Supporting Materials for article

Molecular Structure Features and Acid–Base Ionization of the 5–(4`–Aminophenyl)–10,15,20–tris(4`–sulfophenyl)porphine Conjugate with H–acid in Water

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Особенности молекулярного строения и кислотно–основная ионизация коньюгата 5–(4`–аминофенил)–10,15,20–трис(4`–сульфофенил)порфина с Аш–кислотой в воде

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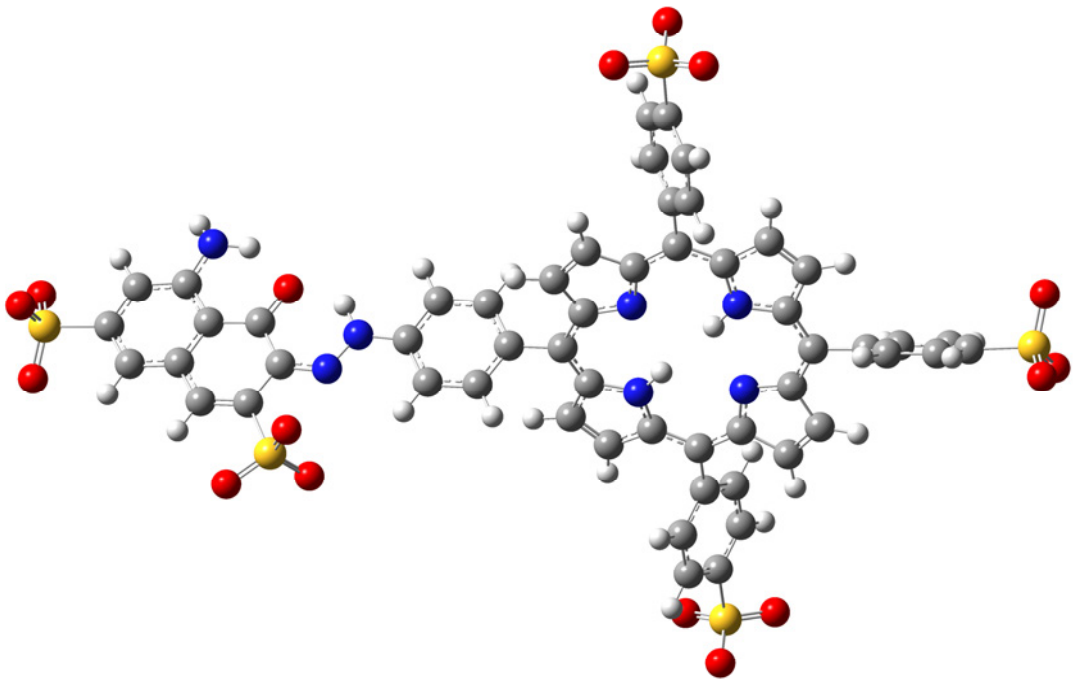
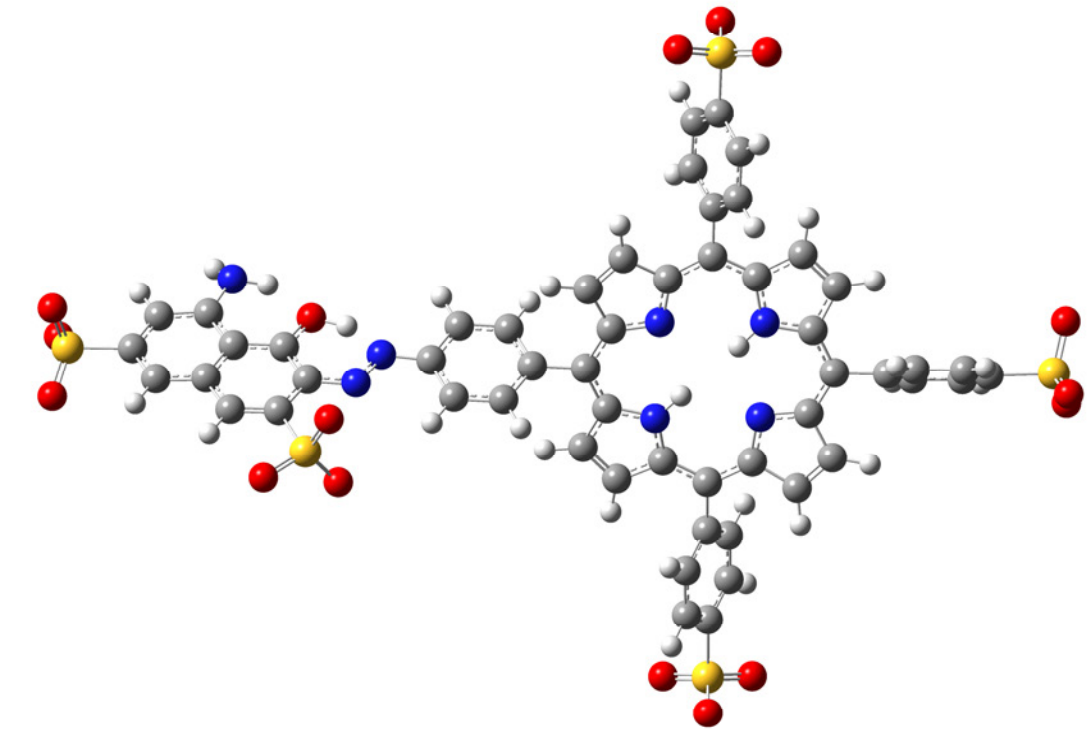
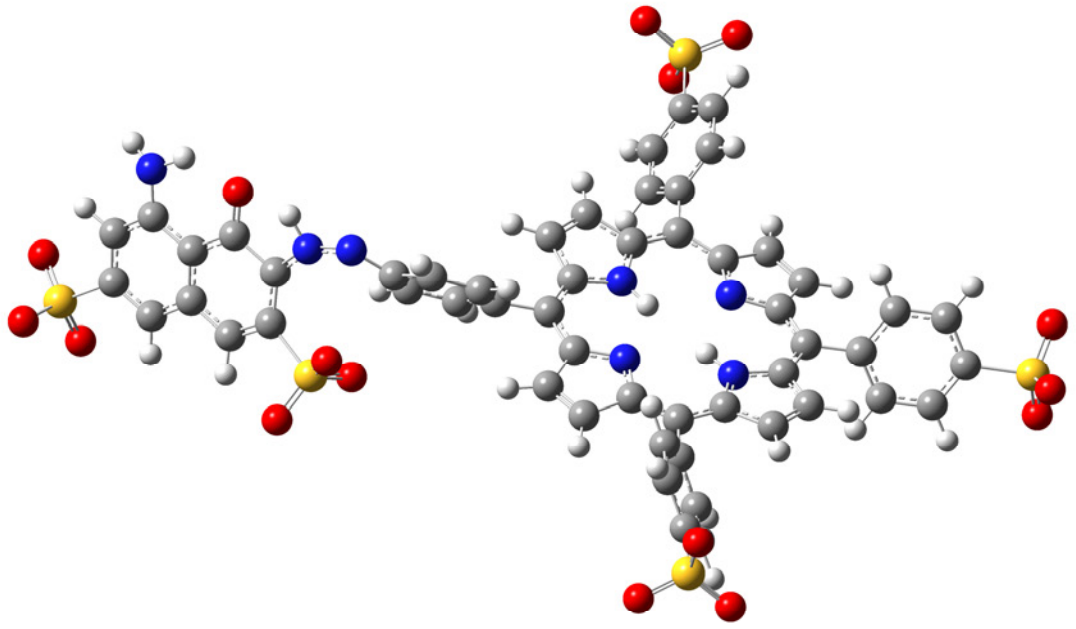


