Q)/[TZ3P+f(Mg), aug-cc-pVQZ(N and C)])[c] for the Renner-degenerate electronic states. Previous calculations of vibronic energies[c] employing the same *ab initio* data in conjunction with perturbation expressions[d] suggested that an observed band belonging to the $\tilde{A}\ ^2\Pi \leftarrow \tilde{X}\ ^2\Sigma^+$ electronic transition[e] should be reassigned. The present work confirms this conclusion which is further substantiated by the rotational structures calculated in the vibronic states, and by Franck-Condon theory predicting relative intensities. $\tilde{A}\ ^2\Pi$ MgNC affords an example of the "classic" Renner effect[f] involving component electronic states with linear equilibrium geometries. We present detailed analyses of rovibronic wavefunctions aimed at providing further insight into the nature of the Renner interaction.

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[b] See, for example, P. Jensen, G. Osmann, and P. R. Bunker, *in: "Computational Molecular Spectroscopy"* (P. Jensen and P. R. Bunker, eds.), Wiley, Chichester, 2000, and references therein.

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