Table 1. *Details of data collection and structure refinement*

Apparatus	Syntex *R*3
Monochromator	Graphite plate
Wavelength (Å)	Mo *Kα*, 0.7107
No. of reflections, θ range (°) for cell parameter determination	25, 5–30
Absorption correction	Yes
Transmission-factor range	0.139–0.084
Scan mode	$\omega/2\theta$
Scan width (°)	1.2
θ range (°)	2–35 ($-18 \leq h \leq 18$, $-8 \leq k \leq 8$, $-11 \leq l \leq 11$)
No. of collected reflections	5706
No. of independent reflections	1411 in $Pna2_1$ and 759 in *Pnma*
No. of parameters	64 in $Pna2_1$ and 41 in *Pnma*
Crystal size (mm)	0.126
Weighting scheme	$w = [\sigma^2(F) + 0.0002F^2]$
Extinction correction factor	0.047
Program used	*SHELXTL* (Sheldrick, 1983)
R and (*wR*)	0.0182 (0.0179) in $Pna2_1$ 0.0207 (0.0214) in *Pnma*
$(\Delta/\sigma)_{\max}$	0.004
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	2.13, −0.62

Table 2. *Atom coordinates* ($\times 10^4$) *and temperature factors* (Å$^2 \times 10^3$) (*e.s.d.'s are in parentheses and refer to the final digits quoted*)

Equivalent isotropic U_{eq} defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Cd	2158 (1)	2500	450 (1)	11 (1)
P	9108 (1)	2500	−1048 (1)	9 (1)
O(1)	9064 (2)	2500	2131 (4)	14 (1)
O(2)	10443 (2)	2500	−2263 (4)	13 (1)
O(3)	8443 (1)	4455 (2)	−2355 (3)	13 (1)
Li	0	0	5000	28 (2)

Table 3. *Interatomic distances* (Å) *and angles* (°) *in the* LiCdPO$_4$ *structure*

PO$_4$ tetrahedron			
P—O(1)	1.528 (2)	P—O(3,3^{i}) 2 ×	1.554 (1)
P—O(2)	1.546 (2)		
O(1)—P—O(2)	113.9 (1)	O(2)—P—O(3,3^{i}) 2 ×	105.8 (1)
O(1)—P—O(3,3^{i}) 2 ×	112.9 (1)	O(3)—P—O(3^{i})	104.6 (1)
CdO$_6$ octahedron			
Cd—O(1^{vi})	2.352 (2)	Cd—O(3^{ii,iv}) 2 ×	2.218 (1)
Cd—O(2^{iii})	2.254 (2)	Cd—O(3^{vi,vii}) 2 ×	2.371 (1)
O(1^{vi})—Cd—O(2^{iii})	174.3 (1)	O(3^{ii})—Cd—O(3^{vi,vii}) 2 ×	151.1 (1)
O(1^{vi})—Cd—O(3^{ii,iv}) 2 ×	92.8 (1)	O(3^{ii})—Cd—O(3^{iv})	119.4 (1)
O(1^{vi})—Cd—O(3^{vi,vii}) 2 ×	78.7 (1)	O(3^{ii})—Cd—O(3^{iv,vi}) 2 ×	88.8 (1)
O(2^{iii})—Cd—O(3^{ii,iv}) 2 ×	90.1 (1)	O(3^{vii})—Cd—O(3^{vi})	62.5 (1)
O(2^{iii})—Cd—O(3^{vi,vii}) 2 ×	96.4 (1)		
LiO$_6$ octahedron*			
Li—O(1^{ii,iii}) 2 ×	2.319 (1)	Li—O(3^{iv,v}) 2 ×	2.126 (1)
Li—O(2^{iv,v}) 2 ×	2.104 (1)		
O(1^{iii},2^{v},3^{iv})—Li—O(1^{ii},2^{iv},3^{v}) 3 ×	180.0 (1)	O(1^{iii},1^{ii})—Li—O(3^{v},3^{iv}) 2 ×	84.6 (1)
O(1^{iii},1^{ii})—Li—O(2^{v},2^{iv}) 2 ×	87.9 (1)	O(2^{v},2^{iv})—Li—O(3^{iv},3^{v}) 2 ×	108.4 (1)
O(1^{iii},1^{ii})—Li—O(2^{iv},2^{v}) 2 ×	92.1 (1)	O(2^{v},2^{iv})—Li—O(3^{v},3^{iv}) 2 ×	71.6 (1)
O(1^{iii},1^{ii})—Li—O(3^{iv},3^{v}) 2 ×	95.4 (1)		

