Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information (ESI) for

The useful properties of H_2O as a ligand of a hydrogenases mimic

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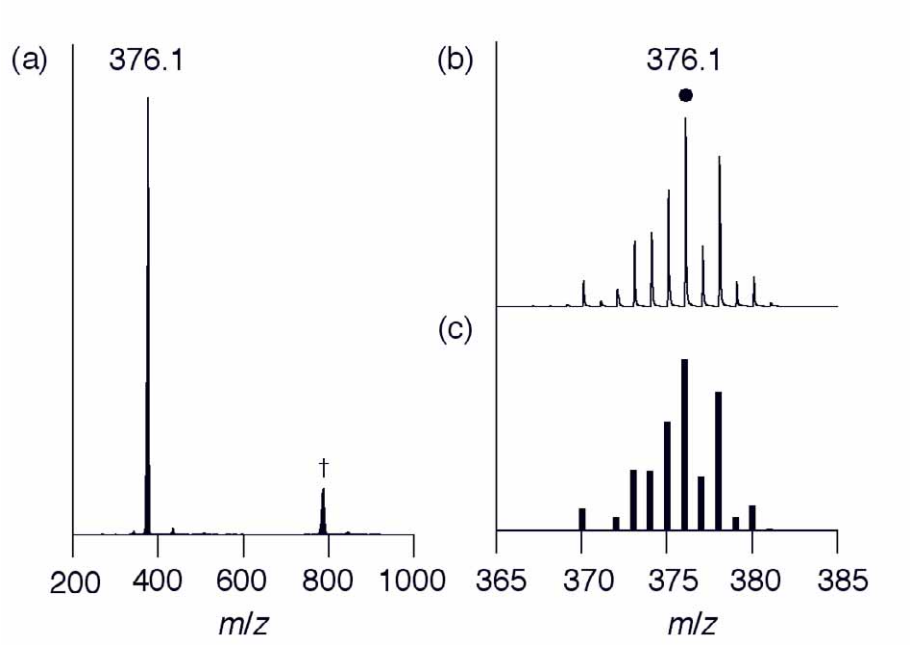

Fig. S1. (a) Positive-ion ESI mass spectrum of **1** in methanol. (b) Signal at *m/z* 376.1 for $[\mathbf{1} - Cl]^+$. (c) Calculated isotopic distribution for $[\mathbf{1} - Cl]^+$. †: the signal of $[2(\mathbf{1}) - Cl]^+$.

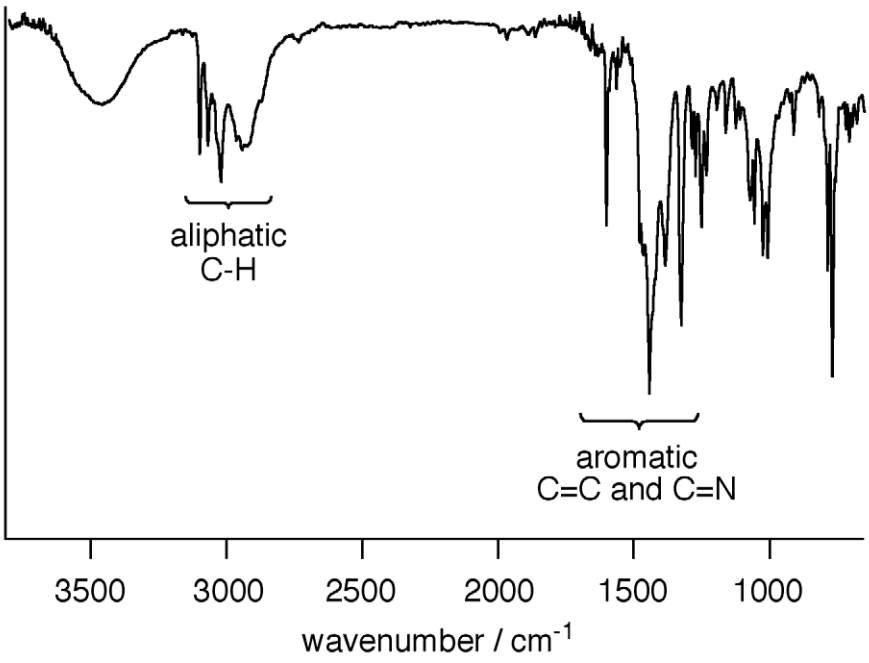

Fig. S2. IR spectrum of **1** as a KBr disk.

