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A one-dimensional coordination polymer with alternating CeN_3O_6 and $SrNO_7$ polyhedra

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The structure of the title compound, (pyridine-2,6-dicarboxylic acid)triaquastrontium(II) tris(pyridine-2,6-dicarboxylato)cerium(IV) hexahydrate, $[Sr(C_7H_5NO_4)(H_2O)_3][Ce(C_7H_3NO_4)_3]\cdot 6H_2O$ or $[Sr(dipicH_2)(OH_2)_3][Ce(dipic)_3]\cdot 6H_2O$, consists of a one-dimensional chain of alternate tricapped trigonal prismatic and square antiprismatic polyhedra made up of $[Ce(dipic)_3]^{2-}$ and $[Sr(dipicH_2)(OH_2)_3]^{2+}$ ions, respectively, linked by the carboxylate groups.

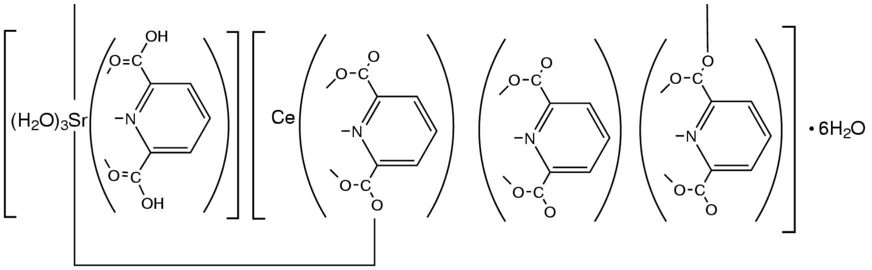
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
H-atom completeness 44%
Disorder in solvent or counterion
R factor = 0.067
wR factor = 0.197
Data-to-parameter ratio = 13.1

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

Comment

Rapid progress in the field of coordination polymers is due to their unusual and desirable properties in the field of materials science (Chen & Suslick, 1993; Swiegers & Malefetse, 2000). Ligands capable of bridging metal centers are well suited for assembling the metal centers to form chains (Sailaja & Rajasekharan, 2000). Dipicolinic acid ($dipicH_2$) is a multifunctional ligand which can act as a bridging as well as a chelating ligand. Mononuclear and three-dimensional networks have been observed in many compounds containing $dipicH_2$, a trivalent lanthanide ion and the Na^+ ion (Albertson, 1970; 1972*a*,*b*,*c*). A linear chain involving alternate coordinate and hydrogen-bond bridges was found in $Na_3Yb(dipic)_3\cdot NaClO_4\cdot 10H_2O$ (Albertson, 1972*b*). A fully coordinatively bridged infinite linear chain involving Ce^{4+}, Ca^{2+} and $dipicH_2$ was reported previously from our laboratory, *viz.* $[Ca(dipicH_2)(OH_2)_3][Ce(dipic)_3]\cdot 5H_2O$ (Swarnabala & Rajasekharan, 1998). In this paper, we report the Sr analog of this compound, *viz.* $[Sr(dipicH_2)(OH_2)_3][Ce(dipic)_3]\cdot 6H_2O$, (I).



(I)

Compound (I) consists of alternating nine-coordinate Ce^{4+} and eight-coordinate Sr^{2+}, assembled in the form of a one-dimensional chain, by the bridging carboxylate groups of $dipic^{2-}$. Three tridentate $dipic^{2-}$ ligands coordinate to Ce^{4+} in a slightly distorted tricapped trigonal prismatic mode. One tridentate $dipicH_2$ and three water molecules are coordinated to Sr^{2+}. Eight-coordination around Sr^{2+} is achieved by sharing

