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ORIGINAL RESEARCH PAPER

A New Gd(III) Complex for Economical Use in MRI

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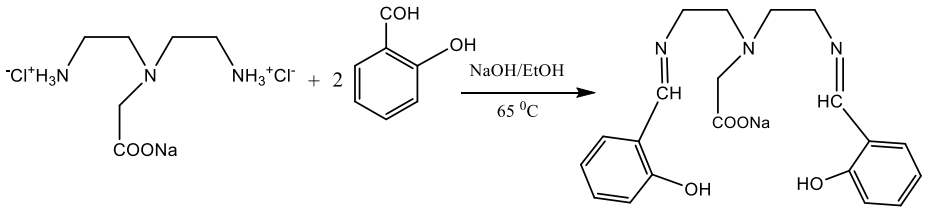
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A B S T R A C T

One of the most important using of the synthesis and characterization of new compounds is their application for the mean of decreases the costs and this application as green materials in the different small and big industrial factories. For this mean we tried to do a new work that can be used in industry systems. One of important methods is the synthesis of applicable new compounds. By this idea we tried to involve the applied researches and also the works that help to industries and improve the economy. In this manuscript we report the synthesis and characterization of a new Gd(III) complex of a polyamine that can be used in MRI to increase the resolution of images. The Schiff base imine was synthesized by the condensation reaction of a new tripodal N_3O donor amine and salsylaldehyde, after synthesis the mentioned compound it was characterized by spectroscopy methods such as microanalysis and IR for complex and NMR for ligand.



1. Introduction

Gadolinium(III) complexes are among the most widely used magnetic resonance imaging (MRI) contrast agents. Owing to its distinctive electronic configuration, particularly in the trivalent oxidation state, Gd^{3+} exhibits strong paramagnetic behavior. Paramagnetism is the property of certain atoms, ions, and molecules that enables them to become weakly magnetized when exposed to an external magnetic field as a result of the partial alignment of their magnetic moments [1–6]. Gadolinium is also one of the few elements that can exhibit significant magnetization at room temperature; the other well-known examples are iron, nickel, and cobalt [1–6].

The strong paramagnetic properties of Gd^{3+} make gadolinium chelates highly effective MRI contrast agents. Gadolinium is not detected directly in an MR image. Instead, its presence is observed indirectly through its ability to accelerate the relaxation of nearby hydrogen nuclei, particularly water protons. At clinically relevant concentrations, gadolinium-based contrast agents predominantly reduce the longitudinal relaxation time (T_1) of tissues in which they accumulate. Consequently, these tissues appear hyperintense on T_1-weighted MR images [7–12]. Although paramagnetism can occur across a broad range of systems—including subatomic particles, atoms, ions, molecules, and bulk materials—the nuclear magnetic moments responsible for the nuclear magnetic resonance (NMR) signal produce a relatively weak form of magnetism. Therefore, although nuclear magnetism is essential for MRI, it cannot account for the pronounced paramagnetic effects associated with gadolinium-based contrast agents [7–12].

The paramagnetism of gadolinium compounds arises primarily from the unpaired electrons in the 4f orbitals of the Gd^{3+} ion. In this ion, seven 4f lectrons remain unpaired, resulting in a large permanent electronic magnetic moment. The magnetic moment of an electron per unit of angular momentum is approximately 658 times greater than that of a proton. Consequently, unpaired electron spins can generate strong, fluctuating local magnetic fields that influence nearby nuclei. These field fluctuations substantially enhance nuclear relaxation, particularly longitudinal (T_1) relaxation, and thereby account for the effectiveness of gadolinium complexes as MRI contrast agents [7–12].

Spectroscopy is one of the most important analytical approaches in chemistry because it provides valuable information about the structural and electronic properties of chemical compounds. Among the various spectroscopic techniques, nuclear magnetic resonance (NMR) spectroscopy is particularly important for determining the types and numbers of atoms, as well as their chemical environments and molecular connectivity [13–16]. Accordingly, the synthesis of new compounds followed by the investigation of their spectroscopic properties is an essential aspect of coordination and inorganic chemistry. In the present study, a new macrocyclic Schiff-base ligand, denoted as HL, was synthesized through the condensation reaction of a tripodal N_3O -donor amine with salicylaldehyde. The ligand was characterized using infrared (IR), ^1H NMR, and ^{13}C NMR spectroscopy. In addition, the corresponding gadolinium(III) complex was prepared and characterized by IR spectroscopy and elemental analysis. The spectroscopic and analytical results obtained for the synthesized compounds were consistent with their proposed structures and

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indicated that the prepared compounds were obtained in a satisfactory degree of purity [13–16].

