

Conformational study of protonated noradrenaline by UV-UV and IR dip double resonance laser spectroscopy combined with an electrospray and a cold ion trap methods

Hiromichi Wako[‡], Shun-ichi Ishiuchi^{‡*}, Daichi Kato[‡], Géraldine Féraud^{#§}, Claude Dedonder-Lardeux[#], Christophe Jouvet[#], Masaaki Fujii^{‡*}

[‡] Laboratory for Chemistry and Life Science, Institute of innovative research, Tokyo Institute of Technology, 4259, Nagatsuta-cho, Midori-ku, Yokohama, Japan.

[#] CNRS, Aix-Marseille Université, PIIM UMR 7365, Avenue Escadrille Normandie-Niémen, 13397 Marseille Cedex 20, France

[§] Present address: LERMA, Sorbonne Universités, UPMC Univ. Paris 06, Observatoire de Paris, PSL Research University, CNRS, F-75252, Paris, France.

* Corresponding authors: ishiuchi.s.aa@m.titech.ac.jp (SI), mfujii@res.titech.ac.jp (MF)

Table S1 Contribution ratios of the $\pi\sigma^*$ configurations in the S_1 - S_0 transition

conformer	contribution ratio / %
G1-STR1	12.1
G1-STR2	20.4
G1-STR3	2.4
G1-STR4	1.4
T-STR1	3.4
T-STR2	5.8
T-STR3	4.0
T-STR4	4.5
G2-STR1	3.2
G2-STR2	7.6
G2-STR3	12.0
G2-STR4	8.8

Fig S1 Ground state optimized structures of NAdH^+

