

Poly[tetra- μ_2 -L-lactato-indium(III)-sodium(I)]

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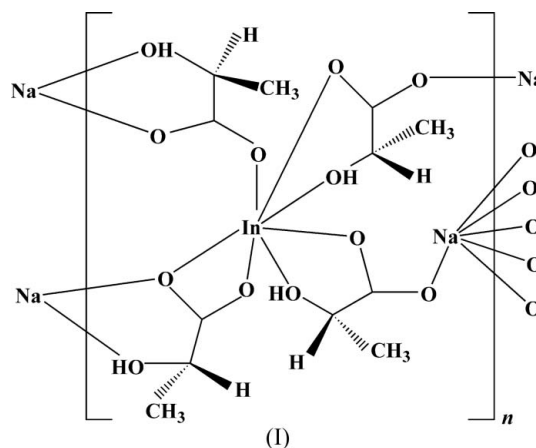
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The asymmetric unit of the title compound, $[\text{InNa}(\text{C}_3\text{H}_5\text{O}_3)_4]_n$, consists of one In^{III} ion, one Na^{I} ion and four crystallographically independent L-lactate monoanions. The coordination of the In^{III} ion is composed of five carboxylate O and two hydroxy O atoms in a distorted pentagonal-bipyramidal coordination geometry. The Na^{I} ion is six-coordinated by four carboxylate O atoms and two hydroxy O atoms from four L-lactate ligands in a distorted octahedral geometry. Each In^{III} ion is coordinated by four surrounding L-lactate ligands to form an $[\text{In}(\text{L-lactate})_4]^-$ unit, which is further linked by Na^{I} ions through $\text{Na}-\text{O}$ bonds to give a two-dimensional layered structure. Hydrogen bonds between the hydroxy groups and carboxylate O atoms are observed between neighbouring layers.

Comment

The construction of coordination polymers with desired properties from multifunctional ligands with metal ions is of current interest and great importance because these materials can exhibit a variety of physical properties, such as catalysis, molecular magnetism, photoluminescence, adsorption and phase separation (Janiak, 2003; Kitagawa *et al.*, 2004; O'Keeffe *et al.*, 2000). The rational synthesis of these materials, however, remains a great challenge. Ionothermal synthesis, a new synthetic methodology developed recently involving the use of an ionic liquid as both solvent and template in the preparation of crystalline solids, offers many advantages over traditional hydrothermal and solvothermal materials synthesis methods (Parnham & Morris, 2007; Reichert *et al.*, 2006). Compared with traditional hydrothermal and solvothermal methods, the change from molecular to ionic reaction media leads to new types of materials being accessible, with structural properties that may be traced directly to the chemistry of the ionic liquid (IL) (Chen *et al.*, 2008; Zhang *et al.*, 2010). Therefore, the ionic species of ILs may control the structures of the materials formed in ionothermal synthesis. There are some examples in which ILs have been successfully applied to the syntheses of novel coordination compounds (Chen *et al.*, 2009; Xu *et al.*,

2007). Of particular interest is a recent study by Morris and co-workers (Lin *et al.*, 2007) on the use of an enantiopure anion as one component of the IL to induce homochirality in a nickel(II) structure constructed of entirely achiral building blocks, despite the fact that the anion of the IL is not occluded by the material. Nevertheless, there are still relatively few examples of coordination polymers prepared by ionothermal reaction to date.



The In^{III} ion is liable to hydrolysis, which limits its use in the construction of coordination compounds under hydrothermal or solvothermal conditions. However, In^{III} ions can be used to construct new frameworks under ionothermal conditions because the In^{III} ion will not hydrolyse in IL solvents. A series of In compounds prepared under ionothermal reaction conditions has been reported recently (Zhang *et al.*, 2008). We report here the title indium compound, poly[tetra- μ_2 -L-lactato-indium(III)sodium(I)], (I). To the best of our knowledge, no indium compound based on the lactate ligand has been reported previously.

