Syntheses, and Crystal and Molecular Structures of [Enneakis(chloroacetato)-tetrakis(dimethyl sulfoxide)trineodymium(III)], $[Nd_3(ClCH_2CO_2)_9\{(CH_3)_2SO\}_4]$, and of the Isomorphous Lanthanum(III) and Praseodymium(III) Salts

Yoshihiko SUGITA and Akira OUCHI*
Department of Chemistry, College of Arts and Sciences, The University of Tokyo, Komaba, Meguro-ku, Tokyo 153
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The crystal and molecular structures of the chloroacetato–dimethyl sulfoxide (dmso) mixed complex of neodymium(III) indicated in the title were determined by the single-crystal X-ray diffraction method. The crystal is monoclinic, space group $P2_1/n$, a=21.106(21), b=15.871(8), c=15.748(7) Å, β=93.29(5)°, Z=4 (including 12 metal atoms in a unit cell). There are three kinds of crystallographically independent metal atoms, Nd(1), Nd(2), and Nd(3): Nd(1) and Nd(3) are ennea-coordinated (approximately tricapped trigonal-prism geometry), and Nd(2) is deca-coordinated (approximately bicapped square-antiprism geometry) including a slightly long M–O bonding. All dmso molecules are directly coordinated to the metal atoms as unidentate, while all the carboxylate ions bridge metal atoms acting as bidentate or tridentate ligands. The bridging atoms are arranged in a chain which is approximately formed along the [101] axis. Also, the isomorphous lanthanum(III) and praseodymium(III) complexes were obtained and their structures were elucidated.

The variety of polymeric structures as well as the high coordination numbers of the metal atoms are characteristic of carboxylato complexes of lanthanoids.[1-10] Among them, the structures of the hydrated chloroacetates of more than half the lanthanoids and yttrium, as well as of the scandium salt (anhydride) have been reported in previous papers.[1-3] The light lanthanoids (La—Eu), the heavy lanthanoids (Gd—Yb) and yttrium, and the scandium salts have the respective types of chain structures.

It is well-known that many transition metals can form Lewis base adducts of their salts. Many of them are mixed complexes in which Lewis base molecules are also directly coordinated to the metal atoms; however, in the other adducts, the base molecules are not bonded to the metal atoms directly. In cases of lanthanoid complexes, although a great variety of adducts have already been synthesized,[11-16] only a few reports have so far been published concerning their structures.

On the line of our structural research concerning the lanthanoid(III) carboxylates, we could synthesize the dimethyl sulfoxide (dmso) adducts of some lanthanoid(III) chloroacetates, which did not include water.

It is interesting to compare their structures with those of the hydrated salts, which have already been elucidated, as well as of other carboxylates. Therefore, the authors have tried to determine the structures of the title complexes by the single-crystal X-ray diffraction method.

Experimental

Synthesis of the [Enneakis(chloroacetato)tetrakis(dimethyl sulfoxide)trineodymium(III)], $[Nd_3(ClCH_2CO_2)_9\{(CH_3)_2SO\}_4]$, and its Isomorphous Complexes. The hydrated neodymium(III) chloroacetate, $Nd(ClCH_2CO_2)_3\cdot 5/3H_2O$ (0.90 g, 2.5 mmol)[1] were dissolved into ethanol (10 cm³), then dmso (0.40 g, 5.1 mmol) as well as benzene (10 cm³) were added to it. The solution was evaporated off by a vacuum rotary evaporator at about 80 °C. To the gummy residue, 15 cm³ of the ethanol–benzene mixture (1:1=v/v) was added and was evaporated once more in the same way. The residue was dissolved into 10 cm³ of methanol, and left standing in a desiccator over silica gel until about two-thirds of the solvent was evaporated off. The deposited crystals were separated, washed with a small portion of methanol, and dried in a silica gel desiccator. Yield, 0.9 g (6.7 mmol, 68%). By the same method, the isomorphous praseodymium(III) and lanthanum(III) mixed complexes were obtained (the yields of the lanthanum and praseodymium complexes were, 1.1 g (2.1 mmol, 75%) and 1.8 g (3.4 mmol, 85%), starting at 1.0 g (2.8 mmol) and 1.4 g (4.0 mmol) of the respective hydrated salts).

