Related literature. The solid solution is isostructural with α-BaB_2O_4 (Mighell, Perloff & Block, 1966) and its structure is stable down to room temperature (Block, Perloff & Weir, 1964). Various other compounds $M$$Ba_2[B_3O_6]_2$ where M = Ca, Cd, Co, Ni and Mg have also been found and their structures (Liebertz & Fröhlich, 1984) also shown to be more closely related to α-BaB_2O_4 than to β-BaB_2O_4. The crystal structure of the solid solution of $Sr_xBa_{3-x}(B_3O_6)_2$ ($x = 1.16$) reported here enables us to define a similar relationship for $M$$Ba_2(B_3O_6)_2$ where M is an alkaline-earth metal.

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New Refinement of $LiCdPO_4$

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Abstract. Cadmium lithium phosphate, $M_r = 214.31$, orthorhombic, *Pnma*, but previously reported as $Pna2_1$ by the present authors [Elammari, Elouadi & Depmeier (1988). *Acta Cryst.* C**44**, 1357–1359], $a = 10.724\,(4)$, $b = 6.288\,(1)$, $c = 4.804\,(1)$ Å, $V = 323.9\,(1)$ Å^3, $Z = 4$, $D_x = 4.40$ g cm^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0.7107$ Å, $\mu = 70.4$ cm^{-1}, $F(000) = 392$, $T = 298$ K, $R = 0.0207$ for 759 independent reflections. The revised structure is less distorted but is otherwise comparable, with discrete PO_4 tetrahedra linked by distorted CdO_6 (c site symmetry m) and LiO_6 (b site symmetry 1) octahedra as described previously.

Experimental. X-ray diffraction data were collected under the conditions reported in Table 1. The refinement of the structure in both space groups, $Pna2_1$ and *Pnma*, gives comparable indicators in each ($R = 0.0182$ and $wR = 0.0172$ for $Pna2_1$; $R = 0.0207$ and $wR = 0.0214$ for *Pnma*). Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).

Related literature. New results of second-harmonic generation (SHG) tests performed with very sensitive equipment (Dougherty & Kurtz, 1976) on as-grown crystals suggest the centrosymmetric space group *Pnma*, since no SHG signal was detected (Williams, 1989). No significant difference is observed between the values of atomic coordinates and interatomic distances given in our former study (Elammari, Elouadi & Depmeier, 1988) and those shown in Tables 2† and 3. It is however surprising that the SHG test performed earlier gave a positive result. This was probably an artefact not related to $LiCdPO_4$.

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† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54492 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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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 *Pna*2$_1$ and 759 in *Pnma*
No. of parameters	64 in *Pna*2$_1$ 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 *Pna*2$_1$ 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* (× 10^4) *and temperature factors* (Å^2 × 10^3) (*e.s.d.'s are in parentheses and refer to the final digits quoted*)

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

	x	*y*	*z*	$U_{\rm eq}$
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*′).

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Structure of 1,3-Propanediammonium Tetrachlorocobaltate(II)

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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$^{\rm II}$ 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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