

# CHEMISTRY

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### Supporting Information

#### **Proton Transfer Accompanied by the Oxidation of Adenosine**

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Shunichi Miyamoto,<sup>[c]</sup> Kazuo Kobayashi,<sup>[c]</sup> Hyotcherl Ihee,<sup>\*, [a, b]</sup> and Tetsuro Majima<sup>\*, [c]</sup>

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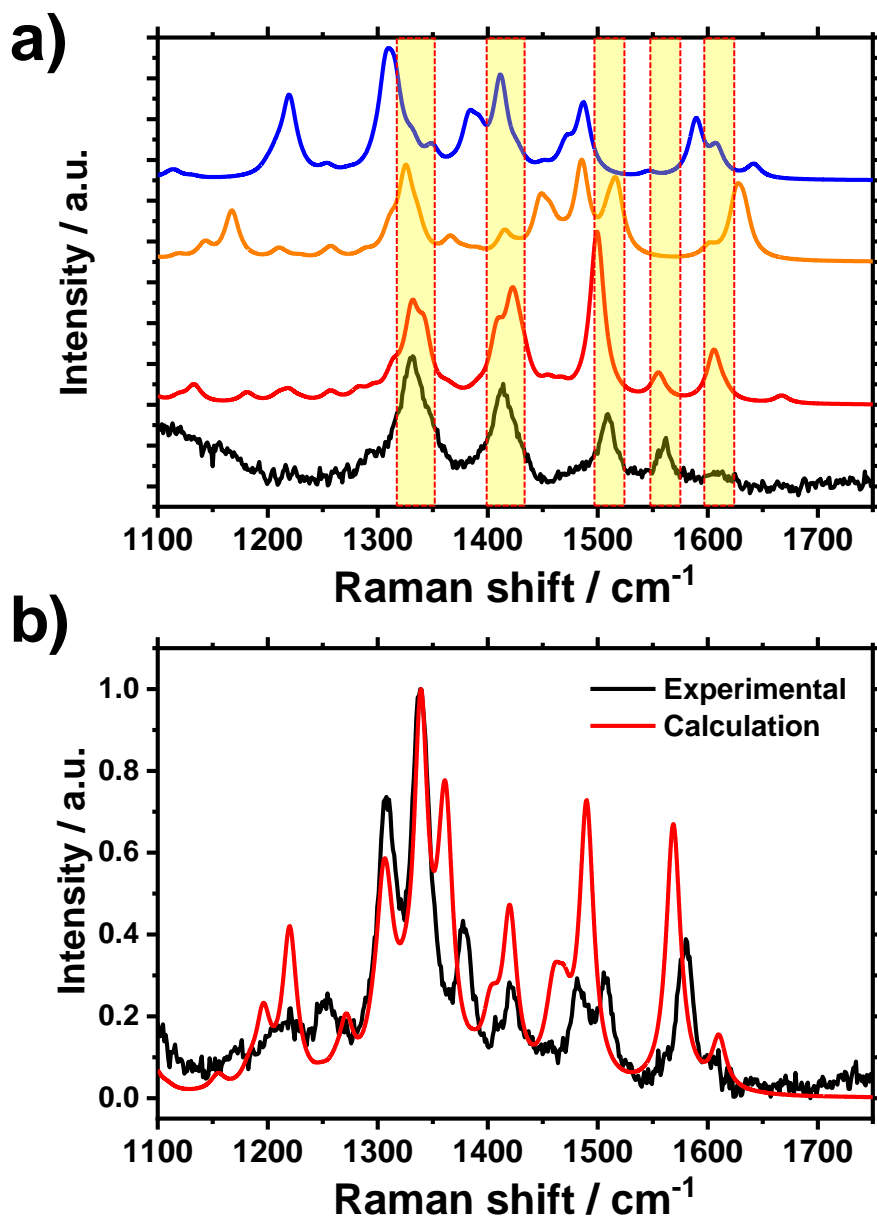
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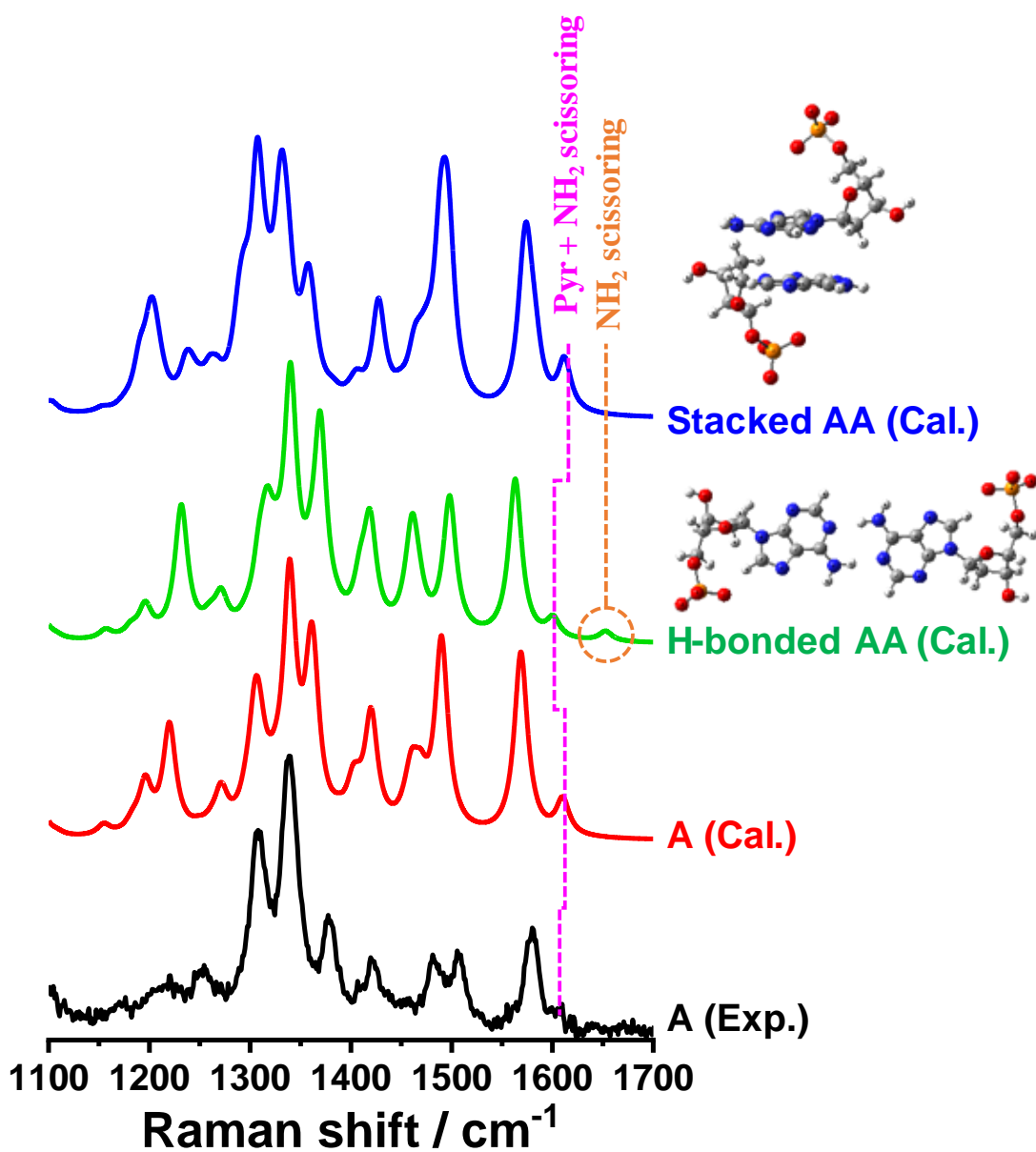
