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Spectroscopic and DFT study of a glutamic acid Nd(III) complex

Issei Takahashi [1], Daisuke Nakane [1], Takashiro Akitsu [1,*] and Chittaranjan Sinha [2]

[1] *Department of Chemistry, Faculty of Science, Tokyo University of Science, Tokyo, 162-8601, Japan*
[2] *Department of Chemistry, Jadavpur University, Kolkata, 700032, India*

* *Corresponding author at: Department of Chemistry, Faculty of Science, Tokyo University of Science, Tokyo, 162-8601, Japan.*
e-mail: akitsu2@rs.tus.ac.jp (T. Akitsu).

RESEARCH ARTICLE

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ABSTRACT

Due to the large number of electrons occupying 4*f* orbitals, the computational chemistry of lanthanide complexes is not as easy as that of *d*-block ones. As a result, even though lanthanide molecules have attracted attention in various fields in recent years, there has been little research on their spectrochemical properties or computational science in detail. In this study, we experimentally measured electronic, circular dichroism (CD), fluorescence, and infrared (IR) spectra as well as the direct current (DC) magnetic susceptibility curves (magnetization (M) versus magnetic field (H) curves (MH) and magnetization (M) versus temperature (T) curves (MT)) of a mononuclear Nd(III) complex with a glutamic acid ligand and to test the density functional theory (DFT) calculation conditions that can be performed from the structure optimization. Bands of C=O and N-H were observed in the IR spectrum, and paramagnetism was confirmed by measurements. The fluorescence intensity of the DMSO solution at 300 K was very weak. Ultraviolet-visible (UV-vis) and CD spectra showed a strong intraligand transition at 200-250 nm and relatively strong sharp *f-f* transitions at 581, 742, and 801 nm (like the solvated Nd(III) ion). Thus, herein we synthesized lanthanide Nd(III) complexes coordinated with amino acids and conducted structure estimation research by comparing experimental measurement results such as electron microscopy, spectroscopy, and magnetism with DFT calculations (optimized structure). Lanthanide complexes are difficult to study because their coordination numbers are large, their solution structures are unclear, and their large number of electrons makes computational chemistry difficult. In general, metals have large ionic radii, and thus can potentially have high coordination numbers. Metal ions of hard Lewis acids prefer hard-base ligands (especially oxygen atoms in water and amino acids). Therefore, it is interesting to try to easily understand the structure in solution by comparing spectroscopic experiments with computational chemistry.

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1. Introduction

Unlike the story about the *d* transition element, the properties of the *f*-block transition element, its oxidation state, complex formation, color, magnetism and fluorescence spectrum show unique chemistry [1,2]. Lanthanoid elements are utilized in various fields due to their spectroscopic and magnetic properties based on the 4*f* orbitals. By being shielded by the 5*p* orbitals, there is no overlap with the coordination pathway, and the line behaves as an isolated electronic system with less division by the ligand field [1]. In that case, it is difficult to obtain a single crystal because the coordination number is also diverse and a relatively high provisional coordination number can be obtained compared to the first advanced metal complex, making it very difficult to analyze the structure of the complex [1].

On the other hand, the absorption and emission characteristics of specific wavelengths are based on transitions between 4*f* orbitals, and the magnetic properties based on the orbital angular momentum and spin angular momentum of electrons in 4*f* orbitals are unique to lanthanides and can be used to detect rare earth elements and create functional materials [3]. As mentioned above, the electrons in the 4*f* orbitals are hardly involved in bonds and the effect of the ligand field is small, so the absorption is due to a weak transition due to the Laborte forbidden, but when the excited state is reached, the emission lifetime is very long due to the small transition probability, and a very sharp peak is observed when observed [4]. Ingenuity for creating luminescent complexes includes introducing antenna ligands to transfer electrons to the excited level by intersystem crossing or energy transfer and introducing appropriate multidentate ligands to reduce the quenching process in which electrons move to the energy levels of the C-H, O-H, and N-H stretching vibrations of surrounding ligands such as water [1].

For magnetic properties, in addition to spin angular momentum, the effective magnetic moment is calculated by considering the influence of orbital angular motion, which is not considered for first transition metals. Because 4*f* electrons do not participate in bonding, there is almost no overlap between the 4*f* orbitals and ligands, and in many cases, they exhibit paramagnetic properties based on dipole-dipole interactions [1].

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Table 1. The selected bond lengths and angles of the optimized molecular structure.

