

University of Groningen

Hexagonal LuMnO₃ revisited

van Aken, B.B.; Meetsma, Auke; Palstra, Thomas T.M.

Published in:
Acta Crystallographica Section E-Structure Reports Online

DOI:
[10.1107/S1600536801015896](https://doi.org/10.1107/S1600536801015896)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2001

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):
van Aken, B. B., Meetsma, A., & Palstra, T. T. M. (2001). Hexagonal LuMnO₃ revisited. *Acta Crystallographica Section E-Structure Reports Online*, 57, 1101 - 1103.
<https://doi.org/10.1107/S1600536801015896>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Hexagonal LuMnO₃ revisited

Bas B. van Aken, Auke Meetsma*
and Thomas T. M. Palstra

Solid State Chemistry Laboratory, Materials
Science Centre, University of Groningen,
Nijenborgh 4, NL-9747 AG Groningen, The
Netherlands.

Correspondence e-mail: a. meetsma@fwn.rug.nl

Key indicators

Single-crystal X-ray study

$T = 293$ K

Mean $\sigma(\text{Mn}-\text{O}) = 0.007$ Å

R factor = 0.027

wR factor = 0.065

Data-to-parameter ratio = 26.0

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The crystal structure of hexagonal LuMnO₃ at room temperature is isomorphous with YMnO₃ and deviates in important details from the early work of Yakel *et al.* [*Acta Cryst.* (1963), **16**, 957–962]. Mn is near the centre of its oxygen coordination environment. On the threefold axes, the apical O–Lu bonds have alternating long and short bond lengths, leading to ferroelectric behaviour. The sample studied was composed of almost equal volumes of inversion twins.

Comment

As part of a programme to investigate the origin of the ferroelectric behaviour in the hexagonal LnMnO₃ family, we have determined accurate structural parameters for single crystals of this series (Van Aken *et al.*, 2001a,b,c). Here we report the structure of LuMnO₃. Single-crystal growth of LuMnO₃ has frequently been reported (Yakel *et al.*, 1963; Bertaut *et al.*, 1963) and the structure was reported by Yakel *et al.* Our refinement shows small but significant differences from the work of Yakel *et al.* (1963), as discussed below. The hexagonal LnMnO₃ family has been described in great detail previously (Van Aken *et al.*, 2001d).

The M –O bond lengths are given in Table 1. The non-equivalent Mn–O atomic distances, both within the basal plane and to the apices, have smaller differences than in previous reports on LuMnO₃ (Yakel *et al.*, 1963). In-plane differences are 0.023 (7) Å (this work) and 0.09 Å (Yakel *et al.*, 1963), apical 0.031 (7) Å (this work) and 0.08 Å (Yakel *et al.*, 1963). As a result Mn is approximately in the centre of its oxygen environment. Likewise, the equatorial Lu–O1 and Lu–O2 bond lengths show less variation than the result of Yakel *et al.* (1963). Our data yield equatorial bond lengths of 2.227–2.294 Å, whereas Yakel *et al.* report 2.18–2.35 Å. The differences in apical bond distances of Lu1 and Lu2 are larger [1.192 (14) and 0.879 (10) Å] respectively, than those reported by Yakel *et al.* (0.84 and 0.96 Å).

Yakel *et al.* (1963) only measured reflections of one asymmetric hkl set, *i.e.* no Bijvoet pairs. Based on the observation of ferroelectricity (Bertaut *et al.*, 1963) and systematic absences, the non-centrosymmetric space group $P6_3cm$ was chosen. Our experiment included over 90% of the Friedel pairs and subsequent analysis confirmed this space group. Yakel *et al.* also discuss the possibility of the existence of domains with reversed polar direction. Our refinement indicated that our sample contained roughly equal volumes of twin domains.

