SPECTROSCOPIC ANALYSIS OF 2,3-DIFLUOROBENZYL RADICAL

Chang Soon Huh
Applied Chemistry Major, Division of
Chemical and Environmental
Engineering, College of Engineering
/Dong-eui University
South Korea
0411black@deu.ac.kr

ABSTRACT

The vibronically cooled electronic emission spectra of the 2,3-difluorobenzyl radical was observed in a corona excited supersonic expansion (CESE) apparatus. Several fundamental modes of methyl- and trimethylbezene were assigned on the basis of previous infrared and Raman values of the precursor and calculation. The spectrum was analyzed in terms of progressions of the fundamental vibrational modes and molecular structures of 2,3-difluorobenzyl and 2,6-difluorobenzyl were calculated and compared with experimental data. The fluoro-substitution effect is first suggested by this group. The substitution effect is that each fluoro substituted position of benzyl radical affect the energy level and also the band shape of the benzyl radical independently. We have generated for the first time the 2,3-difluorobenzyl radical in a jet from which the vibronic emission spectra in the $D_1 \rightarrow D_0$ transition have been recorded.

Keywords: 2,3-difluorobenzyl, 2,6-difluorobenzyl, CESE, *ab initio* calculation.