

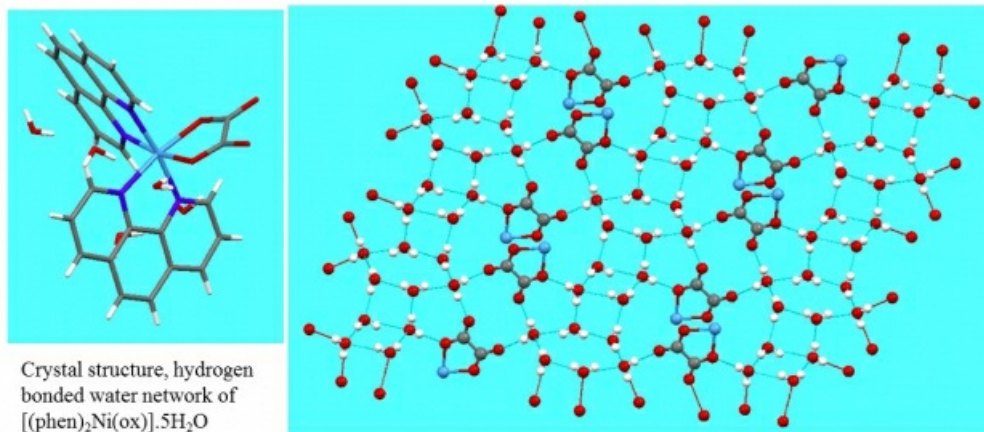
*Synthesis, characterization, crystal structure of bis(phenanthroline)oxalatonickel(II) pentahydrate*Krishnan Rangan¹¹Department of Chemistry, BITS Pilani Hyderabad Campus, Hyderabad, India

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Heterolytic polyazine-oxalate-nickel complex bis(1,10-phenanthroline)oxalatonickel(II) complex is prepared from dichlorobis(1,10-phenanthroline)nickel(II) and potassium oxalate. The complex crystallized from methanol as red block crystals in pentahydrate form, $[(\text{phen})_2\text{Ni}(\text{ox})] \cdot 5\text{H}_2\text{O}$. The compound crystallized in to a triclinic crystal system with P-1 space group with cell parameter $a=10.2780(3) \text{ \AA}$, $b=10.4962(3) \text{ \AA}$, $c=12.5235(3) \text{ \AA}$, $\alpha=77.997(2)^\circ$, $\beta=86.305(2)^\circ$, $\gamma=73.132(2)^\circ$, $V=1264.63(6) \text{ \AA}^3$, $Z=2$, $F(000)=620.0$ and $R_{\text{int}}=2.7\%$. The nickel center of the $[(\text{phen})_2\text{Ni}(\text{ox})]$ complex is surrounded by four nitrogen atoms of two 1,10-phenanthroline ligands and two oxygens of a terminally coordinated oxalate dianion adopting a distorted octahedral geometry. Two of the four oxygens of an oxalate ions are terminally coordinated to the metal center forming a five membered ring and rest of the two oxygens are unbound to any metal center. In this tris-chelate complex the metal complexes is observed in both of the two possible enantiomeric form. The crystal structure shows the presence of five water molecules per $[(\text{phen})_2\text{Ni}(\text{ox})]$ molecule which are not directly coordinated to nickel metal center but connecting the individual complexes through hydrogen bondings. Two uncoordinated and one nickel coordinated oxygen atoms out of the four oxygen atoms of an oxalate ions are involved in hydrogen bonding with water molecules. The water molecules form network of supramolecular extended architecture step ladders like structure with extended R6, R4, R4, R4 oxygen atoms fused ring system with hydrogen bonding. The adjacent water network step ladders are connected and supported by both hydrogen bonding through the coordinated oxalate ligands of the metal complex as well us through the pi-pi interactions between phenanthroline rings of adjacent molecules. The complexes $[(\text{phen})_2\text{Ni}(\text{ox})] \cdot 5\text{H}_2\text{O}$ tend to lose the water either through heating around $50 \text{ }^\circ\text{C}$ or under dry nitrogen gas.

References:

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Keywords: [nickel](#), [oxalate](#), [hydrogen bond](#)