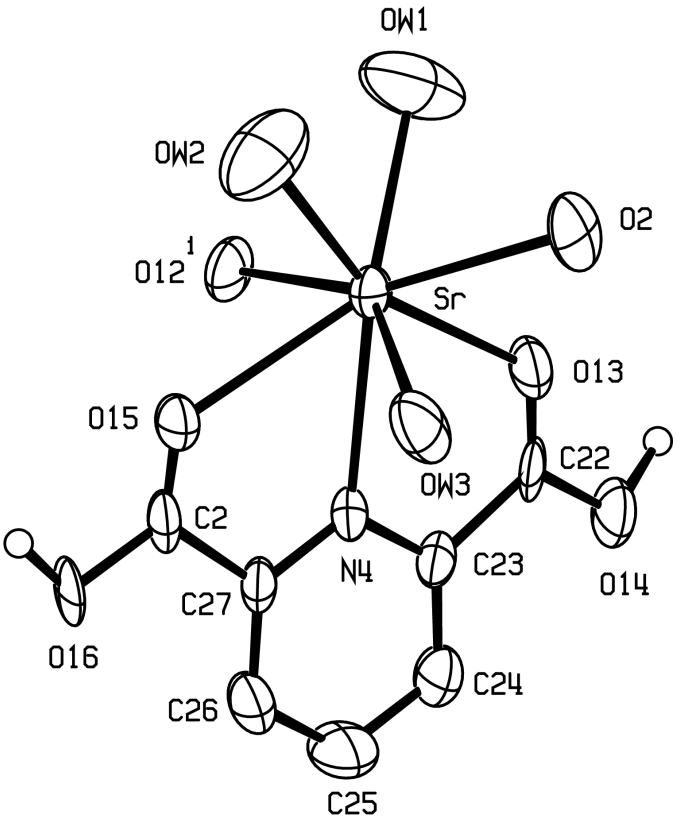


Figure 1
*ORTEP*III view (Burnett & Johnson, 1996) of the cationic unit with the atom numbering. Displacement ellipsoids are shown at the 50% probability level. Ring and water H atoms have been omitted for clarity. [Symmetry code: (i) $1 + x, 1 + y, z$.]

the carboxylate O atoms from two dipic^{2-} ligands of adjacent $[Ce(dipic)_3]^{2-}$ units. This results in a distorted square antiprismatic geometry for the Sr^{2+} unit. Along the chain, the Ce...Sr distances alternate between 5.04 (16) and 6.02 (18) Å.

The cerium coordination polyhedron is essentially the same as that found in the calcium analog. As expected, the Sr—(O,N) distances are longer (by about 0.1 Å) than the Ca—(O,N) distances. The structure is essentially isomorphous with that of the calcium analog (Swarnabala & Rajasekharan, 1998). In both structures, six out of the total eight solvent water sites have partial occupation factors. Refinement suggests the present compound to be a hexahydrate, while the calcium structure was a pentahydrate.

Experimental

To a 5 ml aqueous solution of $SrCl_2·6H_2O$ (0.267 g, 1.00 mmol) and $(NH_4)_2Ce(NO_3)_6$ (0.550 g, 1.00 mmol), 40 ml of a methanolic solution of dipicH_2 (0.668 g, 4.00 mmol) was added slowly while stirring. As the methanolic solution was being added, the colour changed from deep-red to orange to pale-yellow. After stirring for about 5 min, the precipitate which formed was separated by filtration. The clear filtrate gave a yellow crystalline material. Yield 0.696 g (0.661 mmol, 66%). Recrystallization from hot water yielded pale-yellow single crystals of (I) suitable for X-ray data collection.

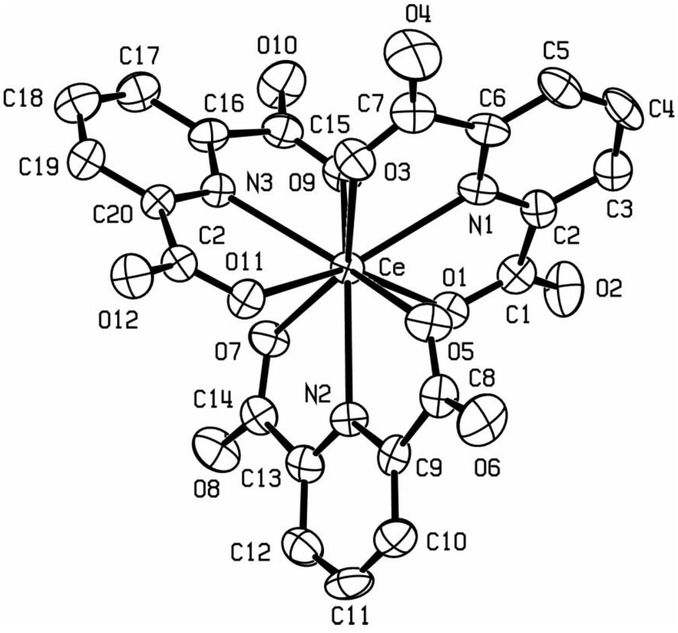


Figure 2
*ORTEP*III view (Burnett & Johnson, 1996) of the anionic unit with the atom numbering. Displacement ellipsoids are shown at the 50% probability level. Ring H atoms have been omitted for clarity.

