Quantum-mechanical H/D–CO_2 collisions and their impact on atmospheric escape and evolution of CO_2-rich planets

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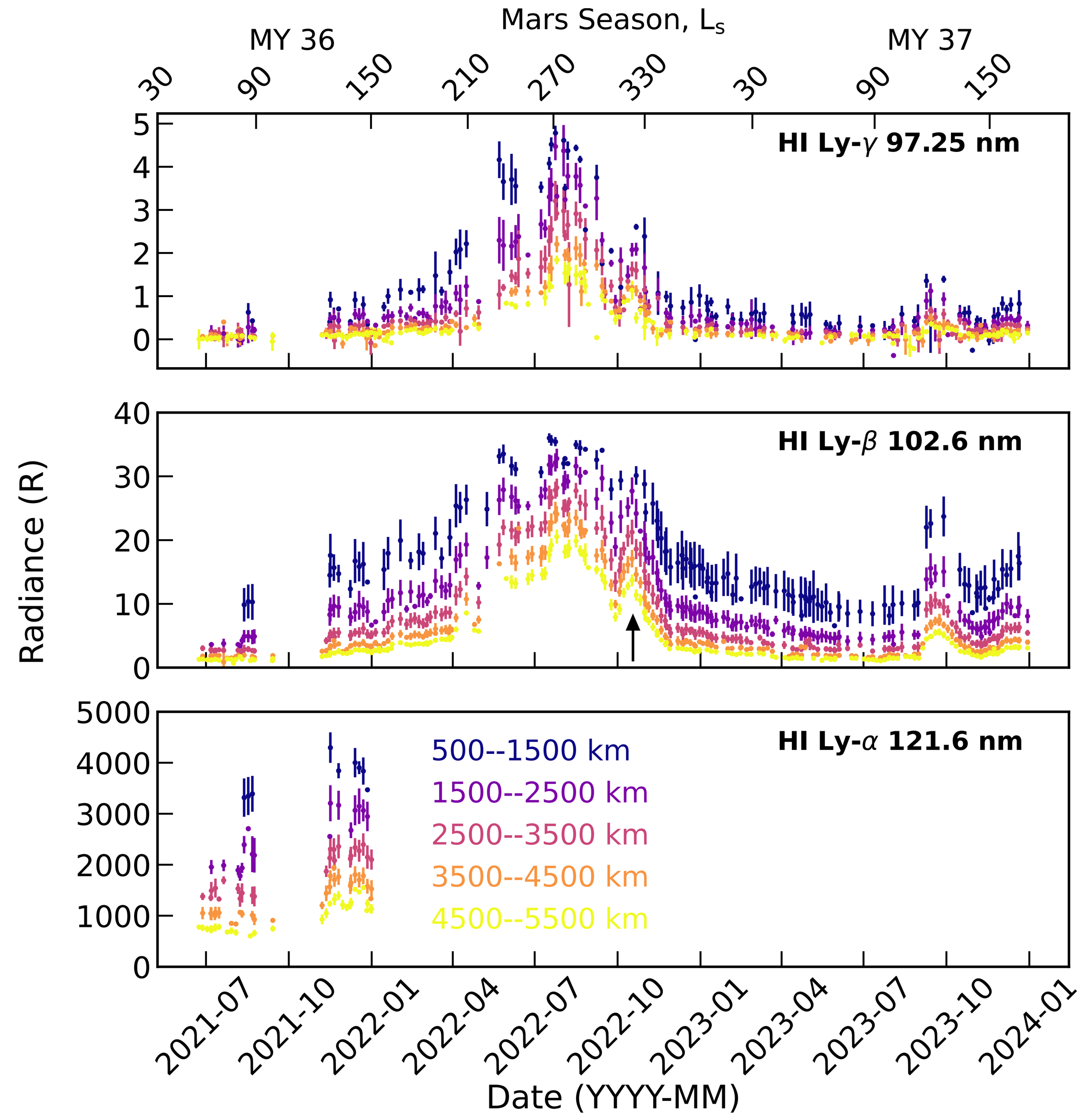
Core message

H/D–CO_2 collisions are not hard-sphere-like: they are strongly forward-peaked, so many collisions barely redirect hot H and D atoms. Classical and mass-scaled collision models therefore overestimate momentum loss and thermalisation. The consequence is macroscopic: revised exobase structure, escape rates, and D/H fractionation on Mars, early Venus/Earth, and CO_2-rich exoplanets.

Why this matters

Hydrogen escape controls long-term water loss and isotopic evolution on Mars, Venus, early Earth, and CO_2-rich exoplanets. In the upper thermosphere, suprathermal H/D atoms undergo only a limited number of collisions before escaping or thermalising. Therefore, the **angular distribution** and **momentum-transfer efficiency** of each collision matter more than the total collision probability alone.