Atom-Atom	Bond distances (Å)	Atom-Atom-Atom	Bond angles (°)
1Nd-2O	2.36417	1Nd-7O-8N	95.74287
1Nd-3O	2.39427	1Nd-6O-8N	96.25274
1Nd-4O	2.38506	6O-8N-7O	114.53292
1Nd-5O	2.36332	6O-8N-9O	122.62689
1Nd-6O	2.41810	7O-8N-9O	122.84018
1Nd-7O	2.43074	6O-1Nd-2O	114.56809
6O-8N	1.29805	6O-1Nd-3O	135.58966
7O-8N	1.29514	6O-1Nd-4O	111.77473
8N-9O	1.20244	6O-1Nd-5O	144.72675
2O-10C	1.27643	7O-1Nd-2O	144.41366
3O-10C	1.27671	7O-1Nd-3O	106.94010
10C-11C	1.52381	7O-1Nd-4O	138.63884
11C-20N	1.46137	7O-1Nd-5O	111.57180
20N-21H	1.01915	2O-1Nd-3O	55.17787
20N-22H	1.01834	3O-1Nd-4O	106.81875
11C-12H	1.09482	4O-1Nd-5O	55.17868
11C-13C	1.56724	5O-1Nd-2O	94.91431
13C-14H	1.09728	2O-1Nd-4O	76.00244
13C-15H	1.09514	3O-1Nd-5O	76.81008
13C-16C	1.55300	6O-1Nd-7O	53.47065
16C-17H	1.09353	2O-10C-3O	119.35976
16C-18H	1.09732	2O-10C-11C	119.56197
16C-19C	1.51919	3O-10C-11C	120.17752
19C-4O	1.27557	10C-11C-20N	108.31275
19C-5O	1.28075	10C-11C-13C	110.23093
		13C-11C-20N	113.21160
		11C-13C-16C	119.16993
		13C-16C-19C	112.01323
		4O-19C-5O	118.70126
		4O-19C-16C	121.35550
		5O-19C-16C	118.98591

The computational science of lanthanide complexes is not as straightforward as that of *d*-block metal complexes due to the presence of electrons occupying 4*f* orbitals. We previously performed DFT calculations under various conditions using the semiempirical PM6 method for a binuclear Sm(III) complex with 3*d*-4*f* orbitals based on the crystal structure obtained [5]. In this study, we prepared a mononuclear Nd(III) complex with glutamic acid as a ligand and experimentally measured electronic spectra such as CD , fluorescence, and IR, as well as DC magnetic susceptibility measurements (MH and MT), and performed structure optimization to verify [1].

In this paper, a Glu-Nd(III) complex was prepared, and the elements were confirmed by SEM-EDS, and the magnetism was confirmed by magnetic measurements (Superconducting Quantum Interference Device, SQUID). Then, for qualitative analysis, IR, UV-vis, and CD spectra were measured, and simulations were performed based on DFT calculations, and the peaks themselves were observed, but with deviations in position and intensity. On the other hand, no fluorescence spectrum was observed at 300 K. The Nd(III) complex is unreliable because it contains the multidentate ligand glutamic acid and the coordination number varies greatly, making it difficult to perform spectral simulations based on the optimized structure , especially to discuss the intensity under these conditions.

2. Experimental

2.1. Materials and instrumentation

A Nd(III) complex with glutamic acid was synthesized by stirring neodymium(III) nitrate and glutamic acid in a mixture of methanol, a small amount of water, and a small amount of acetone. SEM-EDS were measured with a JSM-IT800SHL (JEOL). Magnetic susceptibility was measured at variable temperature (5000 Oe, 5-300K) or variable field (5K, 0-50000 Oe) using a SQUID magnetometer (MPMS-XL7AC, Quantum Design). IR spectra were recorded as KBr pellets on a FT-IR 4200 spectrophotometer (JASCO) in the range of 4000-400 cm^{-1} at 25 °C. Electronic (UV-vis) spectra were measured on a JASCO V-650 UV-vis spectrophotometer in the range of 800-200 nm at 25 °C. CD spectra were acquired on a JASCO J-820 spectropolarimeter in the same range and temperature. Fluorescence spectra were recorded on a JASCO FP-6200 spectrophotometer at 298 K.

2.2. Theory/calculation

First, the Karlsruhe/Ahlrichs basis sets (def-TZVP) have been excluded because they are already outdated. According to general information, the def2 basis set is more systematic and works better. However, it also has the disadvantage of being generally larger in size. The main difference between def-TZVP and def2-TZVP is that def2 is polarized by one additional angular momentum compared to the def basis set. As a result, benchmark test research reports are expected to convince people to use the def2 basis set. That is, the error of the double zeta def2-SVP is usually smaller than that of the old triple zeta def-TZVP. On the basis of this knowledge, we selected def-svp and def-tzvp, looked at the actual calculation results, and selected the appropriate basis functions.