Analyses of the complexes (the calculated values were obtained assuming the formula of $M_3C_{26}H_{42}O_{22}Cl_9S_4$): M=Nd, Found, Nd, 27.36; C, 19.40; H, 2.59%. Calcd, Nd, 27.27; C, 19.68; H, 2.67%. M=La, Found, La, 26.70; C, 19.70; H, 2.59%. Calcd, La, 26.53; C, 19.88; H, 2.70%. M=Pr, Found, Pr, 26.68; C, 19.77; H, 2.68%. Calcd, Pr, 26.81; C, 19.81; H, 2.69%.

Single Crystal X-Ray Structure Analysis. Their crystallographic data are shown in Table 1, together with some experimental conditions regarding the collection of intensity data. The reflections were collected on a Rigaku AFC-6A automated 4-circle X-ray diffractometer with graphite-monochromated Mo $K\alpha$ radiation (λ=0.71073 Å; scan speed, 4° min^{-1} (θ)). During the preliminary intensity data-collection process, since some (though only a few) peaks were found to overlap partially with the vicinal ones, the ω-scan technique was used.

Structure Determination. The structure of the neodymium(III) complex was solved by the heavy-atom method. The positions of metal and some chlorine atoms were deduced from a three-dimensional Patterson map, while all the other non-hydrogen atoms were located by means of successive Fourier syntheses, and refined by a block-diagonal least-squares method. In the last-cycle of the

Table 1. Crystallographic Data and Some Experimental Conditions to Obtain Their Intensity Data of Lanthanum(III), Praseodymium(III), and Neodymium(III) Chloroacetate Dimethyl Sulfoxide, $[M_3(ClCH_2CO_2)_9\{(CH_3)_2SO\}_4]$ Monoclinic; Space Group, $P2_1/n$

	La	Pr	Nd
F. W.	1570.66	1576.65	1586.65
$a(l/Å)$	21.169(12)	21.125(14)	21.106(21)
$b(l/Å)$	15.965(8)	15.888(7)	15.871(8)
$c(l/Å)$	15.885(6)	15.788(5)	15.748(7)
$\beta(\phi/°)$	93.12(4)	93.27(4)	93.29(5)
$U(v/Å^3)$	5361(5)	5290(5)	5267(8)
Z	4	4	4
$D_m(d/g\,cm^{-3})$	1.96(3)	1.97(3)	1.98(3)
$D_x(d/g\,cm^{-3})$	1.95	1.98	2.00
μ(Mo $K\alpha$)(n/cm^{-1})	30.4	33.8	36.0
Number of reflection measured	9882	7372	10513
Reflections used for the calculation[a]	7757	5093	7155
Measured range $(2\theta/°)$	3—50	3—45	3—50
Scan width $(\theta/°)$	1.08	1.03	1.00
Size of the crystal (v/mm^3)	0.28×0.25×0.22	0.30×0.27×0.15	0.35×0.30×0.20
R[b]	0.057	0.061	0.048

a) Reflections with $|F_o|>3\sigma(|F_o|)$ were used. b) $R=\sum||F_o|-|F_c||/\sum|F_o|$.