The asymmetric unit of (I) consists of one In^{III} ion, one Na^{I} ion and four L-lactate monoanions. As depicted in Fig. 1, the In1 ion is seven-coordinated by five carboxylate O atoms (O1, O4, O7, O8 and O10) and two hydroxy O atoms (O3 and O6)

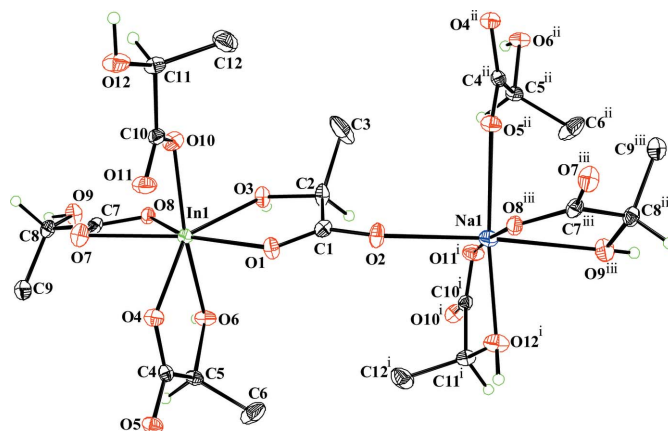
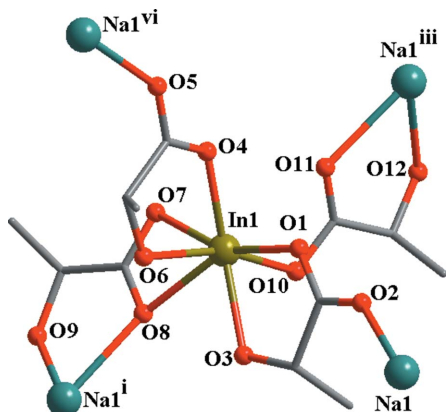


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Methyl H atoms have been omitted for clarity. [Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x - 1, y, z$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.]

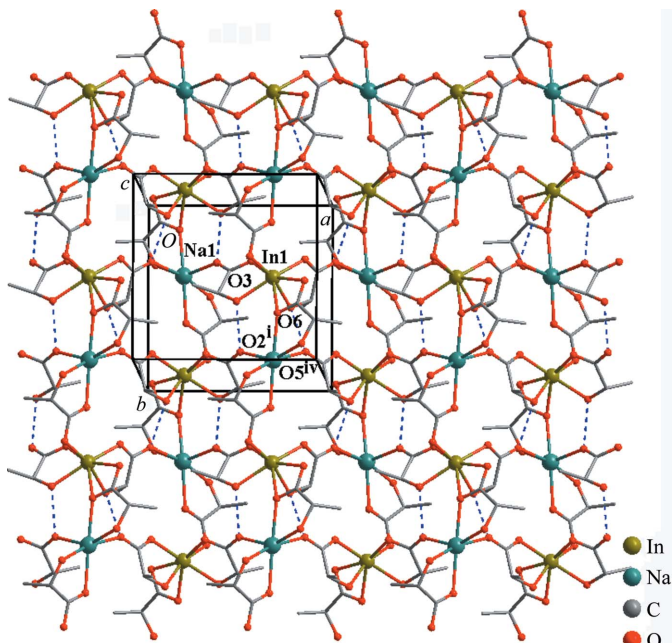

Figure 2

A view of the $[\text{In}(\text{L-lactate})_4]^-$ unit surrounded by four Na^{I} ions. [Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (vi) $x + 1, y, z$.]

from four L-lactate ligands in a pentagonal-bipyramidal coordination environment, with atoms O6 and O10 occupying the apical positions. The In–O bond lengths range from 2.133 (2) to 2.356 (2) Å and the O–In–O bond angles vary from 55.29 (8) to 164.80 (9)° (Table 1). The Na1 ion is six-coordinated by two carboxylate O atoms [O2 and O5ⁱⁱ; symmetry code: (ii) $x - 1, y, z$] and two hydroxy O atoms [O12ⁱ and O9ⁱⁱⁱ; symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$] in a distorted square-planar geometry, with two carboxylate O atoms (O8ⁱⁱⁱ and O11ⁱ) in the apical positions. The Na1 ion is surrounded by four L-lactate ligands, with Na1–O distances varying from 2.364 (3) to 2.476 (3) Å (Fig. 1 and Table 1). The $[\text{NaO}_6]$ octahedron is distorted, with O–Na–O bond angles varying from 65.13 (8) to 175.47 (11)° (Table 1).

Though all the L-lactate ligands bridge one In^{III} ion and one Na^I ion, the four crystallographically independent L-lactate ligands display three different coordination modes. The first type of L-lactate ligand chelates an In^{III} ion through its hydroxy O atom (O3) and one carboxylate O atom (O1), and bridges an Na^I ion through its second carboxylate O atom (O2) (Fig. 2). The second type of L-lactate ligand coordination is similar to the first; it chelates an Na^I ion through its hydroxy O atom (O12) and one carboxylate O atom (O11), and bridges an In^{III} ion through its second carboxylate O atom (O10). The third type of L-lactate ligand employs its carboxylate group (O7 and O8) to chelate an In^{III} ion, and its hydroxy O atom (O9) and one of its carboxylate O atoms (O8) to chelate an Na^I ion. Therefore, there is a μ_2 -O (O8) bridge present in this type of L-lactate ligand.

