VIBRONIC EMISSION SPECTRA OF DIFLUOROBENZYL RADICALS OBSERVED IN A CORONA EXCITED SUPERSONIC EXPANSION

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With a technique of corona excited supersonic expansion (CESE) developed in this laboratory, difluorobenzyl radicals have been generated from difluorotoluenes seeded in a large amount of inert carrier gas He and vibronically excited in a jet using a pinhole-type glass nozzle. The vibronically well-resolved emission spectra of difluorobenzyl radicals recorded with a long path monochromator in the $D_1 \rightarrow D_0$ transition show several vibronic bands originating from the ground vibrational state of the lowest excited electronic state, together with the origin band of the electronic transition. The vibronic spectra have been analyzed to give the electronic transition and vibrational mode frequencies in the ground electronic state of the radicals by comparing with not only those from the precursor but also with those of an ab initio calculation using Gaussian 98 program. The analysis provides the spectra tendency of electronic transition of difluorobenzyl radicals.