Table 2. Final Atomic Coordinates ($\times10^4$) of the Non-Hydrogen Atoms and Their Equivalent Isotropic Temperature Factors of the Neodymium(III) Complex (Estimated Standard Deviations in Parentheses)

Atom	x	y	z	$B_{eq}/Å^2$[a]	Atom	x	y	z	$B_{eq}/Å^2$[a]
Nd(1)	2989.5(2)	7627.6(3)	163.2(3)	2.1_5	O(31)	4916(3)	6490(4)	629(4)	3.9_9
Nd(2)	6426.2(2)	7109.1(3)	3137.0(3)	2.3_2	O(32)	4202(3)	7452(4)	249(4)	2.9_5
Nd(3)	4617.8(2)	7459.0(3)	1821.1(3)	2.2_0	O(33)	3813(3)	6371(4)	1786(4)	3.5_8
S(1)	2240(1)	7800(2)	2127(2)	3.9_6	O(34)	3252(3)	6177(4)	566(4)	3.4_3
S(2)	6837(2)	5677(2)	1483(2)	5.1_0	O(35)	4371(3)	8986(4)	1773(5)	3.7_1
S(3)	4343(1)	8020(2)	4001(2)	4.1_5	O(36)	3534(3)	8219(4)	1479(4)	2.7_0
S(4)	3694(2)	9228(2)	−1094(2)	4.7_6	C(1)	2455(6)	7150(8)	3031(7)	5.1_5
Cl(11)	6846(2)	4442(3)	5692(3)	9.7_7	C(2)	1390(6)	7779(10)	2172(9)	6.2_7
Cl(12)	8164(2)	7858(5)	1286(3)	12.9_9	C(3)	7365(6)	4799(8)	1465(9)	6.1_6
Cl(13)	5616(2)	9090(3)	5570(2)	6.9_8	C(4)	6126(5)	5171(9)	1105(8)	5.7_9
Cl(21)	4975(3)	4445(4)	3858(4)	16.1_1	C(5)	3610(7)	8370(11)	4409(8)	7.3_9
Cl(22)	6103(2)	8362(2)	−602(2)	6.7_8	C(6)	4568(6)	7221(9)	4785(7)	5.4_5
Cl(23)	5865(2)	10455(2)	3317(2)	4.9_7	C(7)	4433(7)	9698(10)	−792(11)	7.4_4
Cl(31)	5321(2)	6089(3)	−1071(2)	7.7_9	C(8)	3222(7)	10148(9)	−1327(9)	6.5_5
Cl(32)	2875(2)	4424(2)	931(2)	6.4_4	C(11)	7037(4)	5930(6)	4879(6)	2.8_0
Cl(33)	3609(3)	10312(3)	2540(3)	10.2_0	C(12)	6664(6)	5104(7)	4811(7)	5.2_5
O(1)	2366(3)	7237(4)	1378(4)	3.8_0	C(13)	8026(4)	7645(6)	2988(5)	2.9_3
O(2)	6739(4)	5825(5)	2427(4)	4.3_4	C(14)	8518(6)	7786(12)	2325(7)	7.2_2
O(3)	4134(3)	7535(5)	3205(4)	3.9_4	C(15)	6506(4)	8191(6)	4756(5)	3.0_0
O(4)	3449(3)	8931(4)	−265(4)	3.5_3	C(16)	6410(5)	8967(7)	5295(7)	4.1_5
O(11)	7287(3)	6182(5)	5566(4)	3.8_4	C(21)	5291(5)	5922(6)	3146(6)	3.2_1
O(12)	7082(3)	6327(4)	4194(4)	3.1_6	C(22)	4805(6)	5223(8)	3117(9)	6.0_5
O(13)	8266(3)	7722(4)	3724(4)	3.5_1	C(23)	5992(4)	7732(6)	1026(6)	2.9_3
O(14)	7469(3)	7474(5)	2777(4)	4.0_9	C(24)	6399(5)	7726(8)	259(7)	4.9_2
O(15)	7072(3)	8095(4)	4553(4)	3.3_1	C(25)	5744(4)	8756(6)	2996(5)	2.6_1
O(16)	6072(3)	7721(4)	4498(4)	3.2_0	C(26)	5380(4)	9535(6)	3199(7)	3.5_3
O(21)	5702(3)	6028(5)	3733(4)	4.0_6	C(31)	4622(4)	6901(6)	76(6)	2.9_4
O(22)	5264(3)	6386(4)	2515(4)	3.9_9	C(32)	4727(5)	6839(8)	−869(7)	4.8_2
O(23)	6250(4)	7346(5)	1645(4)	4.6_4	C(33)	3462(4)	5960(6)	1281(6)	2.8_5
O(24)	5471(3)	8083(5)	993(4)	3.6_3	C(34)	3270(6)	5109(8)	1670(8)	5.4_9
O(25)	6322(3)	8729(4)	3009(4)	3.1_7	C(35)	3795(4)	8918(6)	1635(5)	2.7_4
O(26)	5408(3)	8098(4)	2880(4)	2.8_3	C(36)	3357(5)	9682(7)	1673(7)	4.4_0

