

## Supporting Information

### Photochromic Inorganic-Organic Hybrid: A New Approach for Switchable photoluminescence in the Solid State and Partial Photochromic Phenomenon

Gang Xu,<sup>a</sup> Guo-Cong Guo,<sup>a,\*</sup> Jin-Shuang Guo,<sup>a</sup> Sheng-Ping Guo,<sup>a</sup> Xiao-Ming Jiang,<sup>a</sup> Chen Yang,<sup>a</sup> Ming-Sheng Wang,<sup>a</sup> and Zhang-Jing Zhang<sup>a</sup>

<sup>a</sup> State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

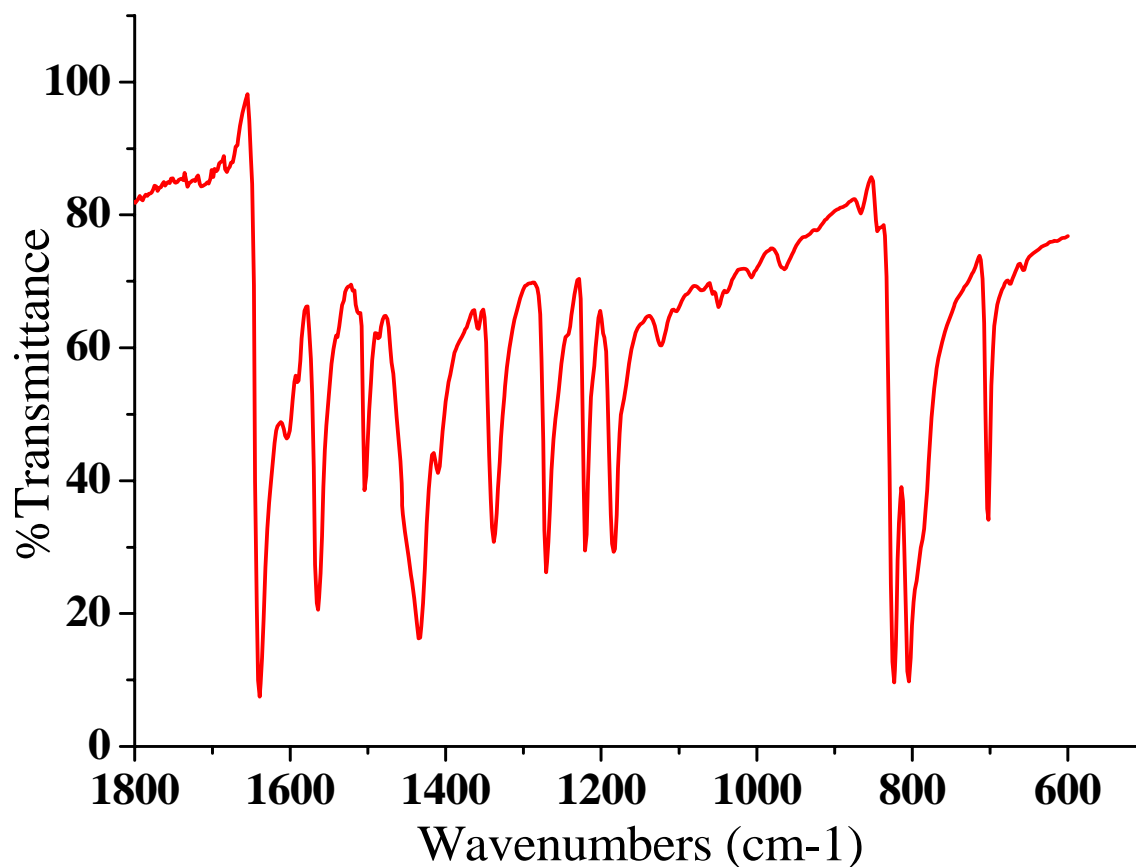


Figure S1. The IR spectrum for **1**.

\* Corresponding author. Tel.: +86 591 83705882; fax: +86 591 83714946.

E-mail address: gcguo@fjirsm.ac.cn (G.-C. Guo).

