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# Nd$(CO_3)$(OH) from single-crystal data

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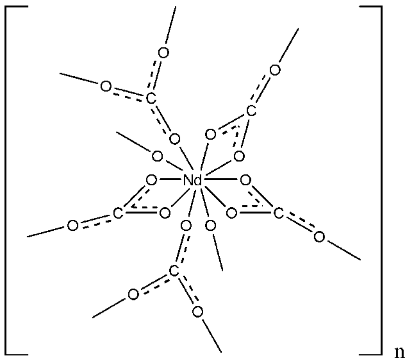
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(O–C) = 0.005 Å; $R$ factor = 0.020; $wR$ factor = 0.050; data-to-parameter ratio = 11.2.

The title compound, poly[$\mu$-hydroxido-$\mu$-carbonato-neodymium], $[Nd(CO_3)(OH)]_n$, has a three-dimensional framework structure assembled from $NdO_{10}$ polyhedra and $CO_3^{2-}$ groups. The Nd atom is coordinated by eight O atoms from $CO_3^{2-}$ groups and two OH anions, while the C atom is coordinated by three O atoms. Nd, two O atoms and C are located on mirror planes.

## Related literature

For an earlier structure determination of the title compound from powder data, see: Dexpert & Caro (1973). For a high-temperature modification, see: Christensen (1973). For similar framework materials, see: Li *et al.* (1998); Lin *et al.* (2003); Plévert *et al.* (2001); Xu, Fan, Chino *et al.* (2004); Xu, Fan, Elangovan *et al.* (2004); Xu, Cheng & You (2006); Xu, Ding *et al.* (2006). For related literature, see: Abrahams *et al.* (2004); Gier *et al.* (1996).



## Experimental

### *Crystal data*

$[Nd(CO_3)(OH)]$
$M_r$ = 221.26
Orthorhombic, *Pnma*
$a$ = 7.231 (5) Å
$b$ = 4.964 (4) Å
$c$ = 8.489 (6) Å
$V$ = 304.7 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 16.86 mm$^{-1}$
$T$ = 293 (2) K
0.08 × 0.08 × 0.06 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min}$ = 0.346, $T_{max}$ = 0.431 (expected range = 0.292–0.364)
1730 measured reflections
424 independent reflections
399 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.050
$S$ = 1.07
424 reflections
38 parameters
1 restraint
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 1.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.09 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Nd1—O2$^{i}$ | 2.346 (4) | Nd1—O1$^{i}$ | 2.587 (3) |
| Nd1—O2 | 2.353 (4) | Nd1—O1$^{ii}$ | 2.616 (4) |
| Nd1—O3 | 2.535 (2) | Nd1—O1 | 2.750 (3) |

Symmetry codes: (i) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 1997*a*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2039).

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# supplementary materials

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# Nd($CO_3$)(OH) from single-crystal data

**W.-J. Feng, G.-P. Zhou, Z.-B. Liu and Y. Xu**

## Comment

Recently, the synthesis of three dimensional frameworks with new topological structures has received great attention, due to their functional applications in catalysis, adsorption, ion-exchange, and radioactive waste remediation. As the building elements of open-frameworks, not only silicon, but germanium and carbon have been choosen to synthesize new open-frameworks (Li *et al.*, 1998; Lin *et al.*, 2003; Plévert *et al.*, 2001; Xu, Fan, Chino *et al.*, 2004; Xu, Fan, Elangovan *et al.*, 2004; Xu, Cheng & You, 2006; Xu, Ding *et al.*,2006). In the last few years, an important advance in porous materials has been achieved by the study of transition metal carbonates. The diamond-type $Na_2Zn_3(CO_3)_4{\cdot}3H_2O$ was reported by Gier *et al.* (1996), while the face-centered (FC) cubic $[Zn_6(CO_3)_{12}(CH_6N_3)_8Na_3[N(CH_3)_4]{\cdot}2H_2O$ was synthesized by Abrahams *et al.* (2004). Compared with other transition metals, the rare-earth elements adopt a large range of coordination numbers. The structure of title compound has been determined by powder diffraction (Dexpert & Caro, 1973). Even a hexagonal high-temperature modification is known (Christensen, 1973). In this work, we synthesized the title compound as single crystals suitable for a structure determination.