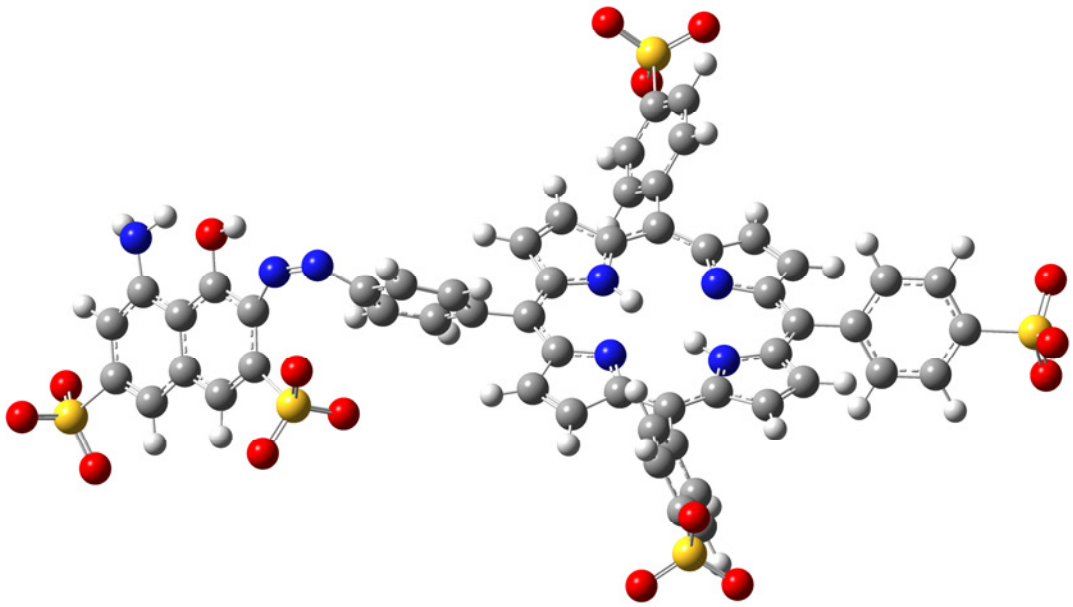
E_0



E_0 + 6.47

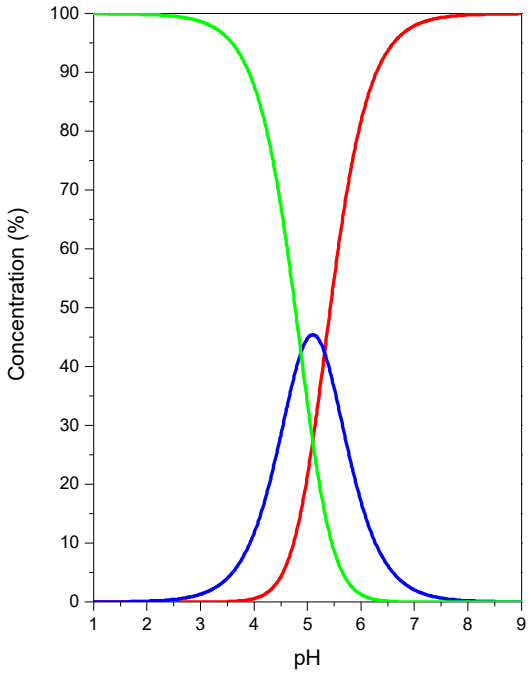


E_0 + 35.47



E_0 + 41.47

Figure S1. Molecular structure and the difference in the total formation energies of various forms of *H*-conjugate (E, kcal/mol) according to the DFT/B3LYP/631G(d,p) method.



$$C_{\mathbf{H_2P}} = \frac{100\%}{1 + K_{b1}\cdot 10^{-pH} + K_{b1}\cdot K_{B2}\cdot 10^{-2pH}} \quad \text{SM(1)}$$

$$C_{\mathbf{H_4P^{2+}}} = \frac{100\%\cdot K_{b1}\cdot K_{B2}\cdot 10^{-2pH}}{1 + K_{b1}\cdot 10^{-pH} + K_{b1}\cdot K_{B2}\cdot 10^{-2pH}} \quad \text{SM(2)}$$

$$C_{\mathbf{H_3P^{+}}} = \frac{100\%\cdot K_{b1}\cdot 10^{-pH}}{1 + K_{b1}\cdot 10^{-pH} + K_{b1}\cdot K_{B2}\cdot 10^{-2pH}} \quad \text{SM(3)}$$

Figure S2. p*H*-dependent distribution of current concentrations of *H*-conjugate conjugated forms: **H_2P**(---), **H_3P^+**(---) and $(H_2O)_2$[**H_4P^{++}**] (---), calculated by the equations SM (1)-(3).