

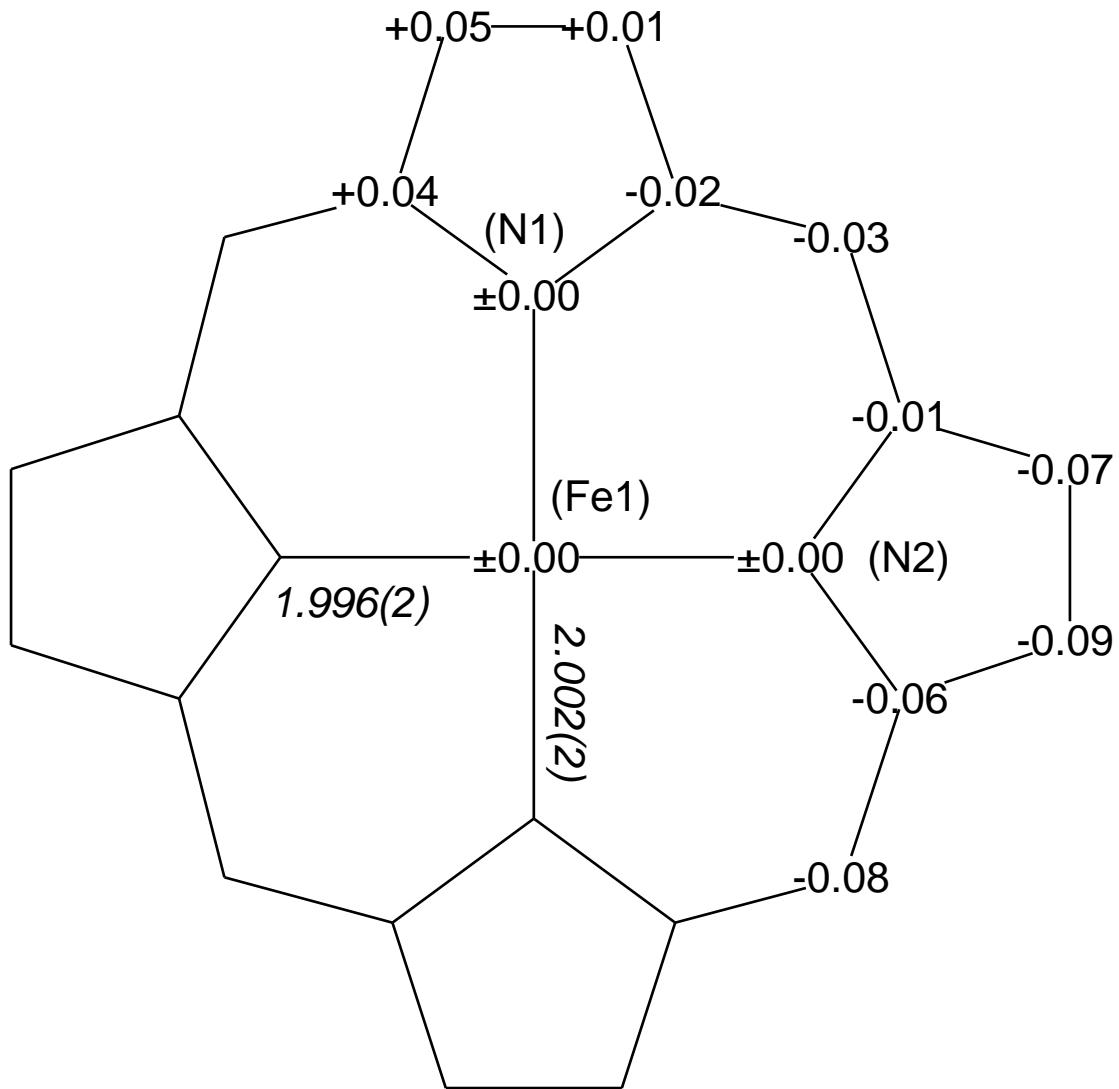
# *Electronic Supplementary Information*

## **Title**

Structure, Optical and Magnetic Behaviour of *meso*-Tetraphenylporphyrinatoiron(III) Tetracyanoethanide,  $[\text{Fe}^{\text{III}}\text{TPP}]^+[\text{TCNE}]^-$ .

