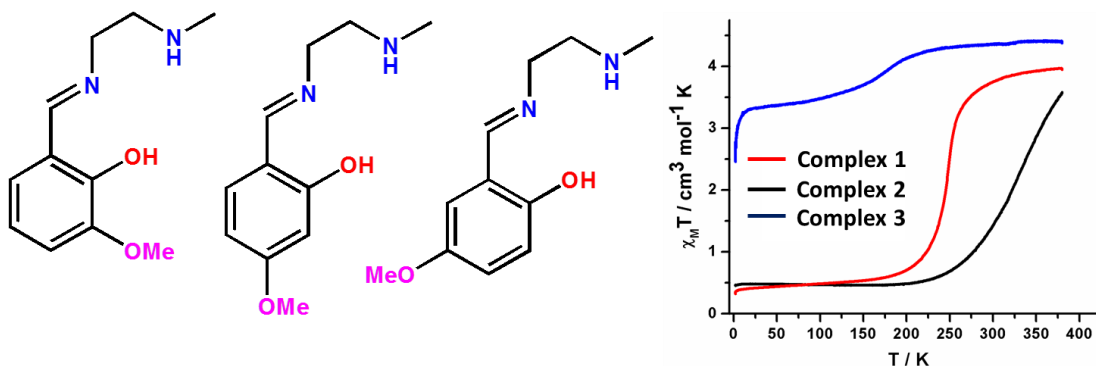


# Differential Electron Donation Leading to Different Spin Crossover Behaviour in Fe(III) Complex

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A detailed experimental and theoretical study has been performed to quantify the effect of electron donation of a ligand substitution from different positions. The reaction of  $\text{Fe}(\text{NCSe})_3$  prepared in situ in MeOH with X-OMe-salEen (X-OMe-salEen = condensation product of ortho, meta and para methoxy substituted salicylaldehyde and N-ethylethylenediamine) in MeOH provided three Fe(III) complexes,  $[\text{Fe}(\text{X-OMe-salEen})_2]\text{NCSe}$ , X = 3-OMe (1), 4-OMe (2), 5-OMe (3) (Figure 1). Complex 1 shows hysteric spin crossover behavior and interestingly it also shows a rate dependence of widening of hysteresis loop. Complex 2 shows spin crossover in half region due to the presence of two crystallographic independent Fe(III) centers. Complex 3 shows abrupt spin transition around room temperature. Complex 1 and 3 are free of any solvent molecules while complex 2 having two water molecules in the molecular structure. The effect of electron donating substitution on the magnetic property has been studied in depth by theoretical and experimental methods for the first time in a solvent free series of complexes.



1

Figure 2 Schematic drawing of the ligands (left) and Magnetic data (right)

## References.

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