

THE COMPLETE ROTATIONAL SPECTRUM OF CH₃NCO UP TO 376 GHz

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The methylisocyanate molecule, CH₃NCO, is of interest as a potential astrophysical species and as a model system for the study of quasisymmetric behavior. The rotational spectrum is made very complex by the presence in CH₃NCO of two large-amplitude motions: an almost free internal rotation and a low barrier skeletal bending motion. This challenging spectrum has, nevertheless, been assigned at 8-38 GHz by Stark spectroscopy^a and has been measured at 117-376 GHz with the broadband FASSST technique.^b

We presently report the results of measuring this spectrum also in supersonic expansion for the transitions below 40 GHz, and at room-temperature in the region between 40 and 120 GHz. In this way we are finally able to confirm the assignment of the ground state and of the internal rotation $m=1$ state and to analyse the nitrogen hyperfine splitting structure. It is also possible to confidently transfer the Stark-based assignment to the transition sequences measured in the mm-wave region, and to assign high K_a sequences. Various models for fitting this spectrum are explored but, even without more extensive fits, we are now able to present temperature scalable linelists for astrophysical applications.

^aJ.Koput, *J. Mol. Spectrosc.* **115**, 131 (1986).

^bZ.Kisiel et al., 65th OSU Symposium on Molecular Spectroscopy, The Ohio State University, Ohio 2010, RC-13.