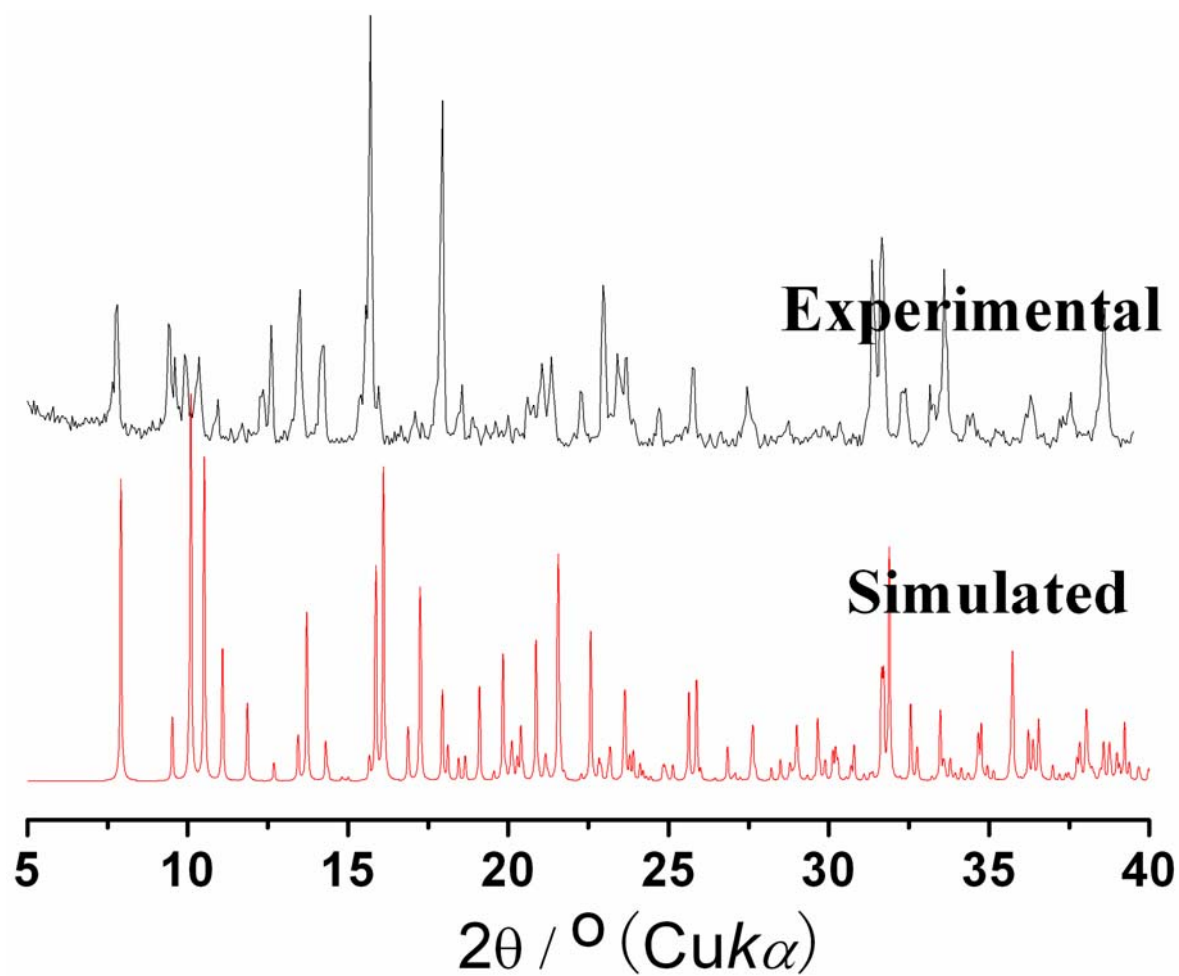
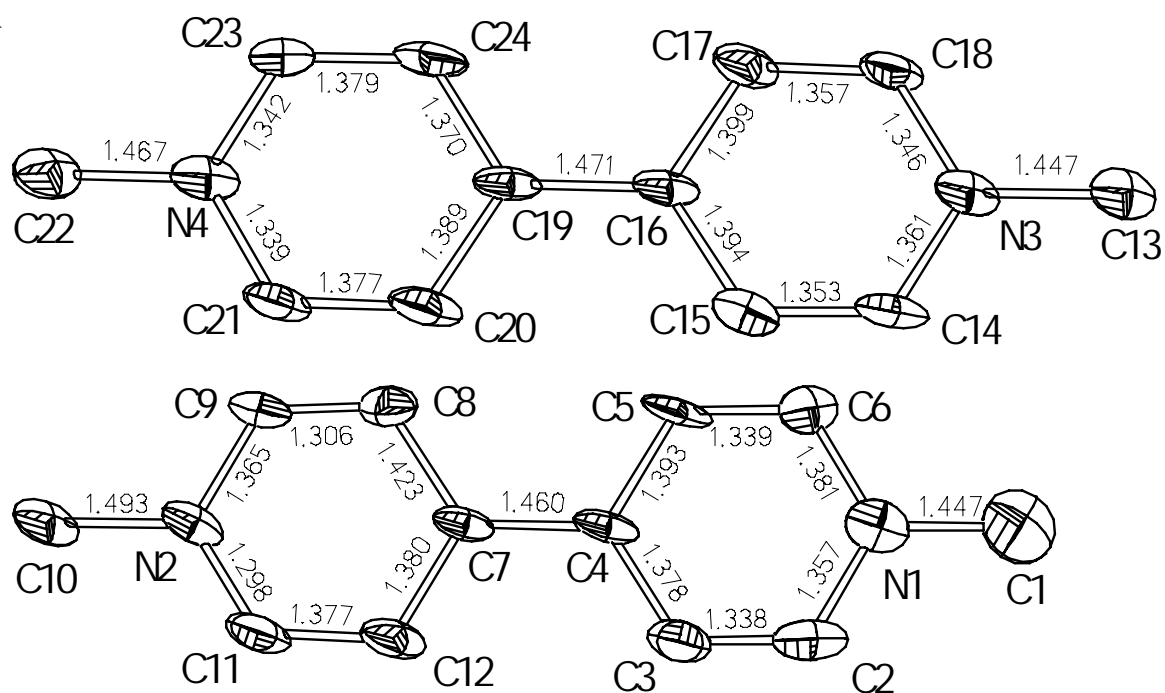