a) The equivalent isotropic temperature factors were computed using the following expression: $B_{eq}=4/3(B_{11}a^2+B_{22}b^2+B_{33}c^2+B_{13}ac\cos\beta)$. The B_{ij}'s are defined by: $T=\exp[-(h^2B_{11}+k^2B_{22}+l^2B_{33}+2hlB_{13}+2klB_{23}+2hkB_{12})]$.

refinement with anisotropic temperature factors for all the non-hydrogen atoms, all the parameter-shifts were less than one-third of the corresponding standard deviations. All hydrogen atoms were excluded from the structure factor calculations. The structures of the isomorphous complexes were solved by starting with the final parameters of the neodymium(III) complex, and were refined in the same way. All of their parameters converged within one-third of the respective standard deviations, too.

Some chlorine atoms of the ligands were found to have relatively large thermal parameters, and some Cl–C bond lengths were a little shorter than the sum of the Pauling's covalent bonding radii (1.76 Å),[17] although the average of the all Cl–C bond lengths of all the three complexes is not short, 1.76 Å. We tried to divide the positions of some such chlorine atoms into disordered structures, but failed. Probably their large temperature factors are due to their low positional restrictions: no atoms are very near such chroline atoms in the crystal. Such a phenomenon has also been found in other lanthanoid complexes, about the atoms in the tail part of the coordinating ligands.[18,19]

All the calculations were carried out on a HITAC M-682H apparatus at the Computer Center of the University of Tokyo, using the local version of the UNICS program.[20] The atomic scattering factors are taken from Ref. 21.

Infrared Spectrum Measurements. Their infrared spectra were obtained by means of a JASCO A202 grating infrared spectrophotometer, using liquid paraffin or hexachloro-1,3-butadiene mull.

Results and Discussion

The final atomic parameters of the neodymium(III) complex are listed in Table 2, while selected bond lengths and bond angles as well as some inter-metal-atomic distances are tabulated in Table 3.[22] The perspective drawing of the neodymium(III) complex around the metal atoms (Nd(1), Nd(2), and Nd(3)), as well as the numbering scheme of the atoms are shown in Figs. 1—3, and the projection of the unit cell to the ac-plane in Fig. 4, respectively.

The Nd(1) and Nd(3) atoms are ennea-coordinated being approximately in a tricapped trigonal-prism geometry, while the Nd(2) atom is deca-coordinated being approximately in a cis-bicapped square-antiprism geometry;[24] however, Nd(2)–O(15) (2.988(8) Å) is a little longer than the other Nd–O bonds. The averages of the Nd–O bond lengths, together with those of the other isomorphous complexes are summarized in Table 4. The average Nd–O bond lengths around Nd(1) and Nd(3) atoms (2.513 and 2.499 Å) are not much different from each other, and they are approximately the same as the sum of the Shannon's ionic radii, 2.51 Å (where the coordination number of the Nd atoms is 9).[25] The Nd(1,3)–O(dmso)$_{av.}$ (from now on, "av." means the average of the values) is