Simulations of various spectroscopic spectra were performed using the basic methods described in the software's manual and the official manual, and no special methods were used. In this study, the exchange-correlation functional was fixed to B3LYP, and calculations were performed using Def-SVP and Def-TZVP for the neodymium atom and 6-31G(d) for other atoms. as basis functions. Unlike the case of Def-TZVP, when calculating with Def-SVP as the basis function, the calculation did not finish and the optimization structure could not be obtained. Among several proposed structures, the most stable proposed structure was optimized by DFT (Gaussian09 [6], Nd: Def2-TZVP functional [5], other atoms: 6-31G(d) [7]) for spectral simulation (Table 1). Sum of electronic and zero-point energies = -1392.206326, Sum of electronic and thermal energies = -1392.190886 where zero-point correction = 0.146202, thermal correction to energy = 1.161642, thermal correction to enthalpy = 0.162586, thermal correction to Gibbs free energy = 0.100441 (Hartree / particle) (Figure 1).

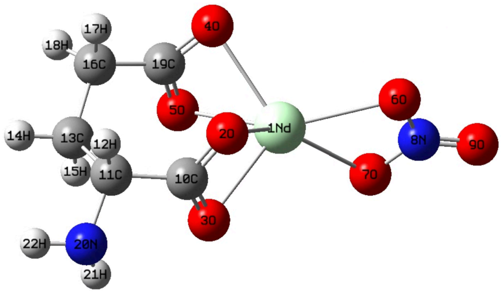

Figure 1. Optimized molecular structure of the Glu-Nd(III) complex.