2. Experimental

2.1. Materials and measurements

All reagents and solvents used in this study were of analytical grade and were purchased from commercial suppliers. They were used as received without further purification. FT-IR spectra were recorded using a STOE IPDS-II spectrometer in the range of 400–4000 cm^{-1} with KBr pellets. NMR spectra were recorded on a Bruker DPX 90 spectrometer [17–20].

2.2. Synthesis of 1,2,2-{N[(CH₂CH₂NH₂)₂CH₂COOH]}.2HCl.2H₂O Ethyl-2-bis (2-phthalimido ethyl)Amino)Acetate, L

2,2-diphthalimidoethylamine (32.8 mmol) was dissolved in 20 ml of acetonitril (100 ml) and added slowly to a stirred solution of Ethylbromoacetate (32.8 mmol) in 30 ml of absolute ethanol and K_2CO_3 and was refluxed for 48 h. After 48 hours the mixture was filtrated and the solution redused and was cooled, the white single crystals were formed. Yield: 61%, m.p. IR (KBr, cm^{-1}): 1714, 1771(νC=O), NMR ($CDCl_3$, ppm, 90 MHz,): 1.1 (t, 3H); 2.92 (t, 4H); 3.46 (s, 1H, CH); 3.62 (t, 4H); 3.95 (q, 4H); 7.57 (s, 8H). ^{13}C NMR ($CDCl_3$, ppm, 90 MHz): 13.64, 35.27, 51.14, 122.29, 116.17, 131.47, 133.10, 167.36, 170.31.

2.2.1.Synthesis of ligand HL, Ethyl-2-bis (2 ethyl)Amino)Acetate (Fig.1)

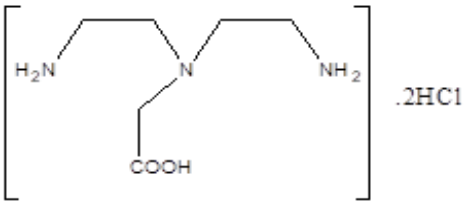


Figure 1. The structure of ligand HL

L (5 g) was dissolved in HCl (150 ml) and refluxed for 12 h, after cooling and evaporation the solution the yellow oil as production was extracted. Yield: 79%. IR (KBr, cm^{-1}): 1734, (νC=O). ^1H NMR (DMSO-d_6, ppm, 90 MHz): 2.24 (m, 2H); 3.08 (m, 4H); 3.55 (m, 4H). ^{13}C NMR ($CDCl_3$, ppm, 90 MHz): 20.92, 33.78, 36.08, 50.85, 51.93, 53.64.

2.2.2.Synthesis of Schiff base H₃L (Fig. 2)

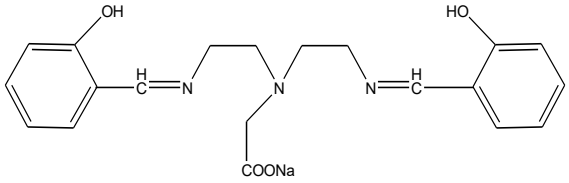


Figure 2. The structure of ligand H_3L

HL (1 mmol) and Salcylaldehyde (2 mmol) were mixed and heated under reflux for 30 min in ethanol (15 ml). The solution was filtered and the filtrate was reduced to ca 10 cm^3. A yellow-colored purified powder was obtained by slow diffusion of Et_2O vapor into this solution. Yield: 54%. IR (KBr, cm^{-1}): 1638, (νC=N Schiff base), 1575, (ν C-O acid). ^1H NMR (DMSO-d_6, ppm, 90 MHz,): 2.8 (m, 4H); 3.24 (m, 4H); 3.76 (s, 2H); 3.24 (m, 8H); 8.38 (s, 2H, Schiff base) . ^{13}C NMR (DMSO-d_6, ppm, 300 MHz,): 41.19, 49.41, 56.82, 117.03, 117.60, 118.65, 131.36, 132.36, 161.15, 165.98, 169.63.

2.2.3. Synthesis of [Gd(H₃L)] Complex

HL (2 mmol) and Salcylaldehyde (2 mmol) were mixed and heated under reflux for 30 min in ethanol (15 ml). The solution was filtered and the filtrate was reduced to ca 10 cm^3. A yellow-colored purified powder was obtained by slow diffusion of Et_2O vapor into this solution. Yield: 67%. 55%. IR (KBr, cm^{-1}): 1643, (νC=N Schiff base), 1608, (νC-O).