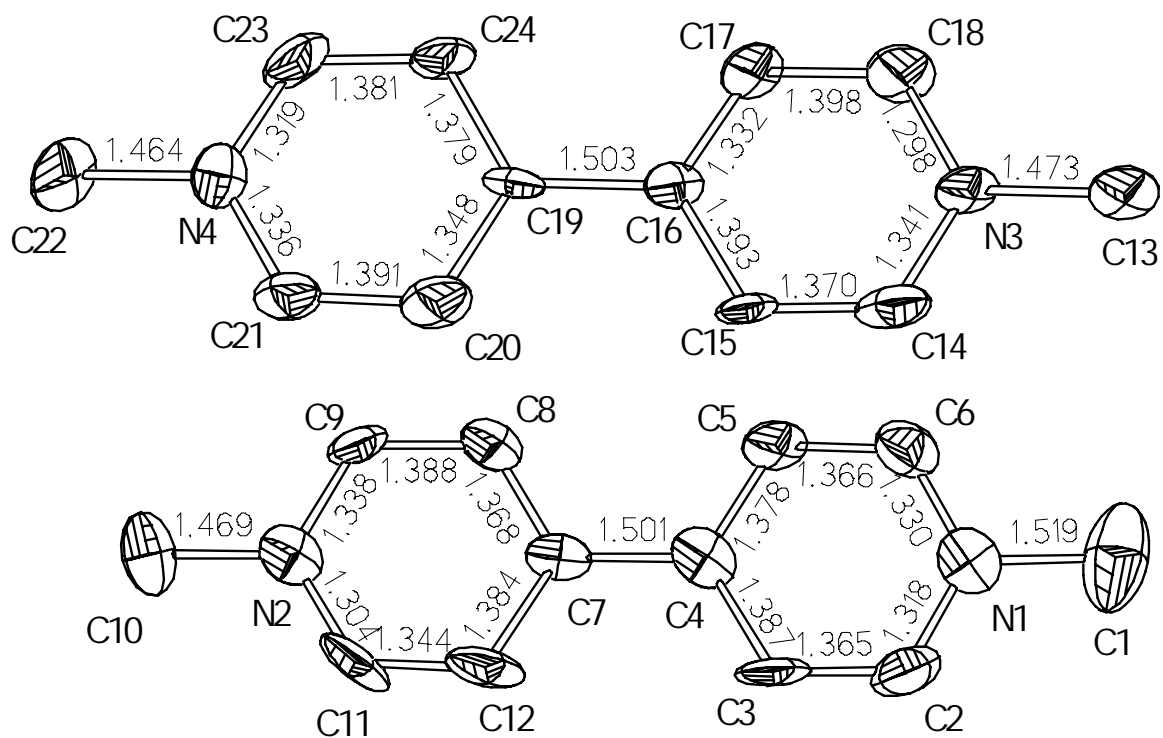


