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# Poly[[aquaneodymium(III)]-$\mu_5$-citrato]

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.017 Å
$R$ factor = 0.046
$wR$ factor = 0.109
Data-to-parameter ratio = 11.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the title complex is composed of $Nd^{III}$ cations, citrate trianions and water molecules, and is formulated as $[Nd(C_6H_5O_7)(H_2O)]_n$, isostructural with the lanthanum analogue [Baggio & Perec (2004). *Inorg. Chem.* **43**, 6965–6968].

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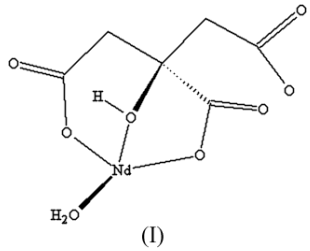
## Comment

The structures and properties of binary rare-earth citrates are of special significance because of the relevance of rare-earth compounds in biomedical applications (Wang *et al.*, 1999). Through a hydrothermal reaction, we have successfully synthesized the title crystalline $Nd^{III}$ binary citrate compound, (I). The compound is isostructural with the lanthanum analogue (Baggio & Perec, 2004).




(I)

The $Nd^{III}$ cation of (I) is coordinated by nine O atoms from one aqua molecule [Nd—O = 2.427 (8) Å] and five symmetry-related citrate trianions [mean Nd—O = 2.551 (7) Å]. The citrate trianion is involved in six Nd—O bonds to five different Nd centres in a very compact three-dimensional structure.

## Experimental

The title complex was prepared by the hydrothermal reaction of neodymium(III) nitrate hexahydrate (0.089 g, 0.25 mmol) and citric acid (0.048 g, 0.25 mmol) in water (16 ml) at pH 3.5. After heating at 423 K for 3 d and cooling to room temperature at 10 K $h^{-1}$, colourless crystals of (I) were obtained in 63% yield.

*Crystal data*

$[Nd(C_6H_5O_7)(H_2O)]$
$M_r$ = 351.36
Monoclinic, $C2/c$
$a$ = 16.6409 (11) Å
$b$ = 8.7622 (6) Å
$c$ = 13.9279 (9) Å
$\beta$ = 120.288 (2)°
$V$ = 1753.6 (2) Å$^3$
$Z$ = 8
$D_x$ = 2.662 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1574 reflections
$\theta$ = 2.7–25.0°
$\mu$ = 5.95 mm$^{-1}$
$T$ = 293 (2) K
Prism, colourless
0.25 × 0.19 × 0.18 mm

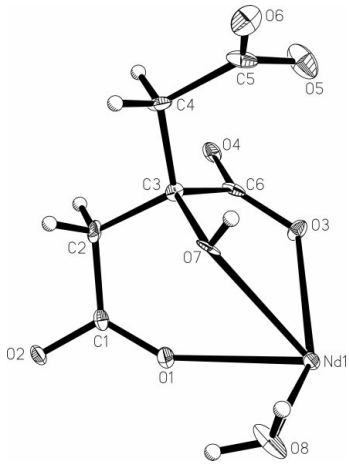



**Figure 1**
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 35% probability level and H atoms are shown as small spheres of arbitrary radii.

*Data collection*

| | |
|---|---|
| Siemens SMART CCD area-detector diffractometer | 1507 independent reflections |
| $\omega$ scans | 1288 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $R_{int} = 0.033$ |
| $T_{min} = 0.245$, $T_{max} = 0.343$ | $\theta_{max} = 25.0°$ |
| 2359 measured reflections | $h = -19 \rightarrow 16$ |
| | $k = -9 \rightarrow 10$ |
| | $l = -16 \rightarrow 14$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0111P)^2 + 116.7406P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.109$ | $\Delta\rho_{max} = 1.31$ e Å$^{-3}$ |
| $S = 1.16$ | $\Delta\rho_{min} = -1.32$ e Å$^{-3}$ |
| 1507 reflections | |
| 136 parameters | |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Nd1—O6$^{i}$ | 2.397 (8) | Nd1—O1 | 2.540 (7) |
| Nd1—O8 | 2.427 (8) | Nd1—O7 | 2.577 (8) |
| Nd1—O3 | 2.495 (7) | Nd1—O1$^{iv}$ | 2.680 (7) |
| Nd1—O2$^{ii}$ | 2.500 (7) | Nd1—O2$^{iv}$ | 2.697 (7) |
| Nd1—O4$^{iii}$ | 2.518 (7) | | |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O7—H7···O3$^{i}$ | 0.82 | 1.89 | 2.668 (10) | 158 |
| O8—H8$B$···O5$^{i}$ | 0.85 | 1.88 | 2.665 (12) | 153 |
| O8—H8$A$···O5$^{ii}$ | 0.85 | 1.97 | 2.653 (12) | 137 |

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

All H atoms were positioned geometrically, with C—H distances of 0.93 Å, citrate O—H distances of 0.82 Å and water O—H distances of 0.85 Å, and were allowed to ride on their carrier atoms, with $U_{iso}$(H) = $1.2U_{eq}$(C,O). The maximum and minimum electron-density peaks are located 0.84 Å from atom O6 and 1.20 Å from atom Nd1, respectively.

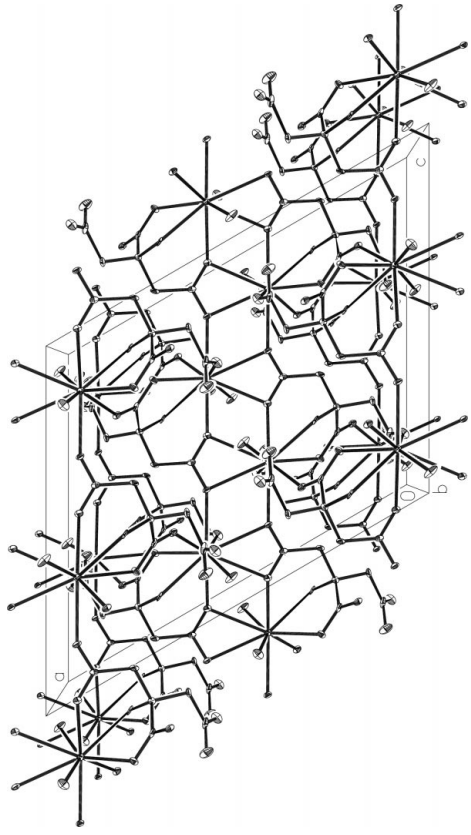



**Figure 2**
Packing diagram for (I), viewed along the $b$ axis. H atoms have been omitted for clarity.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

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