

The near-UV absorber mystery of Venusian atmosphere

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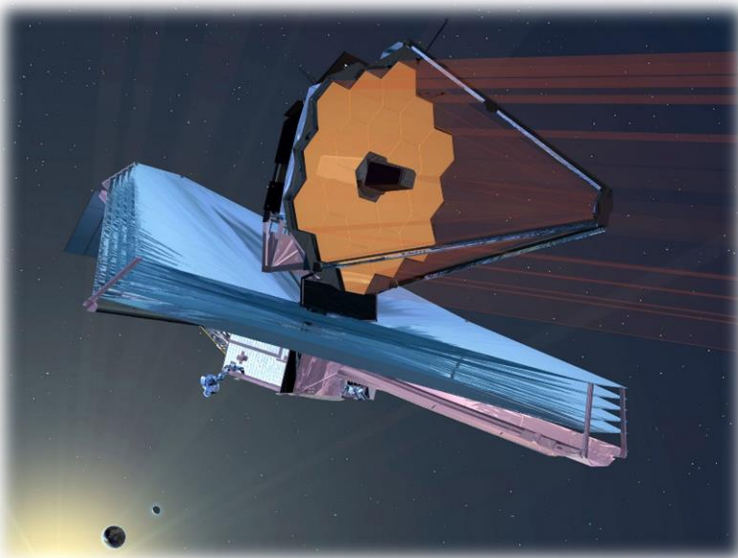
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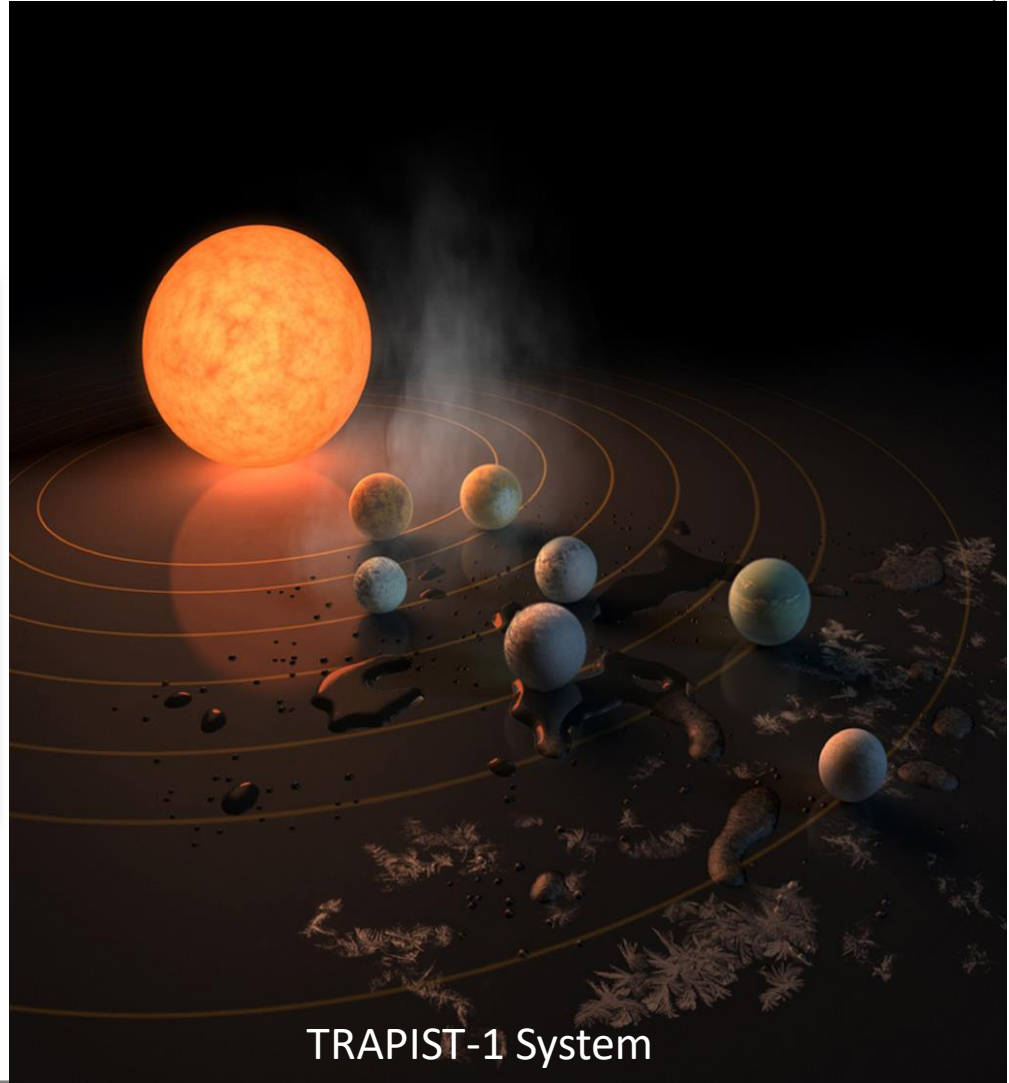
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Spectroscopy



