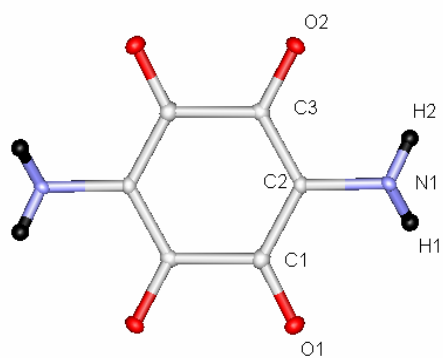


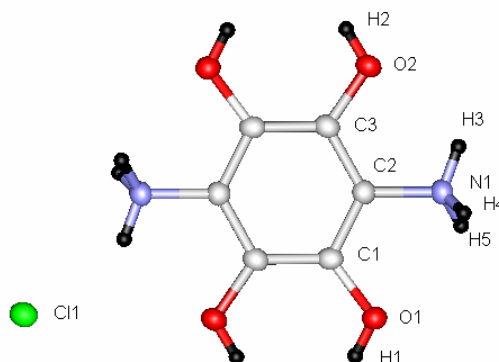
## Supporting Information

Title: Crystal and Electronic Structures of Hydrogen-bonded 2,5-Diamino-3,6-dihydroxy-*p*-benzoquinone

Atomic numbering scheme of compounds 1 and 2.



Compound 1



Compound 2

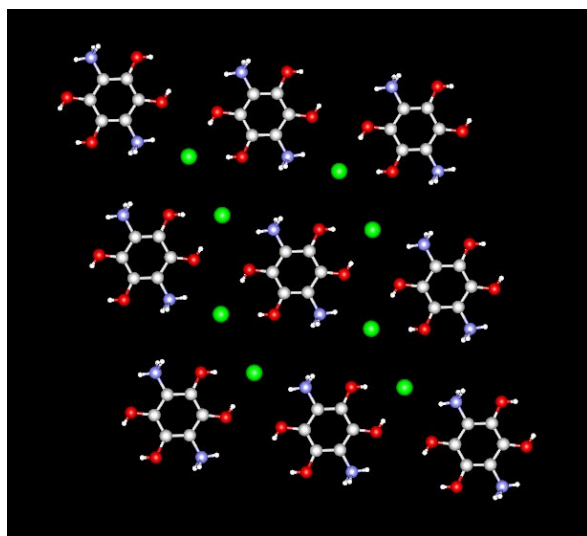
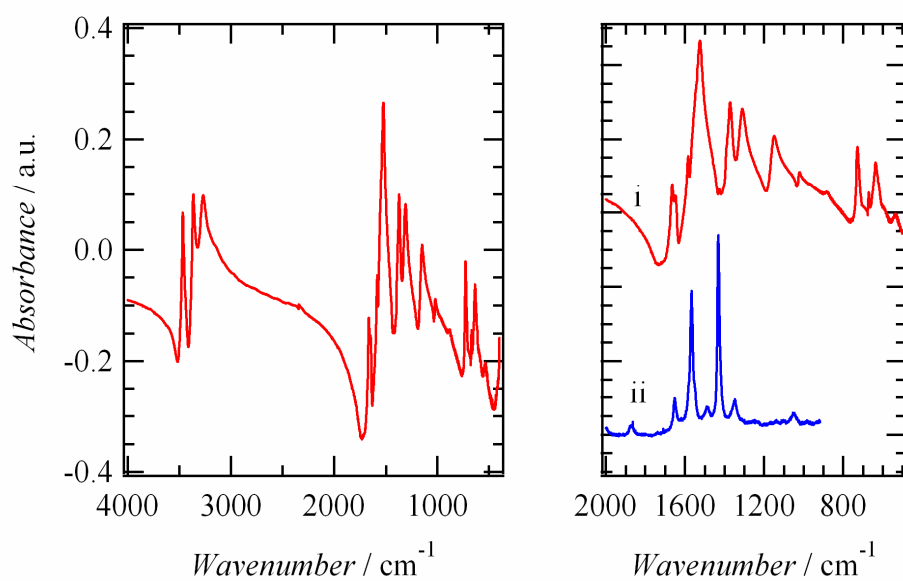
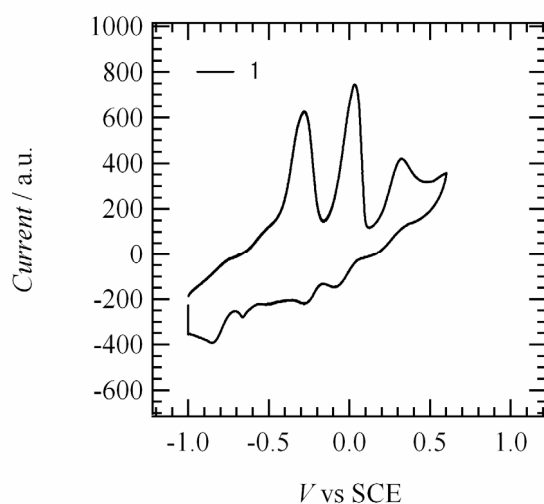


Fig. S1. Molecular packing of (2,3,5,6-tetrahydroxy-*p*-phenylenediammonium)(Cl<sup>-</sup>)<sub>2</sub> **2** in the crystal.



**Fig. S2.** IR (red i) and Raman (blue ii) spectra of molecule **1**.



**Fig. S3.** Cyclic voltammetry of compound **1** in anhydrous DMF using 0.1 M  $(n\text{-Bu}_4\text{N})(\text{BF}_4)$  as the supporting electrolyte, platinum electrodes (working- and counter-electrode), and a saturated calomel electrode (SCE). Three irreversible oxidation peaks were observed at -0.28, 0.03, and 0.32 V.