Legacy models often use hard-sphere, isotropic, or reduced-mass-scaled collision parameters. These approximations miss the strongly forward-peaked nature of H/D–CO_2 scattering.



Observed Martian H exosphere variability and seasonal changes motivate improved escape and thermalisation physics. From Susarla *et al.*, JGR Space Phys 129, e2024JA032525

Quantum scattering calculations

We computed state-resolved, total, differential, and momentum-transfer cross sections for

$$CO_2(j) + H/D \rightarrow CO_2(j') + H/D,$$

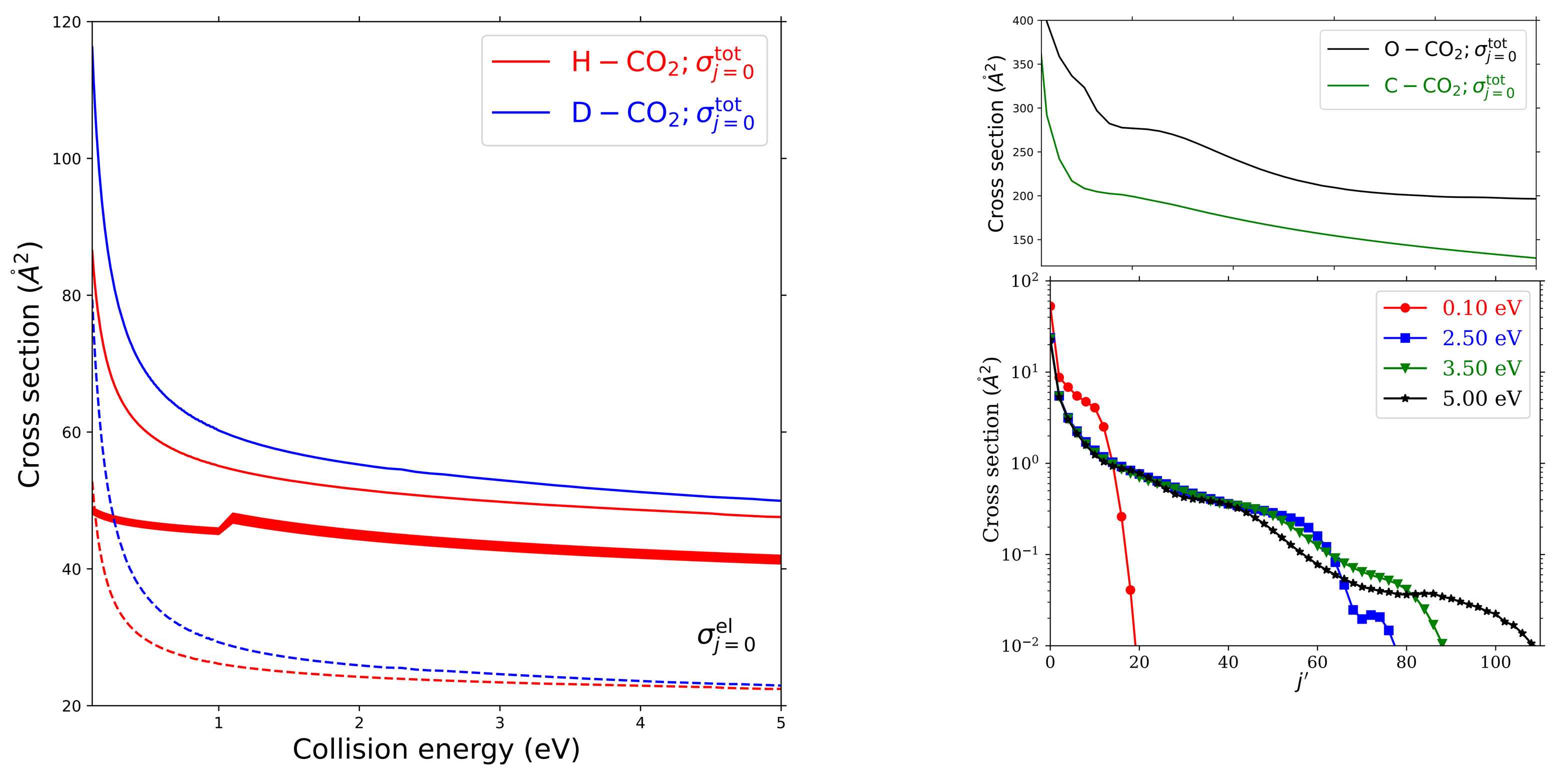
using a time-independent j_z-conserving coupled-states treatment the high-level *ab initio* H–CO_2 potential energy surface of Dagdigian (2015).

- Collision energies up to 5 eV.
- CO_2 rotational basis: $j = 0$–140; up to 241 partial waves, $J = 0$–240.
- Transport cross sections benchmarked against close-coupling calculations to within $\sim 7\%$.

