

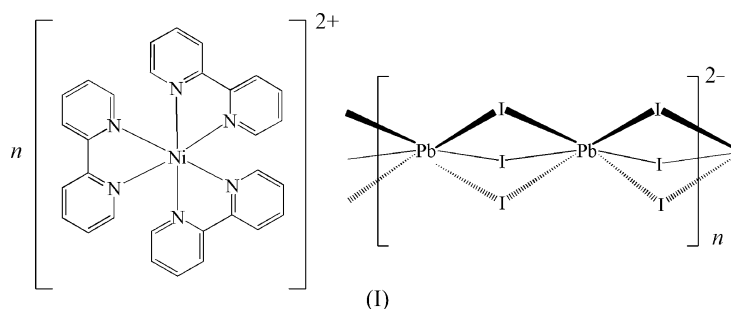
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.028$ Å
 R factor = 0.074
 wR factor = 0.213
Data-to-parameter ratio = 22.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[tris(2,2'-bipyridine)nickel(II)
[hexa- μ -iodo-diplumbate(II)]]**In the title compound, $\{[\text{Ni}(\text{C}_{10}\text{H}_8\text{N}_2)_3][\text{Pb}_2\text{I}_6]\}_n$, each Pb^{II} ion is coordinated by six I^- ions in a distorted octahedral environment. PbI_6 octahedra are connected by common faces to form a one-dimensional anion chain.Received 30 October 2006
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Comment

Lead(II) iodide organic-inorganic hybrid complexes are of special interest because they have significant structural, electrical, non-linear optical, and other physical properties (Mitzi *et al.*, 1995; Guloy *et al.*, 2001; Fan *et al.*, 2006). Their anionic structures range from isolated anions to infinite chains, layered perovskites and three-dimensional polymeric networks, which are modulated by the cations (Li *et al.*, 2005; Mercier, 2005; Poglitsch & Weber, 1987). We report here the crystal structure of the title lead(II) iodide complex, (I), with a one-dimensional anion chain.In (I), there are two crystallographically independent Pb^{II} ions in the asymmetric unit. Each is six-coordinated in a distorted octahedral environment by six I^- ions with $\text{Pb}-\text{I}$ distances ranging from 3.1561 (12) to 3.2830 (14) Å and *cis* $\text{I}-\text{Pb}-\text{I}$ angles from 81.35 (3) to 102.99 (4)° (Table 1). Adjacent octahedra are joined by common faces (I4/I5/I6 and I1/I2/I3) to form a one-dimensional anion chain $[\text{Pb}_2\text{I}_6]_n^{2-}$ along the c axis (Fig. 1). The cation is $[\text{Ni}(\text{bipyridine})_3]^{2+}$, in which each Ni^{II} ion is surrounded by six N atoms from three different bipyridine molecules in a distorted octahedral geometry. The anion chain has no significant hydrogen-bonding interactions with the cations.

Experimental

 PbI_2 (184 mg, 0.4 mmol) and $\text{NaI}\cdot 2\text{H}_2\text{O}$ (74 mg, 0.4 mmol) were dissolved in DMF (10 ml). A solution of 2,2'-bipyridine (94 mg, 0.6 mmol) and $\text{Ni}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (58 mg, 0.2 mmol) in DMF (10 ml) was added and the solution was stirred for 10 min. Vapor of 2-PrOH was diffused slowly into the resulting solution. After about two weeks, orange crystals of (I) were formed.

