

CONTINUOUS SHAPE MEASURE ANALYSIS OF THE CO(II)
COORDINATION GEOMETRY IN $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$

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Abstract

The coordination geometry of Co(II) in $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ was quantitatively assessed using continuous shape measure (CShM) analysis. Five reference six-coordinate geometries were compared to determine the closest idealized polyhedral model. The OC-6 geometry gave the lowest CShM value of 0.852, while considerably higher values were obtained for HP-6, PPY-6, TPR-6, and JPPY-6. These results establish that the Co(II) coordination sphere is predominantly octahedral, with only a small deviation from the ideal geometry.

Introduction

The assignment of coordination geometry is essential for understanding the structural features of transition-metal complexes. For six-coordinate systems, deviations from ideal polyhedra can be quantified using continuous shape measures (CShM), which provide a numerical description of the structural difference between an experimental coordination sphere and an ideal reference geometry [1,2]. The method has been systematically developed for classical coordination polyhedra and subsequently applied to transition-metal complexes and stereochemical analysis [3,4]. In particular, CShM analysis is useful when chelating ligands impose geometrical constraints that lead to deviations from ideal symmetry. 1,10-Phenanthroline is a rigid bidentate N-donor ligand that commonly produces well-defined six-coordinate metal environments. In this work, CShM analysis was applied to $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ to quantitatively establish the preferred geometry of the Co(II) coordination sphere.

Keywords: Co(II) complex, 1,10-phenanthroline, continuous shape measure, coordination geometry, octahedral distortion.

Continuous Shape Measure Analysis of the Co(II) Coordination Environment

The coordination geometry of the Co(II) center in $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ was examined quantitatively by continuous shape measure (CShM) analysis [Fig. 1; Table 1]. The method is particularly useful for distinguishing between closely related six-coordinate geometries because the calculated value directly reflects the deviation of the experimental coordination environment from an ideal reference polyhedron. For the Co(II) center, the CShM values obtained for the selected six-coordinate models are 28.663 for HP-6, 26.636 for PPY-6, 0.852 for OC-6, 14.181 for TPR-6, and 30.218 for JPPY-6. A pronounced difference is therefore observed between the octahedral model and the remaining reference geometries. The OC-6 value of 0.852 is considerably lower than the values calculated for the other models, indicating that the experimental coordination sphere is very close to an ideal octahedral arrangement. This result is consistent with the crystal structure, in which Co(II) is coordinated by six nitrogen donor atoms belonging to three bidentate 1,10-phenanthroline ligands.

Table 1. Calculated the continuous shape measure value for $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$.

Label	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
Co	28.663	26.636	0.852	14.181	30.218

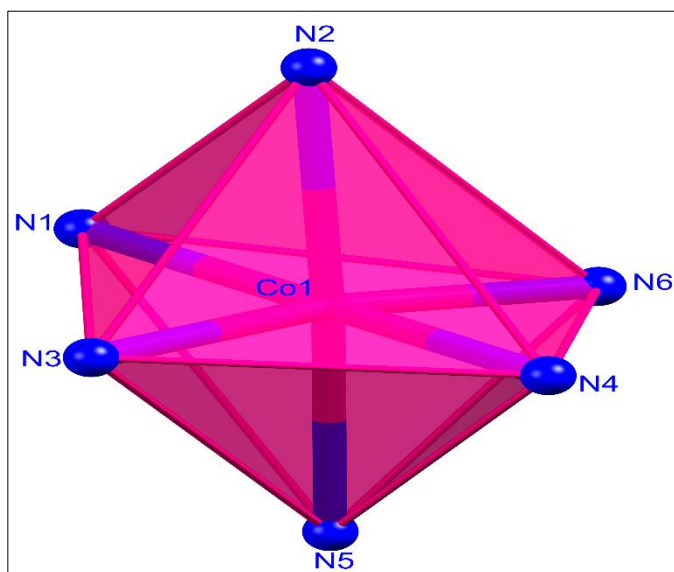


Figure 1. CShM analysis of the Co(II) coordination

The chelating nature of phenanthroline restricts the N-Co-N angles and introduces a measurable deviation from perfect octahedral symmetry. Nevertheless, this distortion is relatively small compared with the deviations associated with the other six-coordinate reference polyhedra. The CShM results therefore provide quantitative structural evidence that the Co(II) site adopts a slightly distorted octahedral geometry.

Conclusion

The CShM analysis provides a quantitative basis for assigning the coordination geometry of Co(II) in $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$. Among the investigated six-coordinate reference geometries, OC-6 gives the lowest value (0.852), whereas HP-6, PPY-6, TPR-6, and JPPY-6 show substantially larger deviations. The pronounced difference between the OC-6 value and those of the alternative models indicates that the experimental coordination sphere is much closer to an ideal octahedron. The non-zero OC-6 value reflects a limited distortion from ideal octahedral symmetry,

consistent with the geometrical restrictions imposed by three chelating 1,10-phenanthroline ligands. The CShM results therefore support the assignment of a slightly distorted octahedral environment around the Co(II) center.

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