Main result: mass scaling fails for light projectiles

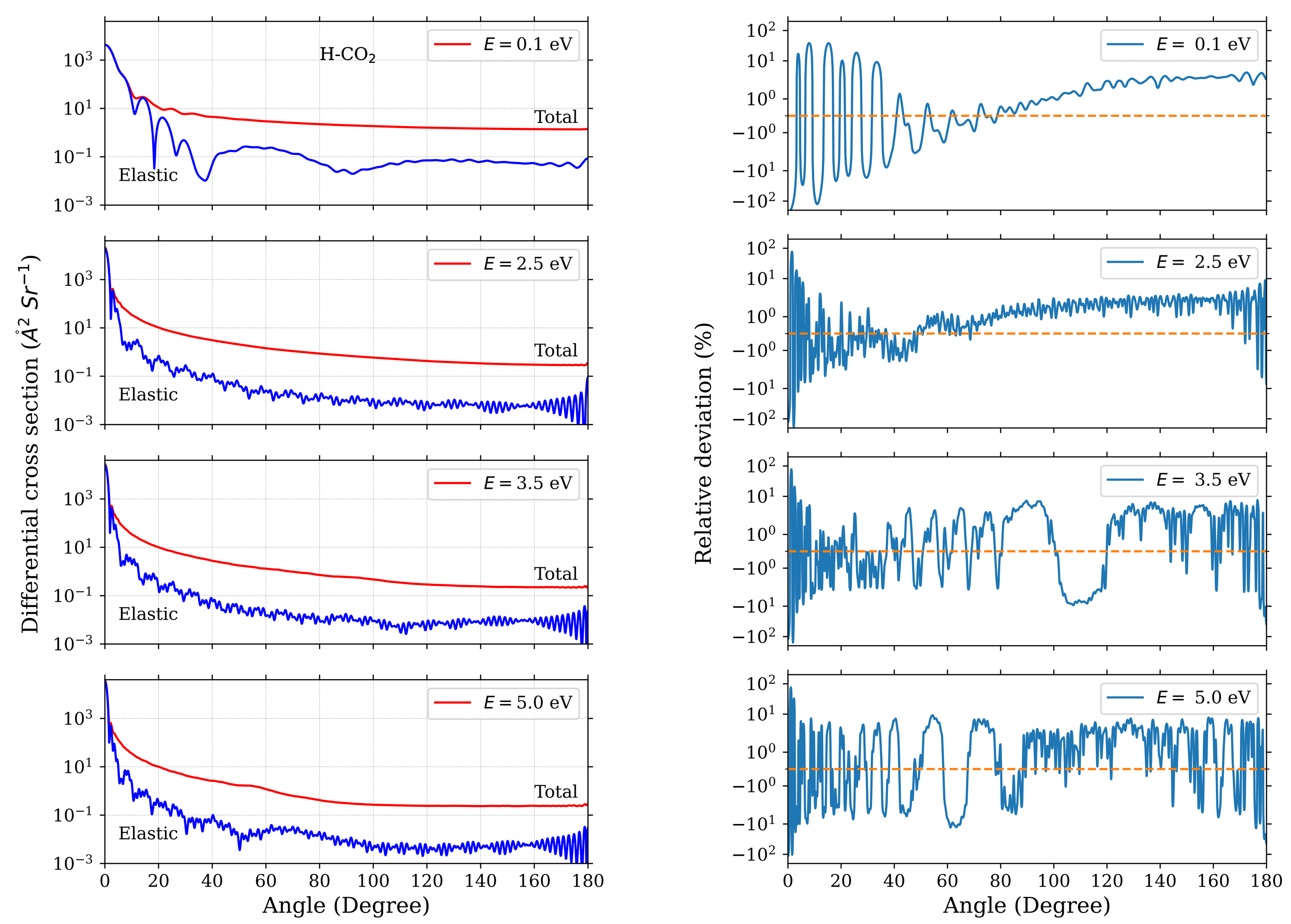
Reduced-mass scaling from O–CO_2 and C–CO_2 overestimates true H–CO_2 cross sections by factors of $\sim$ 30–45. H/D isotope effects are also energy dependent, reaching $\sim$ 35% at low energies, so a single scaling factor is not physically reliable.

