Tetragonal
$P4/mmm$
$a = 3.8827\,(10)$ Å
$c = 7.546\,(2)$ Å
$V = 113.75\,(5)$ Å$^3$
$Z = 1$
$D_x = 6.265$ Mg m$^{-3}$
$D_m$ not measured

Cell parameters from 22 reflections
$\theta = 21–50°$
$\mu = 29.4$ mm$^{-1}$
$T = 124\,(2)$ K
Irregular plate
0.30 × 0.20 × 0.01 mm
Lustrous black

*Data collection*

Siemens $P4$ four-circle diffractometer
$\omega$ scans
Absorption correction: $\psi$ scan (*XEMP*; Sheldrick, 1984)
$T_{\min} = 0.066$, $T_{\max} = 0.779$
682 measured reflections
254 independent reflections

245 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.0387$
$\theta_{\max} = 39.9°$
$h = -1 \rightarrow 7$
$k = -1 \rightarrow 7$
$l = -1 \rightarrow 13$
3 standard reflections every 97 reflections intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.064$
$S = 1.316$
254 reflections
17 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0370P)^2 + 0.0088P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 3.09$ e Å$^{-3}$
$\Delta\rho_{\min} = -3.08$ e Å$^{-3}$
Extinction correction: *SHELXL*96 (Sheldrick, 1996)
Extinction coefficient: 0.061 (8)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å$^2$)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $U_{\rm eq}$ |
|---|---|---|---|---|
| Ba | 1/2 | 1/2 | 0 | 0.01124 (15) |
| Y | 1/2 | 1/2 | 1/2 | 0.00696 (15) |
| Cu1† | 0 | 0 | 0.73395 (12) | 0.0134 (2) |
| Co1‡ | 0 | 0 | 0.73395 (12) | 0.0134 (2) |
| O1 | 0 | 0 | 0 | 0.0132 (8) |
| O2 | 1/2 | 0 | 0.6871 (4) | 0.0101 (4) |

† Site occupancy = 0.55 (3). ‡ Site occupancy = 0.45 (3).

Table 2. *Selected geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ba—O1 | 2.7455 (7) | Cu1—O2 | 1.9733 (7) |
| Ba—O2$^{\rm i}$ | 3.057 (2) | Cu1—O1$^{\rm ii}$ | 2.0075 (10) |
| Y—O2 | 2.4002 (16) | | |
| O2$^{\rm iii}$—Cu1—O2 | 159.34 (17) | Cu1$^{\rm v}$—O1—Cu1$^{\rm vi}$ | 180.0 |
| O2$^{\rm iv}$—Cu1—O2 | 88.16 (3) | Cu1$^{\rm vii}$—O2—Cu1 | 159.34 (17) |
| O2—Cu1—O1$^{\rm ii}$ | 100.33 (8) | | |

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

The composition of the mixed Cu,Co site was determined by refinement (Sheldrick, 1996) with common positional and displacement parameters and a total unit-cell content of 2 [Cu 1.10 (5), Co 0.90 (5)]. The final maximum difference peaks are less than 0.6 Å from the Ba atom and are expected to reflect errors introduced by the absorption correction and crystal quality. The $\psi$ scan absorption method (Sheldrick, 1984) was used because the crystal shape, and its smallest dimension, precluded accurate measurement and boundary-edge definitions.

Data collection: *XSCANS* (Fait, 1991). Cell refinement: *XSCANS*. Data reduction: *XSCANS* and *SHELXTL* (Sheldrick, 1984). Program(s) used to solve structure: *SHELXS*90 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*96 (Sheldrick, 1996). Molecular graphics: *STRUPLO* (Fischer *et al.*, 1990). Software used to prepare material for publication: *SHELXL*96 *CIFTAB*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1169). Services for accessing these data are described at the back of the journal.

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*Acta Cryst.* (1997). C**53**, 1730–1733

# The First Cadmium Rare Earth Borates $CdLn[B_5O_{10}]$ with Ln = La, Sm, Eu

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(*Received 22 January 1997; accepted 2 June 1997*)

## Abstract

Single crystals of the new compounds $CdLn[B_5O_{10}]$ ($Ln = La^{3+}$, $Sm^{3+}$, $Eu^{3+}$) were obtained in silver ampoules at 1073 K by using a $B_2O_3$ flux technique.

