RELIABLE IR LINE LISTS FOR SO_2 AND CO_2 ISOTOPOLOGUES COMPUTED FOR ATMOSPHERIC MODELING ON VENUS AND EXOPLANETS

XINCHUAN HUANG, *Carl Sagan Center, SETI Institute, Moutain View, CA, USA*; DAVID SCHWENKE, *MS 258-2, NAS Facility, NASA Ames Research Center, Moffett Field, CA, USA*; TIMOTHY LEE, *Space Science and Astrobiology Division, NASA Ames Research Center, Moffett Field, CA, USA*; ROBERT R. GAMACHE, *Department of Environmental, Earth, and Atmospheric Sciences, University of Massachusetts, Lowell, MA, USA*.

For SO_2 atmospheric characterization in Venus and other Exoplanetary environments, recently we presented Ames-296K line lists for 626 (upgraded) and other 4 symmetric isotopologues: 636, 646, 666 and 828. For CO_2, we reported Ames-296K (1E-42 cm/molecule) and Ames-1000K (1E-36 cm/molecule) IR line lists up to E'=18000 cm^{-1} for 13 CO_2 isotopologues, including symmetric species 626, 636, 646, 727, 737, 828, 838, and asymmetric species 627, 628, 637, 638, 728, 738. CO_2 line shape parameters were also determined for four different temperature ranges: Mars, Earth, Venus, and higher temperatures. General line position prediction accuracy up to 5000 cm^{-1} (SO_2) or 13000 cm^{-1} (CO_2) is 0.01 – 0.02 cm^{-1}. Most transition intensity deviations are less than 5-10%, when compare to experimentally measured quantities. With such prediction accuracy, these SO_2 and CO_2 isotopologue lists are the best available alternative for those wide spectra region missing from spectroscopic databases such as HITRAN and CDMS. For example, only very limited data exist for SO_2 646/636 and no data at all for other minor isotopologues. They should greatly facilitate spectroscopic analyses in future laboratory or astronomical observations. Our line list work are based on "Best Theory + Reliable High-Resolution Experiment" strategy, i.e. using an ab initio potential energy surface refined with selected reliable high resolution experimental data, and high quality CCSD(T)/aug-cc-pVQ(or Q+d)Z dipole moment surfaces. Note that we have solved a convergence defect on SO_2 Ames-1 PES and further improved the quality and completeness of the Ames-296K SO_2 list by including most recent experimental data into the refinement. We will compare the Ames-296K SO_2 and CO_2 lists to latest experiments and HITRAN/CDMS models. We expect more interactions between experimental and theoretical efforts. Currently the Ames-296K lists are available at http://huang.seti.org/.