TORSION-ROTATION-VIBRATION EFFECTS IN THE v_{20}, $2v_{21}$, $2v_{13}$ AND v_{21}+v_{13} STATES OF CH_3CH_2CN

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Ethyl cyanide, CH_3CH_2CN, is a highly abundant molecule in hot cores associated with massive star formation where temperatures often approach 200 K. Astrophysicists would like to use the many thousands of observed lines to evaluate thermal equilibrium, temperature distributions, heating sources, and radiative pumping effects. In spite of a recent partial success in characterizing the v_{20} and v_{12} vibrational states[a], many aspects of the spectroscopy of the v_{20} state are not adequately characterized. Torsional splittings in the b-type spectrum of v_{20} are typically a few MHz and many a-type transitions also show resolved torsional splittings, both are incompatible with the expected 1200 cm^{-1} barrier to internal rotation in a v_t = 0 state. Additionally all K values above 2 show some obvious perturbations. The three states that lie just above v_{20} are $2v_{21}$, $2v_{13}$ and v_{21} + v_{13}. It has been determined that v_{20} interacts weakly with both $2v_{21}$ and $2v_{13}$ and that $2v_{21}$ interacts weakly with $2v_{13}$, in spite of their common symmetry and very close proximity. However, all the interactions of v_{21} + v_{13} appear to be very strong, making assignments of the combination band particularly problematic. The numerous interactions result in wide spread anomalous torsional splittings. These splittings provide valuable insight into the nature of the interactions, however without a reasonable model, assignment of A or E to a torsional component is far from obvious. There remains no reasonable quantum mechanical description of how to proceed with a torsion-rotation-vibration analysis involving large and small amplitude motions. We present what is known and unknown in this quartet of CH_3CH_2CN states.

[a]Daly, A. M., Bermúdez, C., López, A., et al., 768, 1, ApJ, 2013