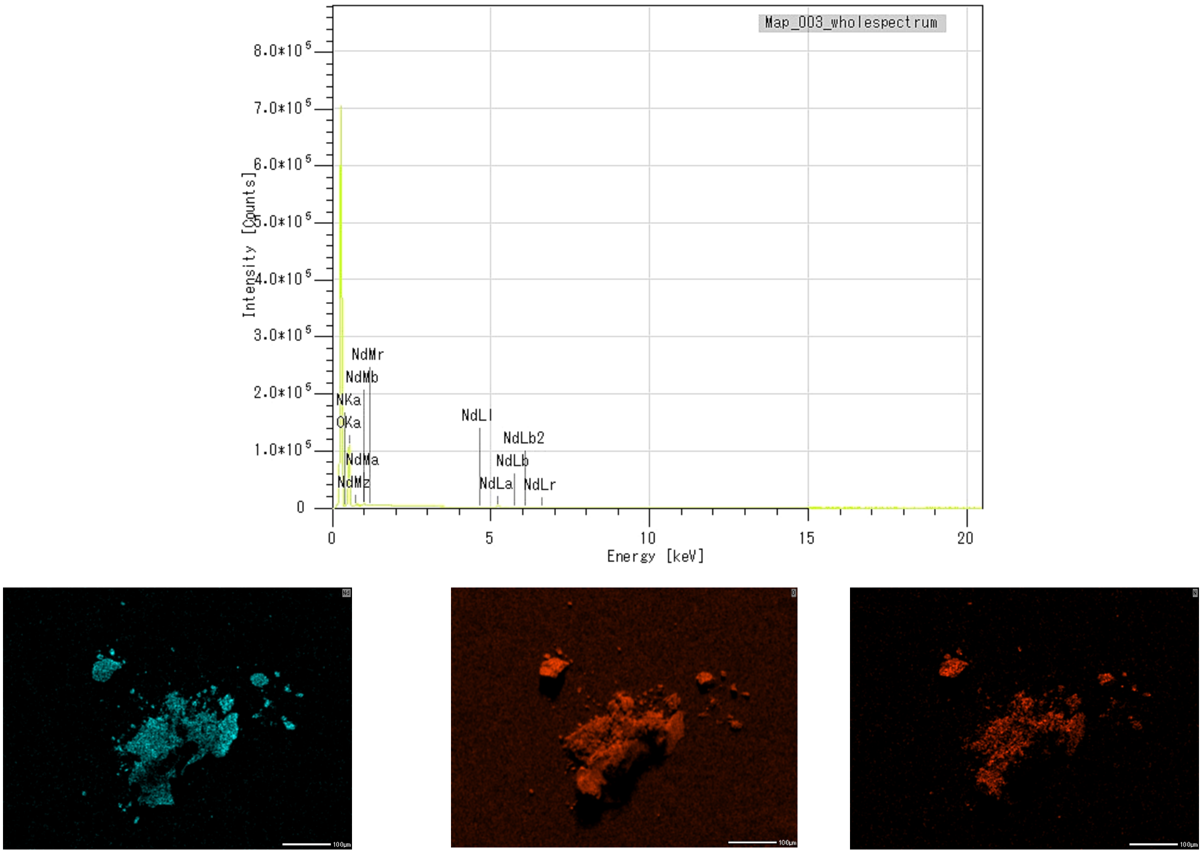

Figure 2. SEM images with EDX elemental analysis of the Nd(III) complex.

3. Results and discussion

Morphology and containing Nd was confirmed with Scanning Electron Microscope (SEM) and Energy Dispersive X-ray Spectroscopy (EDX) elemental mapping, respectively. The peaks derived from the carbon atom and nitrogen atom were weak, suggesting that their amount was lower relative. SEM-EDS, an elemental analysis of the Nd(III) complex coordinated with glutamic acid was performed on the carbon tape and the presence of Nd atoms was confirmed (Figure 2). Note that the nitrogen atom and carbon atom are contained in the carbon tape and the polyimide adhesive, so they appear in most of the image. From these data, the external shape of the crystal of the rare-earth compound and the types of elements contained were analyzed. Due to the synthesis of rare earth complexes [8], the equilibrium of dissociation in solution, and hydration, chemical species may differ from those that can be isolated in solid form [9].

The paramagnetic characteristics of the mononuclear Nd(III) complex (S = 3/2) were confirmed by MH and MT measurements (Figure 3). Direct-current magnetic susceptibility (DC) measurements of the Nd(III) complex coordinated with glutamic acid, MH measurements at a constant temperature of 5 K, and MT measurements at a constant magnetic field of 5000 Oe were performed. As a result, magnetic susceptibility increased with increasing magnetic field in MH measurements, while the magnetic susceptibility decreased with increasing temperature from near absolute zero in the MT measurements, indicating that the complex has paramagnetic properties [10]. However, since the contribution of orbital angular momentum cannot be ignored [10], the results of plotting the MT curve with values related to the effective magnetic moment have no quantitative meaning [10]. It should be noted that the spin-only formula can be used to calculate the magnetic moment only for La^{3+} (f^0), Gd^{3+} (f^7), and Lu^{3+} (f^{14}). This suggested that it was at least a mononuclear complex [10]. The effective magnetic moment must be calculated from the Lande g-factor and the description of the electron and orbital angular momentum in terms of J [9].

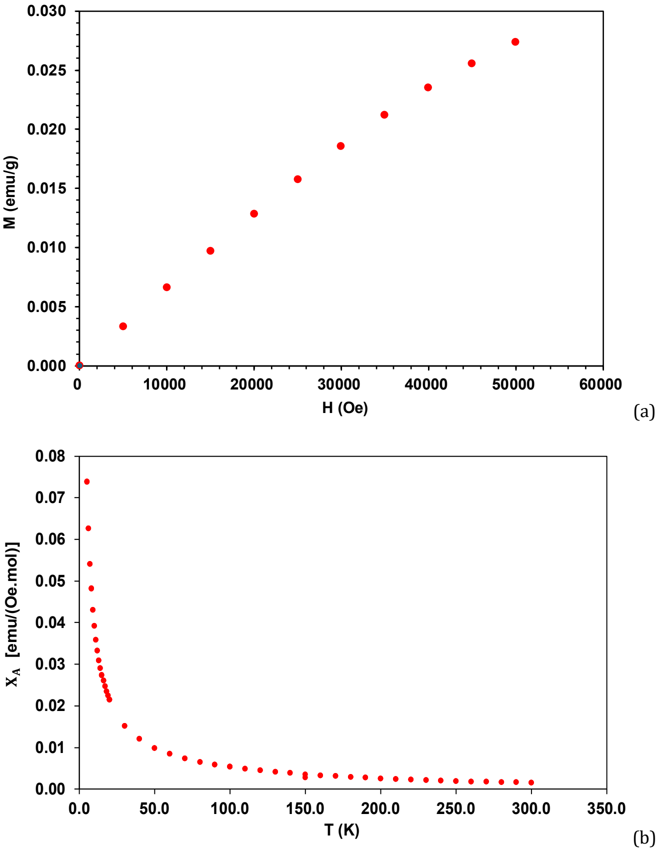

Figure 3. Results of (a) MH and (b) MT magnetic measurements.

