



POLYHEDRAL DISTORTION IN A TRIS(1,10-PHENANTHROLINE)COBALT(II) DINITRATE DIHYDRATE COMPLEX

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Abstract

The crystal structure of $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ was analyzed with emphasis on the Co(II) coordination geometry. The Co(II) center is coordinated by three bidentate 1,10-phenanthroline ligands, forming a distorted octahedral CoN_6 environment. Co-N distances range from 2.073(4) to 2.097(4) Å, with an average of 2.0830 Å. The low bond-length distortion index (0.00301) and quadratic elongation (1.0121) indicate minor bond-length distortion, while the bond-angle variance (42.9745°) points to more pronounced angular distortion. Thus, the CoN_6 unit is predominantly distorted through bond angles.

Introduction

1,10-Phenanthroline is a rigid bidentate N-donor ligand that readily forms stable chelate complexes with transition-metal ions. Cobalt(II) complexes containing three phenanthroline ligands are commonly described as six-coordinate species with distorted octahedral metal environments [1,2]. Related crystal structures demonstrate that the $[\text{Co}(\text{phen})_3]^{2+}$ unit can persist with different counter-anions and lattice-water contents while retaining the characteristic CoN_6 coordination motif [3,4]. Beyond conventional bond-length and bond-angle descriptions, quantitative distortion parameters provide a more objective assessment of coordination geometry. In particular, quadratic elongation and bond-angle variance allow deviations from an ideal polyhedron to be evaluated independently of its absolute size [5]. Here, the structural parameters of $[\text{Co}(\text{phen})_3](\text{NO}_3)_2 \cdot 2\text{H}_2\text{O}$ are analyzed to distinguish bond-length and angular contributions to the distortion of the CoN_6 coordination polyhedron.

Keywords: Cobalt(II), 1,10-phenanthroline, crystal structure, octahedral coordination, polyhedral distortion

2. Polyhedral geometry and coordination environment

The molecular structure of tris(1,10-phenanthroline)cobalt(II) dinitrate dihydrate shows that the Co(II) ion is coordinated by six nitrogen atoms belonging to three bidentate 1,10-phenanthroline ligands, forming a distorted octahedral CoN_6 coordination environment [Fig. 1]. The Co-N bond



lengths vary from 2.073(4) to 2.097(4) Å, with an average value of 2.0830 Å [Table 1]. The relatively small difference between the shortest and longest Co-N bonds indicates that the coordination sphere is not strongly distorted in terms of bond lengths. This is also supported by the low bond-length distortion index of 0.00301 and the quadratic elongation of 1.0121, both of which are close to the values expected for an approximately regular octahedral environment.

Table 2. Polyhedral parameters for Co(II) [Co(phen)₃](NO₃)₂·2H₂O

Bond	Distance (Å)
Co(1)-N(5)	2.073(4)
Co(1)-N(3)	2.074(4)
Co(1)-N(1)	2.082(4)
Co(1)-N(6)	2.085(4)
Co(1)-N(4)	2.086(4)
Co(1)-N(2)	2.097(4)
Average bond length	2.0830
Polyhedral volume (Å ³)	11.8352
Distortion index (bond length)	0.00301
Quadratic elongation	1.0121
Bond angle variance (° ²)	42.9745
Effective coordination number	5.9970

The calculated effective coordination number (5.9970) is consistent with six-coordinate geometry. In contrast, the bond-angle variance of 42.9745°² indicates a more noticeable angular deviation from an ideal octahedron. Such angular distortion can reasonably be associated with the chelating nature of the 1,10-phenanthroline ligands, which impose geometric constraints within the CoN₆ coordination sphere. The calculated polyhedral volume of 11.8352 Å³ further describes the spatial characteristics of the coordination environment. The structural parameters confirm that the Co(II) center adopts a slightly distorted octahedral geometry, with the deviation expressed predominantly through bond angles rather than substantial differences in Co-N bond lengths.



Conclusion

The structural analysis confirms that the Co(II) center in Co(II) [Co(phen)₃](NO₃)₂·2H₂O adopts a six-coordinate, distorted octahedral geometry defined by three bidentate 1,10-phenanthroline ligands. The Co-N distances are closely grouped around the mean value of 2.0830 Å, consistent with the low bond-length distortion index of 0.00301 and quadratic elongation of 1.0121. In contrast, the bond-angle variance of 42.9745°² demonstrates that angular deviations contribute more strongly to the departure from ideal octahedral geometry. Thus, the CoN₆ polyhedron can be described as structurally regular with respect to bond lengths but noticeably distorted in its angular arrangement.

References

1. Srivastava, A.K., 2026. A review on versatile applications of metal complexes incorporating fenamate NSAIDs. *Journal of the Iranian Chemical Society*, 23(7), p.185.
2. Das, S., Das Pattanayak, P., Mohapatra, D. and Dinda, R., 2026. Mixed-ligand oxidovanadium complexes with anticancer potential. *Dalton Transactions*, 55(21), pp.8087-8118.
3. Zhao, S.Z., Zhou, H.W., Qin, C.Y., Zhang, H.Z., Li, Y.H., Yamashita, M. and Wang, S., 2023. Anion effects on spin crossover systems: from supramolecular chemistry to magnetism. *Chemistry–A European Journal*, 29(44), p.e202300554.
4. kizi Toirova, G.K., Turaev, K.K., Karimova, K.B., Prasad, A.A., ugli Kholturaev, K.B., Ruzmetov, A.K., Musurmonov, M., Normamatov, A.S., Ibragimov, A.B., Nazarov, Y.E. and kizi Ochildieva, Y.B., 2026. Structural insights, Hirshfeld surface analysis and antimicrobial activity of a supramolecular bis (1, 10-phenanthroline) cobalt (II) complex containing sulfate and sulfanilate species. *Journal of Molecular Structure*, p.146809.
5. kizi Toirova, G.K., Turaev, K.K., Ibragimov, A.B., Prasad, A.A., Ruzmetov, A.K., Yakubov, D.R., Turgunaliyev, E., Togasharov, A.S., Shukurov, Z.S., Ibragimov, A.B. and Chellakarungu, B., 2026. Polymorphic packing hierarchy in dichlorido-bis (1, 10-phenanthroline) manganese (II): interplay of π - π stacking and C-H $\cdots$ Cl interactions and consequences for lattice stabilization and crystal morphology. *Journal of the Indian Chemical Society*, p.102783.