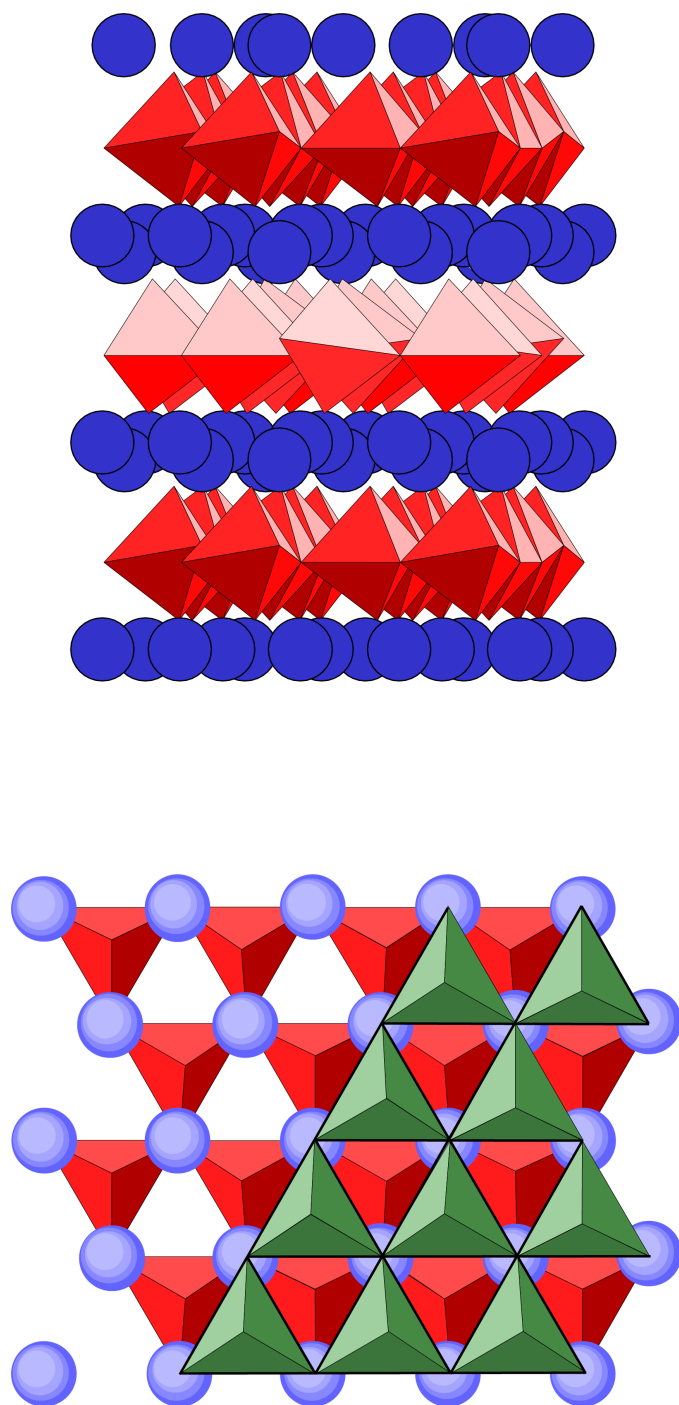
Experimental

Single crystals of LuMnO₃ were obtained using a flux method by weighing appropriate amounts of Lu₂O₃ and MnO₂ with Bi₂O₃ in a