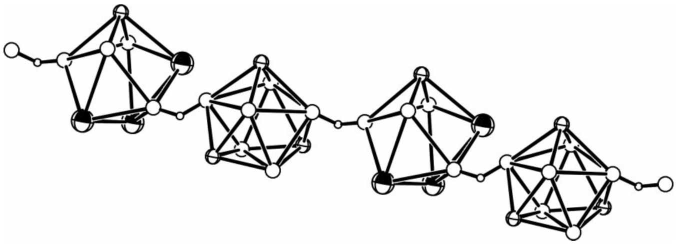


Figure 3
The polymeric chain showing alternating coordination polyhedra. N atoms are shown as ellipsoids, water O atoms are shown as large shaded ellipsoids and carboxyl O atoms are shown as large open circles.

Crystal data

$[Sr(C_7H_5NO_4)(H_2O)_3]$-
$[Ce(C_7H_3NO_4)_3]·6H_2O$
$M_r = 1052.32$
Triclinic, $P\bar{1}$
$a = 11.206$ (4) Å
$b = 12.811$ (2) Å
$c = 16.208$ (4) Å
$\alpha = 96.032$ (17)°
$\beta = 103.54$ (2)°
$\gamma = 113.191$ (16)°
$V = 2028.0$ (9) Å^3

$Z = 2$
$D_x = 1.723$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 15.0–18.0°$
$\mu = 2.52$ mm^{-1}
$T = 293$ (2) K
Hexagonal prism, pale yellow
0.40 × 0.40 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega–2\theta$ scans
Absorption correction: semi-empirical (North *et al.*, 1968)
$T_{min} = 0.575$, $T_{max} = 0.900$
7320 measured reflections
7217 independent reflections
5483 reflections with $I > 2\sigma(I)$

$R_{int} = 0.020$
$\theta_{max} = 25.4°$
$h = -13 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = 0 \rightarrow 19$
2 standard reflections
every 250 reflections
frequency: 90 min
intensity decay: none