Table 3. Selected Bond Lengths and Bond Angles of the Neodymium Complex, with the Standard Deviations in Parentheses

Bond length	(l/Å)	Bond length	(l/Å)
Nd(1)–O(1)	2.461(9)	Nd(1)–O(4)	2.399(7)
Nd(1)–O(32)	2.570(6)	Nd(1)–O(34)	2.444(7)
Nd(1)–O(36)	2.495(8)	Nd(1)–O(11^{i})[a]	2.506(7)
Nd(1)–O(12^{i})	2.901(6)	Nd(1)–O(13^{i})	2.437(9)
Nd(1)–O(15^{i})	2.403(7)	Nd(2)–O(2)	2.434(8)
Nd(2)–O(12)	2.442(7)	Nd(2)–O(14)	2.376(8)
Nd(2)–O(15)	2.988(8)	Nd(2)–O(16)	2.505(9)
Nd(2)–O(21)	2.515(8)	Nd(2)–O(22)	2.832(8)
Nd(2)–O(23)	2.387(10)	Nd(2)–O(25)	2.588(7)
Nd(2)–O(26)	2.673(6)	Nd(3)–O(3)	2.462(10)
Nd(3)–O(22)	2.405(7)	Nd(3)–O(24)	2.489(8)
Nd(3)–O(26)	2.505(7)	Nd(3)–O(31)	2.534(9)
Nd(3)–O(32)	2.579(8)	Nd(3)–O(33)	2.420(7)
Nd(3)–O(35)	2.479(7)	Nd(3)–O(36)	2.614(6)
M(1)···M(3)	4.203(3)	M(3)···M(2)	4.274(4)
M(1)···M(2^{i})	4.476(3)		
Bond angle	**(ϕ/°)**	**Bond angle**	**(ϕ/°)**
Nd(1)–O(11^{i})–C(11^{i})	104.5(7)	Nd(1)–O(12^{i})–C(11^{i})	85.1(7)
Nd(2)–O(12)–C(11)	140.5(7)	Nd(1)–O(13^{i})–C(13^{i})	137.5(8)
Nd(2)–O(14)–C(13)	150.6(7)	Nd(1)–O(15^{i})–C(15^{i})	135.0(7)
Nd(2)–O(15)–C(15)	81.7(6)	Nd(2)–O(16)–C(15)	105.3(6)
Nd(2)–O(21)–C(21)	103.2(7)	Nd(2)–O(22)–C(21)	87.9(7)
Nd(3)–O(22)–C(21)	141.9(7)	Nd(2)–O(23)–C(23)	151.8(9)
Nd(3)–O(24)–C(23)	118.0(7)	Nd(2)–O(25)–C(25)	96.6(5)
Nd(2)–O(26)–C(25)	91.4(5)	Nd(3)–O(26)–C(25)	140.8(7)
Nd(3)–O(31)–C(31)	93.8(7)	Nd(1)–O(32)–C(31)	139.4(6)
Nd(3)–O(32)–C(31)	90.3(6)	Nd(3)–O(33)–C(33)	141.4(7)
Nd(1)–O(34)–C(33)	124.3(7)	Nd(3)–O(35)–C(35)	97.1(5)
Nd(1)–O(36)–C(35)	132.1(7)	Nd(3)–O(36)–C(35)	89.9(5)

a) Key to the symmetry operation: $-0.5+x$, $1.5-y$, $-0.5+z$.

