Permanent Electric Dipole Moments of Four Tryptamine Conformers in the Gas Phase. A New Diagnostic of Structure and Dynamics.¹

DAVID PRATT, TRI V. NGUYEN, University of Pittsburgh — Rotationally resolved electronic spectroscopy in the gas phase, in the absence and presence of an applied electric field, has been used to determine the charge distribution of a cross section of the energy landscape of tryptamine (TRA). We report the magnitude and direction of the permanent electric dipole moments of the four TRA conformers GPyout, GPyup, GPhup and Antiup in their S₀ and S₁ electronic states. Each dipole moment is unique, providing a powerful new tool for conformational analysis of biomolecules in the gas phase. A comparison of the results for the different conformers of TRA reveals that the position and orientation of the ethylamine side chain plays a major role in determining both the permanent and induced electric dipole moments of the different species in both electronic states.

¹This work has been supported by NSF.