Vibronic Spectroscopy of Chlorofluorobenzyl Radicals Generated in Corona Discharge

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The technique of corona excited supersonic expansion (CESE) was employed to produce vibronically excited but jet-cooled benzyl-type radicals from corona discharge of precursors using a pinhole-type glass nozzle developed in this laboratory. Stable precursor molecules such as chlorofluorotoluene and chlorofluorobenzyl chloride were used for the production of jet-cooled chlorofluorobenzyl radicals[1-5], in which the methyl C-H and C-Cl bonds dissociate in corona discharge. The vibronic emission spectra were recorded in the visible region using a long-path monochromator.

From the analysis of the vibronic emission spectra observed from the corona discharge of precursor molecules with a large amount of carrier gas helium, we found the spectroscopic evidence of chlorofluorobenzyl radicals as well as fluorobenzyl radicals which suggest that there might be a displacement reaction of Cl by H of methyl group during corona discharge. By comparing of the spectra observed from different precursors, we can obtain the possible mechanism of bond dissociation process for the production of benzyl-type radicals.

In this presentation, we will discuss the dissociation process of chlorofluorotoluenes in corona discharge and spectroscopic analysis of the substituent effect on electronic transition energy of benzyl-type radicals. The red-shift of the electronic transition energy is sensitive to the types of substituents and positions on the benzene ring. The substituent effect devised in this work could be useful for identification of isomeric benzyl-type radicals.

References

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