Received 8 May 2001

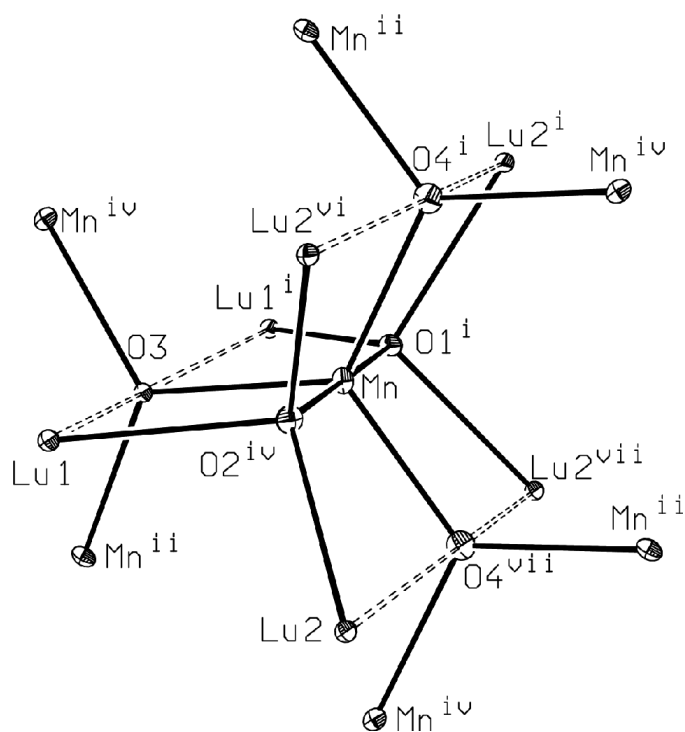
Accepted 26 September 2001

Online 27 October 2001


Figure 1

Schematic view of the crystallographic structure of LuMnO_3 . The top panel shows a view along the basal plane. Lu is represented by shaded spheres, and the MnO_5 clusters are represented by trigonal bipyramids. This panel highlights the two-dimensional nature of the structure. The lower panel depicts a view along the c -axis of two layers to show the stacking of the bipyramids.

1:12 ratio (Yakel *et al.*, 1963). The powders were thoroughly mixed and heated for 48 h at 1523 K in a Pt crucible. The crystals were separated from the flux by increasing the temperature to 1723 K and evaporating the Bi_2O_3 flux (Bertaut *et al.*, 1963).


Figure 2

Perspective ORTEPII (Johnson, 1976) drawing of all inequivalent atoms. All atoms are represented by atomic displacement ellipsoids drawn to encompass 50% of the electron density.

Crystal data

LuMnO_3
 $M_r = 277.90$
 Hexagonal, $P6_3cm$
 $a = 6.038 (1) \text{ \AA}$
 $c = 11.361 (1) \text{ \AA}$
 $V = 358.70 (9) \text{ \AA}^3$
 $Z = 6$
 $D_x = 7.719 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 Cell parameters from 22 reflections
 $\theta = 28.0\text{--}28.8^\circ$
 $\mu = 46.03 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Platelet, black
 $0.120 \times 0.100 \times 0.004 \text{ mm}$

Data collection

Enraf–Nonius CAD-4F diffractometer
 $\omega/2\theta$ scans
 Absorption correction: analytical (de Meulenaer & Tompa, 1965)
 $T_{\min} = 0.084$, $T_{\max} = 0.759$
 4711 measured reflections
 833 independent reflections
 610 reflections with $F > 4\sigma(F)$

$R_{\text{int}} = 0.094$
 $\theta_{\text{max}} = 40.0^\circ$
 $h = -10 \rightarrow 9$
 $k = 0 \rightarrow 10$
 $l = -20 \rightarrow 20$
 3 standard reflections
 frequency: 180 min
 intensity decay: none

Refinement

Refinement on F^2
 $R(F) = 0.027$
 $wR(F^2) = 0.065$
 $S = 1.05$
 833 reflections
 32 parameters
 $w = 1/[\sigma^2(F_o^2) + (0.0293P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 2.0 (4) \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -5.6 (4) \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick, 1997)
 Extinction coefficient: 0.0024 (2)

Table 1Selected geometric parameters (\AA , $^\circ$).

Lu1—O1	2.234 (9)	Lu2—O4 ⁱⁱ	3.279 (10)
Lu1—O2 ⁱ	2.294 (10)	Lu2—O2 ⁱⁱⁱ	2.277 (12)
Lu1—O3 ⁱ	2.244 (14)	Mn—O1	1.882 (7)
Lu1—O3	3.436 (14)	Mn—O2	1.859 (7)
Lu2—O1	2.227 (12)	Mn—O3	2.050 (6)
Lu2—O4	2.401 (10)	Mn—O4	2.019 (7)
O1—Mn—O2	179.6 (6)	O4—Mn—O4 ^{iv}	119.4 (3)
O1—Mn—O3	93.6 (5)	Mn—O3—Mn ^v	117.7 (3)
O1—Mn—O4	86.2 (5)	Mn—O4—Mn ^{vi}	118.8 (3)
O3—Mn—O4	120.2 (3)		

Symmetry codes: (i) $x - y, x, \frac{1}{2} + z$; (ii) $-1 - x + y, y, \frac{1}{2} + z$; (iii) $x - y - 1, x, \frac{1}{2} + z$; (iv) y, x, z ; (v) $-y, x - y, z$; (vi) $-1 - y, x - y, z$.

