FT–IR SPECTROSCOPIC CHARACTERIZATION OF THE COORDINATION POLYMER $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$

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Abstract

A novel manganese (II) tartrate-based coordination polymer, $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$ (Tar =tartrate), was characterized by Fourier-transform infrared (FT-IR) spectroscopy in the range of 4000-400 cm^{-1}. The spectrum exhibited a broad absorption band at 3326 cm^{-1} corresponding to O-H stretching vibrations of coordinated and lattice water molecules as well as hydroxyl groups involved in hydrogen bonding. Strong absorption bands observed at 1555 and 1374 cm^{-1} were assigned to the asymmetric and symmetric stretching vibrations of coordinated carboxylate groups, respectively. The difference between these bands ($\Delta\nu$=181 cm^{-1}) indicates the participation of carboxylate oxygen atoms in coordination with Mn (II) centers. Furthermore, absorption bands in the 592-522 cm^{-1} region were attributed to Mn-O stretching vibrations, confirming the formation of metal-oxygen coordination bonds. The FT-IR results support the successful synthesis of a manganese–tartrate coordination polymer containing μ_4- and μ_3-bridging tartrate ligands.

Keywords: manganese(II), tartrate ligand, coordination polymer, FT-IR spectroscopy, carboxylate coordination, metal-organic framework.

Introduction

Coordination polymers constructed from transition metal ions and multifunctional organic ligands have attracted considerable attention because of their structural diversity and potential applications in catalysis, adsorption, magnetism, and material science. Among various organic ligands, tartrate ions are particularly interesting owing to the presence of multiple oxygen donor sites originating from hydroxyl and carboxylate groups. Tartrate ligands can adopt different coordination modes and bridge several metal centers simultaneously, resulting in multidimensional coordination frameworks. In the title compound, $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$, the tartrate ligands act as both μ_4- and μ_3-bridging units, connecting neighboring manganese centers and generating an extended polymeric structure. FT-IR spectroscopy is a valuable technique for investigating coordination behavior in metal-organic systems because it provides information about the involvement of functional groups in metal binding. Therefore, FT-IR analysis was performed to confirm the coordination of tartrate ligands to manganese ions and to identify the characteristic vibrational features of the synthesized coordination polymer.

Results and Discussion

The FT-IR spectrum of the coordination polymer $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$ was recorded in the range of 4000-400 cm^{-1} to investigate the coordination behavior of the tartrate ligand and to confirm the formation of the manganese-based polymeric framework. The observed absorption bands provide valuable information regarding the functional groups present in the structure and their involvement in metal coordination. A broad absorption band centered at **3326 cm^{-1}** was observed in the high-frequency region of the spectrum. This band is attributed to the stretching vibrations of hydroxyl groups originating from the tartrate ligand together with coordinated and lattice water molecules.