3. Results and Discussion

3.1. Synthesis and characterization

The mentioned Schiff base ligand was synthesized according to the experimental section. By this way first of all the related protected amine was prepared then was reacted with bromo ethyl acetate and after hydrolysis in aqueous HCl the protected amines were realized and ligand was ready for another step. The production of each step was characterized by the different spectroscopy methods like IR, NMR etc. For instance all spectrums are listed in Figes (3-8). Finally by the condensation reaction of Schiff base and Gd(III) metal ion the related complex was synthesized and characterized by IR spectroscopy.

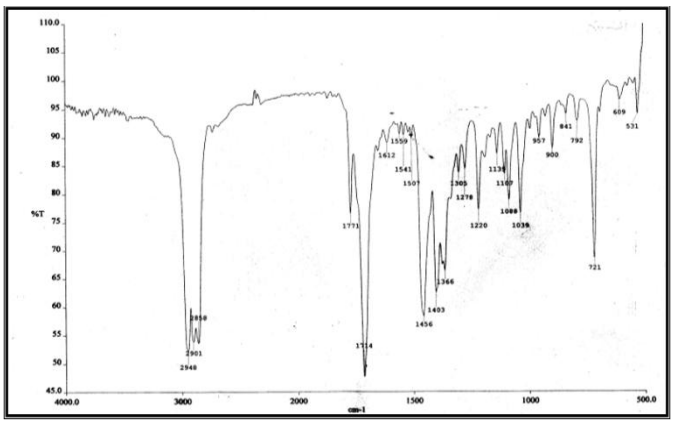


Figure 3. IR spectra of HL ligand

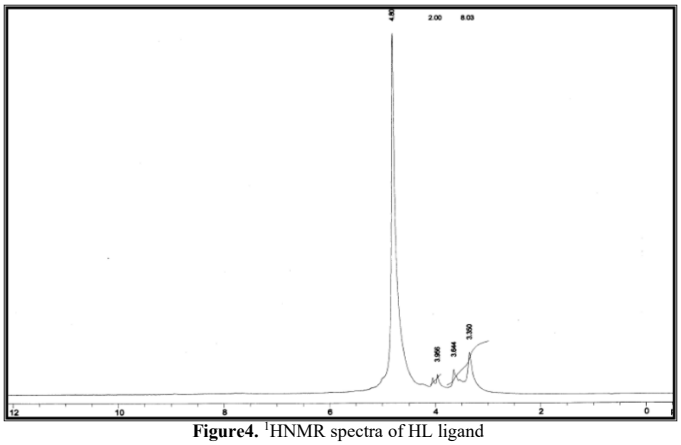


Figure4. ^{1}HNMR spectra of HL ligand

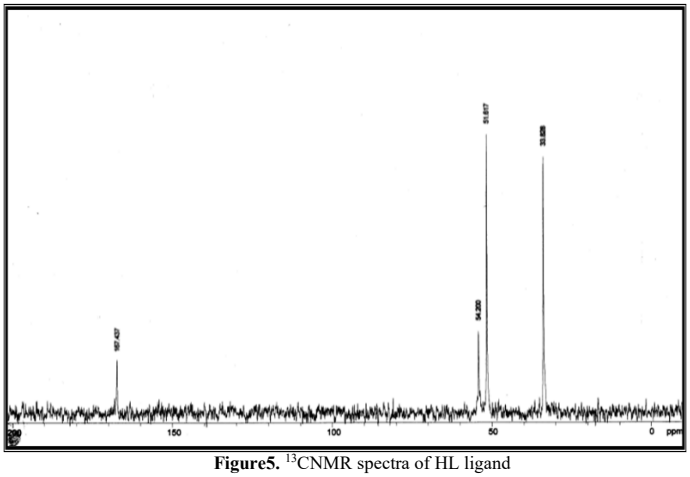


Figure5. ^{13}CNMR spectra of HL ligand

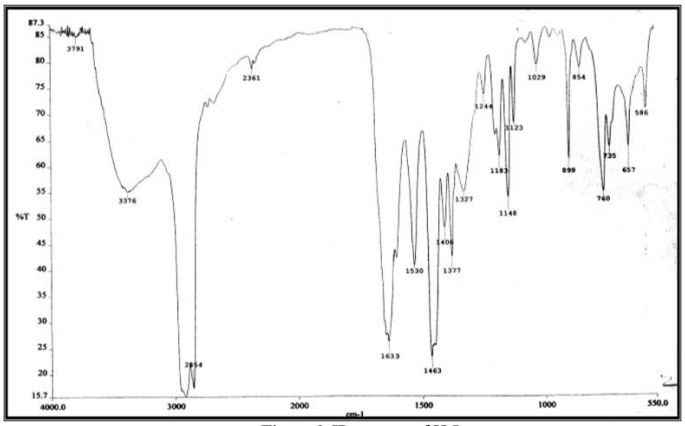


Figure6. IR spectra of H_3L

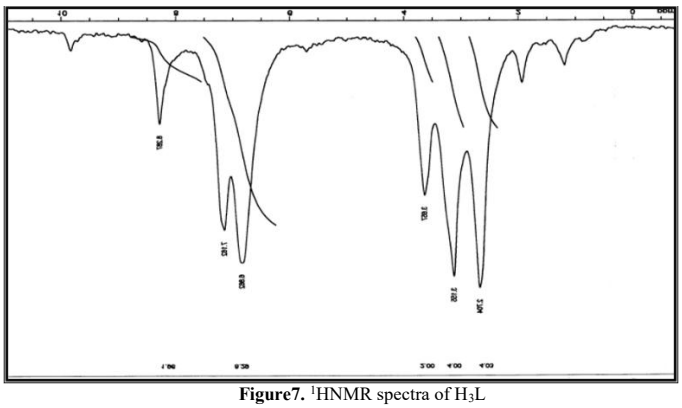


Figure7. ^{1}HNMR spectra of H_3L

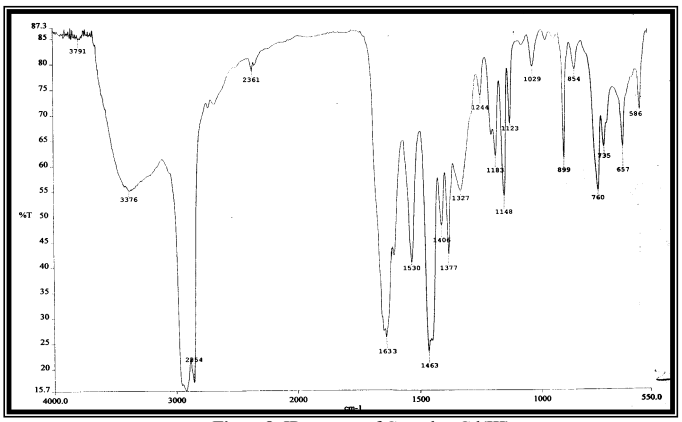


Figure8. IR spectra of Complex Gd(III)

In the case of ligand HL condensation of all the primary amino groups is confirmed by the lack of N–H stretching bands in the IR spectra (3150–3450 cm^{-1}) and the presence of strong C-O (Carbonyl) stretching bands at 1734 cm^{-1}. The presence of a band in 1638 cm^{-1} in the IR spectrum of Schiff base is related to the imine group.

After preparation of Complex the imine group band was appeared in 1643 cm^{-1}. The ^{1}H,^{13}CNMR spectra are confirmed to the structure of both lignads HL and H_3L.

3.2. NMR studies

NMR spectroscopy is one of the most effective techniques for the characterization of new compounds. In this study, ^{1}H, and ^{13}CNMR spectroscopy were used to determine the type and number of protons and carbons in the synthesized products and to confirm that the observed signals were consistent with the proposed molecular