The space group is determined to be $P6_3cm$, taking into consideration the unit cell parameters, statistical analyses of intensity distributions and systematic extinctions ($h-hl: l \neq 2n$; $00l: l \neq 2n$). Attempts to fit the intensities with a crystal structure in space group $P6_3/mcm$ were unsuccessful. Anisotropic displacement parameters and *SHELXL97* indicated that the Lu ions should be shifted away from the mirror plane perpendicular to the c axis.

The integrated intensities were measured in 'flat mode' as the absorption is very large. In 'flat mode' every reflection is measured in the orientation that minimizes the path length through the crystal and thus the absorption. The minimum transmission factor is therefore larger than expected from the crystal size.

The structure was solved by using initial co-ordinates which were taken from a previous reported hexagonal manganite, YMnO_3 (Van Aken *et al.*, 2001a). The positional and anisotropic displacement parameters were refined.

The final difference Fourier map showed a peak of $2.0(4) \text{ e \AA}^{-3}$ near the Lu position and a hole of $5.7(4) \text{ e \AA}^{-3}$ also near the Lu position. No other significant peaks having chemical meaning above the general background (0.9 e \AA^{-3}) were observed in the final difference Fourier map.

The Flack parameter (Flack, 1983) of an initial refinement indicated that the crystal was twinned. Therefore an inversion twin was

added to the structure model, similar to the one reported for YMnO_3 (Van Aken *et al.*, 2001a). An initial attempt gave a twin fraction near 50%. We expect a 50%–50% distribution because this yields no net electrical polarization. We fixed the twin fraction at 50%, which had no significant influence on any other parameter.

Data collection: *CAD-4-UNIX Software* (Enraf–Nonius, 1994); cell refinement: *SET4* (de Boer & Duisenberg, 1984); data reduction: *HELENA* (Spek, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 2000); software used to prepare material for publication: *PLATON* (Spek, 2001).

This work is supported by the Netherlands Foundation for the Fundamental Research on Matter (FOM).

References

- Bertaut, E. F., Forrat, E. F. & Fang, P. (1963). *C. R. Acad. Sci.* **256**, 1958–1961.
- Boer, J. L. de & Duisenberg, A. J. M. (1984). *Acta Cryst.* **A40**, C410.
- Enraf–Nonius (1994). *CAD-4-UNIX Software*. Version 5.1 Utrecht modified version October 1994. Enraf–Nonius, Delft, The Netherlands.
- Farrugia, L. J. (2000). *J. Appl. Cryst.* **30**, 565.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Meulenaer, J. de & Tompa, H. (1965). *Acta Cryst.* **19**, 1014–1018.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (1997). *HELENA*. Utrecht University, The Netherlands.
- Spek, A. L. (2001). *PLATON*. Utrecht University, The Netherlands.
- Van Aken, B. B., Meetsma, A. & Palstra, T. T. M. (2001a). *Acta Cryst.* **C57**, 230–232.
- Van Aken, B. B., Meetsma, A. & Palstra, T. T. M. (2001b). *Acta Cryst.* **E57**, i38–i40.
- Van Aken, B. B., Meetsma, A. & Palstra, T. T. M. (2001c). *Acta Cryst.* **E57**, i87–i89.
- Van Aken, B. B., Meetsma, A. & Palstra, T. T. M. (2001d). *cond-mat/0106298*, available at xxx.lanl.gov.
- Yakel, H. L., Koehler, W. C., Bertaut, E. F. & Forrat, E. F. (1963). *Acta Cryst.* **16**, 957–962.

supporting information

Acta Cryst. (2001). E57, i101–i103 [doi:10.1107/S1600536801015896]

