

C5	0.5866 (5)	0.061 (1)	0.1601 (3)	5.2 (2)
C6	0.5741 (4)	0.050 (1)	0.2221 (3)	3.9 (1)
C7	0.5209 (4)	0.223 (1)	0.2421 (3)	4.1 (1)
C8	0.4435 (4)	0.425 (1)	0.3066 (3)	3.7 (1)
C9	0.3932 (4)	0.572 (1)	0.2589 (3)	4.5 (2)
C10	0.3396 (5)	0.745 (1)	0.2727 (3)	5.1 (2)
C11	0.3350 (5)	0.776 (1)	0.3347 (3)	5.3 (2)
C12	0.3836 (5)	0.631 (1)	0.3829 (3)	4.8 (2)
C13	0.4376 (4)	0.452 (1)	0.3694 (3)	4.0 (1)
C14A†	0.7206 (6)	-0.147 (2)	0.4655 (4)	4.0 (2)
C15A†	0.757 (1)	-0.346 (4)	0.5085 (9)	4.7 (4)
C16A†	0.861 (1)	-0.311 (3)	0.5477 (7)	8.4 (4)
C17A†	0.884 (1)	-0.094 (3)	0.5771 (7)	8.1 (4)
C18A†	0.855 (2)	0.112 (4)	0.536 (1)	6.0 (5)
C19A†	0.7568 (8)	0.083 (2)	0.4875 (5)	5.7 (3)
C14B†	0.697 (1)	-0.103 (3)	0.4912 (8)	4.1 (4)
C15B†	0.7399 (7)	-0.305 (2)	0.5288 (5)	5.1 (2)
C16B†	0.832 (2)	-0.267 (4)	0.582 (1)	5.5 (5)
C17B†	0.903 (1)	-0.114 (3)	0.5653 (8)	4.1 (4)
C18B†	0.8735 (8)	0.071 (2)	0.5117 (5)	5.6 (2)
C19B†	0.776 (1)	0.003 (4)	0.463 (1)	5.5 (5)

† Atoms with suffix A have occupancies of 0.66 and those with suffix B have occupancies of 0.34.

Table 2. Selected geometric parameters (Å, °)

Ni—S1	2.148 (2)	Ni—N1	1.874 (5)
Ni—O1	1.845 (5)	Ni—N2	1.948 (5)
S1—Ni—O1	174.2 (1)	O1—Ni—N1	96.1 (2)
S1—Ni—N1	89.6 (2)	O1—Ni—N2	83.4 (2)
S1—Ni—N2	91.0 (2)	N1—Ni—N2	178.7 (2)

The H atoms of the Schiff base ligand were attached to their C atoms geometrically (C—H 0.95 Å). The H atoms of the cyclohexylamine ligand were not attached. Displacement parameters of all H atoms were constrained at 1.3 times those of the corresponding atoms and a riding model was used for all H atoms. During the early stages of refinement, disorder was evident for the cyclohexyl ring. Resolution of the disorder was made possible by restraining all the bonding C—C (1.54 Å) and the non-bonding C14···C18 and C15···C17 (2.51 Å) distances in the ring. After some isotropic refinement of the disordered C atoms, without the H atoms, new coordinates were obtained and these were kept fixed to refine the relative occupancy factors. At this point, a difference map started to show the second ring. The coordinates of the second ring were treated in the same way as described above. Finally, both components were refined isotropically with the coordinates of some atoms being constrained (C16B, C17A, C18A, C17B, C19B).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1993). Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SIMPEL* in *MolEN*. Program(s) used to refine structure: *LSFM* in *MolEN*. Molecular graphics: *ORTEP* (Johnson, 1965) in *MolEN*. Software used to prepare material for publication: *MolEN*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: BM1052). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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[N-(2-Amino-κN-ethyl)piperaziniumyl-N¹]-tetrachloroindium(III)

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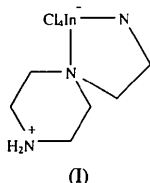
Abstract

The crystal structure of the title compound consists of molecules of [InCl₄{(NH₂CH₂CH₂)₂C₄H₁₀N₂}] held together in buckled sheets by a network of hydrogen bonds. The In atom has a distorted octahedral coordination geometry with the *N*-(2-aminoethyl)piperazinium cation behaving as a bidentate ligand.