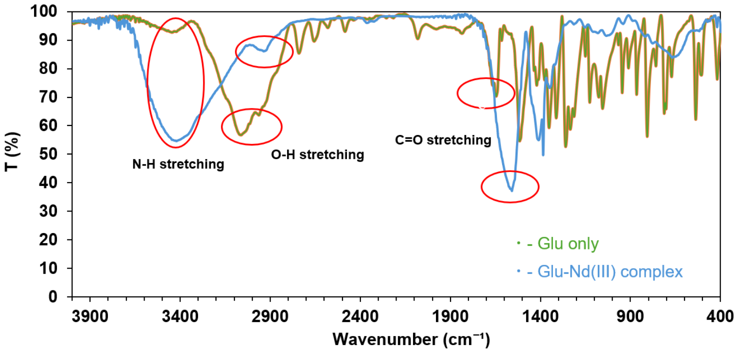

Figure 4. Experimental IR spectra of the Glu (green) and Glu-Nd(III) complex (blue).

Magnetic properties depend on the number of unpaired electrons, and Ln can be paramagnetic or diamagnetic [10]. Based on the Russell–Saunders coupling [10], the quantum numbers S and L are coupled to form a total angular momentum J. This is a kind of angular momentum coupling method in atomic physics that considers the interaction of orbital angular momentum and spin angular momentum (the contrasting method is called *j-j* coupling) [4]. This coupling is important in describing the energy levels of multi-electron atoms, especially those in which the orbital angular momentum cannot be ignored (except in 3*d* metal complexes) [10]. Specifically, the orbital angular momentum and the spin angular momentum of each electron are coupled to form the total orbital angular momentum L and the total spin angular momentum S, respectively. These L and S are then further combined to form the total angular momentum *J*. This *J* is conserved against external perturbations (e.g. magnetic fields) [1].

The IR spectra of glutamic acid alone and of a Nd(III) complex with glutamic acid as a ligand were measured with the KBr method (Figure 4). As a result, it was confirmed that various vibrational peaks shifted to the lower wavenumber side due to coordination of C=O vibration before and after coordination [11]. Furthermore, although the peak intensity was weakened, the OH vibration of the carboxyl group was observed, confirming the presence of uncoordinated carboxyl groups in the precipitate [11]. In the IR spectrum of a lanthanide complex, the vibration peaks of the metal bond between the lanthanide and the ligand are difficult to observe because the bonds are formed by electrons from the f orbital, and the vibrations specific to the ligand become stronger [11, 12]. In this vibration spectrum, although there is a phenomenon of OH peaks that is believed to be due to loss of hydrogen atoms due to coordination, it can be seen that the peak intensities of C=O vibrations and N-H vibrations are stronger than those of original glutamic acid alone [11].

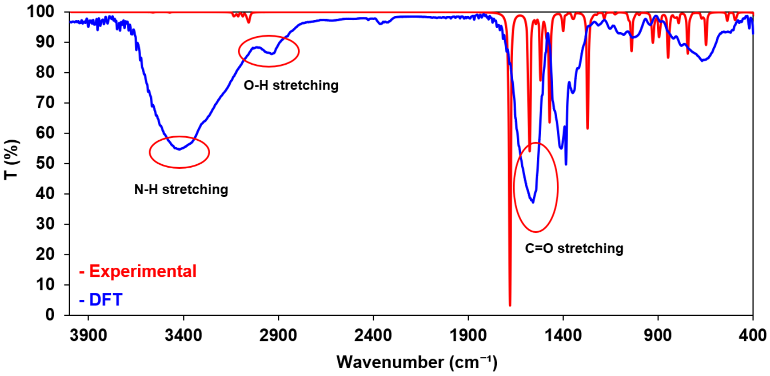

Figure 5. Experimental (red) and DFT simulated (blue) IR spectra of Glu-Nd(III) complex.

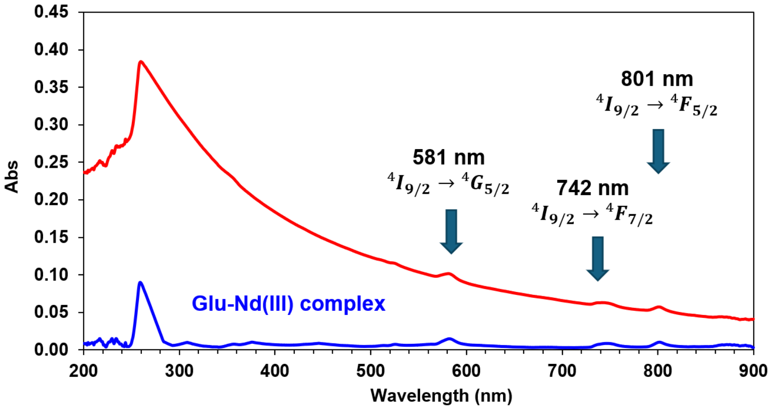

Figure 6. UV-vis spectra were measured using a solution of neodymium nitrate in methanol and a solution of a glutamic acid-ligand Nd(III) complex in methanol.