Hexagonal LuMnO₃ revisited

Bas B. Van Aken, Auke Meetsma and Thomas T. M. Palstra

S1. Comment

As part of a program to investigate the origin of the ferroelectric behaviour in the hexagonal LnMnO₃ family, we have determined accurate structural parameters for single crystals of this series (Van Aken *et al.*, 2001a,b,c). Here we report the structure of LuMnO₃. Single crystal growth of LuMnO₃ has frequently been reported (Yakel *et al.*, 1963; Bertaut *et al.*, 1963) and the structure was reported by Yakel *et al.* Our refinement shows small but significant differences from the work of Yakel *et al.* as discussed below. The hexagonal LnMnO₃ family has been described in great detail previously (Van Aken *et al.*, 2001 d).

The metal-oxygen bond lengths are given in Table 1. The non-equivalent Mn—O atomic distances, both within the basal plane and to the apices, have smaller differences than in previous reports on LuMnO₃ (Yakel *et al.*, 1963). In-plane differences are 0.023 (7) Å (this work) and 0.09 Å (Yakel *et al.*), apical 0.031 (7) Å (this work) and 0.08 Å (Yakel *et al.*). As a result the Mn is approximately in the centre of its oxygen environment. Likewise, the equatorial Lu—O1 and Lu—O2 bond lengths show less variation than Yakel *et al.*'s result. Our data yield equatorial bond lengths of 2.227–2.294 Å, whereas Yakel *et al.* report 2.18–2.35 Å. The differences in apical bond distances of Lu1 and Lu2 are larger [1.192 (14) and 0.879 (10) Å] respectively, than those reported by Yakel *et al.* (0.84 and 0.96 Å).

Yakel *et al.* (1963) only measured reflections of one asymmetric *hkl* set, *i.e.* no Bijvoet pairs. Based on the observation of ferroelectricity (Bertaut *et al.*, 1963) and systematic absences, the non-centrosymmetric space group P6₃cm was chosen. Our experiment included over 90% of the Friedel pairs and subsequent analysis confirmed this space group. Yakel *et al.* also discuss the possibility of the existence of domains with reversed polar direction. Our refinement indicated that our sample contained roughly equal volume of twin domains.

S2. Experimental

Single crystals LuMnO₃ were obtained using a flux method by weighing appropriate amounts of Lu₂O₃ and MnO₂ with Bi₂O₃ in a 1:12 ratio (Yakel *et al.*, 1963). The powders were thoroughly mixed and heated for 48 h at 1523 K in a Pt crucible. The crystals were separated from the flux by increasing the temperature to 1723 K and evaporating the Bi₂O₃ flux, (Bertaut *et al.*, 1963).

S3. Refinement

The space group is determined to be P6₃cm, taking into consideration the unit cell parameters, statistical analyses of intensity distributions and systematic extinctions (*h*-*h*l: $l \neq 2n$; 00 *l*: $l \neq 2n$). Attempts to fit the intensities with a crystal structure in space group P6₃/*mcm*, were unsuccessful. Anisotropic displacement parameters and *SHELXL97* indicated that the Lu ions should be shifted away from the mirror plane perpendicular to the *c* axis.

The integrated intensities were measured in 'flat mode' as the absorption is very large. In 'flat mode' every reflection is measured in the orientation that minimizes the path length through the crystal and thus the absorption. The minimum

transmission factor is therefore larger than expected from the crystal size.

The structure was solved by using initial co-ordinates which were taken from a previous reported hexagonal manganite, YMnO₃ (Van Aken *et al.*, 2001*a*). The positional and anisotropic displacement parameters were refined.

The final difference Fourier map showed a peak of 2.0 (4) e Å⁻³ near the Lu position and a hole of 5.7 (4) e Å⁻³ also near the Lu position. No other significant peaks having chemical meaning above the general background (0.9 e Å⁻³) were observed in the final difference Fourier map.

The Flack parameter (Flack, 1983) of an initial refinement indicated that the crystal was twinned. Therefore an inversion twin was added to the structure model, similar to the one reported for YMnO₃ (Van Aken *et al.*, 2001*a*). An initial attempt gave a twin fraction near 50%. We expect a 50%-50% distribution because this yields no net electrical polarization (Rao & Gopalakrishnan, 1997). We fixed the twin fraction at 50%, which had no significant influence on any other parameter.