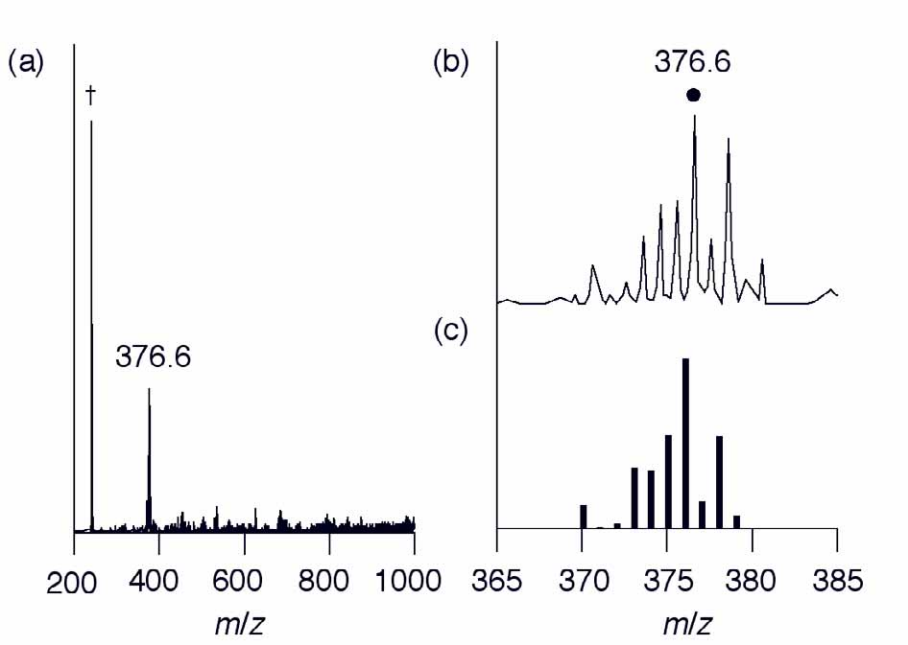

Fig. S3. (a) Positive-ion ESI mass spectrum of [**2**]$(BF_4)_2$ in methanol. (b) Signal at *m/z* 376.6 for [**2** - H]$^+$. (c) Calculated isotopic distribution for [**2** - H]$^+$. †: the signal of Bz^py.

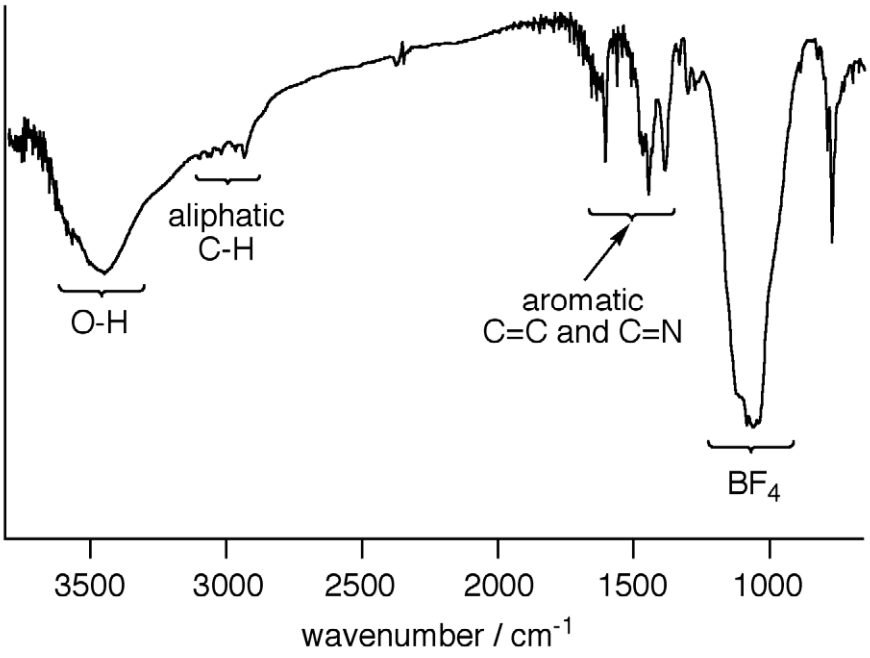

Fig. S4. IR spectrum of [**2**]$(BF_4)_2$ as a KBr disk.