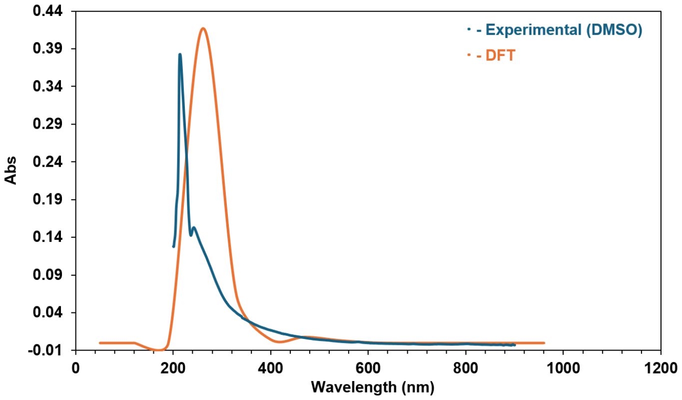

Figure 7. UV-vis spectra of the Nd(III) complex in DMSO (blue) and DFT calculated one (orange).

The IR spectrum of the Nd(III) complex with glutamic acid as a ligand was calculated and assigned by DFT as follows: (i) NH vibration: 3421 cm^{-1} (measured value) *vs.* loss (calculated value), (ii) OH vibration: 2935 cm^{-1} (actual value) *vs.* loss (calculated value), (iii) C=O vibration: 1558 /cm (measured value) *vs.* 1579 cm^{-1} (calculated value).

The actual C=O vibration peak was predicted. In the DFT calculation, the functionals used were Nd: def2-TZVP, C, H, N, O: 6-31G(d), and the bond order of the C=O of the carboxyl group was established (Figure 5). Furthermore, the calculated peak at 1682 cm^{-1} was the assumed N=O vibration of the nitrate ion. These are reasonable results that correspond to typical peak values for amino acid compounds or metal complexes containing glutamic acid [11].

Furthermore, UV-vis spectra were measured using a solution of neodymium nitrate in methanol and a solution of a glutamic acid-ligand Nd(III) complex in methanol (Figure 6). The spectra showed a strong intra-ligand transition at 200-250 nm and relatively strong sharp *f-f* transitions at 581, 742, and 801 nm (like the solvated Nd(III) ion). These results confirmed the presence of Nd atoms in the complex [12].

In addition, the UV-vis spectra of the glutamic acid liganded Nd (III) complex was measured in DMSO (200-700 nm) and compared with the calculated DFT spectrum (50-950 nm) (Figure 7). Strong peaks were observed at 262 and 240 nm in the measured and DFT-calculated spectra, respectively. The DFT simulation of the spectrum did not show the *f-f* transition peaks expected from the 4*f* orbital splitting.

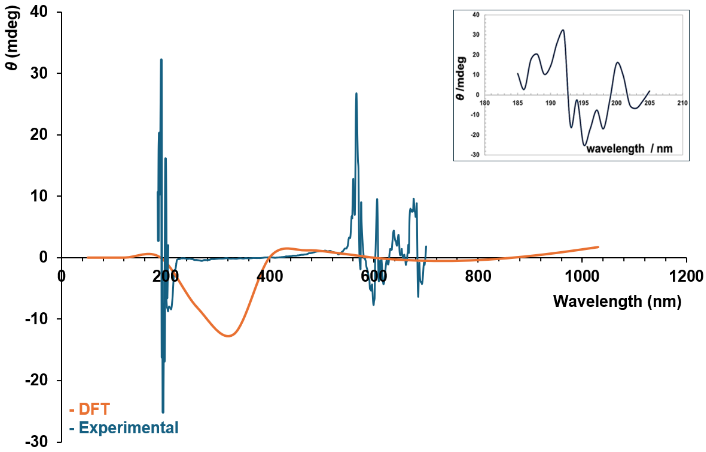

Figure 8. CD spectra of the Nd(III) complex in DMSO (blue) and calculated by DFT (orange).