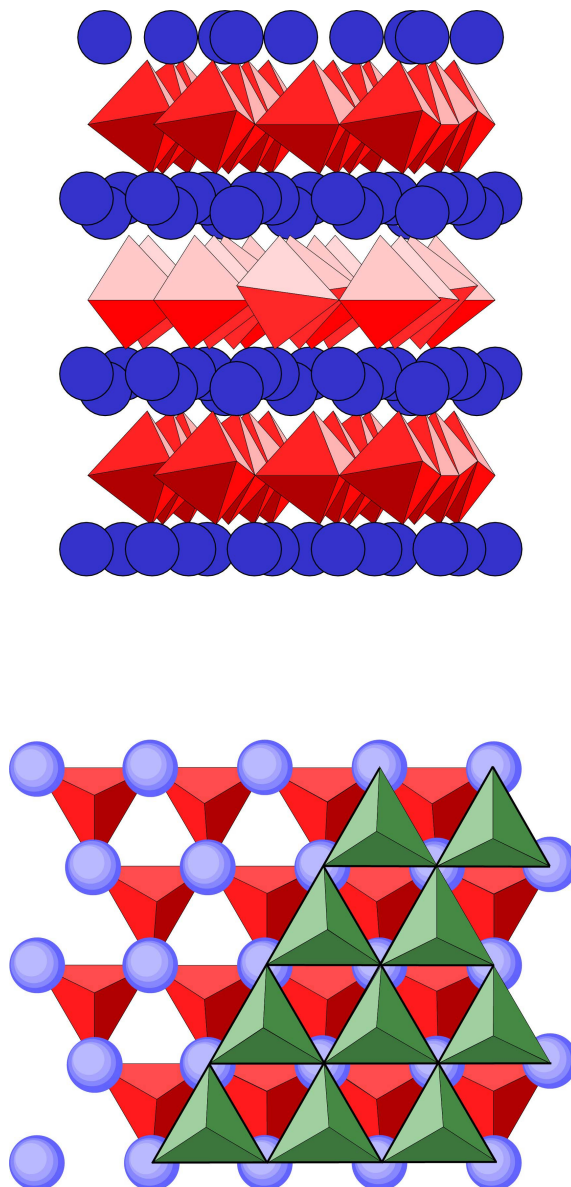
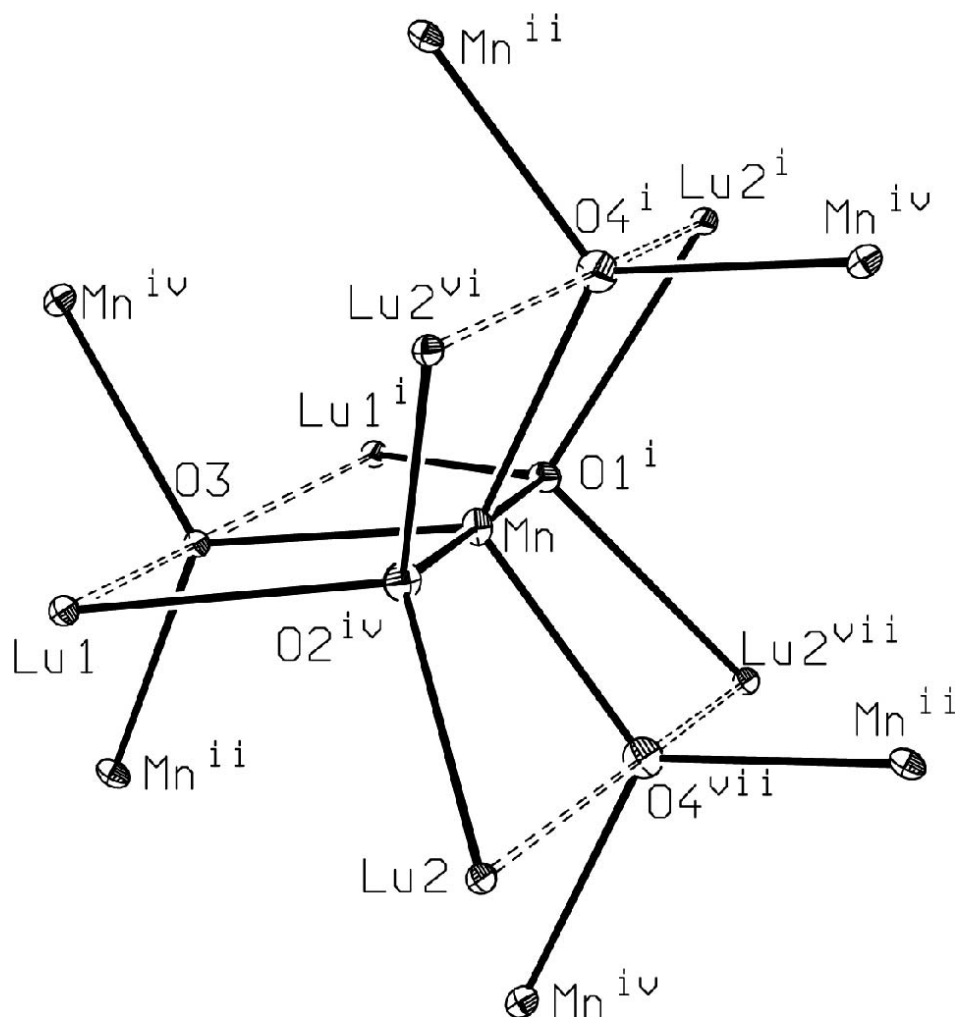


