LABORATORY DETECTIONS OF CYANOTHIOFORMALDEHYDE (HCSCN) AND MERCAPTOACETONITRILE ($HSCH_2CN$) BY CP-FTMW SPECTROSCOPY

DANIEL P. ZALESKI, JUSTIN L. NEILL, MATT T. MUCKLE, NATHAN A. SEIFERT, AMANDA A. STEBER, BRENT J. HARRIS, AND BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904*; VALERIO LATTANZI AND MICHAEL MCCARTHY, *Harvard-Smithsonian Center for Astrophysics, 60 Garden St., Cambridge, MA 02138, and School of Engineering and Applied Sciences, Harvard University, 29 Oxford St., Cambridge MA 02138.*; ANTHONY J. REMIJAN, *National Radio Astronomy Observatory, 520 Edgemont Rd., Charlottesville, VA 22904.*.

We have previously reported results for reaction product screening of potential interstellar molecules using broadband rotational spectroscopy. This approach was applied to the reaction products created in an electrical discharge of CH_3CN and H_2S [a]. By screening the product mixture with molecular rotational spectroscopy it is possible to directly compare laboratory and observatory surveys to identify overlapping transitions. Also, as the product molecules are identified, it becomes possible to propose the formation mechanism in the experiment and use this chemical insight to propose new candidate products. For the electrical discharge chemistry of CH_3CN and H_2S radical-radical recombination reactions followed by elimination of molecular hydrogen were inferred to be important and has led to the laboratory identification of additional products HCSCN and $HSCH_2CN$. A previous mm-wave study of HCSCN motivated by its possibility as an interstellar species reported a pure rotational spectrum different form the one we obtain [b]. A Kraitchman substitution structure confirms the assignment of our spectrum to HCSCN. Possible causes for the discrepancy in microwave and mm-wave rotational spectroscopy results will be discussed. The $HSCH_2CN$ rotational spectrum shows two low-lying torsional levels that can interact through proton tunneling as is observed in the structurally similar propargyl alcohol. The design of a 40-60 GHz CP-FTMW, used to aid in the laboratory analysis of HCSCN, is also briefly presented.

[a] D.P. Zaleski *et al.* 66th OSU ISMS: WF01.

[b] M. Bogey *et al. JACS*, 111, (1989), 7399.