Symmetry code: (i) x, $0.5-y$, z; (ii) $-x$, $-y$, $-z$; (iii) $1-x$, y, z; (iv) $1-x$, $y-0.5$, $-z$; (v) $x-1$, $0.5-y$, $1+z$; (vi) $x-1$, y, $-(0.5+z)$; (vii) $x-0.5$, $0.5-y$, $-(0.5+z)$.

* For reading the values of O—Li—O angles the following rule should be used: the notation O(*A*,*B*,*C*)—Li—O(*A*′,*B*′,*C*′) means that the angles concerned are O(*A*)—Li—O(*A*′), O(*B*)—Li—O(*B*′) and O(*C*)—Li—O(*C*′).

We are greatly indebted to Professor Dr H. Wondratschek who allowed the data collection in his Laboratory at Karlsruhe, to Dr I. D. Williams who performed the second-harmonic generation tests in Professor S. K. Kurtz's Laboratory and also to Professor S. C. Abrahams for fruitful discussions and particularly for recommending us to continue the refinement in space group *Pnma*.

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Structure of 1,3-Propanediammonium Tetrachlorocobaltate(II)

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(*Received* 3 *February* 1991; *accepted* 18 *July* 1991)

Abstract. [CoCl$_4$(C$_3$H$_{12}$N$_2$)], $M_r = 276.87$, monoclinic, $P2_1/n$, $a = 10.703$ (2), $b = 10.653$ (1), $c = 10.852$ (2) Å, $\beta = 118.46$ (1)°, $V = 1087.8$ Å^3, $Z = 4$, $D_x = 1.69$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 22.60$ cm^{-1}, $F(000) = 556$, $T = 298$ K, final $R = 0.059$ for 1068 unique reflections [$I > 3\sigma(I)$]. The Co$^{\mathrm{II}}$ ion is coordinated by four Cl atoms in a tetrahedral geometry. The paraffinic chains which bridge the tetrahedra have a nearly planar zigzag configuration.

Experimental. The blue plate-shaped crystals of [CoCl$_4$(C$_3$H$_{12}$N$_2$)] were grown at room temperature

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Table 1. *Fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal displacement parameters* ($\text{Å}^2 \times 10^3$)

$U_{eq} = (8\pi^2/3)$ trace **U**.

	x	y	z	U_{eq}
Co	2450 (1)	3639 (1)	4956 (1)	31 (1)
Cl(1)	3485 (2)	1905 (2)	4616 (2)	36 (1)
Cl(2)	4129 (2)	4994 (2)	6478 (2)	45 (1)
Cl(3)	1210 (2)	4564 (2)	2841 (2)	43 (1)
Cl(4)	1042 (3)	2966 (2)	5868 (3)	53 (1)
N(11)	1699 (7)	2003 (6)	1205 (6)	34 (3)
C(12)	1949 (8)	3570 (8)	−342 (7)	36 (3)
C(13)	2744 (8)	2779 (8)	995 (8)	39 (4)
C(14)	3026 (8)	4381 (8)	−567 (8)	43 (4)
N(15)	2179 (7)	5218 (6)	−1811 (6)	40 (3)