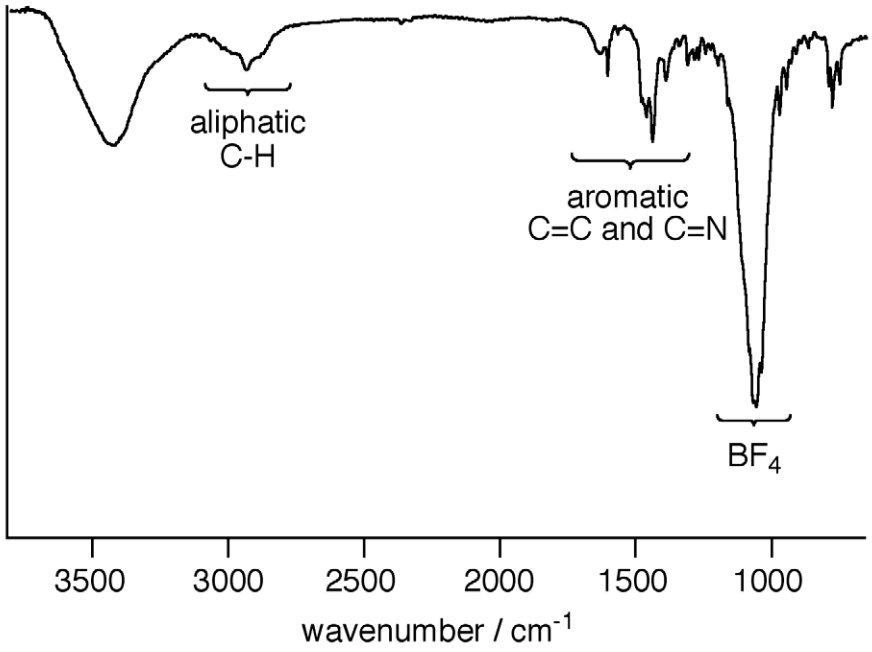

Fig. S5. IR spectrum of [**3**]$(BF_4)_2$ as a KBr disk.

