AOGS 2005

Quantum Mechanics and Planetary Atmospheres

BRENTON R. LWEIS[1]

[1]*Research School of Physical Sciences and Engineering, The Australian National University*

Parametric models of molecular photoabsorption and photodissociation are routinely employed in the radiative-transfer and photochemical codes for planetary atmospheres. While such models are based, as far as possible, on the latest experimental data, it is impractical to perform experiments over the full range of pressure and temperature conditions applicable to planetary atmospheres. Thus, the accuracy of the inevitable interpolation and extrapolation required depends critically on the model validity. In the vacuum-ultraviolet (VUV) and extreme-ultraviolet (XUV) spectral regions, where highly excited coupled molecular states, which eventually dissociate, are accessed in electronic transitions, simple parametric models cannot be expected to be realistic.

The development of a new, physically-based, quantum-mechanical model for diatomic molecular photoabsorption and photodissociation is described, together with the state-of-the-art high-resolution laser-spectroscopic experiments used for model calibration. The advantages of this model include simultaneous computation of the total photodissociation cross section and the branching ratios for dissociation into all energetically-accessible channels, and a seamless treatment of isotopic and temperature effects. Applications of the model to N_2 in the XUV, of particular relevance to the current encounter of *Cassini-Huygens* with Titan, and O_2 in the VUV, [1], [2] are discussed.

Quantum-interference effects are found to lead to far-wing lineshape asymmetry not predicted by the simple models. These effects may have a significant bearing on the penetration of solar radiation into planetary atmospheres and the consequent photochemistry, including isotopic fractionation, [3] together with the quality of retrievals of species distributions from planetary missions.

Keywords: Planetary atmospheres; quantum mechanics; molecular photodissociation; vacuum-ultraviolet; nitrogen; oxygen; Titan; photochemistry.

References

[1] B. R. Lewis, S. T. Gibson, *et al., Phys. Chem, Earth C* **26**, 519 (2001).
[2] J. Lacoursiere, S. A. Meyer, *et al., J. Chem. Phys.* **110**, 1949 (1999).
[3] M. C. Liang, G. A. Blake, B. R. Lewis, and Y.L. Yung, unpublished.