Comment

Few crystal structures of octahedral indium(III) mixed-ligand chloro complexes of the form [InCl_xL_{6-x}]^{3-x}, where *L* is a coordinating ligand with an N-donor atom, have been reported in the literature. Examples include, for *x* = 1, [HB(3,5-Me₂pz)₃In{H₂B(pz)₂}Cl] (pz is pyrazolyl) (Reger, Mason, Reger, Rheingold & Ostrander, 1994), for *x* = 2, [NH₂Et₃][InCl₂(dpt)₂] (dpt is 1,3-diphenyltriazene), [InCl₂(dpt)(bipy)] and [InCl₂(dpt)(3,5-Me₂py)₂] (bipy is bipyridyl, py is pyridyl) (Leman, Roman & Barron, 1992), for *x* = 3, [mer-InCl₃(py)₃].py (Jeffs, Small & Worrall, 1984) and [{HB(pz)₃}₂InCl₃][{HB(pz)₃}₂In].thf.CH₂Cl₂ (thf

is tetrahydrofuran) (Reger, Mason, Rheingold & Ostrander, 1994), and for $x = 4$, $[\text{InCl}_4(\text{bipy})]^-$ and $[\text{InCl}_4(4\text{-Mepy})_2]^-$ (Tsapkov *et al.*, 1992). The title compound, (I), is the third example to be found for which $x = 4$ and is rather unusual in that it contains the *N*-(2-aminoethyl)piperazinium cation behaving as a bidentate ligand. The Cambridge Structural Database (1995) does not contain any examples of bidentate behaviour for this ligand.



The asymmetric unit contains one $[\text{InCl}_4\{(\text{NH}_2\text{CH}_2\text{CH}_2)_4\text{N}_2\text{H}_{10}\}]$ molecule which has distorted octahedral geometry around the In atom (Fig. 1). The *N*-(2-aminoethyl)piperazinium cation is disordered over two orientations, with refined occupancies of 0.666 (4) for N2, N3, C2–C6 and 0.334 (4) for N12, N13, C12–C16; both show chair conformations of the piperazinium ring. The molecules are linked to form buckled sheets through a network of hydrogen bonds involving the protonated N atoms of the piperazinium rings (N3 and N13) and two of the four chlorides (Cl1 and Cl4) on adjacent molecules $[\text{Cl1}\cdots\text{N3}^i$ 3.234 (5), $\text{Cl1}\cdots\text{N13}^i$ 3.192 (9), $\text{Cl4}\cdots\text{N3}^{ii}$ 3.175 (5) and $\text{Cl4}\cdots\text{N13}^{ii}$ 3.20 (1) Å; symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$] (Fig. 2). These $\text{N}\cdots\text{Cl}$ distances are close to that of 3.142 (9) Å observed for a hydrogen bond between nitrogen and chlorine in $[\text{NHEt}_3][\text{InCl}_2(\text{dpt})_2]$ (Leman, Roman & Barron, 1992). As expected, the hydrogen bonding leads to an increase in the In—Cl distances In—Cl1 [2.529 (1) Å] and In—Cl4 [2.517 (1) Å],

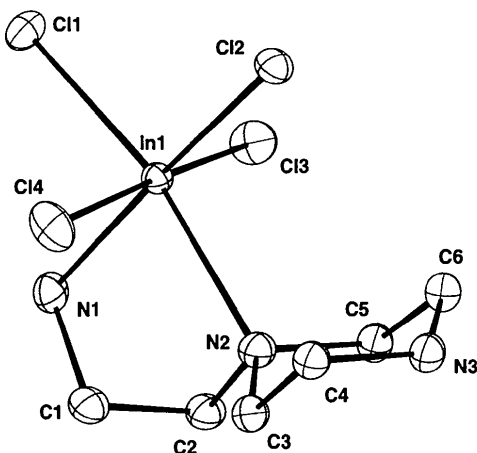


Fig. 1. CAMERON (Watkin, Prout & Pearce, 1996) plot of (I) showing the major component of the piperazinium ring disorder [occupancy of 0.666 (4)]. Displacement ellipsoids are plotted at the 50% probability level and H atoms have been omitted for clarity.

compared with In—Cl2 [2.453 (1) Å] and In—Cl3 [2.464 (1) Å]. The latter distances are in good agreement with those reported in a recent survey of $\text{In}^{\text{III}}\text{—Cl}$ bond lengths (Knop, Cameron, Adhikesavalu, Vincent & Jenkins, 1987). The In—N1 distance [2.252 (3) Å] is considerably shorter than the In—N2 and In—N12 distances [2.468 (5) and 2.453 (8) Å, respectively], due in part to the reduced steric hindrance around N1 compared with N2 and N12.