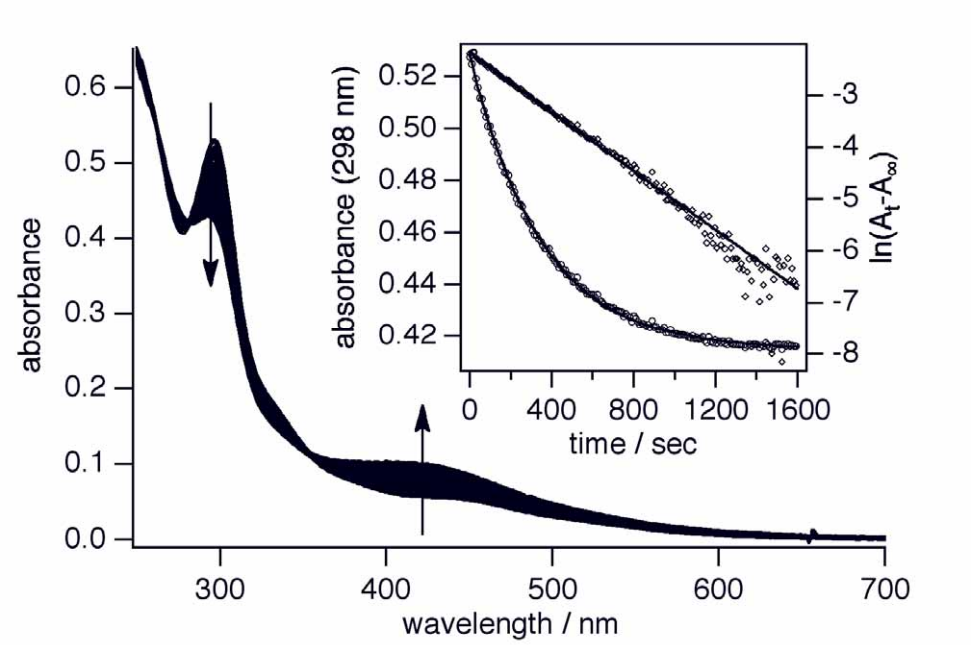

Fig. S6. UV-vis spectral change for the reaction of $[\mathbf{A}_{aqua}](NO_3)_2$ with H_2 (0.1 MPa) in water at pH 7.0 at 25 ºC. Inset shows the reaction time profile of the absorbance at 298 nm and the first-order plot.

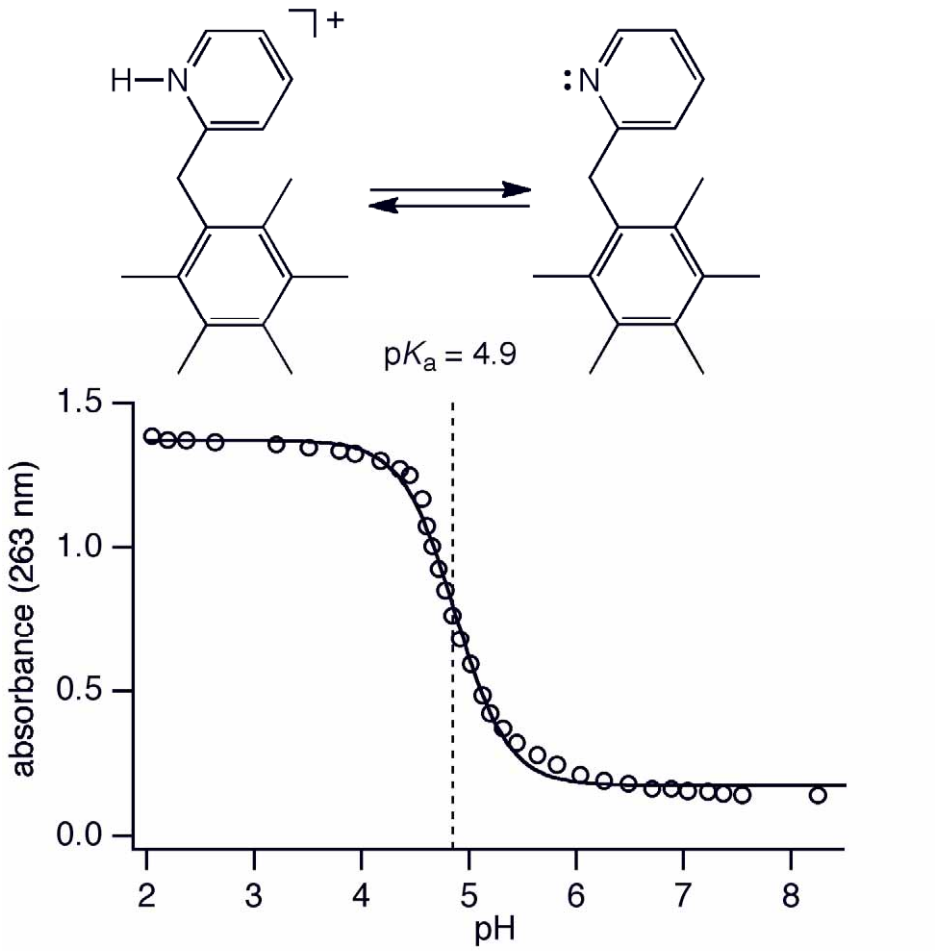

Fig. S7. A plot of absorbance (l = 263 nm) *versus* pH. Experiments were performed by the titration of Bz^py with 0.1 HNO_3/H_2O and 0.1 M $NaOH/H_2O$ in water at 25 °C.