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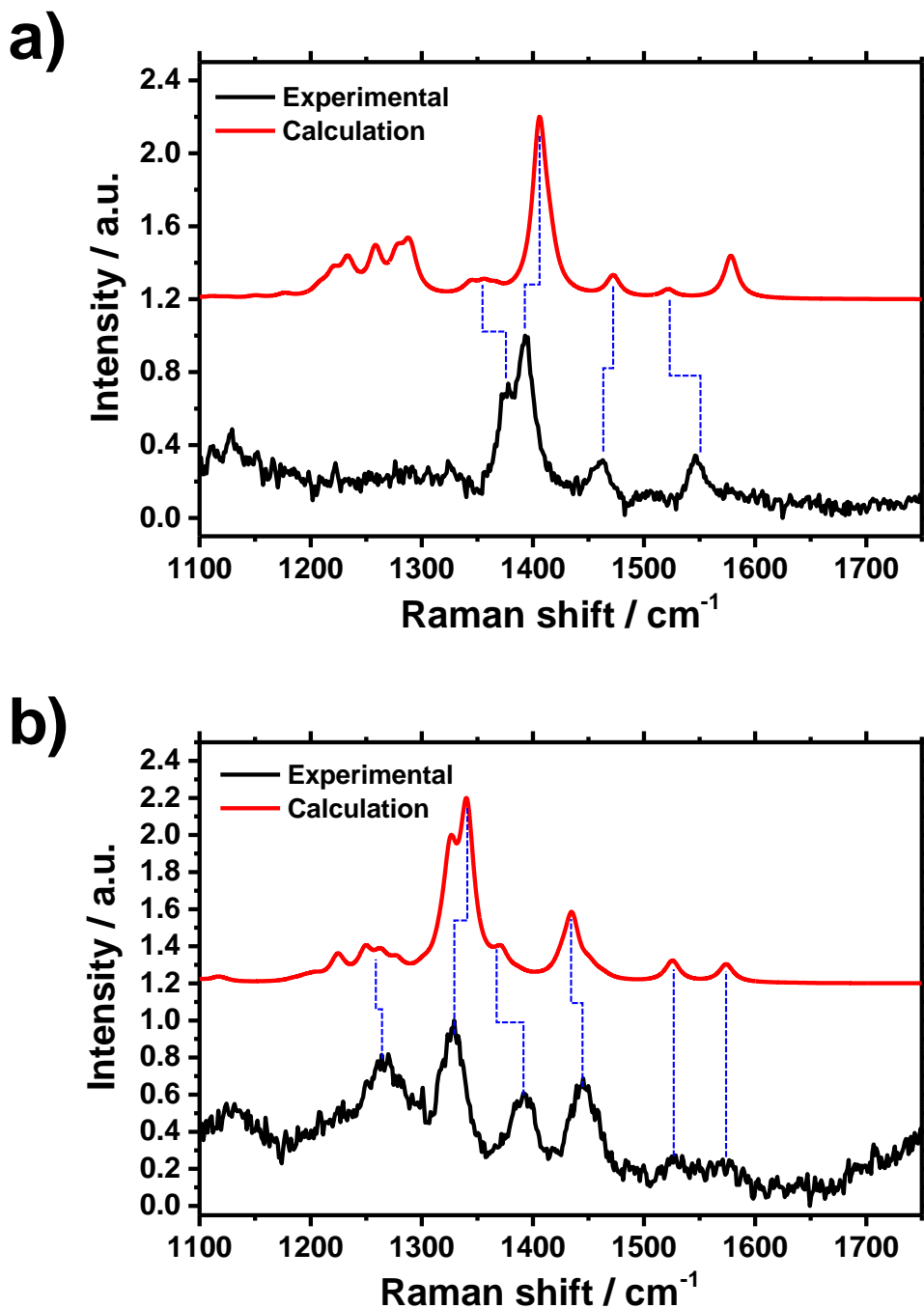
**Figure S1.** a) Experimental Raman spectrum of  $\text{AH}^+$  (black line) and theoretical Raman spectra of  $\text{AH}^+$  (red line:  $\text{AH}^+(\text{N1}+\text{H}^+)$ , orange line:  $\text{AH}^+(\text{N1}+\text{H}^+)$ , and blue line:  $\text{AH}^+(\text{N7}+\text{H}^+)$ ). b) Experimental and theoretical Raman spectra of **A**. All simulated Raman spectra were calculated with B3LYP-D3/6-311++G(d,p) method. Scaling factor: 0.982 for  $\text{AH}^+(\text{N1}+\text{H}^+)$  and **A**.