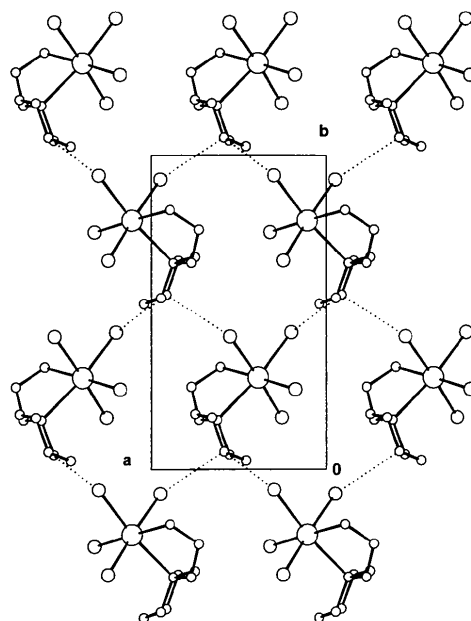


Fig. 2. View along the *c* axis showing the hydrogen-bonding network linking the $[\text{InCl}_4\{(\text{NH}_2\text{CH}_2\text{CH}_2)_4\text{N}_2\text{H}_{10}\}]$ molecules to form a sheet structure.

Experimental

The title compound was formed as a by-product during the synthesis of a microporous indium phosphate. Indium(III) chloride (0.5 g) was dispersed in 2-butanol (10 ml) by stirring and then orthophosphoric acid (0.37 ml) and *N*-(2-aminoethyl)piperazine (T) (0.59 ml) were added to give a $\text{InCl}_3/\text{H}_3\text{PO}_4/\text{T}/\text{butan-2-ol}$ mixture in the molar ratio 1:2.4:2:25.6. The mixture was sealed in a Teflon-lined stainless steel autoclave and heated at 433 K for 5 d. After slow cooling, the product was filtered, washed in ethanol and dried in air at 353 K. The product was polyphasic, containing white polycrystalline material and colourless rectangular plates of the title compound. Energy-dispersive analytical electron microscopy on a hand-picked sample of the crystals showed that they contained indium and chlorine in the ratio 1:4, but no phosphorus could be detected.

Crystal data

$[\text{InCl}_4(\text{C}_6\text{H}_{16}\text{N}_3)]$
 $M_r = 386.85$

Mo $K\alpha$ radiation
 $\lambda = 0.71073 \text{ \AA}$

Monoclinic
 $P2_1/n$
 $a = 7.326(1) \text{ \AA}$
 $b = 12.868(1) \text{ \AA}$
 $c = 14.098(1) \text{ \AA}$
 $\beta = 94.49(1)^\circ$
 $V = 1325.0(2) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.94 \text{ Mg m}^{-3}$
 D_m not measured

Data collection

Enraf–Nonius DIP2020
 image-plate diffractometer
 Image-plate scans
 Absorption correction:
 see text
 6781 measured reflections
 1590 independent reflections

Cell parameters from 124
 reflections
 $\theta = 5\text{--}25^\circ$
 $\mu = 2.54 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Rectangular plate
 $0.24 \times 0.11 \times 0.08 \text{ mm}$
 Colourless

1423 observed reflections
 $[I > 3\sigma(I)]$
 $R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 25^\circ$
 $h = -8 \rightarrow 8$
 $k = -14 \rightarrow 14$
 $l = -15 \rightarrow 15$
 No standard reflections

Refinement

Refinement on F
 $R = 0.0211$
 $wR = 0.0206$
 $S = 1.1659$
 1423 reflections
 191 parameters
 H atoms placed geometrically
 after each cycle
 Weights: five-term Chebyshev
 polynomial (Carruthers & Watkin,
 1979)

$(\Delta/\sigma)_{\text{max}} = 0.008$
 $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
 Extinction correction: none
 Atomic scattering factors
 from *International Tables*
 for *X-ray Crystallography*
 (1974, Vol. IV, Table
 2.2B)