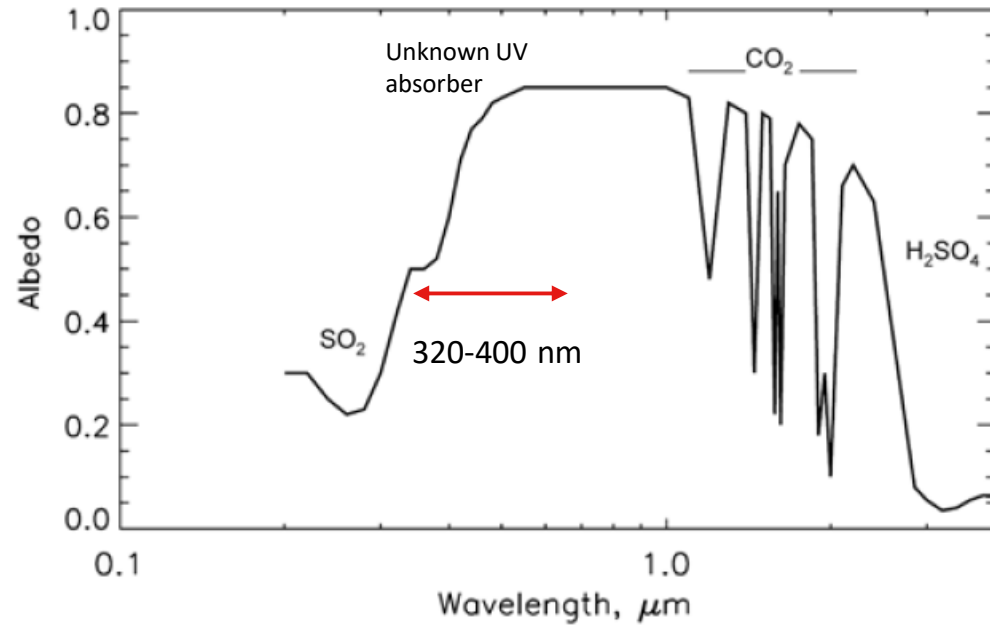
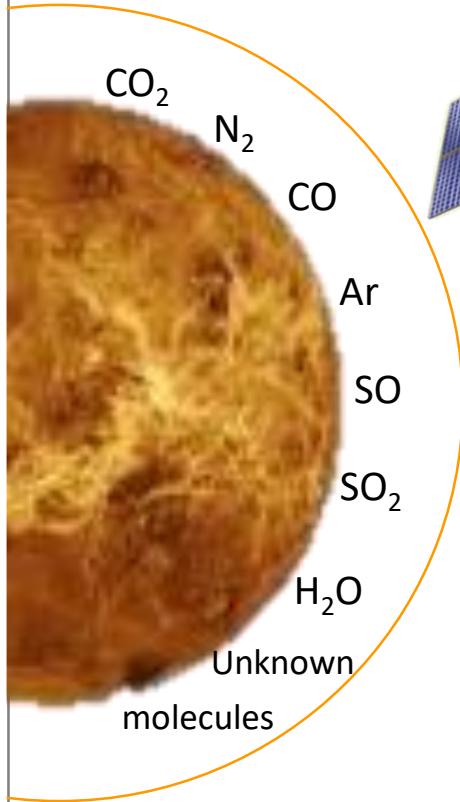
James Webb Space Telescope

