

Formation of H-bonding networks in the solid state structure of a trinuclear cobalt(III/II/III) complex with N₂O₂ donor Schiff base ligand and glutaric acid as bridging co-ligand: Synthesis, structure and DFT study

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Physical measurement

A PerkinElmer 240C elemental analyzer was used to get the data of the elemental analysis (carbon, hydrogen and nitrogen). A PerkinElmer RX-1 FTIR spectrophotometer was used to run the IR spectra in KBr (4500-500 cm⁻¹). A SHIMADZU (UV-1900i) UV-Vis-spectrofluorometer was used to record the electronic spectra in acetonitrile. The magnetic susceptibility was measured with an EG&PAR vibrating sample magnetometer, model 155 at room temperature and diamagnetic corrections was made using Pascal's constants. Effective

magnetic moments was calculated using the formula $\mu_{\text{eff}} = 2.828(\chi_{\text{M}}T)^{1/2}$, where χ_{M} = corrected molar susceptibility.

X-Ray crystallography

Suitable single crystals of the complexes were used for data collection by means of a 'Bruker D8 QUEST area detector' diffractometer equipped with graphite-monochromated Mo K_{α} radiation ($\lambda = 0.71073 \text{ \AA}$) at 273 K. A direct method was used to solve the molecular structures and full-matrix least squares on F^2 (SHELX-16/6 package)^{S1} was used for refinement. Anisotropic thermal parameters were used to refine the non-hydrogen atoms. Hydrogen atoms bonded to carbon and nitrogen atoms were refined in fixed geometric positions as were hydrogen atoms in -OH groups. Hydrogen atoms in water molecules were located in difference Fourier maps and refined with distance constraints. The $-(\text{CH}_2)_3\text{COOH}$ group was disordered over two sets of positions and the two parts were refined with 50% occupancy. The SADABS^{S2} program was used to perform Multi-scan absorption corrections.

Hirshfeld surface analysis

Hirshfeld surfaces^{S3-S5} offer a three-dimensional representation of close contacts in a crystal, which can be viewed in a fingerprint plot.^{S6-S8} These were calculated using Crystal Explorer,^{S9} with bond lengths to hydrogen atoms set to standard values.^{S10} For each point on the Hirshfeld isosurfaces, two distances d_e , the distance from the point to the nearest nucleus external to the surface and d_i , the distance to the nearest nucleus internal to the surface, were defined. The normalized contact distance (d_{norm}) based on d_e and d_i is defined as:

$$d_{\text{norm}} = \frac{(d_i - r_i^{\text{vdw}})}{r_i^{\text{vdw}}} + \frac{(d_e - r_e^{\text{vdw}})}{r_e^{\text{vdw}}}$$

Where, r_i^{vdw} and r_e^{vdw} are the van der waals radii of the atoms. The value of d_{norm} may be negative or positive depending on intermolecular contacts being shorter or longer than the van der Waals separations. The parameter d_{norm} displays a surface with a red-white-blue colour, where blue regions are indicative of no close contacts, while bright red spots and white areas represent shorter contacts and contacts around the van der Waals separation respectively. The Hirshfeld surface is unique for a fixed CIF.^{S11}

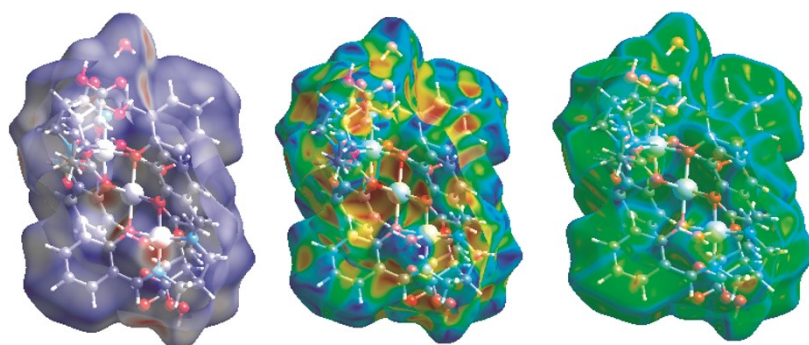


Figure S1: Hirshfeld surface of the complex mapped with d_{norm} (left), shape index (middle) and curvedness (right).

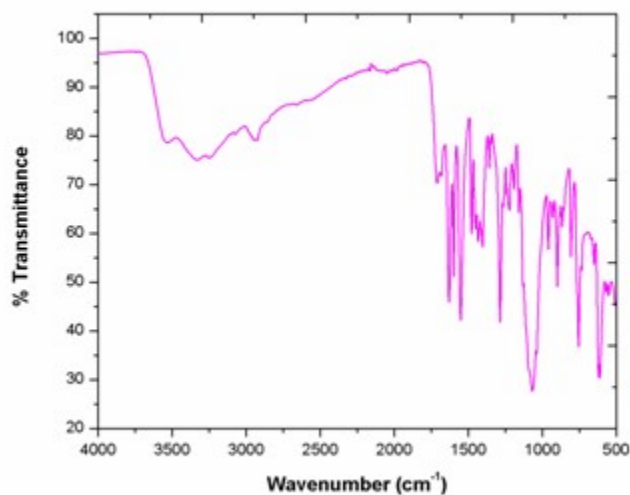


Figure S2: IR spectrum of the complex.

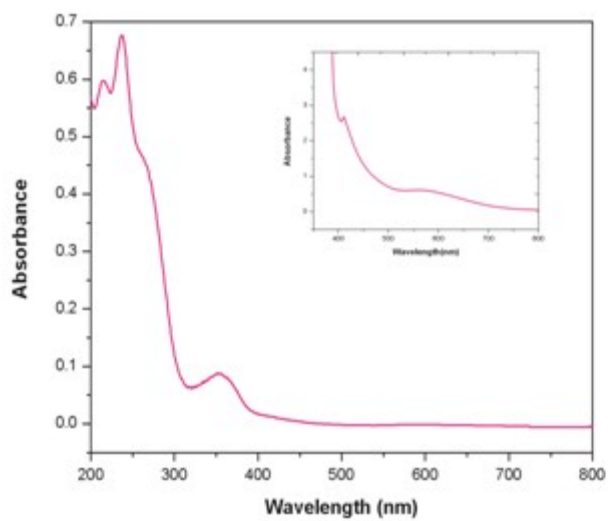


Figure S3: Electronic spectrum of the complex. Inset shows the absorption band for low spin cobalt(III) center in the complex.

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