In1—Cl4	2.517 (1)	N12—C12	1.506 (8)
In1—N1	2.252 (3)	N12—C13	1.496 (9)
In1—N2	2.468 (5)	N12—C15	1.471 (9)
In1—N12	2.453 (8)	N13—C14	1.492 (9)
N1—C1	1.473 (5)	N13—C16	1.491 (9)
C1—C2	1.466 (6)	C3—C4	1.496 (7)
C1—C12	1.465 (8)	C5—C6	1.505 (7)
N2—C2	1.506 (6)	C14—C13	1.508 (9)
N2—C3	1.476 (6)	C15—C16	1.503 (9)
C11—In1—C12	95.97 (3)	In1—N2—C3	116.1 (3)
C11—In1—C13	90.31 (4)	C2—N2—C3	108.8 (5)
C12—In1—C13	94.91 (4)	In1—N2—C5	116.9 (4)
C11—In1—C14	90.46 (4)	C2—N2—C5	105.8 (4)
C12—In1—C14	89.16 (4)	C3—N2—C5	106.6 (5)
C13—In1—C14	175.76 (4)	C4—N3—C6	111.2 (5)
C11—In1—N1	87.61 (8)	In1—N12—C13	118.1 (7)
C12—In1—N1	175.04 (9)	C12—N12—C13	103.2 (8)
C13—In1—N1	88.49 (9)	In1—N12—C15	116.1 (7)
C14—In1—N1	87.38 (9)	C12—N12—C15	109.8 (9)
C11—In1—N2	163.6 (1)	C13—N12—C15	108.4 (9)
C12—In1—N2	100.0 (1)	C14—N13—C16	109.7 (9)
C13—In1—N2	84.9 (1)	C1—C2—N2	112.5 (4)
C14—In1—N2	93.2 (1)	N2—C3—C4	110.6 (5)
N1—In1—N2	76.7 (1)	N3—C4—C3	110.2 (5)
C11—In1—N12	164.5 (2)	N2—C5—C6	114.0 (5)
C12—In1—N12	98.0 (2)	N3—C6—C5	109.0 (5)
C13—In1—N12	95.0 (2)	N13—C14—C13	110.1 (9)
C14—In1—N12	83.2 (2)	N12—C13—C14	111.9 (9)
In1—N1—C1	111.7 (2)	N12—C15—C16	109.5 (9)
N1—C1—C2	112.0 (4)	N13—C16—C15	108.3 (9)
In1—N2—C2	101.9 (3)		

The absorption correction was not derived explicitly but by scaling of equivalent reflections through 90 image frames. A total of 102 restraints were applied to the parameters of the *N*-(2-aminoethyl)piperazinium moieties; the C—C and N—C bond lengths were restrained to their common mean values and the U_{ij} parameters of adjacent atoms were restrained to their mean values. Anisotropic displacement parameters were refined for all non-H atoms and isotropic displacement parameters for all H atoms, which were placed geometrically after each refinement cycle. The two components of the piperazinium ring disorder are related approximately by a local mirror plane which does not extend further into the structure.

Data collection: *DIP2000 User Manual* (Enraf–Nonius, 1995). Cell refinement: *DIP2000 User Manual*. Data reduction: *DIP2000 User Manual*. Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *CRYSTALS* (Watkin, Prout, Carruthers & Betteridge, 1996). Molecular graphics: *CAMERON* (Watkin, Prout & Pearce, 1996). Software used to prepare material for publication: *CRYSTALS*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BM1077). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

	$U_{\text{eq}} = (U_1U_2U_3)^{1/3}$			
	x	y	z	U_{eq}
In1	0.10949 (3)	0.79241 (2)	0.10689 (2)	0.0258
Cl1	0.2987 (1)	0.93571 (8)	0.04076 (7)	0.0384
Cl2	0.3222 (1)	0.75532 (8)	0.24585 (7)	0.0365
Cl3	0.2457 (1)	0.66511 (9)	0.00260 (8)	0.0441
Cl4	-0.0502 (2)	0.92270 (9)	0.20473 (8)	0.0473
N1	-0.1055 (4)	0.8256 (2)	-0.0122 (2)	0.0370
C1	-0.2716 (5)	0.7630 (3)	-0.0037 (3)	0.0388
N2†	-0.1227 (7)	0.6567 (4)	0.1263 (3)	0.0342
N3†	-0.0847 (7)	0.5568 (5)	0.3118 (4)	0.0374
N12‡	-0.142 (1)	0.6786 (7)	0.1472 (7)	0.0351
N13‡	-0.044 (2)	0.5084 (8)	0.2741 (7)	0.0346
C2†	-0.2283 (7)	0.6575 (4)	0.0303 (4)	0.0369
C3†	-0.2507 (8)	0.6761 (5)	0.2002 (4)	0.0356
C4†	-0.1551 (9)	0.6651 (5)	0.2974 (4)	0.0363
C5†	-0.0542 (9)	0.5475 (4)	0.1409 (4)	0.0375
C6†	0.0411 (8)	0.5281 (5)	0.2378 (5)	0.0380
C12‡	-0.300 (1)	0.7332 (9)	0.0943 (6)	0.0369
C14‡	-0.060 (2)	0.616 (1)	0.3121 (8)	0.0353
C13‡	-0.193 (2)	0.678 (1)	0.2478 (8)	0.0349
C15‡	-0.133 (2)	0.5703 (8)	0.1145 (8)	0.0343
C16‡	0.013 (2)	0.513 (1)	0.1749 (8)	0.0345

† Site occupancy of 0.666(4). ‡ Site occupancy of 0.334(4).