Photos from NASA's image gallery



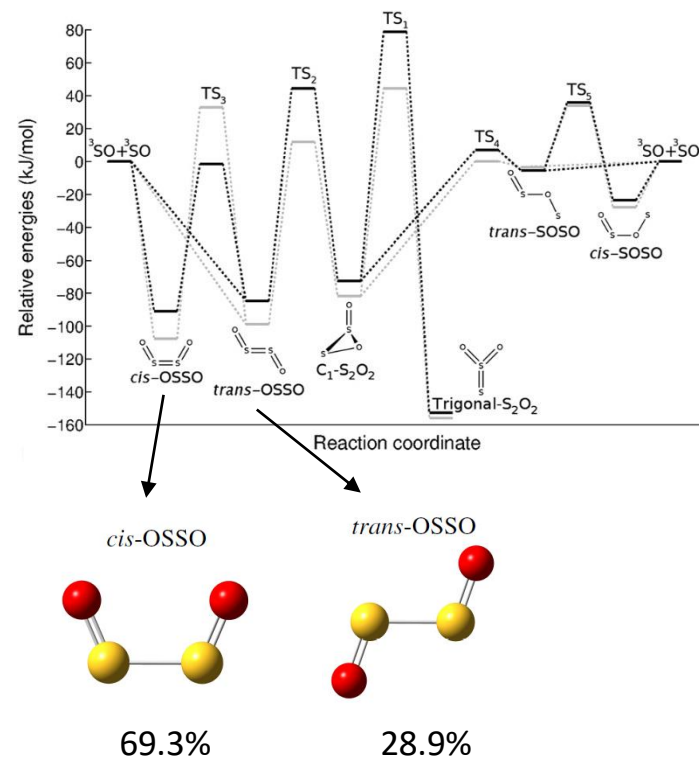
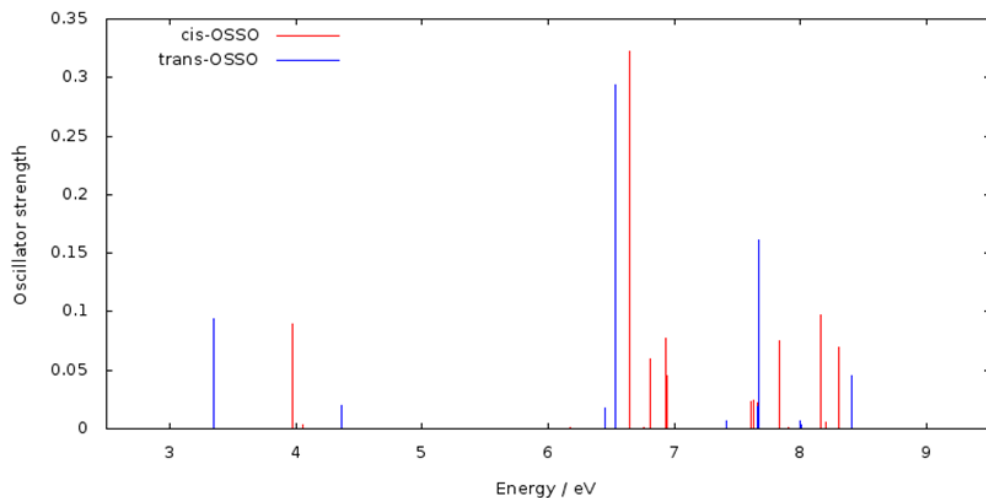
TRAPIST-1 System

Atmosphere of Venus



Previous study ¹ on S₂O₂

- Identified two cis-OSSO and trans-OSSO isomers
- Calculated the vertical excitations



[1] B. N. Frandsen, P. O. Wennberg, and H. G. Kjaergaard, "Identification of OSSO as a near-UV absorber in the Venesian atmosphere.", *Geophysical Research Letters* **11**, 146–155 (2016).

