Supporting Information

Excited-state Triple-Proton Transfer in 7-Azaindole(H_2O)$_2$ and Reaction Path Studied by Electronic Spectroscopy in the Gas Phase and Quantum Chemical Calculations

[1]Kenji Sakota, [2]Christophe Jouvet*, [2]Claude Dedonder, [3]Masaaki Fujii, [1]Hiroshi Sekiya*

[1]Department of Chemistry, Faculty of Sciences, and Department of Molecular Chemistry, Graduate School of Science, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581, Japan

[2]Institut des Sciences Moléculaires d'Orsay and Centre Laser de L'université Paris Sud, Université Paris-Sud 11, 91405 Orsay Cedex, France

[3]Chemical Resources Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku,
Yokohama 226-8503, Japan

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*Corresponding author.
E-mail: christophe.jouvet@u-psud.fr , sekiya@chem.kyushu-univ.jp

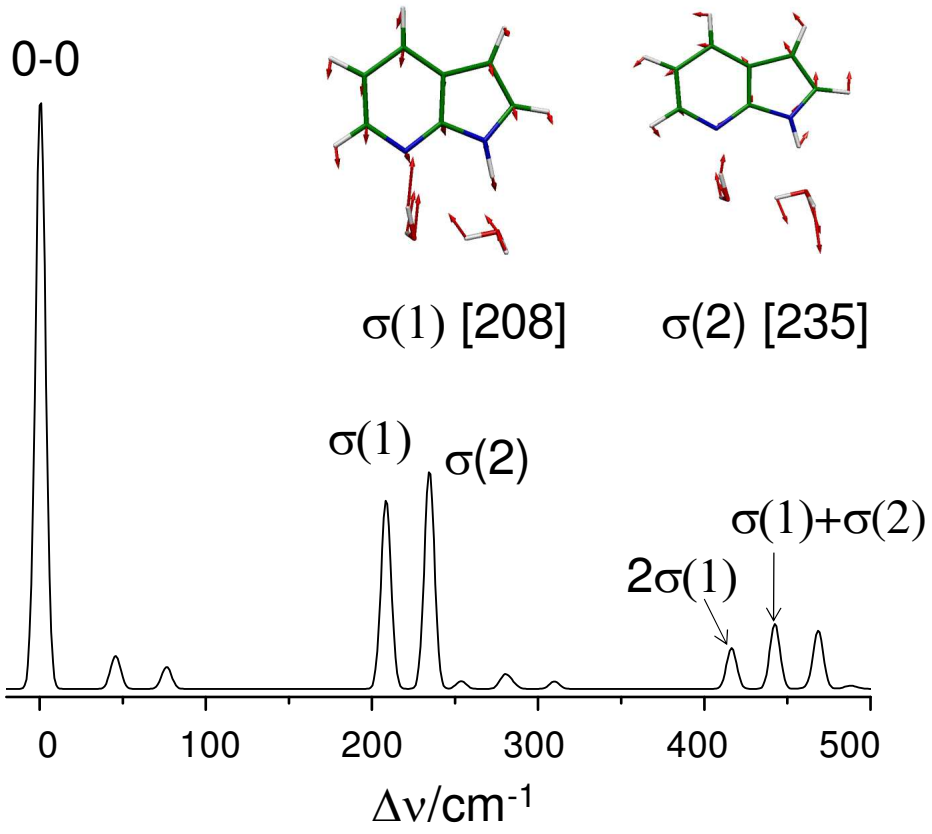

Figure SI

Figure SI The S_1-S_0 electronic spectrum of the cyclic 7AI$(H_2O)_2$ in the $\Delta\nu$=0-500 cm^{-1} region has been obtained by TD/DFT calculations using the cc-pVDZ basis set. The Franck-Condon analysis is carried out using the Pgopher software[33]. The displacments of two intermolecular modes σ(1) and σ(2) and their frequencies in units of cm^{-1} are inserted.