

# Spectroscopic properties and ligand field analysis of chromium(III) compounds

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The low temperature emission, absorption and excitation spectra, and 298 K infrared spectra of *cis*-[Cr(cyclam)L<sub>2</sub>]X (cyclam=1,4,8,11-tetraazacyclotetradecane; L=NH<sub>3</sub>, en/2, pn/2, F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, ONO<sup>-</sup>, N<sub>3</sub><sup>-</sup>, NCS<sup>-</sup>, ONO<sub>2</sub><sup>-</sup>) have been measured. The vibrational intervals of the electronic ground state are extracted from the far-infrared and emission spectra. Chromium (III) complexes show sharp line spectral features in the visible region of the optical spectrum that are not usually seen in other metal complexes. These sharp metal-centred transitions are sensitive to the immediate metal environment and can be used as a structural probe for the local geometry about the metal centre. The electronic bands due to spin-allowed and spin-forbidden transitions are assigned. Using the observed electronic transitions, a ligand field analysis was performed in the framework of the angular overlap model (AOM). We propose to develop experimental and theoretical techniques to extract two kinds of geometric information from sharp line spectra of chromium(III) complexes. The first is the actual angular positions of the coordinating atoms, particularly with reference to the bite angles subtended by chelating ligands. The second has to do with the orientation of the coordinated atom, if the latter has an orbital capable of bonding, the orientation will affect the metal d-orbital energies. The method would open the significant possibility of obtaining structural information for molecules in non-crystalline environments, e.g., in solution or adsorbed on a surface, or a transition metal binding site imbedded in a large biological molecule.

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