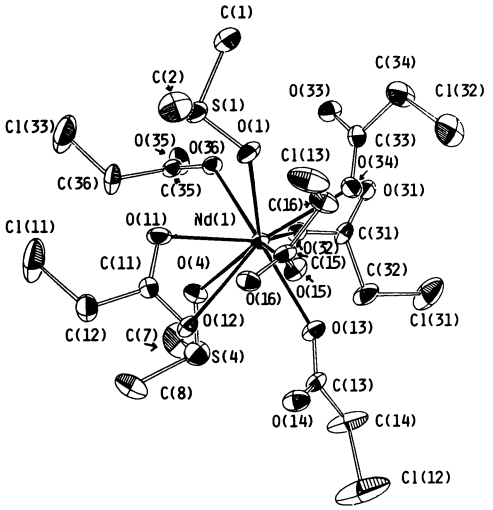

Fig. 1. A perspective drawing of the neodymium(III) complex around the Nd(1) atom. Here the atoms of the acidato ligands including Cl(11), Cl(12), and Cl(13) are the ones symmetry operated by $-0.5+x$, $1.5-y$, $-0.5+z$.

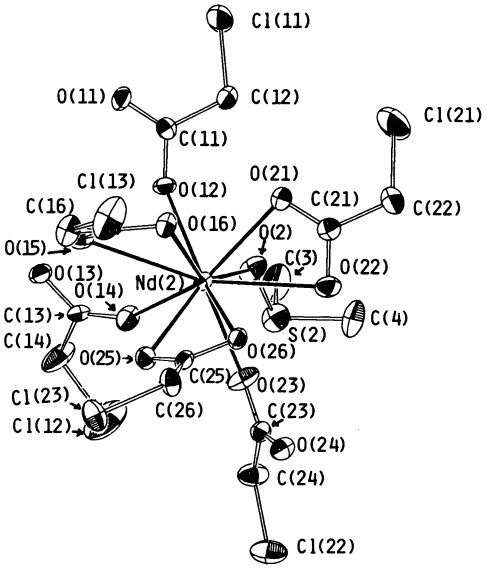

Fig. 2. A perspective drawing of the neodymium(III) complex around the Nd(2) atom.

Table 4. Comparison of the M–O Bondings of the Complexes (l/Å)

M=	La	Pr	Nd
M(1)-O(all)$_{av.}$[a]	2.562	2.526	2.513
M(3)-O(all)$_{av.}$	2.556	2.515	2.499
M(2)-O(all except 15)$_{av.}$	2.586	2.540	2.528
M(2)-O(all)$_{av.}$	2.618	2.584	2.574
M(1,3)-O(dmso)$_{av.}$	2.486	2.457	2.441
M(1,3)-O(acid)$_{av.}$	2.573	2.534	2.519
M(2)-O(acid)$_{av.}$	2.632	2.601	2.590
Sum of Shannon's ionic radii[b]			
M(IX)-O(II)	2.57	2.53	2.51
M(X)-O(II)	2.62	(2.58)	(2.56)

a) av. means the average of the M–O bond lengths between the metal atom and the group of coordinating oxygen atoms. b) See Ref. 25. II, X, IX means their coordination number.

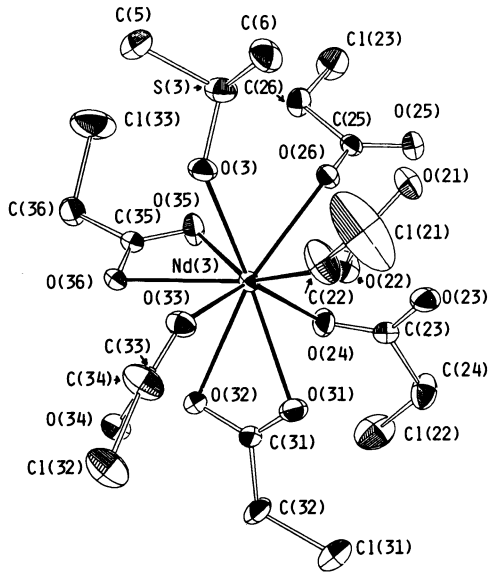

Fig. 3. A perspective drawing of the neodymium(III) complex around the Nd(3) atom.