Spectra simulation²

- Trajectory surface hopping technique

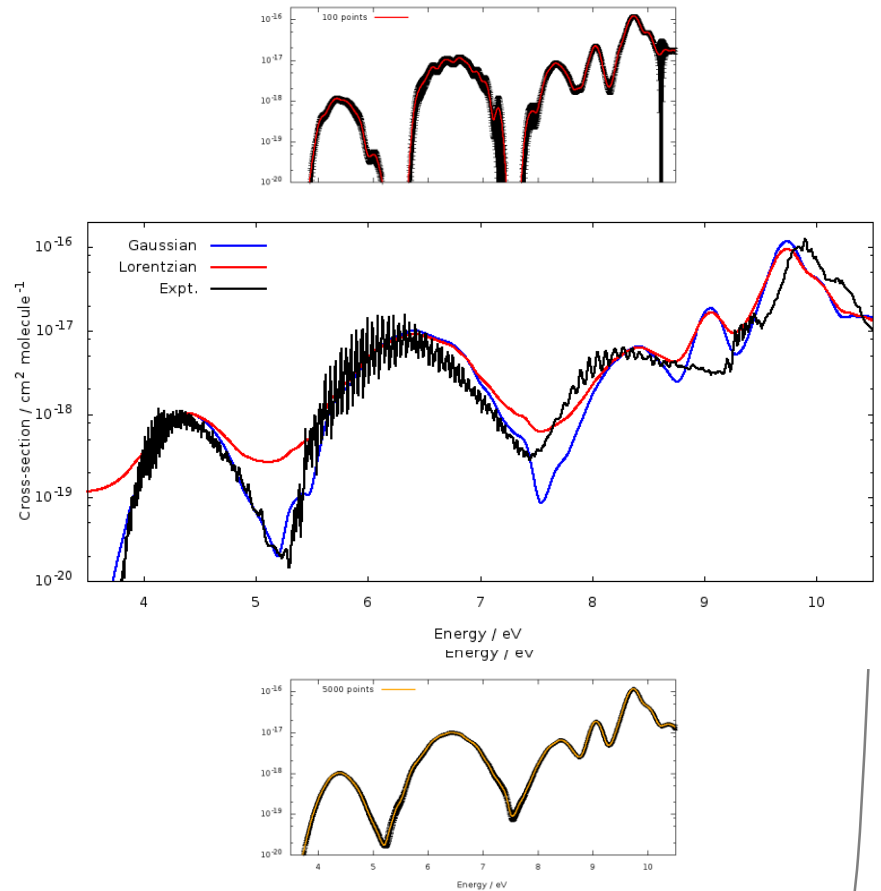
Simulation parameters

- Newton-X parameters
- Electronic structure parameters

[2] S. Farahani, B. N. Frandsen, H. G. Kjaergaard, and J. R. Lane, "Simulated Electronic Absorption Spectra of Sulfur-Containing Molecules Present in Earth's Atmosphere." Accepted in The Journal of Physical Chemistry A (2019).

SO₂ Newton-X parameters

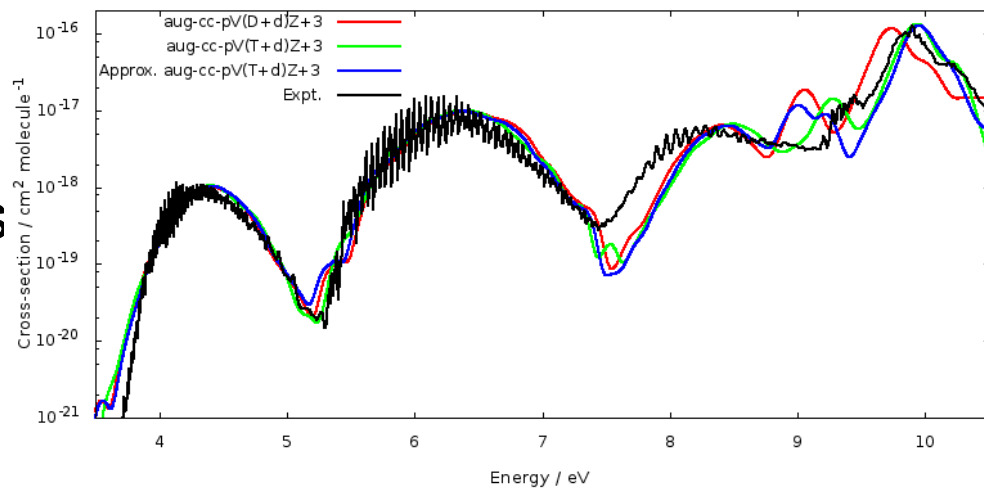
- Distribution
- Number of points
- Band shape
- Phenomenological broadening of the spectrum (δ)