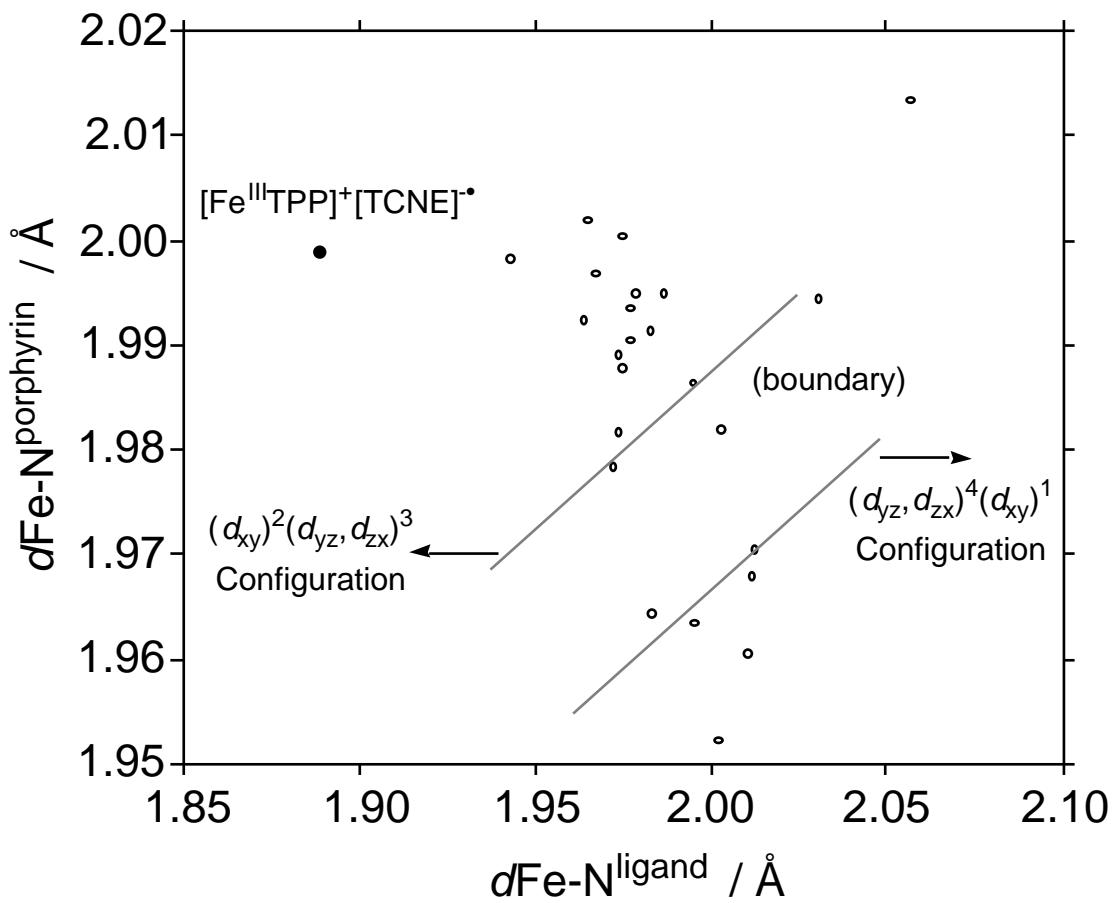
## **Authors**

Shinji Mikami, Ken-ichi Sugiura,\* Tatsuo Maruta, Yonezo Maeda, Masaaki Ohba, Naoki Usuki, Hisashi Ōkawa, Tomoyuki Akutagawa, Sadafumi Nishihara, Takayoshi Nakamura, Kentaro Iwasaki, Nobuyuki Miyazaki, Shojun Hino, Eiji Asato, Joel S. Miller,\* and Yoshiteru Sakata,\*



**Figure-S1**

Deviations of the atoms from the least squares plane formed by the iron and four nitrogen atoms. All displacements are given in unit of 0.01 Å. The bond distances of *d*Fe-Nporphyrin are given in italic (Å).



**Figure-S2**

Plott of  $d_{\text{Fe-Nporphyrin}}$  and  $d_{\text{Fe-NTCNE}}$  of  $[\text{Fe}^{\text{III}}\text{TPP}]^+[\text{TCNE}]^{\bullet}\bullet 2\text{PhCl}$  on *Silver's-Map* ( $\bullet$ :  $[\text{Fe}^{\text{III}}\text{TPP}]^+[\text{TCNE}]^{\bullet}\bullet 2\text{PhCl}$ ,  $\circ$ : reference data).<sup>43</sup> Each electronic configuration region was surrounded using the reference data.<sup>43</sup>