

**Emission properties and DFT calculations of protonated DNA bases****Naokazu Yoshikawa***Nara Women's University, Japan*

**Abstract:** Protonated DNA bases, [AdenineH<sub>2</sub>]Cl<sub>2</sub> (ACl<sub>2</sub>), [AdenineH]H<sub>2</sub>PO<sub>4</sub> (AP), [Cytosine]Cl (CCl), [Cytosine]H<sub>2</sub>PO<sub>4</sub> (CP), [GuanineH]Cl (GCl) and [GuanineH]H<sub>2</sub>PO<sub>4</sub> (GP) were newly prepared by the reaction of (Adenine, Cytosine, Guanine) with concentrated HCl or H<sub>3</sub>PO<sub>4</sub> in water and characterized by X-ray analysis and UV-vis spectroscopy.

Relatively intense blue emissions were obtained by the interaction between protonated DNA bases and the adjacent H<sub>2</sub>PO<sub>4</sub><sup>-</sup>. These compounds have hydrogen bonds, which restrain the nonradiative decay to produce emission. Six single crystals for ACl<sub>2</sub>, AP, CCl, CP, GCl and GP were newly obtained. Comparison of calculated bond lengths and angles for compounds ACl<sub>2</sub>, AP, CCl, CP, GCl and GP between ground states and singlet excited states were examined using DFT. In AP and CP, relatively intense emission in acetonitrile were obtained by forming two hydrogen bonds to the anion H<sub>2</sub>PO<sub>4</sub><sup>-</sup>.

**Biography:** I am researcher from 2000. I have completed PhD in 2008 from Nara Women's University and continued postdoctoral studies with Osaka University and Nara educational University. I have published more than 40 papers in reputed journals. I have a interest in iridium complexes and ruthenium complexes. Recently I am also interested in metal free emission product.

**Publications:**

1. Anion Influence of Emission Properties and DFT Calculations of Diprotonated and Triprotonated Terpyridines
2. Syntheses, X-Ray Crystal Structures, Emission Properties and DFT Calculations of Monoprotonated Polypyridines
3. Study of the triplet excited states and DFT calculations of iridium(III) complexes with mixed ligands
4. Emission property and DFT calculation for the 3MLCT luminescence of Ru(bpy)<sub>2</sub>(L)<sub>2</sub><sup>2+</sup> complex
5. Transition states of the 3MLCT to 3MC conversion in Ru(bpy)<sub>2</sub>(phen derivative)<sub>2</sub><sup>2+</sup> complexes

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