National Aeronautics and Space Administration

Laboratory Spectral Simulations of Exoplanet Atmospheres

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Program: Strategic Initiatives

Project Objective:

The objectives of our laboratory investigations are to:

1. Produce high resolution infrared spectroscopy data for equilibrium atmospheres
2. Follow photochemistry and aerosol formation in hot-Jupiter-type exoplanet atmospheres as they evolve under high temperatures and UV radiation

Our work will help understanding the role of UV-photochemistry in exoplanet atmospheres in addition to thermochemistry.

FY18/19 Results:

- Studied thermochemistry in H_2:CO (300:1) and H_2:CO:H_2O (400:1:1) atmospheres using the **CAAPSE (Cell for Atmospheric and Aerosol Photochemistry Simulations of Exoplanets)** experiment from 1173 K to 1473 K and the photochemistry using UV-radiation at Ly-α (121.6nm).
- Formation of CO_2 in the gas-phase with thermochemistry
- Formation of CO_2 and H_2O in the gas-phase with photochemistry with H_2O being more important at T>1200 K
- Determine the source of oxygen to be CO for the formation of CO_2 under UV irradiation

3. Approach:

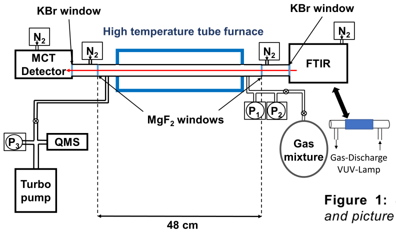

Figure 1: *Scheme of the CAAPSE experiment (left) and picture of the CAAPSE in action at JPL (right).*

The CAAPSE setup is presented in Figure 1. The cell is filled with 15 mbar of D_2:^{13}CO (300:1) or D_2:^{13}CO:D_2O (400:1:1) gas mixtures to simulate hydrogen-dominated atmosphere with C/O ratios of 1 and 0.5. The gases are heated at temperatures up to 1473 K. When the gaseous mixture has reached the thermal equilibrium composition, it is irradiated using a microwave discharge hydrogen flow lamp (Ly-α (121.6 nm) emission band plus a broad emission band in the 140–170 nm range, mimicking the VUV solar flux received in simulated exoplanet atmospheres).

4. Source of Oxygen for the formation of CO_2 in H_2/CO atmospheres:

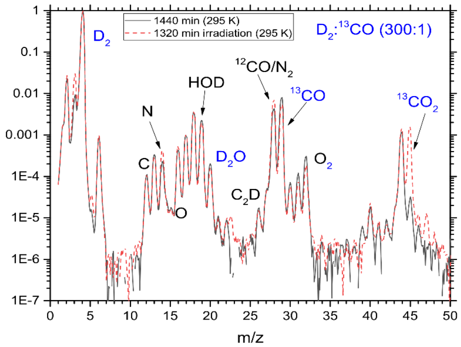

Figure 2: Evolution of the gas phase composition after 1320 min of UV irradiation of D_2:^{13}CO (300:1) gas mixture at room temperature, monitored with in situ mass spectrometry. These results showed that for two ^{13}CO molecules consumed, one $^{13}CO_2$ molecule is formed, while H_2O or O_2 depletion observed cannot account for $^{13}CO_2$ formed. These results highlight that CO is the source of oxygen in the photochemical formation of CO_2.

- We shown that CO_2 could be formed photochemically in H_2:CO atmospheres (Fleury et al. 2019)
- Figure 2 shows the mass spectra of the D_2:^{13}CO gas mixture at 295 K before and after irradiation. We observed the consumption of ^{13}CO (*m/z* 29) and the formation of $^{13}CO_2$ (*m/z* 45).
- We found that CO is the source of oxygen for the formation of CO_2.

5. Thermochemistry and Photochemistry in H_2/CO/H_2O atmospheres:

Figure 3 shows the IR-Absorption spectra (irradiated and unirradiated) in the 1800-3000 cm^{-1} (3.3-5.5 μm) range with a resolution of 0.25 cm^{-1} at different temperatures.

The room-temperature spectrum contains the absorption band of the initial ^{13}CO (2095 cm^{-1}) and D_2O (2780 cm^{-1}).

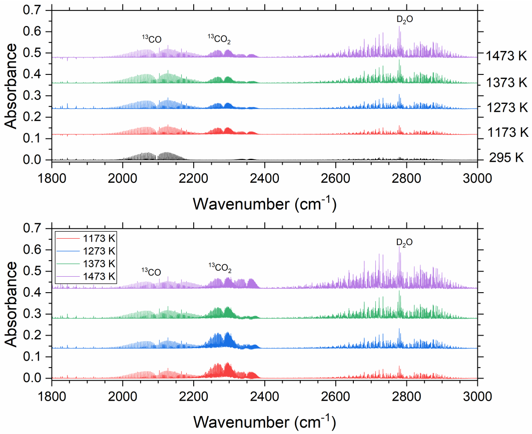

Figure 2: *IR spectra of the initial gaseous mixture of H_2:^{13}CO (99.7%:0.3%) at 295 K and at the equilibrium for different set oven temperatures: 573 K, 873 K, 1173 K, 1273 K, 1373 K, and 1473 K (top) and after 18 hours of irradiations at 121.6 nm (Ly-α) (bottom); spectra are offset for clarity,*

The spectra of the heated gases reveal the formation of bands due to two new (thermally-generated) molecular species: $^{13}CO_2$ (2284 cm^{-1}) and D_2O (2780 cm^{-1}). CO_2 is isotopically labelled with ^{13}C, highlighting that it is formed during thermal chemistry from the initial ^{13}CO.

UV (121,6 nm, Ly-α) irradiation of the heated gases leads to a decrease of [CO], an increase of [CO_2], and the formation of water. Photochemistry can strongly influence the composition of H_2:CO:H_2O warm exoplanet atmospheres. CO_2 and H_2O can be efficiently produced in these atmospheres despite competitive loss processes. The gas temperature strongly influences the efficiency of the different chemical pathways, notably due to the increase of the absorption cross-sections of CO_2 when the temperature increases.

Benefits to NASA and JPL (or significance of results):

These results highlight the importance of including UV photochemistry in models used to simulate exoplanet atmospheres. Photochemistry and thermochemistry are both heavily involved in the composition of hot-Jupiter-like exoplanet atmospheres, and these results can be used to better interpret ground- and space-based spectroscopic observations of these exoplanet atmospheres. For missions like JWST, our studies will provide much-needed laboratory reference data for atmospheric molecules and aerosols in the infrared and ultraviolet spectral regions.

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Publications:

B. Fleury, M. S. Gudipati, B. L. Henderson, and M. Swain, "Photochemistry in hot H_2-dominated exoplanet atmospheres", (2019), ApJ 871:158

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