Figure S2. The PXRD patterns for 1.

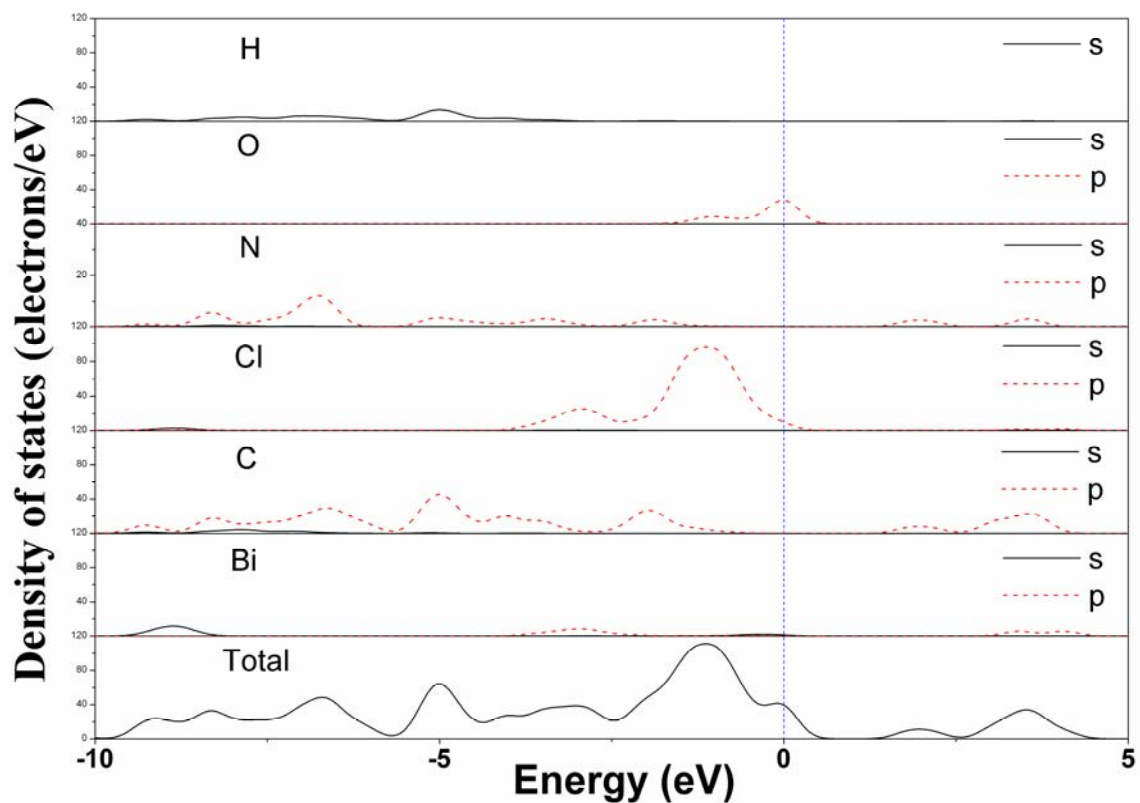


Colourless 1

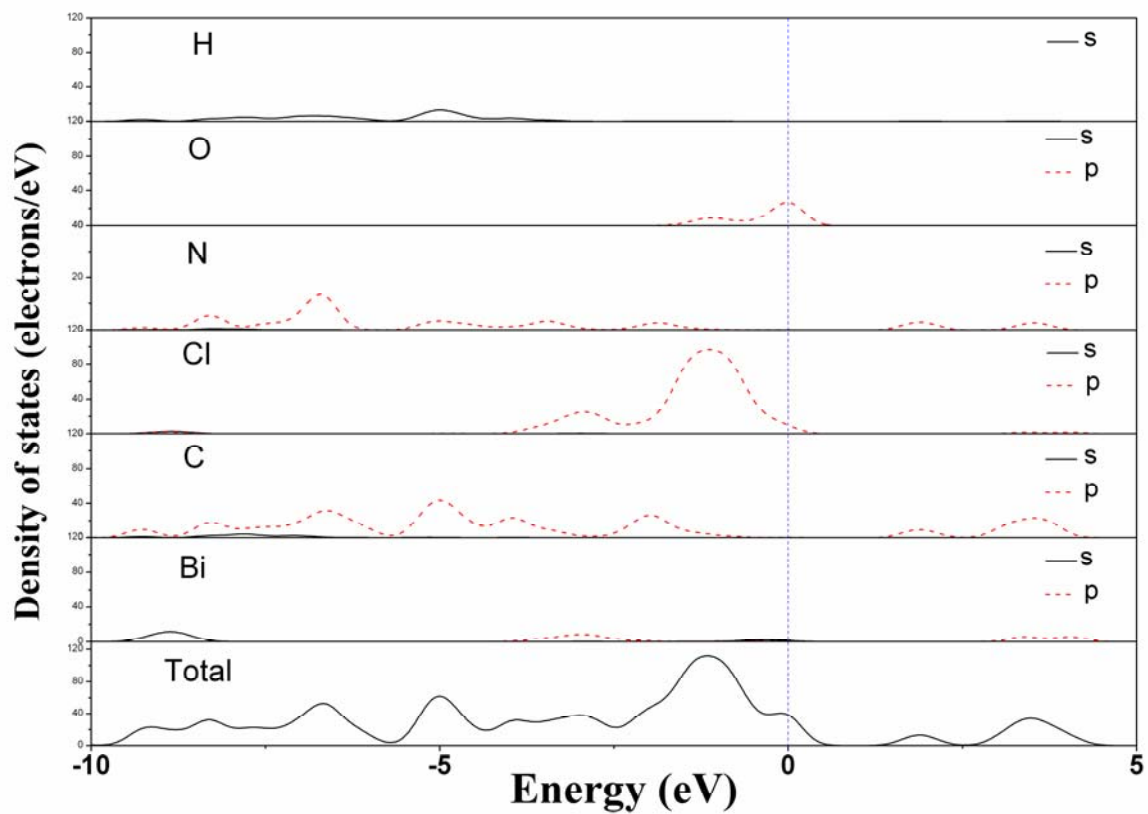


Black 1

Figure S3. Bond lengths of [MV]<sup>2+</sup> of Colourless 1 and Black 1.



Colourless 1



## Yellowish 1

Figure S4. The total and partial DOS of title complex.

Table S1. The intermolecular distances (Å) between inorganic component, organic component and lattice water molecules.

	C...O	N...Cl	C...Cl	O...Cl
<b>Colourless 1</b>	C1...O1W 3.236 C9...O1W 2.881	N3...Cl11 3.318	C18...Cl1 3.410 C9...Cl3 3.336 C4...Cl4 3.368 C5...Cl4 3.412 C7...Cl4 3.438 C19...Cl5 3.446 C21...Cl10 3.438 C16...Cl12 3.390 C19...Cl12 3.372	O1W...Cl8 3.193 O2W...Cl8 3.262
<b>Yellowish 1</b>	C1...O1W 3.214 C9...O1W 3.013	N3...Cl11 3.350	C18...Cl1 3.403 C9...Cl3 3.299 C4...Cl4 3.367 C5...Cl4 3.396 C7...Cl4 3.440 C19...Cl5 3.447 C21...Cl10 3.420 C16...Cl12 3.405 C19...Cl12 3.394	O1W...Cl8 3.233 O2W...Cl8 3.260
<b>Black 1</b>	C1...O1W 3.196 C9...O1W 3.006	N3...Cl11 3.341	C18...Cl1 3.425 C9...Cl3 3.295 C4...Cl4 3.357 C5...Cl4 3.394 C7...Cl4 3.449 C19...Cl5 3.454 C21...Cl10 3.443 C16...Cl12 3.389 C19...Cl12 3.388	O1W...Cl8 3.262 O2W...Cl8 3.231