The structure features a three-dimensional framework constructed from $NdO_{10}$ polyhedra and carbonates. As in the previously reported Sm($CO_3$)(OH), the asymmetric unit of the title compound contains five independent non-H atoms, and all of them belong to the inorganic framework (Fig. 1). The Nd atom is coordinated by ten O atoms from $CO_3^{2-}$ and $OH^-$ anions. The C atom is coordinated by three O atoms with C—O distances ranging from 1.269 (7) to 1.289 (4) Å and angles ranging from 119.4 (5) to 120.2 (2)°. Each C atom makes eight C—O—Nd linkages through bridging O atoms. While each $OH^-$ group acts as a $\mu_2$-bridging ligang linking two Nd atoms to generate a $[Nd—O]_n$ chain. Furthermore, the $[Nd—O]_n$ chains are connected by $CO_3^{2-}$ anions to form a three-dimensional inorganic framework, as shown in Fig. 2. The Nd atom has the typical geometrical parameters, with Nd—O distances in the range 2.346 (4)–2.750 (3) Å. The O—Nd—O angles are between 49.2 (1) and 156.6 (2)°. These bond distances and angles are in agreement with those found in the reported rare-earth compounds (Xu, Ding *et al.*, 2006). The O—H anions are involved in hydrogen bonding with each other; the shortest O···O distance is 3.107 (4)Å and the O—H···O angle is 154 (7)°.

## Experimental

Purple block-shaped crystals were hydrothermally synthesized from a mixture of $Nd(NO_3)_3$ (99%, Shanghai Reagent Company), $Cu(NO_3)_2$ (99.5%, Tianjin Bodi Reagent Company), $HCO_2H$ (88%, Tianjin Taixing Reagent factory), $H_2O$, tetraethylammoniumhydroxide (10%, Beijing chemical factory), and guanidine nitrate (98%, Shanghai Reagent Company). In a typical synthesis, $Nd(NO_3)_3$ (0.3464 g), $Cu(NO_3)_2$ (0.0525 g), guanidine nitrate (0.7882 g) were dissolved in the solvent of water (8.0 g) followed by the addition of $HCO_2H$ (0.7169 g) and tetraethylammoniumhydroxide (0.7131 g) with constant stirring. Finally, the mixture was kept in a 25 ml Teflon-lined steel autoclave at 180 °C for 7 days. The autoclave was slowly cooled to room temperature, and then the product was filtered, washed with distilled water, and dried at room temperature. Purple block-shaped crystals of title compound were obtained.

## Refinement

The highest peak in the difference map is 1.17 e/Å$^3$, and 0.85 (2) Å from $Nd_1$, while the minimum peak is 0.77 (2) Å from $Nd_1$. The H atom was located from the Fourier map.

## Figures

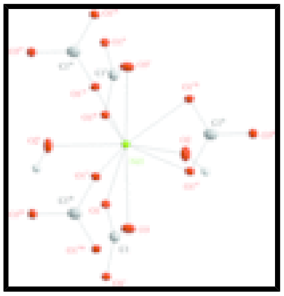

Fig. 1. The coordination of Nd in the title compound. Displacement ellipsoids at the 70% probability level. [Symmetry codes: (i) 1/2 + *x*, *y*, −3/2 − *z*; (ii) *x*, *y* + 1, *z*; (iii) 1/2 + *x*, 1/2 − *y*, 3/2 − *z*; (iv) 1/2, 1/2 + *y*, 1/2 + *z*; (v) 1/2 − *x*, −*y*, 1/2 + *z*; (vi) *x*, 1/2 − *y*, *z*; (vii) 1/2 + *x*, −1/2 − *y*, 3/2 − *z*; (viii) 1/2 + *x*, 1 + *y*, 3/2 − *z*); (ix) 1/2 + *x*, *y*, 3/2 − *z*; (*x*) *x*, −1/2 − *y*, *z*.

