P43K-3911: New O+CO_2 scattering cross sections and their impact on photochemical atmospheric escape of oxygen from Mars

Thursday, 13 December 2018
13:40 - 18:00
Walter E Washington Convention Center - Hall A-C (Poster Hall)

Dissociative recombination of O_2^+ and CO_2^+ molecular ions in the upper atmosphere of Mars is a major source of suprathermal (hot) oxygen atoms. A significant fraction of hot O atoms are sufficiently fast to overcome Mars' gravitational potential and escape to space. This mechanism is known as photochemical escape (PE) and found to be one of the major escape mechanisms presently active on Mars. The Mars Atmosphere and Volatile Evolution Mission (MAVEN) can constrain the PE rate from measurements of electron temperature and density and ion temperature and density. Escape probabilities of hot O can then be constructed from in-situ neutral densities and escaping O flux loss due to collisions with atmospheric background gases. Due to CO_2 abundance in the upper atmosphere, O+CO_2 scattering is the most important sink of the escaping hot O flux that strongly affects estimates of total atomic oxygen escape rate obtained from MAVEN data, as outlined above.

New O+CO_2 elastic and inelastic cross sections were constructed from first principles for collision energies from 0.01-5 eV. O(^3P)+CO_2 collisions were described using new 4D electronic potential energy surfaces (PESs) for restricted geometries. Three lowest triplet states of CO_2 were considered for symmetric, bending, and asymmetric vibrational modes. The cross sections were determined from close-coupling calculations performed on individual surfaces using vibrating rotor approximations for CO_2 molecule[1]. Differential and momentum transfer cross sections, of use in energy transfer atmospheric models, were also constructed. The obtained cross sections are in excellent agreement with published results[2,3]. Our new elastic cross sections are significantly smaller than assumed in earlier atmospheric escape models, resulting in larger photochemical escape rate of O from Mars, as estimated from a 1D escape model. Our results agree well with estimated hot O flux (about 9×10^{25} s^{-1}) derived from altitude profiles of 130.4 nm O emission measured up to ~4,000 km by the Imaging Ultraviolet Spectrograph on MAVEN orbiter[4].

[1] M. Gacesa and V. Kharchenko, Geophys. Res. Lett., 39, L10203 (2012)

[2] L. Yeung et al., J. Phys. Chem. A, 116, 64 (2012)

[3] M.-P. de Lara-Castells et al., J. Chem. Phys. 124, 164302 (2006)

[4] A. Rahmati et al., J. Geophys. Res. 123, 1192 (2018)

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