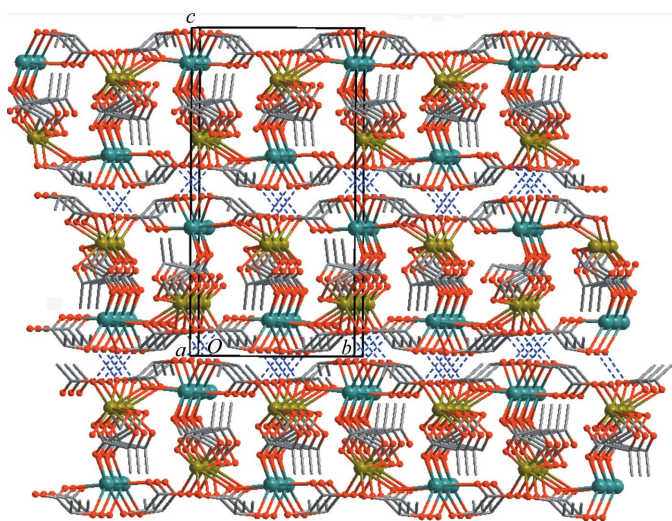
Each In^{III} ion is coordinated by four surrounding L-lactate ligands to form an $[\text{In}(\text{L-lactate})_4]^-$ unit (Fig. 2). Each of these $[\text{In}(\text{L-lactate})_4]^-$ units is linked by four neighbouring Na^I ions through Na–O bonds to generate a two-dimensional layer along the *ab* plane (Fig. 3). Within the layer, there are hydrogen bonds between the hydroxy groups and the carboxylate O atoms [O3···O2ⁱ and O6···O5^{iv}; symmetry code: (iv) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$] (Table 2). The two-dimensional layers are stacked along the *c* direction to produce the crystal


Figure 3

A perspective view of the two-dimensional layered structure of (I). H atoms have been omitted for clarity. Dashed lines between hydroxy O and carboxylate O atoms indicate hydrogen bonds. [Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$.]

packing (Fig. 4). Interlayer hydrogen bonds are observed between the hydroxy groups and the carboxylate O atoms [O9···O10^v and O12···O7^{vi}; symmetry codes: (v) $x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (vi) $x - \frac{1}{2}, -y + \frac{1}{2}, -z$] (Table 2).

Some coordination compounds incorporating the lactate ligand have been reported previously. Most of them are mononuclear structures, such as $[\text{Co}(\text{lactate})_2(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$ (Carballo *et al.*, 2002), $[\text{Mn}(\text{lactate})_2(\text{H}_2\text{O})_2]$ (Lis, 1982) and $[\text{Al}(\text{lactate})_3]$ (Bombi *et al.*, 1990). A few compounds with two-dimensional structures containing bridging lactate ligands


Figure 4

A view of the packing of (I) along the *a* axis. H atoms have been omitted for clarity. Dashed lines between hydroxy O and carboxylate O atoms indicate interlayer hydrogen bonds.

have also been reported. However, all of them are homo-metallic compounds. For example, $[\text{Eu}(\text{lactate})_2(\text{H}_2\text{O})_2]\text{-ClO}_4)_n$ possesses a cationic two-dimensional laminar layer charged with the perchlorate ions (Qu *et al.*, 2008). In the $[\text{Cu}(\text{lactate})_2]_n$ complex (Balboa *et al.*, 2007), the lactate ligand chelates a Cu^{II} ion through its hydroxy O atom and one carboxylate O atom, and bridges one Cu^{II} ion through the second carboxylate O atom, to generate a neutral two-dimensional framework where the basic structural unit is the mononuclear $[\text{Cu}(\text{lactate})_2]$ unit.

Experimental

$\text{In}(\text{NO}_3)_3 \cdot 4.5\text{H}_2\text{O}$ (229.2 mg, 0.6 mmol) and the monosodium salt of 5-sulfoisophthalic acid (53.6 mg, 0.2 mmol) were mixed with 1-ethyl-3-methylimidazolium L-lactate (0.6 g) in a 25 ml Parr Teflon-lined stainless steel vessel. The vessel was sealed and heated to 413 K. The temperature was maintained for 12 d and then the mixture was allowed to cool naturally to obtain colourless crystals of (I) [yield 51%, based on $\text{In}(\text{NO}_3)_3 \cdot 4.5\text{H}_2\text{O}$]. IR (KBr pellet, ν , cm^{-1}): 3465, 3391, 3105, 2950, 1638, 1598, 1564, 1473, 1417, 1254, 1124, 1073, 954, 868, 776, 666, 588, 540, 518.