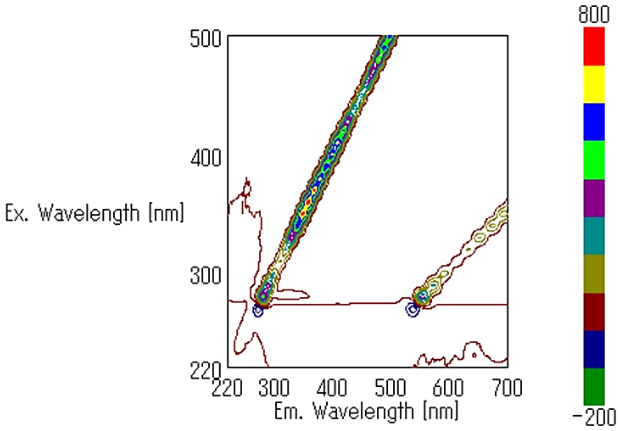

Figure 9. 3D fluorescence spectrum of the Nd(III) complex (not emitted at room temperature).

The transitions expected from experience or calculations are relatively too weak in intensity in actual UV-vis spectra, so they cannot always be observed. The fluorescence spectra described below are similar depending on the temperature and energy transfer conditions [12]. The splitting of the 4f orbital is less affected by the type of ligand or solvent located at the interior angle than the 5*s* orbital, *etc*., so it is thought that the peak position did not change much when the neodymium nitrate hydrate was dissolved in water and when glutamic acid was added [12].

In this way, herein, we synthesized lanthanide Nd(III) complexes coordinated with amino acids and conducted structure estimation research by comparing experimental measurement results such as electron microscopy, spectroscopy, and magnetism with DFT calculations (optimized structure). Even if the crystal structure of the Nd(III) complex is determined and the coordination mode in the solid state (which may be one of many isomers) is confirmed, it is difficult to discuss the exact mode of existence because the ligand dissociates in solution and the equilibrium state is established. As one method, we will compare the available experimental data, promising hypothetical structures, and calculation data and discuss them here. As a tentative rough trend, it may be good to assume that it is the predominant chemical species in solution.

In parallel with the UV-vis spectra, CD spectra were measured from 200 to 700 nm in methanol (Figure 8), and the differences in intensity revealed that the intraligand and *f-f* transitions were observed at different concentrations. CD spectra (in DMSO and DFT) were also compared to discuss (Figure 8) [13]. DFT calculations predicted strong peaks for the intraligand and *f-f* transitions, but no peaks in the vicinity were observed in the experimental data [14]. When the ligand is an amino acid, that is, when it has an amino group and a carboxyl group, a chelate ring is formed and a CD spectrum is observed [15].

Finally, the Glu-Nd(III) complex was dissolved in methanol and the 3D fluorescence spectrum was measured (Ex: 220 to 500 nm, Em: 220 to 700 nm) (Figure 9). Under these conditions (300 K, in MeOH), the intensity of the Glu-Nd(III) complex was very weak. The reason for the very low peak intensity is that the solubility of the Glu-Nd(III) complex in methanol is very low, the number of Nd atoms present in the solution is very small, and the fluorescence emitted by the Nd atoms is close to the excitation energy of the OH vibration of methanol [12], so the fluorescence is absorbed by the methanol molecules surrounding the complex.

4. Conclusions

In summary, a Glu-Nd (III) complex was prepared. Elements and magnetism were confirmed by means of SEM-EDS and magnetic measurement (SQUID), respectively. For qualitative assignments, IR, UV-vis, and CD spectra were measured and simulated based on DFT calculations. However, fluorescence spectra could not be observed at 300 K. In solutions, where the crystal structure is not reliable or available, optimized structure-based spectral simulation is difficult, in particular discussion of the intensity at present conditions.

With regard to lanthanide contraction and the coordination number in a potentially coordinating solvent, we were able to gain a deeper understanding of the fact that the actual in-solution complex structure obtained because of lanthanide contraction is not constant by comparing it with calculations. Based on the UV-VIS and CD spectra that served as the basis for this, it is expected that the color gradation of lanthanides changes as the number of 4*f* electrons increases from La to Gd, and repeats in the same way from Lu to Gd. This time, the trend for Nd(III) was expected, but it was also found that the *f*-*f* transition was not necessarily observed clearly.