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.197$
$S = 1.06$
7217 reflections
552 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1388P)^2 + 0.5844P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.026$
$\Delta\rho_{\max} = 1.67$ e Å^{-3}
$\Delta\rho_{\min} = -3.20$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ce—O7	2.333 (6)	Sr—O2	2.540 (7)
Ce—O9	2.334 (6)	Sr—OW1	2.545 (9)
Ce—O5	2.336 (6)	Sr—O12^{i}	2.547 (6)
Ce—O11	2.346 (6)	Sr—OW2	2.571 (9)
Ce—O3	2.366 (6)	Sr—OW3	2.617 (8)
Ce—O1	2.371 (6)	Sr—O13	2.632 (6)
Ce—N3	2.507 (7)	Sr—O15	2.640 (6)
Ce—N2	2.515 (7)	Sr—N4	2.673 (7)
Ce—N1	2.520 (7)		
O7—Ce—O9	80.2 (2)	O3—Ce—N1	62.9 (2)
O7—Ce—O5	127.1 (2)	O1—Ce—N1	64.1 (2)
O9—Ce—O5	144.5 (2)	N3—Ce—N1	117.8 (2)
O7—Ce—O11	86.3 (2)	N2—Ce—N1	120.2 (2)
O9—Ce—O11	128.1 (2)	O2—Sr—OW1	76.0 (3)
O5—Ce—O11	80.9 (2)	O2—Sr—O12^{i}	144.2 (2)
O7—Ce—O3	147.0 (2)	OW1—Sr—O12^{i}	72.8 (3)
O9—Ce—O3	88.5 (2)	O2—Sr—OW2	90.4 (3)
O5—Ce—O3	78.2 (2)	OW1—Sr—OW2	79.3 (4)
O11—Ce—O3	76.6 (2)	O12^{i}—Sr—OW2	100.5 (3)
O7—Ce—O1	80.0 (2)	O2—Sr—OW3	70.6 (2)
O9—Ce—O1	75.7 (2)	OW1—Sr—OW3	142.8 (3)
O5—Ce—O1	86.4 (2)	O12^{i}—Sr—OW3	143.7 (2)
O11—Ce—O1	150.1 (2)	OW2—Sr—OW3	85.0 (3)
O3—Ce—O1	127.1 (2)	O2—Sr—O13	74.2 (2)
O7—Ce—N3	74.2 (2)	OW1—Sr—O13	84.6 (3)
O9—Ce—N3	64.3 (2)	O12^{i}—Sr—O13	85.7 (2)
O5—Ce—N3	138.4 (2)	OW2—Sr—O13	160.0 (3)
O11—Ce—N3	63.8 (2)	OW3—Sr—O13	101.3 (3)
O3—Ce—N3	73.0 (2)	O2—Sr—O15	141.8 (2)
O1—Ce—N3	135.1 (2)	OW1—Sr—O15	135.9 (3)
O7—Ce—N2	64.0 (2)	O12^{i}—Sr—O15	74.0 (2)
O9—Ce—N2	137.0 (2)	OW2—Sr—O15	79.0 (3)
O5—Ce—N2	63.1 (2)	OW3—Sr—O15	71.9 (2)
O11—Ce—N2	74.7 (2)	O13—Sr—O15	120.9 (2)
O3—Ce—N2	134.5 (2)	O2—Sr—N4	117.4 (2)
O1—Ce—N2	75.4 (2)	OW1—Sr—N4	133.9 (3)
N3—Ce—N2	121.9 (2)	O12^{i}—Sr—N4	74.9 (2)
O7—Ce—N1	139.0 (2)	OW2—Sr—N4	139.1 (3)
O9—Ce—N1	72.6 (2)	OW3—Sr—N4	77.7 (2)
O5—Ce—N1	71.9 (2)	O13—Sr—N4	60.8 (2)
O11—Ce—N1	134.7 (2)	O15—Sr—N4	60.4 (2)

Symmetry code: (i) $1 + x, 1 + y, z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O14—H14···OW4^{i}	0.82	1.71	2.498 (11)	160
O16—H16···O6^{ii}	0.82	1.82	2.607 (10)	161

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

Among the eight water sites, six (OW6, OW7, OW8, OW9, OW10 and OW11) were refined with partial occupation factors. The H atoms of the water molecules were not located.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *Xtal*3.4 (Hall *et al.*, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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References

Albertson, J. (1970). *Acta Chem. Scand.* **24**, 1213–1229.
Albertson, J. (1972*a*). *Acta Chem. Scand.* **26**, 985–1004.
Albertson, J. (1972*b*). *Acta Chem. Scand.* **26**, 1005–1017.
Albertson, J. (1972*c*). *Acta Chem. Scand.* **26**, 1023–1044.
Burnett, M. N. & Johnson, C. J. (1996). *ORTEP*III. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Chen, C.-T. & Suslick, K. S. (1993). *Coord. Chem. Rev.* **128**, 293–332.
Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius. Delft. The Netherlands.
Hall, S. R., King, G. S. D. & Stewart, J. M. (1995). Editors. *Xtal*3.4. University of Western Australia, Perth: Lamb.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sailaja, S. & Rajasekharan, M. V. (2000). *Inorg. Chem.* **39**, 4586–4590.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Swarnabala, G. & Rajasekharan, M. V. (1998). *Inorg. Chem.* **37**, 1483–1485.
Swiegers, G. F. & Malefetse, T. J. (2000). *Chem. Rev.* **10**, 3484–3587.

Acta Cryst. (2001). E**57**, m341–m343 S. Sailaja *et al.* • $[Sr(C_7H_5NO_4)(H_2O)_3][Ce(C_7H_3NO_4)_3]\cdot 6H_2O$ **m343**