Crystal data

$[\text{InNa}(\text{C}_3\text{H}_5\text{O}_3)_4]$	$V = 1737.7$ (4) \AA^3
$M_r = 494.09$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 9.4744$ (12) \AA	$\mu = 1.45$ mm^{-1}
$b = 9.5803$ (12) \AA	$T = 296$ K
$c = 19.145$ (2) \AA	$0.18 \times 0.13 \times 0.09$ mm

Data collection

Bruker APEXII area-detector diffractometer	10916 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	4259 independent reflections
$T_{\text{min}} = 0.781$, $T_{\text{max}} = 0.881$	3680 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.029$

Table 1

Selected geometric parameters (\AA , $^\circ$).

In1—O10	2.133 (2)	Na1—O12 ⁱ	2.364 (3)
In1—O4	2.162 (2)	Na1—O5 ⁱⁱ	2.423 (3)
In1—O1	2.183 (2)	Na1—O2	2.435 (3)
In1—O6	2.217 (2)	Na1—O8 ⁱⁱⁱ	2.437 (2)
In1—O3	2.255 (2)	Na1—O11 ⁱ	2.462 (2)
In1—O8	2.338 (2)	Na1—O9 ⁱⁱⁱ	2.476 (3)
In1—O7	2.356 (2)		
O10—In1—O4	122.10 (9)	O8—In1—O7	55.29 (8)
O10—In1—O1	91.88 (9)	O12 ⁱ —Na1—O2	99.82 (12)
O4—In1—O1	81.77 (10)	O5 ⁱⁱ —Na1—O2	88.19 (8)
O10—In1—O6	164.80 (9)	O12 ⁱ —Na1—O8 ⁱⁱⁱ	110.79 (10)
O4—In1—O6	73.05 (8)	O5 ⁱⁱ —Na1—O8 ⁱⁱⁱ	77.75 (9)
O1—In1—O6	91.77 (10)	O2—Na1—O8 ⁱⁱⁱ	85.24 (10)
O10—In1—O3	83.36 (9)	O12 ⁱ —Na1—O11 ⁱ	66.95 (9)
O1—In1—O3	72.36 (9)	O5 ⁱⁱ —Na1—O11 ⁱ	103.98 (11)
O6—In1—O3	83.70 (9)	O2—Na1—O11 ⁱ	98.95 (12)
O10—In1—O8	93.10 (8)	O8 ⁱⁱⁱ —Na1—O11 ⁱ	175.47 (11)
O6—In1—O8	75.68 (8)	O12 ⁱ —Na1—O9 ⁱⁱⁱ	84.43 (10)
O3—In1—O8	74.12 (8)	O5 ⁱⁱ —Na1—O9 ⁱⁱⁱ	92.82 (11)
O10—In1—O7	87.13 (9)	O8 ⁱⁱⁱ —Na1—O9 ⁱⁱⁱ	65.13 (8)
O4—In1—O7	81.37 (9)	O11 ⁱ —Na1—O9 ⁱⁱⁱ	110.47 (11)
O6—In1—O7	94.55 (9)		

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

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O3—H3 \cdots O2 ⁱ	0.86 (4)	1.76 (4)	2.620 (3)	177 (4)
O6—H6 \cdots O5 ^{iv}	0.82 (4)	1.77 (4)	2.578 (4)	170 (4)
O9—H9 \cdots O10 ^v	0.83 (4)	2.26 (4)	3.087 (4)	173 (4)
O12—H12 \cdots O7 ^{vi}	0.87 (4)	2.05 (4)	2.916 (3)	173 (4)

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

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$	$\Delta\rho_{\text{max}} = 0.45$ e \AA^{-3}
$wR(F^2) = 0.057$	$\Delta\rho_{\text{min}} = -0.42$ e \AA^{-3}
$S = 1.02$	Absolute structure: Flack (1983),
4259 reflections	with 1766 Friedel pairs
247 parameters	Flack parameter: 0.03 (2)
H atoms treated by a mixture of independent and constrained refinement	

H atoms bonded to C atoms were placed in calculated positions and treated using a riding-model approximation, with $\text{C—H} = 0.96$ \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl groups, and $\text{C—H} = 0.98$ \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylidyne groups. Hydroxy H atoms were located in a difference map and refined with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008) and DIAMOND (Brandenburg, 2005); software used to prepare material for publication: SHELXTL.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: LG3055). Services for accessing these data are described at the back of the journal.

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