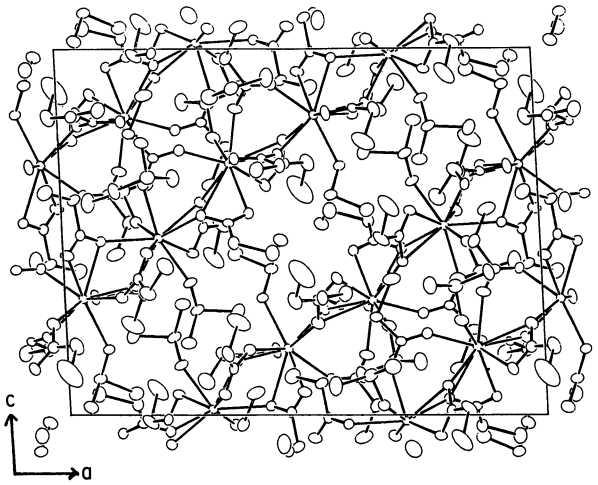

Fig. 4. A projection of the unit-cell to the ac-plane.

2.441 Å, which is shorter than the Nd(1,3)-O(acid)$_{av.}$, 2.519 Å. Therefore, in these complexes, the former bonds are likely to be stronger than the latter ones.

The average of all ten Nd–O bond lengths around the Nd(2) atom is 2.574 Å, which is longer than the sum of the Shannon's ionic radii, 2.56 Å (the coordination number of the Nd atom is 10).[25] Even when the longest bond, Nd(2)–O(15), is rejected, the average of the other nine bond lengths is 2.528 Å, which is longer than the average Nd–O bond lengths around the ennea-coordinated Nd(1) or Nd(3) atoms. Therefore, atom O(15) should be regarded as the ligating atom, or at least, it also affects the coordination geometry around the Nd(2) atom. The Nd-(2)–O(2) (dmso oxygen atom) is 2.434 Å, which is much shorter than the Nd(2)–O(acid)$_{av.}$, 2.590 Å. Consequently, the Nd–O(dmso) bond is stronger than the

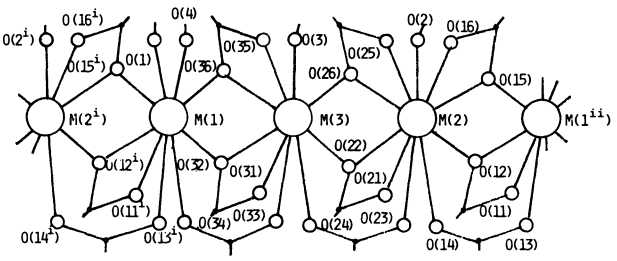

Fig. 5. A schematic presentation of the bridgings between the metal atoms.[23]

Nd–O(acid) bonds around the deca-coordinated Nd(2) atom, too.

The metal atoms are arranged approximately along the [101] axis in the order of Nd(1^{ii}), Nd(2), Nd(3), Nd(1), Nd(2^{i})…,[23] as shown schematically in Fig. 5. The interatomic distance is 4.317 Å (on the average); this is shorter than the average inter-metal-atomic distance of the chain in the hydrated neodymium chloroacetate, 4.435 Å.[1]

It is very interesting that this dmso adduct has an average M…M′ distance of the complex chain shorter than that of the hydrate, though the dmso adduct has a larger unit-cell, and smaller density (5267(8) Å^3 and 2.00 g cm^{-3} for the dmso adduct, and 3986(2) Å^3 and 2.27 g cm^{-3} for the hydrate). Moreover, since the Nd–O(dmso)$_{av.}$ lengths are shorter than the Nd–O(acid)$_{av.}$ lengths in the dmso adduct, while the Nd–O(water)$_{av.}$ lengths are about the same as the Nd–O(acid)$_{av.}$ lengths in the hydrate, the approaching dmso ligands in this adduct are expected to prevent any approaching of neighboring complexes in the linear polymer: however this expectation did not prove to be correct.

