

VIBRONIC EMISSION SPECTRA OF METHYL-SUBSTITUTED BENZYL 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, the 2,4,5-trimethylbenzyl radical has been generated from 1,2,4,5-tetramethylbenzene 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 spectrum of 2,4,5-trimethylbenzyl radical recorded with a long path monochromator in the D_1 - D_0 transition shows 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 structure has been analyzed to give the electronic transition and vibrational mode frequencies in the ground electronic state of the radical by comparing with not only those from the precursor as well as with those of the ab initio calculation using Gaussian 98 program. The analysis provides the spectra tendency of electronic transition with increasing methyl substitution.