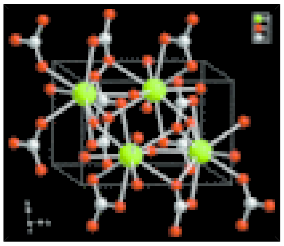

Fig. 2. Threedimensional open framework with 6-membered ring channels viewed along *b* axis.

## poly[μ-hydroxido-μ-carbonato-neodymium]

### *Crystal data*

$[Nd(CO_3)(OH)]$

$M_r = 221.26$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 7.231$ (5) Å

$b = 4.964$ (4) Å

$c = 8.489$ (6) Å

$V = 304.7$ (4) Å$^3$

$Z = 4$

$F_{000} = 396$

$D_x = 4.823$ Mg m$^{-3}$

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 1700 reflections

θ = 3.7–27.0º

μ = 16.86 mm$^{-1}$

$T = 293$ (2) K

Block, pink

0.08 × 0.08 × 0.06 mm

### *Data collection*

Bruker APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2)$ K

424 independent reflections

399 reflections with $I > 2\sigma(I)$

$R_{int} = 0.027$

$\theta_{max} = 28.7$º

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

$T_{\min} = 0.346$, $T_{\max} = 0.431$

1730 measured reflections

$\theta_{\min} = 3.7°$

$h = -3 \rightarrow 9$

$k = -6 \rightarrow 6$

$l = -10 \rightarrow 11$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.050$

$S = 1.07$

424 reflections

38 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 0.2734P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.015$

$\Delta\rho_{\max} = 1.17$ e Å$^{-3}$

$\Delta\rho_{\min} = -1.09$ e Å$^{-3}$

Extinction correction: SHELXL97 (Sheldrick, 1997b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.040 (2)