Crystal data

[Ni(C₁₀H₈N₂)₃][Pb₂I₆]
M_r = 1703.04
 Monoclinic, *P*₂₁/*c*
a = 17.2337 (14) Å
b = 14.7012 (8) Å
c = 16.4273 (12) Å
 β = 101.409 (5)°
V = 4079.7 (5) Å³

Z = 4
D_x = 2.773 Mg m⁻³
 Mo *K*α radiation
 μ = 13.26 mm⁻¹
T = 293 (2) K
 Prism, orange
 0.15 × 0.1 × 0.05 mm

Data collection

Rigaku Mercury CCD
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.332, *T_{max}* = 1.000
 (expected range = 0.171–0.515)

31216 measured reflections
 9307 independent reflections
 6421 reflections with *I* > 2σ(*I*)
R_{int} = 0.058
 θ_{max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.074
wR (*F*²) = 0.213
S = 1.04
 9307 reflections
 406 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0949P)^2 + 47.3372P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.005$
 $\Delta\rho_{max} = 2.23 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{min} = -2.30 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Pb1–I1	3.1561 (12)	Pb2–I6	3.2088 (14)
Pb1–I3	3.2203 (12)	Pb2–I2 ⁱ	3.2332 (14)
Pb1–I5	3.2438 (13)	Pb2–I5	3.2457 (13)
Pb1–I2	3.2560 (14)	Pb2–I3 ⁱ	3.2617 (13)
Pb1–I6	3.2774 (13)	Pb2–I1 ⁱ	3.2624 (13)
Pb1–I4	3.2830 (14)	Pb2–I4	3.2661 (16)
I1–Pb1–I3	87.31 (3)	I6–Pb2–I2 ⁱ	97.81 (4)
I1–Pb1–I5	96.73 (4)	I6–Pb2–I5	85.82 (3)
I3–Pb1–I5	90.72 (3)	I2 ⁱ –Pb2–I5	96.84 (4)
I1–Pb1–I2	84.14 (4)	I6–Pb2–I3 ⁱ	178.89 (4)
I3–Pb1–I2	81.63 (3)	I2 ⁱ –Pb2–I3 ⁱ	81.35 (3)
I5–Pb1–I2	172.26 (4)	I5–Pb2–I3 ⁱ	93.55 (3)
I1–Pb1–I6	87.83 (3)	I6–Pb2–I1 ⁱ	95.76 (3)
I3–Pb1–I6	172.92 (4)	I2 ⁱ –Pb2–I1 ⁱ	82.83 (3)
I5–Pb1–I6	84.73 (3)	I5–Pb2–I1 ⁱ	178.42 (3)
I2–Pb1–I6	102.99 (4)	I3 ⁱ –Pb2–I1 ⁱ	84.87 (3)
I1–Pb1–I4	171.49 (4)	I6–Pb2–I4	85.06 (4)
I3–Pb1–I4	101.19 (4)	I2 ⁱ –Pb2–I4	177.11 (4)
I5–Pb1–I4	83.41 (4)	I5–Pb2–I4	83.64 (4)
I2–Pb1–I4	96.88 (4)	I3 ⁱ –Pb2–I4	95.78 (4)
I6–Pb1–I4	83.70 (4)	I1 ⁱ –Pb2–I4	96.61 (4)

Symmetry code: (i) *x*, −*y* + $\frac{1}{2}$, *z* − $\frac{1}{2}$.

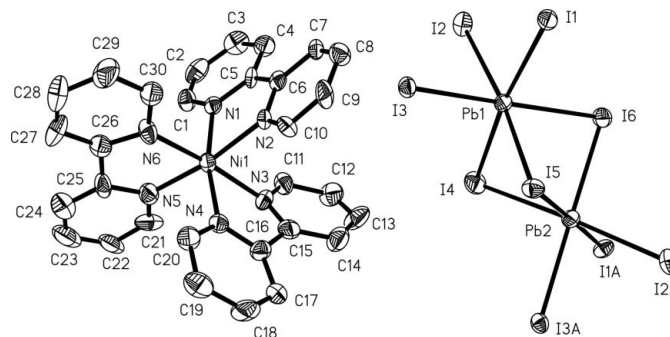


Figure 1

The asymmetric unit of (I), together with additional I atoms to complete the coordination of both Pb atoms. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. [Symmetry code: (A) *x*, $\frac{1}{2}$ − *y*, $-\frac{1}{2}$ + *z*.]

H atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C). The highest peak is located 0.96 Å from atom I4 and deepest hole is located 0.78 Å from atom Pb2.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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