The compounds are isotypic with $CoSm[B_5O_{10}]$ and contain two-dimensional infinite $[B_5O_{10}]^{5-}$ ion chains. Three of five B sites are tetrahedrally coordinated. $Cd^{2+}$ occupies distorted $CdO_6$ polyhedra while $Ln^{3+}$ is tenfold coordinated by O atoms.

## Comment

The synthesis and crystal structure determinations of three different copper lanthanoid borates, $CuLn_2[B_2O_5]_2$ with Ln = $Tm^{3+}$ (Schaefer & Bluhm, 1995*b*), $Er^{3+}$ or $Lu^{3+}$ (Schaefer & Bluhm, 1995*e*), $CuLn_2[B_8O_{16}]$ with Ln = $Tb^{3+}$ (Schaefer & Bluhm, 1995*c*), and $CuLn[B_5O_{10}]$ with Ln = $Tb^{3+}$ (Schaefer & Bluhm, 1995*a*), $Tm^{3+}$ or $Lu^{3+}$ (Schaefer & Bluhm, 1995*d*), have been reported. In spite of having the same formula as $CuLn[B_5O_{10}]$, the $CoLn[B_5O_{10}]$ compounds with Ln = $La^{3+}$ (Abdullaev, Mamedov & Dzhafarov, 1975), $Nd^{3+}$ (Abdullaev, 1976), $Sm^{3+}$ (Abdullaev, Mamedov & Dzhafarov, 1974), $Ho^{3+}$ (Abdullaev *et al.*, 1978), $Y^{3+}$ (Abdullaev, Mamedov, Dzhafarov & Aliev, 1980) or $Yb^{3+}$ (Dzhafarov, Abdullaev & Mamedov, 1985), and $MgLa[B_5O_{10}]$ (Saubat, Vlasse & Fouassier, 1980) have a different crystal structure. Nickel forms two different lanthanoid borates: $NiHo_2[B_2O_5]_2$ (Bluhm & Wiesch, 1996), which is isotypic with the copper compound mentioned above, and $NiLn[B_5O_{10}]$ with Ln = $Nd^{3+}$ or $Gd^{3+}$ (Campa *et al.*, 1995), which belongs to the $CoLn[B_5O_{10}]$ type. The zinc lanthanoid borates $ZnLn[B_5O_{10}]$ with Ln = $Ce^{3+}$, $Nd^{3+}$ or $Tb^{3+}$ (Busche & Bluhm, 1996) are also isotypic with the $CoLn[B_5O_{10}]$ type. Prompted by the unexpected crystal structure of the nickel lanthanoid borates, we decided to investigate the behaviour of cadmium in lanthanoid borates.

The crystal structure analyses of the three title lanthaniod borates demonstrate that they belong to the $CoLn[B_5O_{10}]$ type. The structure contains a distorted octahedrally coordinated Cd site and a tenfold irregular O-atom polyhedron surrounding the lanthanoid site. Two edge-sharing $CdO_6$ octahedra form isolated $Cd_2O_{10}$ units, while lanthanoid polyhedra form chains along [010] *via* common edges. The asymmetric unit contains three tetrahedrally and two trigonally coordinated B-atom sites (Fig. 1). These units form infinite two-dimensional planes along [010] and $[10\bar{1}]$ (Fig. 2). The $BO_4$ tetrahedra form twelve- and four-membered polyhedra rings, and two-thirds of the two neighbouring tetrahedra are additionally connected *via* bridging $BO_3$ groups. The polyborate anions, connected *via* $Cd_2O_{10}$ units, form a framework with tunnels along [010] which are filled with $LnO_{10}$ polyhedra (Fig. 3).