SO₂

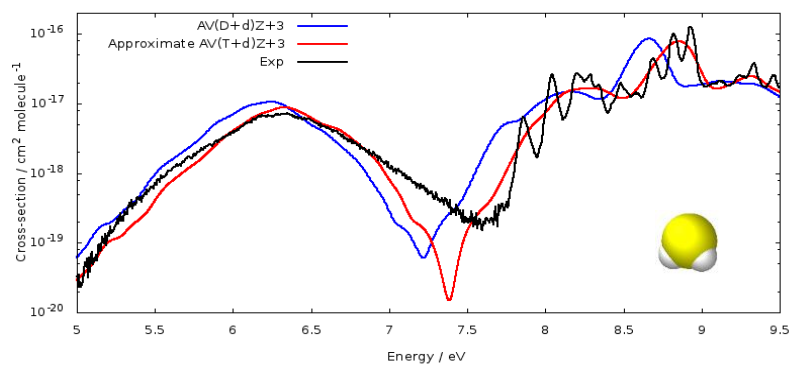
Electronic structure parameters

- *Ab initio* method
- Basis set
- Number of excited states

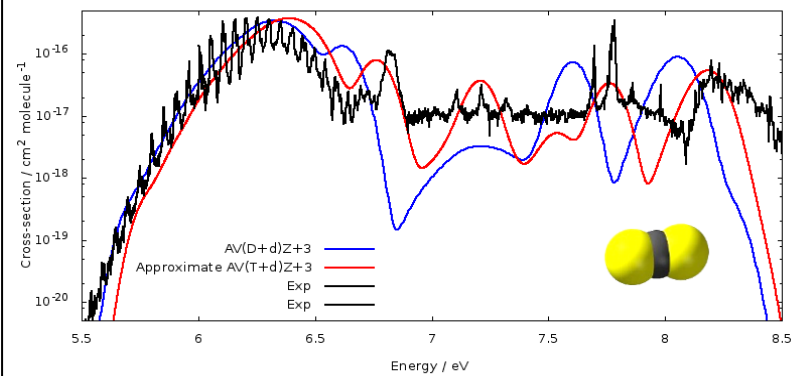


Other benchmarking S-molecules

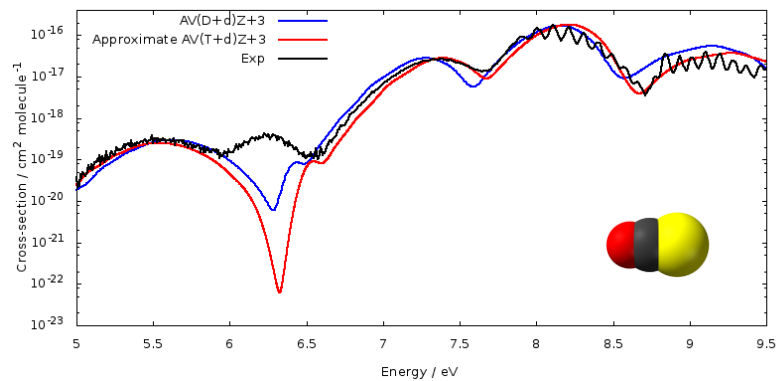
