Abstract Submitted
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Changes in the unoccupied electronic structure of the spin crossover molecule [Co(dpzca)$_2$] YANG LIU, XIN ZHANG, AXEL ENDERS, PETER DOWBEN, JIAN LUO, JIAN ZHANG, Univ of Nebraska - Lincoln, ALPHA NDIAYE, LBNL, Advanced Light Source — We have investigated the changes in the unoccupied electronic structure of the spin crossover molecule - [Co(dpzca)$_2$] using X-ray absorption spectroscopy (XAS) and have compared the results with magnetometry (SQUID) measurements. The studies of the variable temperature of the electronic structure of this cobalt complex with symmetric pyrazine imide ligands, -(2-pyrazylcarbonyl)-2-pyrazinecarboxamide, i.e. [Co(dpzca)$_2$], are consistent with density functional theory (DFT). The temperature dependence of the occupancy of the high-spin state and low-spin state molecular orbital states, the unoccupied e_g/t_{2g} ratio from XAS and high spin state to low spin state ratio from molecular magnetic susceptibility χ_MT indicates that the low spin state is not a zero spin state, but simply a lower moment state that would occur below the spin crossover transition of [Co(dpzca)$_2$].

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