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Assembled complexes with transition metal ion as a center metal can show various chemical and physical properties. And assembled iron(II) complexes bridged by 1,2-bis(4-pyridyl)ethane (bpa), which has *anti-gauche* conformers, as a bridging ligand showed a stereospecific structure depending on the conformer of bpa. For example, the complex $[trans\text{-Fe}(\text{bpa})_2(\text{NCS})_2]_n$ in the case of *gauche*-type bpa shows 1D chain structure, while in the case of *anti*-type bpa shows grid structure and interpenetrated structure (Fig.1). The difference in structures appears depending on the synthetic condition. And Mössbauer spectroscopy revealed that the complexes $[trans\text{-Fe}(\text{bpa})_2(\text{NCX})_2]_n$ ($X = \text{S}, \text{Se}$) have unique quadrupole splitting (Q.S.) values depending on its structure. The Q.S. value of NCS complex is the double of that of NCSe complex in 1D chain structure, while is a half of that of NCSe complex in interpenetrated structure. These results suggest that the electric field gradient (EFG) of those complexes should be reversed. Moreover the assembled system enclathrating organic compound as guest molecule caused a spin-crossover (SCO) phenomenon and the transition temperature changed depending on the anion (NCS^- , NCSe^- , NCBH_3^-). The Q.S. values correlate with the EFG around Fe nucleus. The EFG is mainly determined by 3d orbital population of valence orbitals. And the transition temperature in SCO concerns with the ligand field splitting of the complex molecules. In the present study, we studied the changes in Q.S. value and spin state by using SCF-DV- $X\alpha$ method.

The data of X-ray structure analysis were employed as the present calculation model and the calculation was performed by cutting down the assembled structure to mononuclear complex. As a result of SCF-DV- $X\alpha$ computing, the 3d orbital splitting and the molecular orbital depiction of all complexes showed the pseudo tetragonal distortion shrunk along anion axis. And it could be seen that the crystal field splitting (Δ_o) obtained by simple calculation from its result correlates with the transition temperature (Fig.2). However since it is very difficult to estimate the true ground state of each complex in the molecular orbital calculation including first row transition metals, these results obtained from DV- $X\alpha$ calculation showed that the spin multiplicity of ground state in the present complexes was singlet, namely low-spin state, in spite of non-SCO system.

At this presentation we will report the approach to such problem and the correlation between the Q.S. value of the experimental data and the calculation value obtained by DV- $X\alpha$ method.

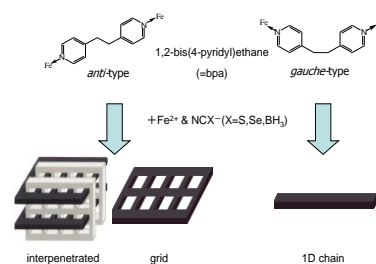


Fig.1 The assembled structures of $[\text{Fe}(\text{bpa})_2(\text{NCX})_2]_n$, depending on the conformer of bpa.

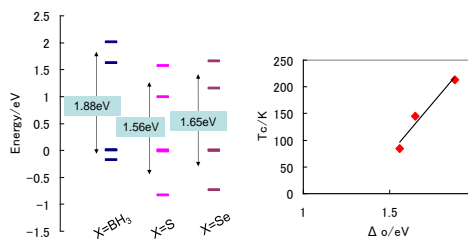


Fig.2 The correlation of $[\text{Fe}(\text{bpa})_2(\text{NCX})_2]$ in SCO system between Δ_o and T_c .