**Figure S2.** Experimental Raman spectrum of A (black) at neutral pH and theoretical Raman spectra of A (red), H-bonded adenosine dimer (green), and stacked adenosine dimer (blue).



**Figure S3.** a) Experimental and theoretical Raman spectra of  $\text{AH}^{\bullet 2+}(\text{N1}+\text{H}^+)$ . b) Experimental and theoretical Raman spectra of  $\text{A}^{\bullet}(\text{N10-H})$ . All simulated Raman spectra were calculated with (U)B3LYP-D3/6-31G(d) method. Scaling factors: 0.93 and 0.982 for  $\text{AH}^{\bullet 2+}(\text{N1}+\text{H}^+)$  and  $\text{A}^{\bullet}(\text{N10-H})$ , respectively.



**Figure S4.** a) Raman spectrum measured at pH 2.3. b) Raman spectra of  $\text{AH}^{2+}(\text{N1}+\text{H}^+)$  calculated with (U)B3LYP-D3/6-31G(d) method. Scaling factor: 0.93. c) Raman spectra of  $\text{A}^{*+}$  calculated with (U)B3LYP-D3/6-31G(d) method. Scaling factor: 0.982. d) Raman spectra of  $\text{A}^{*+}$  calculated with (U)B3LYP-D3/6-31G(d) method. Scaling factor: 0.93.