from alcohol solution containing 1,3-propanediammonium chloride and $CoCl_2.6H_2O$. A platelet of dimensions 0.12 × 0.28 × 0.40 mm was selected for crystal structure determination. Intensity data were collected using a Nicolet *R3M/E* diffractometer. Cell parameters were obtained by a least-squares method using 25 centred reflections with $5.81 < 2\theta < 24.95°$. Data were collected within $1.5 < \theta < 30°$ using the ω-scan method and were corrected for Lorentz–polarization and absorption effects (transmission coefficients, minimum 0.456, maximum 0.691). The range for h was 0 to 16, for k 0 to 15 and for l −16 to 16. The intensity variation of a standard reflection (0,0,16) was ± 2% about the mean value. The main computer program used was *SHELXTL* (Sheldrick, 1983). Of the 3568 reflections measured, 3160 were independent; of these, 1608 were observed $[I > 3\sigma(I)]$ and were used in the refinement. The structure was solved by the heavy-atom method. Full-matrix least-squares refinement on F of positional and anisotropic thermal parameters of non-H atoms. 91 parameters were refined. Final $R = 0.059$, $wR = 0.056$, maximum $\Delta/\sigma = 0.001$, $w = [\sigma^2(F)]^{-1}$. Maximum, minimum $\Delta\rho$ values in final difference synthesis 0.75, $-0.66\,\text{e Å}^{-3}$. H atoms were placed in calculated positions and were assigned isotropic thermal parameters $U = 0.08\,\text{Å}^2$. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV).

Atomic fractional coordinates and equivalent isotropic thermal parameters for the non-H atoms are listed in Table 1.* Fig. 1 shows a view of the unit-cell contents. Bond lengths and angles are given in Table 2. Atomic numbering scheme and thermal ellipsoids for the non-H atoms are shown in Fig. 2.

Table 2. *Bond lengths* (Å) *and angles* (°)

E.s.d.'s in the least significant digits are given in parentheses.

Co—Cl(1)	2.273 (2)	Co—Cl(3)	2.258 (2)
Co—Cl(4)	2.278 (3)	Co—Cl(2)	2.282 (2)
N(11)—C(13)	1.493 (12)	C(12)—C(13)	1.538 (10)
C(12)—C(14)	1.550 (14)	C(14)—N(15)	1.507 (10)
Cl(1)—Co—Cl(3)	106.6 (1)	Cl(1)—Co—Cl(4)	106.8 (1)
Cl(3)—Co—Cl(4)	112.9 (1)	Cl(1)—Co—Cl(2)	110.8 (1)
Cl(3)—Co—Cl(2)	109.8 (1)	Cl(4)—Co—Cl(2)	109.9 (1)
C(13)—C(12)—C(14)	109.6 (6)	N(11)—C(13)—C(12)	109.3 (6)
C(12)—C(14)—N(15)	107.2 (6)		

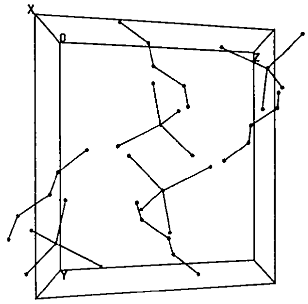

Fig. 1. View of the unit-cell contents.

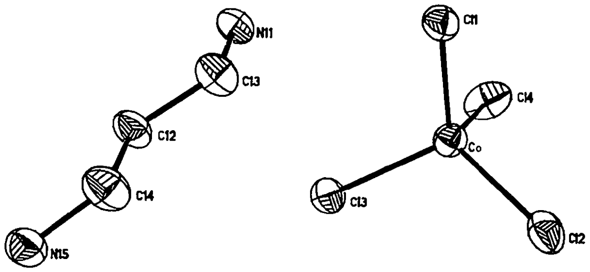

Fig. 2. Atomic numbering scheme and thermal ellipsoids for the non-H atoms.

Related literature. The structure of the title compound is similar to that of $[NH_3(CH_2)_3NH_3]ZnCl_4$ (Kallel, Fail, Fuess & Daoud, 1980). The tetrahedral $CoCl_4^{2-}$ anions are interconnected *via* hydrogen bonding to the 1,3-propanediammonium groups. However, the mean Co—Cl distance is a little less than the corresponding mean Zn—Cl bond length in $ZnCl_4^{2-}$. The $CoCl_4^{2-}$ tetrahedra show angles ranging from 106.6 (1) to 112.9 (1)° indicating a small distortion from tetrahedral symmetry resulting from hydrogen bonding.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54493 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: MU0180]