THE CM-, MM- AND SUBMM-WAVE SPECTRUM OF ALLYL ISOCYANIDE AND RADIOASTRONOMICAL OBSERVATIONS IN ORION KL AND THE PRIMOS LINE SURVEY

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Last year we presented the first rotational analysis of the ground state of the two conformers of allyl isocyanide from 4 GHz to 905 GHz. The analysis of the rotational spectrum of the cis conformer of allyl isocyanide was extended. We resolved Coriolis interactions of a and b types between the excited vibrational states $\nu_1 = 1$ and $\nu_2 = 1$, calculated to be at 156 cm^{-1} ($A^{'}$) and 167 cm^{-1} ($A^{''}$) respectively (MP2/aug-cc-pvtz), from 150 GHz to 600 GHz[a]. Strong perturbations were observed in the 150-310 GHz range for low values of the quantum number K_a starting from $K_a = 0, 1$. The anharmonicities appeared as well at higher frequencies for larger quantum numbers. The two modes were fitted together with the SPFIT/SPCAT[b] suite of programs and a set of Coriolis parameters was accurately determined. The fit contains more than 3000 lines up to $J = 99$ and $K_a = 12$ for both modes. We did not detect these species neither in the IRAM 30-m line survey of Orion KL nor in the PRIMOS survey towards SgrB2. Nevertheless, we provided upper limits to their column density in Orion KL. *This work was supported by the CNES and the Action sur Projets de l'INSU, PCMI.*

[a] I. Haykal et al. *manuscript in preparation*

[b] H. Pickett *J. Mol. Spec.* **148**, 371-377, 1991.