The examples of nickel lanthanoid borates (mentioned above) show that the $CoLn[B_5O_{10}]$ type is only formed when lanthanoids with large ionic radii are employed. Holmium (Bluhm & Wiesch, 1996), which has a rather small ionic radius, forms a different crystal structure containing less nickel. Thus, it is not impossible that

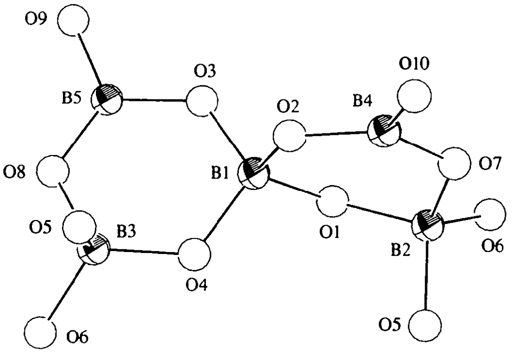

Fig. 1. The asymmetric unit of the title compounds contains three tetrahedrally and two trigonally coordinated B sites. Atoms are plotted with arbitrary isotropic radii.

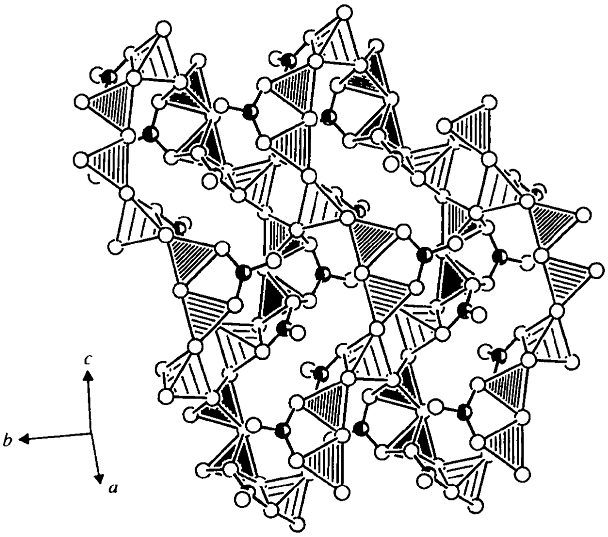

Fig. 2. The planar infinite borate anion $[B_5O_{10}]^{5-}$ forms four- and twelve-membered rings of tetrahedra (hatched).

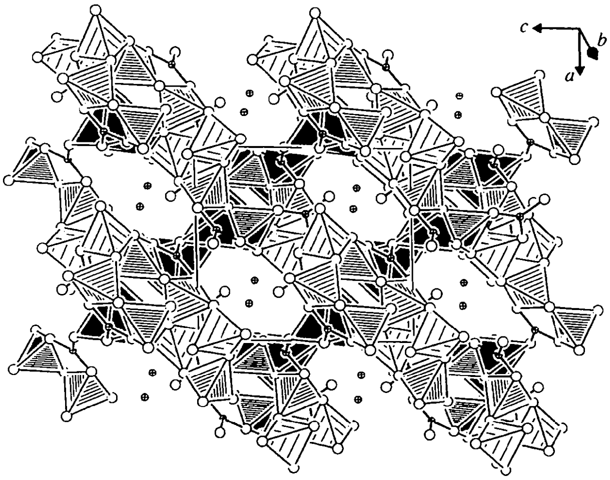

Fig. 3. The polyborate anions along $[10\bar{1}]$, connected *via* closely hatched $Cd_2O_{10}$ units, form a framework with tunnels along [010]. These are filled by the lanthanoid ions, represented as circles with crosses.

lanthanoids with smaller ionic radii might form different cadmium lanthanoid borate structures. Investigations into this are currently in progress.

## Experimental

Single crystals of the title compounds were obtained by using a $B_2O_3$ flux technique. A stoichiometric mixture of CdO and $Ln_2O_3$ and an excess of $B_2O_3$ were heated in a closed silver ampoule to 1073 K and allowed to stay at this temperature for two days. After the samples had been cooled to 573 K at a rate of 5 K $h^{-1}$, the resulting materials were extracted with warm water in order to remove the excess $B_2O_3$. The crystals exhibited irregular shapes. The major phases consisted of $CdB_4O_7$, as judged from powder diffraction (Siemens D500) (Ihara & Krogh-Moe, 1966).