Probably, the dmso methyl groups in this adduct, which are non-polar and are intercalated between complex chains, act to pack the chain in the limited space between the hydrophobic layers of the hydrocarbon groups: the inter-chain separations are kept large, but the inter-metal atomic distances in the chains are shortened.

The bridging structure, the numbers and the types of the bridging carboxylate ions between respective neighboring metal atoms in the chain of the title dmso adduct, is much different from that of the hydrated salt of the same metal;[1] this type of chain structure has not yet been found in any other linear polymeric chains of the other lanthanoid carboxylates. In the titled complex, all the pairs of the neighboring metal atoms are bridged by three carboxylate ions respectively: one in bidentate (approximately in the *Z,Z*-type, but some of them are quite deformed), and two in the tridentate types.[26] In some deformed bidentate bridges between Nd(1) and Nd(3), as well as Nd(3) and Nd(2), one of the C–O–M angles in very small, only about 110—125°, and some atomic positions are much deviated from the mean-square plane of the MOCO′M′ bridging. All the tridentate bridges of these complexes are also more or less deformed from the ideal form (here the ideal form means the bridge, where the three metal-oxygen bondings, M–O, M–O′, and M′–O′, are about the same in their lengths, and the bond angles of M–O–C as well as M–O′–C are about the same (95—100°), while that of M′–O′–C is larger (150—160°)).[26]

Although there are no fundamental differences between their structures, the isomorphous lanthanum(III) and praseodymium(III) complexes have larger unit cells than the neodymium(III) complex: their cell dimensions decrease depending on the atomic number of the central metal atom. The decrease of the cell-volume is mainly caused by packing the coordination sphere around the central metal atom: the M–O bond lengths decrease. Therefore, as shown in Table 4, almost all M–O bond lengths are generally shorter in a higher atomic number metal complex, although the lengths of some weak bonds, such as M(1)–O(15) and M(1)–O(12^{i}), rather increase with the metal atomic number.

The infrared spectra of these complexes were examined, but there are almost no differences between them. The ν_{as}(COO) and ν_{s}(COO) peaks appear as the respective doublets of the maximum wavenumbers of 1598, 1573 cm^{-1}, and of 1418, 1402 cm^{-1}, respectively. In the spectra of the hydrated chloroacetates of lanthanum(III), and neodymium(III), these bands appear at about 1580 and 1415—1420 cm^{-1}, respectively. Therefore, these peak maximum wavenumbers of both types of complexes are not much different from each other.

The ν(SO) band of the titled complexes appear at about 1000 cm^{-1} as a sharp strong peak, while the band of free dmso appears at about 1050 cm^{-1} as a broad band: the peak of the complexes is much red-shifted. This fact corresponds with the strong M–O(dmso) bond in the complexes, as was expected from the results of the X-ray structure analysis.

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23) Key to the symmetry operations: i, $-0.5+x$, $1.5-y$, $-0.5+z$; ii, $0.5+x$, $1.5-y$, $0.5+z$.
24) Around the Nd(1) atom, O(1), O(12^{i}), O(15^{i}), and O(4), O(32), O(36) atoms are at the apexes of the both side triangles of the prism, respectively, while around the Nd(3) atom, O(22), O(24), O(26), and O(32), O(33), O(36) atoms are at the respective apex positions of the both triangles. Around the Nd(2) atom, O(2), O(14), O(25), O(22), and O(12), O(15), O(16), and O(21) are at the apexes of the respective squares, while O(23) (over the former square) and O(26) (over the O(16), O(21), O(22), O(25) side face) are at the cap positions. Around the Nd(2) atom, when the O(15) atom is not regarded, tricapped trigonal-prism geometry can be assumed, where O(16), O(25), O(26), and O(2), O(16), O(22) are at the apexes of the both side triangles of the prism, respectively, while O(14), O(16), and O(22) are at the cap positions.
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