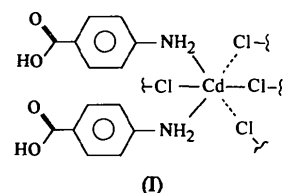
Table 2. Selected geometric parameters (\AA , $^\circ$)

In1—Cl1	2.529 (1)	N2—C5	1.501 (7)
In1—Cl2	2.4528 (9)	N3—C4	1.495 (7)
In1—Cl3	2.464 (1)	N3—C6	1.491 (7)

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The carboxyl groups of the independent ($n = 1, 2$) *p*-aminobenzoic acid residues are linked by pairs of hydrogen bonds [O(11)—H(O11)···O(22') and O(21)—H(O21)···O(12'')]; symmetry codes: (i) $x, y + 1, z$; (ii) $x, y - 1, z$, as is typical in assemblies formed from carboxylic acid synthons (Desiraju, 1995). The two linked carboxyl groups are not, however, related centrosymmetrically. The interatomic distances and angles are close to those observed in *p*-aminobenzoic acid (Lai & Marsh, 1967). In the two structurally distinct organic residues ($n = 1, 2$) of the asymmetric unit, the atoms of the aromatic ring are coplanar to within 0.01 Å and the angle between these planes is 3.8(9)°. The amino and carboxyl groups are displaced significantly from the aromatic plane; atoms C(n4), C(n7), O(n1) and O(n2) ($n = 1, 2$) of the carboxyl groups are coplanar to within 0.01 Å, but these groups are rotated slightly around the C(n4)—C(n7) bonds by *ca* 2–3° out of coplanarity with the aromatic rings.

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Bis(*p*-aminobenzoic acid-*N*)dichloro-cadmium(II)

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Abstract

In crystals of [CdCl₂(C₇H₇NO₂)₂], the Cd atom is octahedrally coordinated by four Cl atoms and two N atoms from two *p*-aminobenzoic acid ligands. Infinite zigzag chains of edge-shared octahedra run along the *a* axis. Pairs of *p*-aminobenzoic acid residues anchored onto the Cd chains form thick organic–inorganic layers parallel to the (011) plane. An N—H···Cl hydrogen-bond network maintains the packing cohesion between the layers.

Comment

Crystals of the title compound, (I), are built from infinite chains of CdCl₄N₂ octahedra interconnected in a three-dimensional manner through pairs of O—H···O hydrogen-bonded *p*-aminobenzoic acid molecules and also by N—H···Cl hydrogen bonds. The main geometrical features of this organic–inorganic assembly are summarized in Tables 2 and 3.

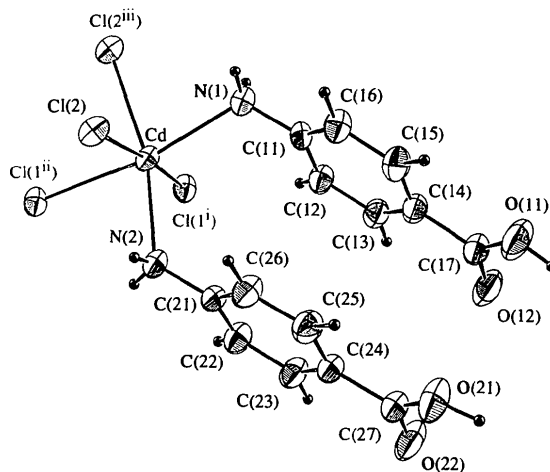


Fig. 1. An ORTEP (Johnson, 1965) drawing of the title compound showing the metal coordination. Displacement ellipsoids for non-H atoms are shown at the 50% probability level.

The coordination of the N atoms is distorted tetrahedral, with a relatively large C(n1)—N(n) distance of 1.42 Å (*cf.* 1.38 Å in *p*-aminobenzoic acid where this bond is already associated with a non-planar coordination at the amino N atom). The angles subtended at the N atom are H(1Nn)—N(n)—H(2Nn) 108(4) and 113(4), H(1Nn)—N(n)—Cd 106(3) and 93(3), C(n1)—N(n)—H(1Nn) 111(3) and 110(3), C(n1)—N(n)—Cd