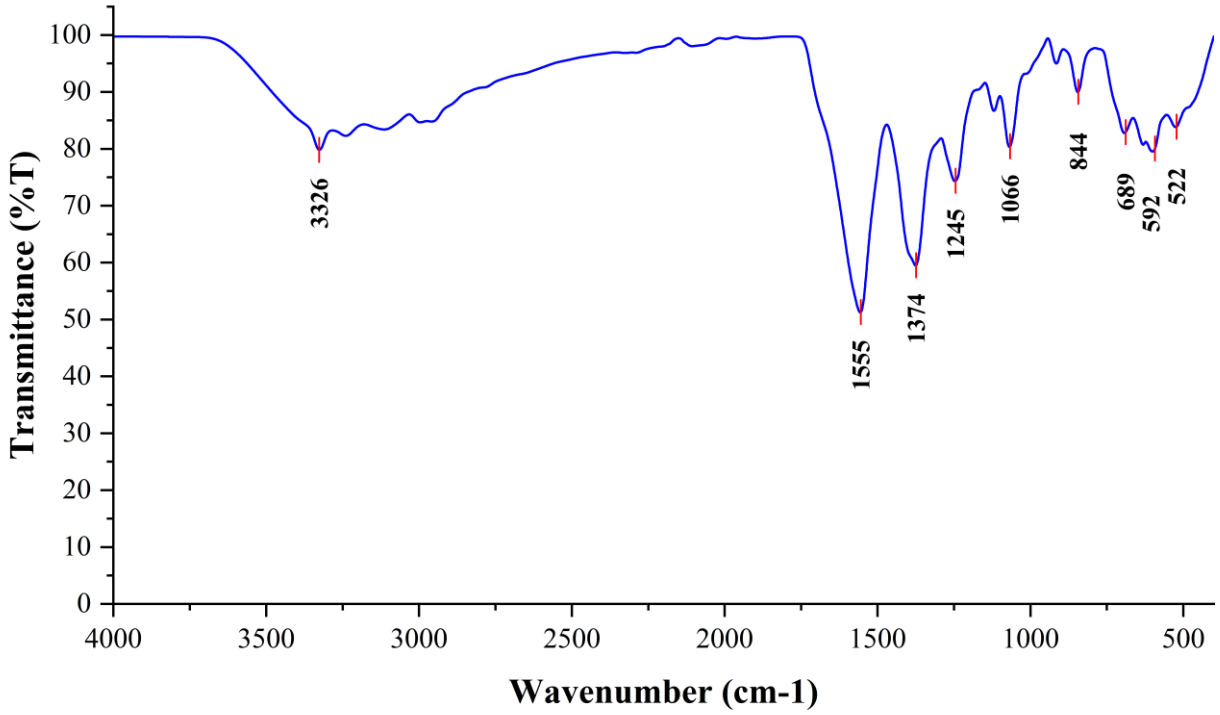

Figure 1. FT-IR spectrum of the coordination polymer $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$ recorded in the range of 4000-400 cm^{-1}.

The considerable broadening of this absorption peak indicates the existence of an extensive hydrogen-bonding network within the crystal structure. Such hydrogen-bond interactions are expected in the title compound because the crystal lattice contains both coordinated water molecules and three crystallization water molecules, which can interact with the hydroxyl and carboxylate oxygen atoms of neighboring tartrate ligands. The spectrum also exhibits two prominent absorption bands at **1555 cm^{-1}** and **1374 cm^{-1}**, which are assigned to the asymmetric stretching vibration, $\nu\_as(COO^-)$, and symmetric stretching vibration, $\nu\_s(COO^-)$, of the carboxylate groups, respectively. The presence of these bands confirms the deprotonation of tartaric acid and the

incorporation of tartrate ligands into the coordination framework. The separation between the asymmetric and symmetric stretching frequencies ($\Delta\nu$ = 181 cm^{-1}) suggests that the carboxylate oxygen atoms are involved in coordination with the Mn(II) centers. This observation is consistent with the crystallographically determined μ_4- and μ_3-bridging coordination modes of the tartrate ligands, where the oxygen atoms serve as donor sites linking adjacent manganese ions into an extended polymeric structure. Furthermore, characteristic absorption bands were observed in the low-wavenumber region between **592 and 522 cm^{-1}**. These bands are attributed to the stretching vibrations of **Mn-O** bonds and provide direct spectroscopic evidence for coordination between manganese ions and oxygen donor atoms. The appearance of these bands confirms the successful formation of the metal-ligand framework and supports the proposed coordination environment around the Mn(II) centers.

Table 1. FT–IR spectral assignments for the coordination polymer $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$

Wavenumber (cm^{-1})	Assignment	Description
3326	ν(O-H)	Stretching vibrations of hydroxyl groups and water molecules involved in hydrogen bonding
1555	νas(COO^-)	Asymmetric stretching vibration of coordinated carboxylate groups
1374	νs(COO^-)	Symmetric stretching vibration of coordinated carboxylate groups
592-522	ν(Mn-O)	Stretching vibrations of manganese–oxygen coordination bonds

The FT-IR analysis therefore provides strong evidence for the successful synthesis of the manganese(II) tartrate coordination polymer and confirms the participation of tartrate oxygen atoms in bridging neighboring metal centers through μ_4- and μ_3-coordination modes.

Conclusion

The FT-IR spectroscopic investigation of $[Mn_2(\mu_4\text{-Tar})(\mu_3\text{-Tar})(H_2O)]_n \cdot 3H_2O$ confirmed the successful formation of a manganese(II)-tartrate coordination polymer. The broad absorption band at 3326 cm^{-1} was attributed to hydrogen-bonded hydroxyl groups and water molecules. Strong bands at 1555 and 1374 cm^{-1} corresponded to the asymmetric and symmetric stretching vibrations of coordinated carboxylate groups,

indicating the involvement of tartrate oxygen atoms in metal coordination. The characteristic Mn-O stretching vibrations observed in the 592-522 cm^{-1} region provided direct evidence for metal-ligand bond formation. The FT-IR data support the existence of an extended coordination framework in which μ_4-tartrate and μ_3-tartrate ligands bridge neighboring Mn(II) centers.

References

1. Nakamoto, K. (2009). *Infrared and Raman Spectra of Inorganic and Coordination Compounds*. Wiley.
2. Socrates, G. (2004). *Infrared and Raman Characteristic Group Frequencies*. Wiley.
3. Housecroft, C.E., Sharpe, A.G. (2018). *Inorganic Chemistry*. Pearson.
4. Cotton, F.A., Wilkinson, G., Murillo, C.A., Bochmann, M. (1999). *Advanced Inorganic Chemistry*. Wiley.
5. Greenwood, N.N., Earnshaw, A. (2012). *Chemistry of the Elements*. Butterworth-Heinemann.
6. Miessler, G.L., Fischer, P.J., Tarr, D.A. (2014). *Inorganic Chemistry*. Pearson.
7. Ferraro, J.R., Nakamoto, K., Brown, C.W. (2003). *Introductory Raman Spectroscopy*. Academic Press.
8. Silverstein, R.M., Webster, F.X., Kiemle, D.J. (2014). *Spectrometric Identification of Organic Compounds*. Wiley.