

Student Talk
Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

An Experimental and Theoretical Investigation on the Easy-Plane Magnetic Anisotropy of Pentagonal Bipyramidal Cobalt(II) Complexes

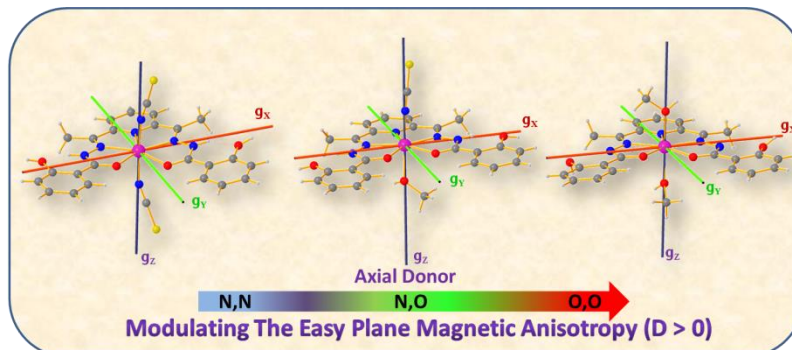
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Abstract: A rational approach of modulating the easy-plane magnetic anisotropy of mononuclear pentagonal bipyramidal Co^{II} single molecule magnets (SMMs) has been revealed.^{1,2} A class of three new pentagonal-bipyramidal complexes with formulae $[\text{Co}(\text{H}_2\text{daps})(\text{MeOH})_2]$ (**1**), $[\text{Co}(\text{H}_4\text{daps})(\text{NCS})(\text{MeOH})] \cdot (\text{ClO}_4) \cdot (\text{MeOH})$ (**2**) and $[\text{Co}(\text{H}_4\text{daps})(\text{NCS})_2] \cdot (\text{MeOH})_2$ (**3**) (H_4daps = 2,6-bis(1-salicyloylhydrazonoethyl) pyridine) were studied.³ In these complexes, the axial positions are successively replaced by different O and N donor ligands in a systematic way. Detailed magnetic measurements disclose the existence of large easy-plane magnetic anisotropy and field induced slow magnetic relaxation behavior. Both experimental and *ab initio* theoretical calculations display that easy-plane magnetic anisotropy is maintained upon variation of coordination environments. Nevertheless, the magnitude of the D value was found to be increased in case of weaker axially coordinated σ -donor ligands and a more symmetrical equatorial ligand. Additionally, from detail investigation of field and temperature dependence of relaxation time it can be concluded that QTM is the predominant process for slow magnetic relaxation and the Raman process is significant which explicates the thermal dependence. Magnetic dilution experiments have been performed to eliminate the possible influence of intermolecular interactions on magnetic behaviors of adjacent Co^{II} centres.



References and Notes:

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Arpan Mondal was born in Kolkata, India, in 1992. He received his bachelor's degree from Behala College, University of Calcutta and master's degree from Presidency University, Kolkata.

He joined Dr. S Konar's group in 2016. His research interests are experimental and theoretical investigation on single ion magnet of radical and metal complexes.