H₂S



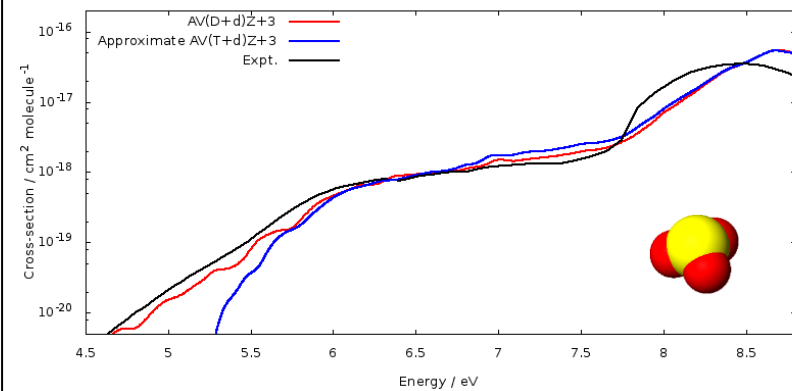
CS₂



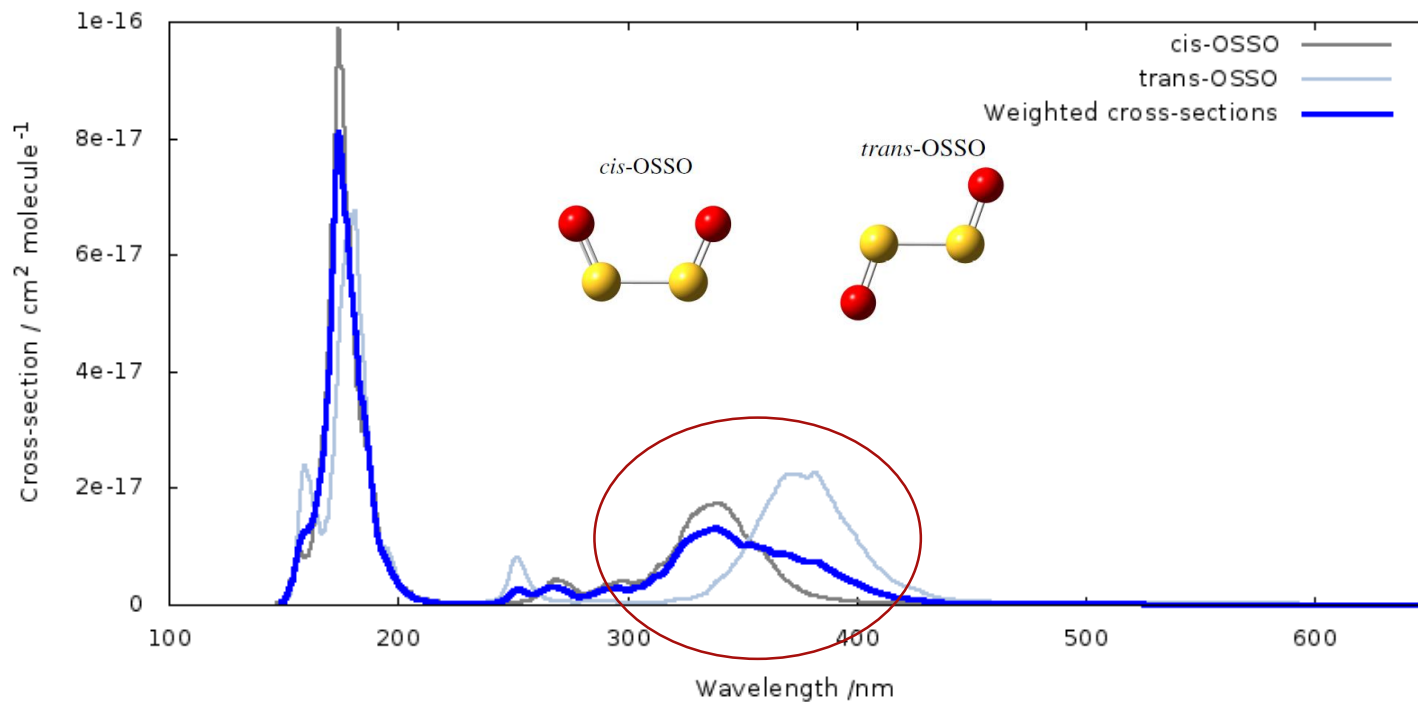
OCS



SO₃



Weighted simulated spectra





Thank you

Venus Transit seen by NASA's Sun-observing TRACE spacecraft

Photos from NASA's image gallery