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{\text{iso}}$*/$U_{\text{eq}}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Nd1 | 0.35584 (4) | 0.2500 | 0.83332 (3) | 0.00774 (18) | |
| O1 | 0.1525 (3) | −0.0258 (6) | 0.6121 (4) | 0.0095 (6) | |
| O2 | 0.0386 (6) | 0.2500 | 0.8949 (5) | 0.0144 (9) | |
| H1 | 0.000 (14) | 0.154 (15) | 0.970 (7) | 0.017* | 0.50 |
| O3 | 0.2941 (7) | −0.2500 | 0.8032 (5) | 0.0141 (9) | |
| C1 | 0.1960 (9) | −0.2500 | 0.6793 (6) | 0.0074 (11) | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Nd1 | 0.0073 (2) | 0.0066 (2) | 0.0093 (2) | 0.000 | 0.00035 (9) | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.0106 (14) | 0.0075 (15) | 0.0103 (14) | 0.0010 (10) | 0.0005 (10) | 0.0007 (13) |
| O2 | 0.010 (2) | 0.024 (2) | 0.0089 (19) | 0.000 | 0.0002 (16) | 0.000 |
| O3 | 0.021 (2) | 0.008 (2) | 0.0140 (19) | 0.000 | −0.0064 (18) | 0.000 |
| C1 | 0.007 (3) | 0.006 (3) | 0.009 (3) | 0.000 | 0.0028 (19) | 0.000 |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Nd1—O2$^{i}$ | 2.346 (4) | Nd1—C1 | 3.034 (4) |
| Nd1—O2 | 2.353 (4) | O1—C1 | 1.289 (4) |
| Nd1—O3 | 2.535 (2) | O1—Nd1$^{vii}$ | 2.587 (3) |
| Nd1—O3$^{ii}$ | 2.535 (2) | O1—Nd1$^{viii}$ | 2.616 (4) |
| Nd1—O1$^{iii}$ | 2.587 (3) | O2—Nd1$^{vii}$ | 2.346 (4) |
| Nd1—O1$^{i}$ | 2.587 (3) | O2—H1 | 0.84 (2) |
| Nd1—O1$^{iv}$ | 2.616 (4) | O3—C1 | 1.269 (7) |
| Nd1—O1$^{v}$ | 2.616 (4) | O3—Nd1$^{ix}$ | 2.535 (2) |
| Nd1—O1 | 2.750 (3) | C1—O1$^{x}$ | 1.289 (4) |
| Nd1—O1$^{vi}$ | 2.750 (3) | C1—Nd1$^{viii}$ | 2.961 (6) |
| Nd1—C1$^{v}$ | 2.961 (6) | C1—Nd1$^{ix}$ | 3.034 (4) |
| O2$^{i}$—Nd1—O2 | 137.14 (12) | O3—Nd1—C1$^{v}$ | 94.45 (10) |
| O2$^{i}$—Nd1—O3 | 90.92 (11) | O3$^{ii}$—Nd1—C1$^{v}$ | 94.45 (10) |
| O2—Nd1—O3 | 81.41 (12) | O1$^{iii}$—Nd1—C1$^{v}$ | 85.83 (13) |
| O2$^{i}$—Nd1—O3$^{ii}$ | 90.92 (11) | O1$^{i}$—Nd1—C1$^{v}$ | 85.83 (13) |
| O2—Nd1—O3$^{ii}$ | 81.41 (12) | O1$^{iv}$—Nd1—C1$^{v}$ | 25.80 (8) |
| O3—Nd1—O3$^{ii}$ | 156.6 (2) | O1$^{v}$—Nd1—C1$^{v}$ | 25.80 (8) |
| O2$^{i}$—Nd1—O1$^{iii}$ | 71.38 (12) | O1—Nd1—C1$^{v}$ | 127.56 (12) |
| O2—Nd1—O1$^{iii}$ | 140.24 (10) | O1$^{vi}$—Nd1—C1$^{v}$ | 127.56 (12) |
| O3—Nd1—O1$^{iii}$ | 133.04 (13) | O2$^{i}$—Nd1—C1 | 81.87 (12) |
| O3$^{ii}$—Nd1—O1$^{iii}$ | 69.26 (14) | O2—Nd1—C1 | 74.00 (13) |
| O2$^{i}$—Nd1—O1$^{i}$ | 71.38 (11) | O3—Nd1—C1 | 24.29 (13) |
| O2—Nd1—O1$^{i}$ | 140.24 (10) | O3$^{ii}$—Nd1—C1 | 133.66 (14) |
| O3—Nd1—O1$^{i}$ | 69.26 (14) | O1$^{iii}$—Nd1—C1 | 145.70 (13) |
| O3$^{ii}$—Nd1—O1$^{i}$ | 133.04 (13) | O1$^{i}$—Nd1—C1 | 87.72 (14) |
| O1$^{iii}$—Nd1—O1$^{i}$ | 63.92 (14) | O1$^{iv}$—Nd1—C1 | 136.82 (12) |
| O2$^{i}$—Nd1—O1$^{iv}$ | 139.50 (10) | O1$^{v}$—Nd1—C1 | 91.91 (12) |
| O2—Nd1—O1$^{iv}$ | 77.08 (11) | O1—Nd1—C1 | 25.14 (11) |
| O3—Nd1—O1$^{iv}$ | 120.24 (12) | O1$^{vi}$—Nd1—C1 | 84.79 (12) |
| O3$^{ii}$—Nd1—O1$^{iv}$ | 70.77 (12) | C1$^{v}$—Nd1—C1 | 112.29 (9) |
| O1$^{iii}$—Nd1—O1$^{iv}$ | 68.40 (10) | C1—O1—Nd1$^{vii}$ | 125.5 (3) |
| O1$^{i}$—Nd1—O1$^{iv}$ | 94.72 (7) | C1—O1—Nd1$^{viii}$ | 92.2 (3) |
| O2$^{i}$—Nd1—O1$^{v}$ | 139.50 (10) | Nd1$^{vii}$—O1—Nd1$^{viii}$ | 111.60 (10) |
| O2—Nd1—O1$^{v}$ | 77.08 (11) | C1—O1—Nd1 | 89.9 (3) |
| O3—Nd1—O1$^{v}$ | 70.77 (12) | Nd1$^{vii}$—O1—Nd1 | 93.30 (11) |

