AB INITIO ROTATION-VIBRATION SPECTRA OF $\tilde{X}\ ^2\Sigma^+$ MgNC

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In 1986 Guélin *et al.*[b] found, in radio astronomical observations, six transitions originating in the circumstellar envelope of the late-type carbon star IRC+10216. No assignment of these lines could be given at the time, but they were later identified[c,d] as belonging to the rotational spectrum of the MgNC radical. Thus, MgNC became the first Mg-containing molecule to be identified in interstellar space. The only rotationally resolved, spectroscopic data presently available for $\tilde{X}\ ^2\Sigma^+$ MgNC comprise the rotational spectrum[c,e] together with a few vibronic bands, all originating in the vibronic ground state and belonging to the $\tilde{A}\ ^2\Pi \leftarrow \tilde{X}\ ^2\Sigma^+$ electronic transition.[f] In the hope of stimulating further characterization of $\tilde{X}\ ^2\Sigma^+$ MgNC by high resolution spectroscopy, we report here *ab initio* simulations of its lowest $\tilde{X}$-state rotation-vibration bands. The calculations are carried out with the MORBID program system,[g] and they are based on a previously calculated potential energy function using ACPF method,[h] supplemented with dipole moment surfaces computed with CASSCF/[TZ3P+f(Mg), aug-cc-pVQZ(N andC)].

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