Total cross sections: surrogate systems are not enough



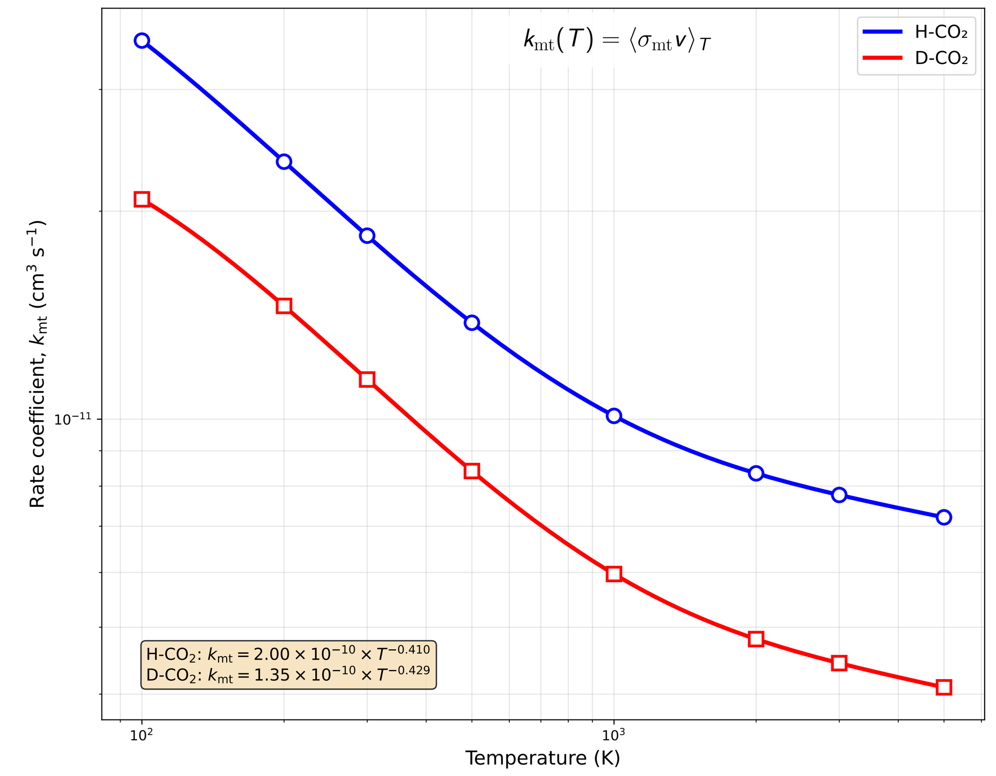
Left: H–CO_2 and D–CO_2 cross sections differ the most at low energy. **Top right:** O–CO_2 and C–CO_2 surrogate systems overestimate H–CO_2. **Bottom right:** Rotationally inelastic channels fall rapidly with j'.

Why transport is small: forward-peaked scattering



Differential cross sections reveal the mechanism. Most scattering occurs at small angles, so total cross sections overstate the efficiency of momentum loss. H/D deviations are angle dependent and cannot be represented by uniform scaling. The collision frequency may be high, but forward-peaked collisions barely redirect hot H/D atoms. This increases the effective momentum-transfer mean free path and makes suprathermal escape more likely than isotropic models would predict.

Rate coefficients for atmospheric models



T (K)	k_H cm^3 s^{-1}	k_D	k_D/k_H
100	3.53×10^{-11}	2.08×10^{-11}	0.589
300	1.84×10^{-11}	1.14×10^{-11}	0.619
1000	1.01×10^{-11}	5.97×10^{-12}	0.590
5000	7.21×10^{-12}	4.09×10^{-12}	0.568

At 300 K, mass-scaling from O–CO_2 would give $k_H \sim 3 \times 10^{-10}$ cm^3 s^{-1}, about 16 times larger than the quantum-mechanical H–CO_2 result. In escape models, this reduces collisional thermalisation efficiency and provides a direct path from quantum cross sections to Mars H/D escape, Venus and early Earth evolution, and CO_2-rich exoplanet atmospheres.

Implications for escape and evolution

- **Mars:** smaller σ_{mt} implies longer effective momentum-transfer mean free paths for hot H/D in the upper thermosphere.
- **Thermal escape:** in simple isothermal exobase estimates, reducing σ_{mt} can shift the exobase by
$$\Delta z_{exo} \simeq H \ln f,$$
giving plausible shifts of ~10–20 km and order-unity changes in Jeans escape rates.
- **Non-thermal escape:** suprathermal atoms undergo only a few collisions, so revised cross sections directly affect escape probabilities.
- **D/H fractionation:** isotope effects are energy and angle dependent; uniform H-to-D scaling is not reliable.
- **Early Earth, Venus, exoplanets:** weaker H–CO_2 momentum transfer may change thermospheric temperature and hydrogen-loss histories.

Take-home points

1. H/D–CO_2 scattering is strongly forward-peaked.
2. O/C–CO_2 mass scaling overestimates H–CO_2 cross sections by up to $\sim$ 30–45.
3. H/D isotope effects reach $\sim$ 35% at low energy.
4. New k_{mt} values are $\sim$ 16× smaller than mass-scaled estimates at 300 K.
5. These corrections can alter exobase structure, escape rates, and atmospheric evolution scenarios.

Data products

Cross sections & Rate coefficients Zenodo/17549249