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Emission Spectra of *p*-Xylene Excited by Ar^+ Ion Beam

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Emission spectra of *p*-xylene were measured under ion-impact excitation. There were a weak band of the S_1-S_0 transition of *p*-xylene itself and several intense bands of excited fragment species. The spectra were similar to those excited by electron impact, but the band intensity of the parent molecule was much weaker under ion-impact excitation.

Emission spectra of many organic compounds excited by electron impact have been investigated to reveal the excitation and dissociation processes in these molecules.1) Aromatic compounds have shown intense bands due to the S_1-S_0 transition of the parent molecules as well as the lines and bands due to excited fragment species.1-3) The S_1-S_0 band shows vibrational structure characteristic of electron excitation (hot bands4) and symmetry forbidden transitions5)). As an extension of these studies, an apparatus for a spectroscopic study on the ion-molecule collision process has been constructed and the optical emission spectra of *p*-xylene have been measured.

The collision chamber has a gas cell and a Colutron Ion Source. It was evacuated with two turbo-molecular pumps (110 dm^3/s). The base pressure was of the order of 4×10^{-6} Torr (1 Torr =133 Pa) and the operating pressure in the gas cell was about 2×10^{-4} Torr. The optical emission was observed at an angle of 90° with respect to the ion beam with a JASCO CT-50 monochromator equipped with a Hamamatsu R585 photomultiplier. Photons were counted with a Hamamatsu C1230 photoncounter. *p*-Xylene (Guaranteed reagent, Wako Pure Chem. Ind.) was frozen and pumped repeatedly to remove any dissolved gasses.

Typical emission spectra excited in collision with Ar^+ ions showed several intense lines and bands of excited fragment species such as H^* (Balmar lines), C^* (A-X), C_2^* (d-a), CH^* (A-X, B-X, C-X), and CH^{+*} (B-A) as well as the lines of Ar produced by charge exchange of the incident Ar^+ ions as shown in Figs. 1 (B) and 2. However, any band assignable to the S_1-S_0 transition of *p*-xylene molecule was hardly visible in Fig. 1 (B), although such a band was clearly visible in the spectrum by electron impact (Fig. 1 (A)).1-3) The emission from the fragment species was relatively more intense with an ion impact than the case by electron impact. The incident ion removes a π-electron from *p*-xylene in a charge exchange reaction, and the dissociation energy of aromatic skeletal bonds would decrease.

The ordinate of Fig. 1 (B) was expanded in the 240-330 nm region as shown in Fig. 2. The spectrum showed a broad band; its band shape was identical to that excited by electron impact,2,3) though an intense CH band overlaps. Since its vibrational structure (indicated in the figure) was same as that obtained by electron impact, we could confirm that this band was due to the S_1-S_0 transition. Direct excitation to the S_1 state of *p*-xylene occurs also by ion impact.

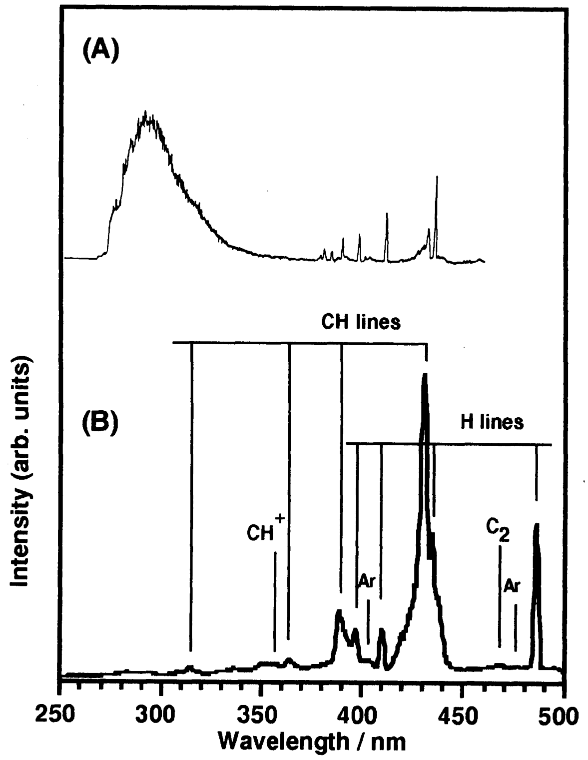

Fig. 1. The optical emission of *p*-xylene by electron impact (A) and by Ar^+ ion impact (B).

(A) From Ref. 3.

(B) Optical resolution: 2.2 nm
Impact energy: 3.0 keV
Ion beam current: 0.4 μA

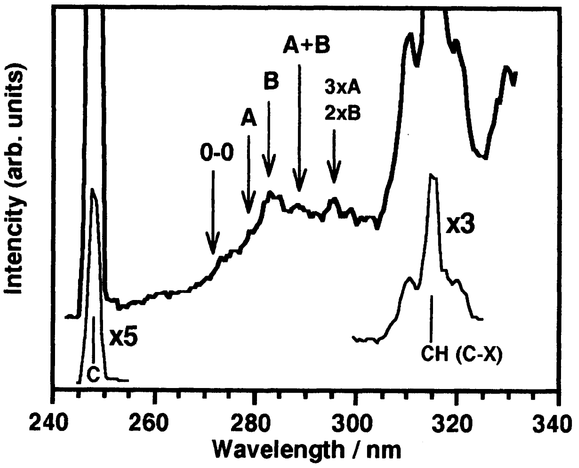

Fig. 2. The S_1-S_0 transition of *p*-xylene excited by Ar^+ ion impact.
Vibrational progression:
A: 829 cm^{-1} B: 1208 cm^{-1}

Optical resolution: 2.2 nm
Impact energy: 3.0 keV
Ion beam current: 0.4 μA

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