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Cumulant Expansion Line Shape Theory Applied to Photoexcitation Spectrum of Protonated Tyrosine[1] MINO YANG, JANG SOOK KWON, CHANG MIN CHOI, NAM JOON KIM, Chungbuk National University, JOONKYUNG JANG, Pusan National University — Photodepletion spectrum of gaseous protonated tyrosine molecules was obtained at 150 K by UV laser spectroscopic technique in conjunction with mass spectrometry and interpreted by theoretical methods. The spectrum exhibits distinct three bands separated each other by about 800 cm^{-1}. The whole pattern of the spectrum was reasonably reproduced by a combination of theoretical methods, the second order cumulant expansion, a semi-empirical quantum chemistry method, molecular dynamics simulation, and a semi-classical time-correlation function approach. The three spectral bands turned out to arise from the vibronic transition of two vibrational modes constituted by the "benzene breathing" mode and a torsional mode of the amino acid backbone. It is suggested that the major factor of the spectral broadening is not conformational disorder nor lifetime broadening but the thermal fluctuation of the stable conformers. The good agreement between the experimental and theoretical spectra exemplifies the validity of the theoretical methods applied for the present molecular system.

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Mino Yang
Chungbuk National University

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