### $CdLa[B_5O_{10}]$

*Crystal data*

$CdLa[B_5O_{10}]$
$M_r = 465.36$
Monoclinic
$P2_1/n$
$a = 8.7652\ (10)$ Å
$b = 7.8844\ (10)$ Å
$c = 9.640\ (2)$ Å
$\beta = 91.468\ (10)^\circ$
$V = 666.0\ (2)$ Å$^3$
$Z = 4$
$D_x = 4.641$ Mg m$^{-3}$
$D_m$ not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 5\text{–}15^\circ$
$\mu = 9.573$ mm$^{-1}$
$T = 293\ (2)$ K
Irregular
$0.1 \times 0.1 \times 0.05$ mm
Flesh coloured

*Data collection*

Siemens AED-2 diffractometer
$\omega\text{–}2\theta$ scans
Absorption correction: $\psi$ scan (*EMPIR*; Stoe & Cie, 1988)
$T_{min} = 0.289$, $T_{max} = 0.620$
3086 measured reflections
2938 independent reflections

2455 reflections with $I > 2\sigma(I)$
$R_{int} = 0.0347$
$\theta_{max} = 35.04^\circ$
$h = -14 \rightarrow 0$
$k = 0 \rightarrow 12$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 120 min
intensity decay: 0.2%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.061$
$S = 1.045$
2938 reflections
130 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.29$ e Å$^{-3}$
$\Delta\rho_{min} = -1.05$ e Å$^{-3}$
Extinction correction: *SHELXL93* (Sheldrick, 1993)
Extinction coefficient: 0.0151 (5)
Scattering factors from *International Tables for Crystallography* (Vol. C)

### $CdSm[B_5O_{10}]$

*Crystal data*

$CdSm[B_5O_{10}]$
$M_r = 476.85$
Monoclinic
$P2_1/n$
$a = 8.588\ (3)$ Å
$b = 7.8819\ (14)$ Å
$c = 9.583\ (2)$ Å
$\beta = 92.34\ (2)^\circ$
$V = 648.2\ (3)$ Å$^3$
$Z = 4$
$D_x = 4.887$ Mg m$^{-3}$
$D_m$ not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 5\text{–}15^\circ$
$\mu = 12.305$ mm$^{-1}$
$T = 293\ (2)$ K
Irregular
$0.1 \times 0.1 \times 0.1$ mm
Pale yellow

*Data collection*

Philips PW1100 diffractometer
$\omega\text{–}2\theta$ scans
Absorption correction: $\psi$ scan (*EMPIR*; Stoe & Cie, 1988)
$T_{min} = 0.052$, $T_{max} = 0.158$
2979 measured reflections
2828 independent reflections

2267 reflections with $I > 2\sigma(I)$
$R_{int} = 0.0186$
$\theta_{max} = 34.98^\circ$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 12$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 120 min
intensity decay: 0.2%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.090$
$S = 1.148$
2828 reflections
130 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.008$

$\Delta\rho_{max} = 2.93$ e Å$^{-3}$
$\Delta\rho_{min} = -2.98$ e Å$^{-3}$
Extinction correction: *SHELXL93* (Sheldrick, 1993)
Extinction coefficient: 0.00145 (8)
Scattering factors from *International Tables for Crystallography* (Vol. C)

### $CdEu[B_5O_{10}]$

*Crystal data*

$CdEu[B_5O_{10}]$
$M_r = 478.41$
Monoclinic
$P2_1/n$
$a = 8.5477\ (12)$ Å
$b = 7.881\ (2)$ Å
$c = 9.580\ (2)$ Å
$\beta = 92.53\ (2)^\circ$
$V = 644.7\ (2)$ Å$^3$
$Z = 4$
$D_x = 4.929$ Mg m$^{-3}$
$D_m$ not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 5\text{–}15^\circ$
$\mu = 12.990$ mm$^{-1}$
$T = 293\ (2)$ K
Irregular
$0.1 \times 0.1 \times 0.1$ mm
Yellow–orange

