Quantum dynamics study on multi channel dissociation and isomerization reactions of formaldehyde

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Competition between various reaction channels including isomerizations and dissociations is observed in many molecular systems, exhibiting multiple potential energy minima and dissociation pathways. Formaldehyde (H$_2$CO) is a prototype of such molecules. The barrier height of isomerization to HCOH intermediate is very close to that of the molecular dissociation channel leading to H$_2$ and CO fragments. The threshold to the radical dissociation to H + HCO is located slightly above the molecular dissociation channel.

We carried out quantum dynamics calculations to study the two dissociation channels as well as isomerization on the ground state $S_0$ surface of H$_2$CO. The branching ratios of the isomerization reaction and radical dissociation to the molecular reaction of formaldehyde at the electronic ground state near reaction threshold energy are treated in the discussion. The energy range examined was set from the molecular dissociation threshold to slightly above the radical channel one. We examine (1) the time scale of intramolecular vibrational energy relaxation (IVR), (2) the role of isomerization in the dissociation reactions, and (3) the branching ratio of the radical channel as the function of energy. For this purpose, we constructed global potential function which describes two dissociation channels as well as isomerization.

We found branching ratio of radical reaction to total dissociation was $\sim 0.2$, which shows plateau behavior within 250 fs. The isomerization branching ratio to molecular dissociation reaction was $2 \sim 6\%$ in the energy range at 250 fs, however increasing feature in time was clearly observed.

The left 6 and right 3 figures correspond to the time-dependent branching ratio of isomerization and radical channel to molecular dissociation for energy filtered states respectively.