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Energy Transfer Rates for Collisions of CO_2 and O Atoms

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The rate coefficients for the vibrational quenching of solar excited carbon dioxide by impacts with atomic oxygen are crucial in modeling the energy budgets of Earth, Mars, and especially Venus. CO_2 is one of the species affected by non-LTE (Non Local Thermodynamic Equilibrium) processes at high altitudes on Earth, Mars and Venus. For the Venus non-LTE CO_2 vibrational populations, a system of chemical kinetic equations (the non-LTE kinetic model) has to be solved, which, due to the abundance of O atoms and their efficiency to activate (de-activate) one or more of the vibrational modes of CO_2, needs to include the O + CO_2 collisional VT (vibrational to translational) energy transfer processes,

CO_2 (0, v_2, 0) + O(^3P) $\rightarrow$ CO_2 (0,v_2 - 1, 0) + O(^3P), v_2=1, 2, 3

CO_2 (0, 0, 1) + O(^3P) $\rightarrow$ CO_2 (0, v_2,0) + O(^3P), v_2=1, 2, 3

The rates of these processes have large uncertainties (or in some cases have not been measured) and they are the primary sources of error in the computed populations of the Venus CO_2 vibrational states. We present here results from recent first principles calculations to obtain the desired rate coefficients. The calculations are performed using Quasi-Classsical Trajectories (QCT) methods, coupled with a spectral analysis step that projects out the vibrational mode populations.