*Data collection*

Siemens AED-2 diffractometer
$\omega\text{–}2\theta$ scans
Absorption correction: $\psi$ scan (*EMPIR*; Stoe & Cie, 1988)
$T_{min} = 0.067$, $T_{max} = 0.161$
2988 measured reflections
2840 independent reflections

2200 reflections with $I > 2\sigma(I)$
$R_{int} = 0.0361$
$\theta_{max} = 35.02^\circ$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 12$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 120 min
intensity decay: 0.2%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.095$
$S = 0.989$
2840 reflections
130 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0640P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.009$
$\Delta\rho_{\max} = 4.14$ e Å$^{-3}$
$\Delta\rho_{\min} = -3.21$ e Å$^{-3}$
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.00055 (8)
Scattering factors from *International Tables for Crystallography* (Vol. C)

All data were processed and corrected for absorption (*EMPIR*; Stoe & Cie, 1988) on an IBM *RS*/6000 series computer. Electronic density residuals of 3–4 e Å$^{-3}$ in the case of CdSm[$B_5O_{10}$] and CdEu[$B_5O_{10}$] are within a distance of 1 Å from the heavy-atom peaks and are due to the irregular crystal shape and the absorption correction method.

For all compounds, data collection: *STADI*4 (Stoe & Cie, 1992); cell refinement: *STADI*4; data reduction: *STADI*4; program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *ORTEP* (Johnson, 1965); software used to prepare material for publication: *SHELXL*93.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1197). Services for accessing these data are described at the back of the journal.

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*Acta Cryst.* (1997). C**53**, 1733–1735

# Structure d'un Monophosphate Synthétique de Magnésium et de Sodium: $Mg_3Na_3(PO_4)_3$

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(*Reçu le 2 octobre 1996, accepté le 24 février 1997*)

## Abstract

The title compound, a new magnesium sodium phosphate, was prepared by hydrothermal methods. The structure is a monophosphate and contains three kinds of Mg—O polyhedra which form two types of infinite chains parallel to the [001] direction. These chains are connected with $PO_4$ tetrahedra by corner-sharing to form a framework. Na atoms occupy the interstices of the framework. The 1/3 substructure appears along the [010] direction.

## Commentaire

Cette étude a été réalisée dans le cadre de l'étude systématique des structures des monophosphates. Ghorbel, d'Yvoire & Dorémieux-Morin (1974) ont fait la synthèse de trois composés: $MgNa_4(PO_4)_2.H_2O$, $MgNa_4(PO_4)_2$ -$\alpha$ et -$\gamma$. Les relations structurales entre eux ont été étudiées par ces auteurs à l'aide de la diffraction des rayons X sur poudre à haute températures. Ben Amara, Vlasse, Olazcuaga, Le Flem & Hagenmuller (1983) ont déterminé la structure de $Mg_4Na(PO_4)_3$; Yamakawa, Yamada & Kawahara (1994) ont fait la détermination de la structure de $Mg_5Na_2(PO_4)_4$. Nous donnons dans cet article la structure d'une nouvelle phase obtenue par synthèse hydrothermale.

La structure appartient au groupe des monophosphates. Il existe trois sortes de Mg: Mg1 et Mg2 sont liés les uns après autre pour former les chaînes de la direction [001], et les polyèdres Mg3 forment aussi les chaînes. Les deux sortes de chaînes sont liées aux tétraèdres $PO_4$ en mettant en commun leurs sommets. Les polyèdres de Na se trouvent dans les interstices des polyèdres de Mg et P. La structure a un sous-réseau suivant [010], trois fois plus court que le réseau original. Le résultat de la détermination de la structure de notre composé est illustré par Fig. 1.

Les distances Mg—O moyennes correspondant aux trois sortes de polyèdres Mg sont 2,063, 2,153 et 2,052 Å, compatible aux résultats antérieurs [2,023, 2,076 et 2,080 Å (Ben Amara *et al.*, 1983); 2,102,

*Acta Crystallographica Section C*
ISSN 0108-2701 © 1997