$O(^3P)+CO_2$ SCATTERING DYNAMICS WITH MCTDH FOR UNDERSTANDING OXYGEN ESCAPE FROM MARS ATMOSPHERE

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We report cross sections for the collision of O(3P) + CO2 scattering at collision energies which are important to understand the O escape from Mars atmosphere. The cross sections were calculated using newly developed state-of-the-art *ab initio* potential energy surfaces (PESs) correlating the lowest energy asymptote of the complex.

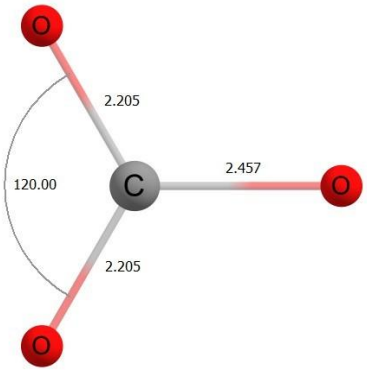

Figure 1: Coordinate fpr O + CO_2 collison with a bending geometry with the <OCO angle at 120 degrees.

The work presented here explores for the first time a fully quantum mechanical approach to providing inelastic cross-sections and rates using Multi-configurational Time Dependent Hartree (MCTDH) method.

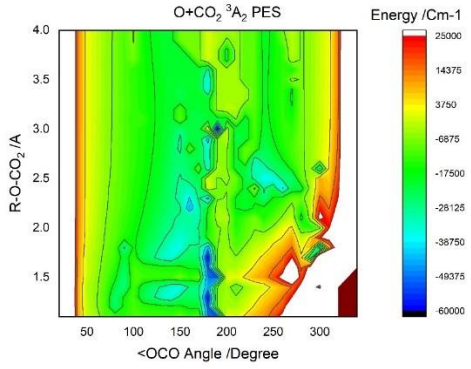

Figure 2: Contour plot of the the 3A2 potential energy surface for the O + CO_2 complex.

The new PES allows us to investigate the influence and importance of in-plane bending vibration of CO_2 and the stretching vibration of CO_2 to the scattering cross-sections of $O(^3P)$-CO_2 compared to that of the rigid rotor approximation previously reported [1]. This also allows for an understanding of rotational and vibrational energy transfer processes in this atom-triatom collision.

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References:

[1] M. Gacesa, R. J. Lillis, and K. J. Zahnle, $O(^3P)+CO_2$ scattering cross-sections at superthermal collision energies for planetary aeronomy, MNRAS **491**, 5650–5659 (2020)