Collisional excitation and collision-induced dissociation of astrochemically relevant molecules by ion impacts

M. Nakamura

Physics Laboratory, College of Science and Technology Nihon University, Japan

The collision-induced dissociation (CID) of small molecules by ion impacts such as

$$X^+ + AB \rightarrow \quad X^+ + A + B$$

plays an important role in the chemical evolution in molecular clouds [1-3]. Here we present a theoretical work on the energy transfer and fragmentation of molecules by ion impacts at hyperthermal energies. The classical trajectory (CT) calculation and the sudden-limit model [4,5] are applied to estimate the energy transfer from translational to internal degrees of freedom. Figure 1 represents the calculated excitation spectrum of CO molecule by proton impacts at the collision energy E=27 eV. The model predicts the energy-transfer from the translational to the internal degrees of freedom with less efficiency. The threshold energy for CID of CO molecule by ion impacts is calculated. The results are listed in Table I. When the projectile is much lighter than the target, the spectator model works well. The probability of CID depends strongly on the orientation angle at the moment of the contact. The CID takes place predominantly when an ion hits the molecule either perpendicular or parallel to the molecular axis. Calculation and analysis would be extended to other astrochemically relevant molecules.

Table I: Threshold energy (eV) for the collision-induced dissociation of CO by ion impacts obtained with the classical trajectory calculation and with the spectator model.

Projectile	CT calculation	Spectator Model
H^+	60	59
D^+	41	31
He^+	29	17
C^+	35	7

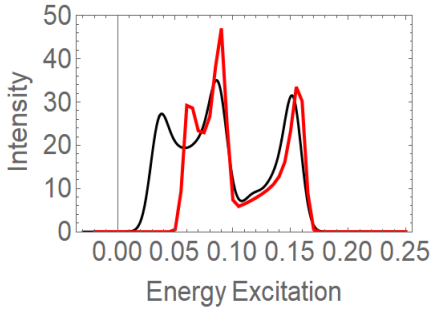

Figure 1: Calculated excitation spectrum of CO molecule by proton impact with incident energy of 27 eV. The black (red) curve is the result obtained with the classical trajectory (sudden limit model).

References

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