formulas. As shown in Figures 4 and 7, the ^{1}HNMR spectra of the tripodal tetraamine ligand and the Schiff base are in good agreement with their expected structures. In Figure 4, three separate signals are observed, all of which appear as triplets and correspond to the methylene groups. Another signal appears as a singlet and is assigned to the methylene group adjacent to the carboxylate functionality. In Figure 5, four peaks are observed, which match the structure of the tripodal ligand. The signals appearing in the aliphatic region correspond to the methylene groups, while the remaining signal is related to the carbonyl-containing fragment. In the case of the Schiff base, as shown in Figure 7, aliphatic, aromatic, and imine protons are present. Therefore, three main types of proton signals are expected. The aliphatic protons appear in the range of 2–4 ppm and integrate for 10 protons. In addition, signals at around 7 ppm correspond to 8 aromatic protons, and the signal at approximately 8 ppm is assigned to 2 imine protons. Overall, the NMR spectra of both the imine precursor and the Schiff-base compound confirm their proposed formulations and structures. Some additional weak peaks are attributable to solvent impurities.

4. Conclusions

A new Schiff-base ligand, H_3L derived from a tripodal N_3O -donor ligand, was successfully synthesized. The corresponding Gd(III) complex was also prepared using this ligand. The Schiff-base ligand was characterized by ^{13}C,1HNMR and IR spectroscopy, whereas the Gd(III) complex was characterized by IR spectroscopy. The spectroscopic results were consistent with the proposed structures of all synthesized compounds reported in this manuscript.

Author Contributions

All authors contributed equally to the conception, preparation, and writing of this manuscript.

Conflict of Interest

The authors, while observing publication ethics in the referencing, declare the absence of interest of conflict.

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