| | | | |
|---|---|---|---|
| O3$^{ii}$—Nd1—O1$^{v}$ | 120.24 (12) | Nd1$^{viii}$—O1—Nd1 | 147.34 (11) |
| O1$^{iii}$—Nd1—O1$^{v}$ | 94.72 (7) | Nd1$^{vii}$—O2—Nd1 | 111.45 (17) |
| O1$^{i}$—Nd1—O1$^{v}$ | 68.40 (10) | Nd1$^{vii}$—O2—H1 | 116 (7) |
| O1$^{iv}$—Nd1—O1$^{v}$ | 50.35 (15) | Nd1—O2—H1 | 119 (7) |
| O2$^{i}$—Nd1—O1 | 74.76 (12) | C1—O3—Nd1 | 100.49 (10) |
| O2—Nd1—O1 | 68.32 (11) | C1—O3—Nd1$^{ix}$ | 100.49 (10) |
| O3—Nd1—O1 | 49.42 (12) | Nd1—O3—Nd1$^{ix}$ | 156.6 (2) |
| O3$^{ii}$—Nd1—O1 | 108.93 (12) | O3—C1—O1$^{x}$ | 120.2 (3) |
| O1$^{iii}$—Nd1—O1 | 146.02 (6) | O3—C1—O1 | 120.2 (3) |
| O1$^{i}$—Nd1—O1 | 107.59 (12) | O1$^{x}$—C1—O1 | 119.4 (5) |
| O1$^{iv}$—Nd1—O1 | 144.81 (6) | O3—C1—Nd1$^{viii}$ | 153.3 (4) |
| O1$^{v}$—Nd1—O1 | 113.18 (5) | O1$^{x}$—C1—Nd1$^{viii}$ | 62.0 (2) |
| O2$^{i}$—Nd1—O1$^{vi}$ | 74.76 (12) | O1—C1—Nd1$^{viii}$ | 62.0 (2) |
| O2—Nd1—O1$^{vi}$ | 68.32 (11) | O3—C1—Nd1 | 55.22 (10) |
| O3—Nd1—O1$^{vi}$ | 108.93 (12) | O1$^{x}$—C1—Nd1 | 171.7 (4) |
| O3$^{ii}$—Nd1—O1$^{vi}$ | 49.42 (12) | O1—C1—Nd1 | 65.0 (2) |
| O1$^{iii}$—Nd1—O1$^{vi}$ | 107.59 (12) | Nd1$^{viii}$—C1—Nd1 | 118.41 (10) |
| O1$^{i}$—Nd1—O1$^{vi}$ | 146.02 (6) | O3—C1—Nd1$^{ix}$ | 55.22 (10) |
| O1$^{iv}$—Nd1—O1$^{vi}$ | 113.18 (5) | O1$^{x}$—C1—Nd1$^{ix}$ | 65.0 (2) |
| O1$^{v}$—Nd1—O1$^{vi}$ | 144.81 (6) | O1—C1—Nd1$^{ix}$ | 171.7 (4) |
| O1—Nd1—O1$^{vi}$ | 59.71 (14) | Nd1$^{viii}$—C1—Nd1$^{ix}$ | 118.41 (10) |
| O2$^{i}$—Nd1—C1$^{v}$ | 152.98 (16) | Nd1—C1—Nd1$^{ix}$ | 109.76 (19) |
| O2—Nd1—C1$^{v}$ | 69.88 (16) | | |

Symmetry codes: (i) *x*+1/2, *y*, −*z*+3/2; (ii) *x*, *y*+1, *z*; (iii) *x*+1/2, −*y*+1/2, −*z*+3/2; (iv) −*x*+1/2, *y*+1/2, *z*+1/2; (v) −*x*+1/2, −*y*, *z*+1/2; (vi) *x*, −*y*+1/2, *z*; (vii) *x*−1/2, *y*, −*z*+3/2; (viii) −*x*+1/2, −*y*, *z*−1/2; (ix) *x*, *y*−1, *z*; (x) *x*, −*y*−1/2, *z*.

