Abstract Submitted
for the DAMOP16 Meeting of
The American Physical Society

Reactive scattering of O and H_2 and quenching of OH at collision energies up to 4.4 eV[1] MARKO GACESA, NASA/Ames Res Ctr, VASILI KHARCHENKO[2], University of Connecticut, Department of Physics — We report new cross sections for the $O(^3P)$ + H_2 reactive scattering as well as quenching rates for rotationally and vibrationally excited OH by H atoms for a range of collision energies from 0.4 and 4.4 eV. These processes are important for understanding non-local thermal equilibrium (non-LTE) regime in astrophysical environment such as photon-dominated regions (PDRs) and evolution of planetary atmospheres in time, including the atmospheres of Earth and Mars. The cross sections were calculated quantum mechanically using coupled-channel formalism implemented in MOLSCAT and ABC computer codes on refitted recent potential energy surfaces for $^3A'$ and $^3A''$, while the surface-hopping effects were estimated from models and similar atom-molecule reactions. A large basis set was used to ensure the convergence at higher energies. Our results agree well with the published data at lower energies and indicate that reduced-dimensionality approach at collision energies higher than about 1.5 eV may not be adequate. Differential cross sections and diffusion cross sections, of interest in transport calculations, are also reported.

[1]This work was been supported by NASA grant NNX10AB88G
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Date submitted: 29 Jan 2016 Electronic form version 1.4