SPECTROSCOPIC IDENTIFICATION OF NEW BENZYL-TYPE RADICALS IN CORONA EXCITATION: CHLORO-α-METHYLBENZYL RADICALS

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Using a pinhole-type glass nozzle coupled with corona excited supersonic expansion (CESE), precursors *o*- and *p*-chloro-ethylbenzenes seeded in a large amount of inert carrier gas helium were corona discharged to produce jet-cooled benzyl-type radicals. The vibronic emission spectra were recorded with a long path monochromator to observe vibronic bands of benzyl-type radicals in the visible region. The analysis of the spectra shows the evidence of the *o*- and *p*-chlorobenzyl radicals as typical products in corona excitation as well as the *o*- and *p*-chloro-α-methylbenzyl radicals as unexpected species.[a] After subtracting the bands belonging to chlorobenzyl radicals, we could construct the vibronic emission spectra of the *o*- and *p*-chloro-α-methylbenzyl radical in the $D_1 \rightarrow D_0$ electronic transition at the gas phase. By comparing with those of *ab initio* calculation and of the known vibrational mode frequencies with similar structures, we could obtain the electronic transition and assign the vibrational modes to the bands observed.

[a]H. G. Ahn, G. W. Lee, and S. K. Lee *J. Phys. Chem. A* **112** (51), 13427 (2008).