Fig. 1

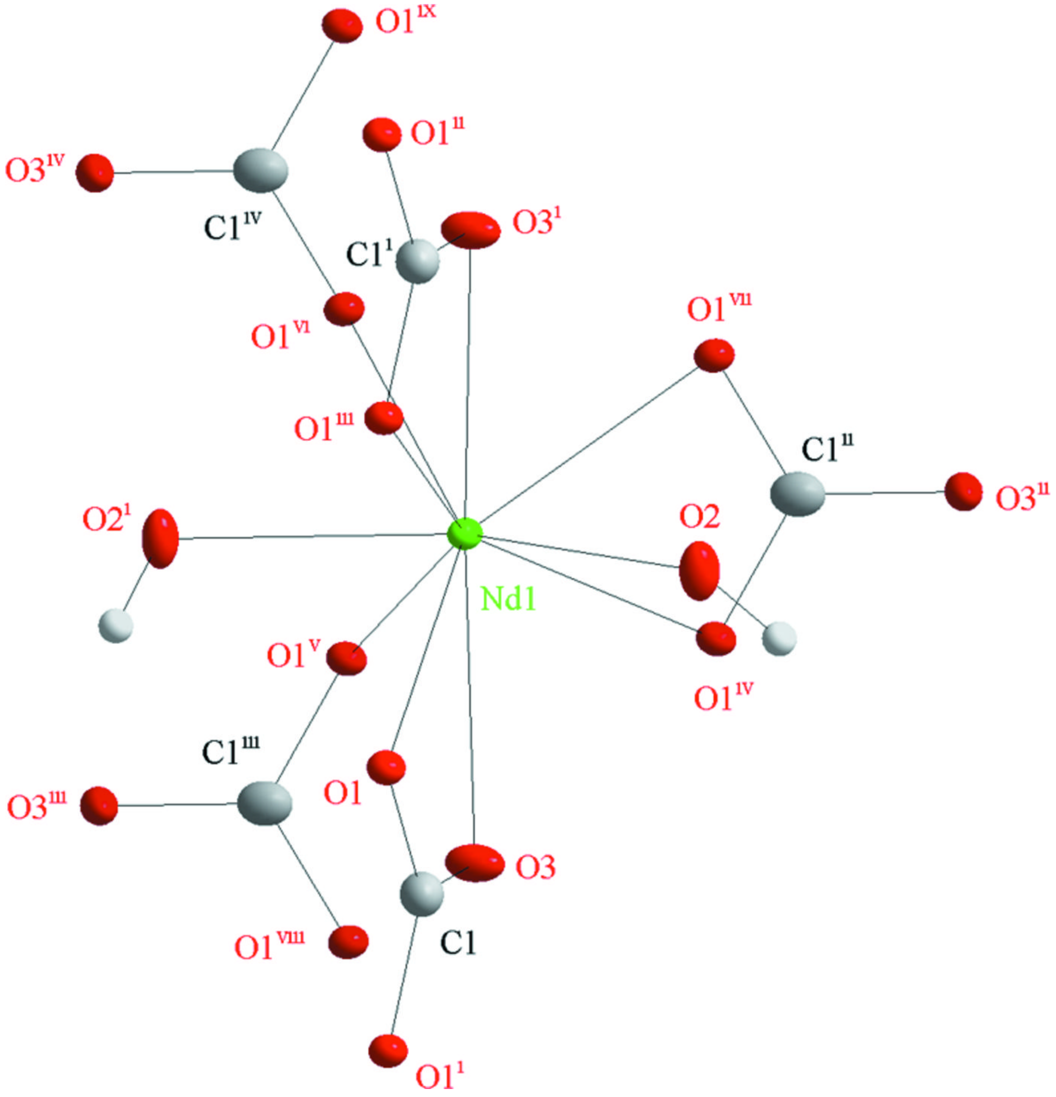
O1IX
O1II
O3IV
C1IV
O3I
C1I
O1VII
O1VI
O1III
C1II
O3II
O2I
O2
Nd1
O1V
O1IV
C1III
O1
O3III
O3
O1VIII
C1
O1I

**Fig. 2**