

## **Pump and Probe the Structure and Electronic Configuration of LIESST State**

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A six-coordinated iron(II) complex,  $\text{t-Fe(tzpy)}_2(\text{NCS})_2$  (tzpy = 3-(2-pyridyl)[1,2,3]triazolo[1,5-*a*]pyridine), undergoes a graduate spin transition from a paramagnetic high spin state ( $^5\text{T}_2$ ,  $S = 2$ , HS-1) above 200K to a diamagnetic low spin state ( $^1\text{A}_1$ ,  $S = 0$ , LS-1) below 75 K according to the magnetic measurement. The crystal structures of both HS-1 and LS-1 are studied at 298 and 40K respectively. Significant differences in Fe-N distances and in coordination geometries of Fe do occur during the spin transition. The electronic configuration of Fe in both HS and LS states is monitored by Fe K- & L-edge absorption. In addition, the ligand C-N stretching frequency can also be followed through the spin transition.

A light-induced-excited-spin-state-trapping phenomenon (LIESST) is observed by pumping the crystal with 532nm laser at 40K, where a relatively long-lived high spin state (HS-2) occurred. The molecular and crystal structure of this HS-2 state is investigated using pump and probe mode. The excitation can be easily detected by XRD, XAS and IR spectroscopy. The molecular structure and electronic configuration of Fe of HS-2 state are very similar to those of HS-1. The relaxation from such HS-2 state to the low spin state (LS-2) is followed via C-N stretching frequency at various temperature.

**Keywords:** spin-crossover, x-ray absorption spectroscopy, excited spin state