# ACCURATE IR INTENSITY PREDICTION FOR $N_2O$ ANALYSIS AS A POTENTIAL BIOSIGNATURE MOLECULE IN PLANETARY AND EXOPLANETARY ATMOSPHERES: UNCERTAINTY AND UPGRADES

XINCHUAN HUANG[a], *Carl Sagan Center, SETI Institute, Moutain View, CA, USA*; DAVID SCHWENKE, *MS 258-2, NAS Facility, NASA Ames Research Center, Moffett Field, CA, USA*.

Accurate IR line lists of astronomically important molecules can help their quantitative analysis and modeling in planetary and exoplanetary atmosphere studies. To minimize the uncertainty of analysis resulting from IR line list or opacity data, the intensity prediction accuracy of semi-empirically computed IR line lists may be improved by using more accurately refined potential energy surface (PES) and more accurate ab initio dipole moment surface (DMS). Recently we reported Ames-1 296K IR line list for $N_2O$ and its isotopologues, based on a PES refinement with $\sigma_{rms}$ = 0.02 $\mathrm{cm}^{-1}$for selected HITRAN2020 levels and band origins, and a DMS fitted from extrapolated CCSD(T)/aug-cc-pV(T,Q,5)Z dipoles in the range of 0 - 20,000 $\mathrm{cm}^{-1}$, with fitting $\sigma_{rms}$ = $2.7\times10^{-5}$ a.u.. It has overall good agreement with published experimental data and effective dipole models, plus more reliable predictions for minor isotopologues. However, relatively larger discrepancies and extra sensitivities have been noticed on several bands, calling for further studies to verify and improve the accuracy of Ames intensity predictions. This investigation focuses on the dipole surface. A new CCSD(T) DMS series are fitted from various dipole sets computed on 8000 - 13,000 geometries with $E_{max}$ = 10,000 - 17,000 $\mathrm{cm}^{-1}$. With fitting $\sigma_{rms}$ in the range of $10^{-5}$ - $10^{-7}$ a.u., we are able to track the DMS impact on IR intensities for each individual band or transition. Results and findings will be presented, e.g., the DMS sensitive predictions for bands like $1113\leftarrow0000$, and the stable predictions for other bands like $\nu_1\leftarrow\nu_2$. The differences among the best performing DMS candidates increases beyond 10,000 $\mathrm{cm}^{-1}$. It probably requires new experimental studies to consolidate a choice of "Ames-2" DMS and line lists. Other potential factors behind the intensity accuracy and uncertainties will also be discussed.

[a]Funded by NASA Grant 18-APRA18-0013 and through NASA/SETI Co-operative Agreement 80NSSC20K1358.