The *f*-block elements are a very interesting field in inorganic chemistry. Ideally or simply, it would be expected that many Ln^{3+} ions are colored in both solid and aqueous solutions and that color depends on the number of unpaired electrons. The mechanism of the correlation between the actual color and the number of unpaired electrons, which was particularly interesting this time (depending on the chemical species in the solution and various conditions), will be necessary to know for practical application. The diverse chemical properties of *f*-block metals influence the formation of various reactions and compounds. Because it is used industrially as a catalyst, it has the ability to accelerate chemical reactions and is indispensable to modern society. It would be great if we could contribute to the development of new technologies and materials.

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Disclosure statement

Conflict of interest: The authors declare that they have no conflict of interest.
Ethical approval: All ethical guidelines have been adhered to.
Sample availability: Samples of the compounds are available from the author.

CRediT authorship contribution statement

Conceptualization: Chittaranjan Sinha; Methodology: Issei Takahashi, Chittaranjan Sinha; Investigation: Issei Takahashi, Chittaranjan Sinha; Writing - Original Draft: Issei Takahashi, Takashiro Akitsu; Review and Editing: Chittaranjan Sinha, Daisuke Nakane; Project Administration: Takashiro Akitsu.

ORCID and Email

Issei Takahashi
1321075@ed.tus.ac.jp
https://orcid.org/0000-0001-5044-1486
Daisuke Nakane
a29776@rs.tus.ac.jp
https://orcid.org/0000-0001-9566-0674
Takashiro Akitsu
akitsu2@rs.tus.ac.jp
https://orcid.org/0000-0003-4410-4912
Chittaranjan Sinha
crsjuchem@gmail.com
https://orcid.org/0000-0002-4537-0609

References

[1]. Cotton, S. *Lanthanide and Actinide Chemistry*; Wiley-Blackwell: Hoboken, NJ, 2006.
[2]. Wybourne, B. G.; Smentek, L. *Optical spectroscopy of lanthanides: Magnetic and hyperfine interactions*; CRC Press: London, England, 2019.
[3]. Akitsu, T. Lanthanide Complexes in Recent Molecules. *Molecules* **2022**, *27* (18), 6019.
[4]. Matsumoto, K. *Chemistry of Lanthanide.* Asakura Shoten Publisher: Tokyo, Japan, 2008.
[5]. Kawahara, K.; Okumura, Y.; Takiguchi, Y.; Nakane, D.; Akitsu, T. Lightening calculations for Schiff base lanthanide complexes. *AIP Conf. Proc.* **2024**, *3030*, 020006.
[6]. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian, Inc., Wallingford CT, 2009.
[7]. Hatanaka, M. Theoretical Study of Lanthanide Luminescence Materials. *Mol. Sci.* **2021**, *15* (1), A0118. https://doi.org/10.3175/molsci.15.A0118
[8]. Shinoda, S.; Tsukube, H. Development of Analytical and Separation Systems Using Ternary Complexation Characteristics of Tris(β-diketonato)lanthanides. *Bunseki Kagaku* **2012**, *61* (3), 169–176.
[9]. Arnesano, F.; Banci, L.; Piccioli, M. NMR structures of paramagnetic metalloproteins. *Quart. Rev. Biophys.* **2005**, *38* (2), 167–219.
[10]. Acharya, J.; Kalita, P.; Chandrasekhar, V. High-Coordinate Mononuclear Ln(III) Complexes: Synthetic Strategies and Magnetic Properties. *Magnetochemistry* **2020**, *7* (1), 1. https://doi.org/10.3390/magnetochemistry7010001
[11]. Roddick-Lanzilotta, A. D.; McQuillan, A. An in situ Infrared Spectroscopic Study of Glutamic Acid and of Aspartic Acid Adsorbed on TiO_2: Implications for the Biocompatibility of Titanium. *J. Colloid Interface Sci.* **2000**, *227* (1), 48–54.
[12]. Nawrocki, P. R.; Sørensen, T. J. Optical spectroscopy as a tool for studying the solution chemistry of neodymium(III). *Phys. Chem. Chem. Phys.* **2023**, *25* (29), 19300–19336.
[13]. Rajabi, A.; Grotjahn, R.; Rappoport, D.; Furche, F. A DFT perspective on organometallic lanthanide chemistry. *Dalton Trans.* **2024**, *53* (2), 410–417.
[14]. Janowski, A.; Wałkuska, I.; Lewandowski, W. Infrared spectra of lanthanide complexes with eriochrome cyanine r. *Anal. Chim. Acta* **1982**, *144*, 289–294.
[15]. Hawkins, C. J.; Lawson, P. J. Circular dichroism spectra of amino acid complexes. Carboxylatopentaamminecobalt(III) compounds. *Inorg. Chem.* **1970**, *9* (1), 6–11.