Figure 1

Schematic view of the crystallographic structure of LuMnO₃. The top panel shows a view along the basal plane. Lu is represented by shaded spheres, and the MnO₅ clusters are represented by trigonal bipyramids. This panel highlights the two-dimensional nature of the structure. The lower panel depicts a view along the *c* axis of two layers to show the stacking of the bipyramids.

**Figure 2**

Perspective *ORTEPII* (Johnson, 1976) drawing of all inequivalent atoms. All atoms are represented by atomic displacement ellipsoids drawn to encompass 50% of the electron density.

Lutetium Manganese Oxide

Crystal data

LuMnO₃
 $M_r = 277.90$
 Hexagonal, $P6_3cm$
 Hall symbol: P 6c -2
 $a = 6.038 (1) \text{ \AA}$
 $c = 11.361 (1) \text{ \AA}$
 $V = 358.70 (9) \text{ \AA}^3$
 $Z = 6$
 $F(000) = 720$

Unit cell parameters (Duisenberg, 1992. *J. Appl. Cryst.* 25, 92-96) and orientation matrix were determined from a least-squares treatment of SET4 (de Boer & Duisenberg, 1984) setting. Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did yield extra symmetry elements (Spek, 1988. *J. Appl. Cryst.* 21, 578-579; Le Page 1987. *J. Appl. Cryst.* 20, 264-269; Le Page, Y. 1988. *J. Appl. Cryst.* 21, 983-984), but they are not compatible with the structure.

$D_x = 7.719 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 22 reflections

$\theta = 28.0\text{--}28.8^\circ$
 $\mu = 46.03 \text{ mm}^{-1}$
 $T = 293 \text{ K}$

Platelet, black
 $0.12 \times 0.10 \times 0.004 \text{ mm}$

Data collection

Enraf Nonius CAD-4F
 diffractometer
 Radiation source: fine focus sealed Philips Mo
 tube
 Perpendicular mounted graphite
 monochromator
 $\omega/2\theta$ scans
 Absorption correction: analytical
 (Meulenaer & Tompa, 1965)
 $T_{\min} = 0.084$, $T_{\max} = 0.759$

4711 measured reflections
 833 independent reflections
 610 reflections with $F > 4\sigma(F)$
 $R_{\text{int}} = 0.094$
 $\theta_{\max} = 40.0^\circ$, $\theta_{\min} = 3.6^\circ$
 $h = -10 \rightarrow 9$
 $k = 0 \rightarrow 10$
 $l = -20 \rightarrow 20$
 3 standard reflections every 180 min
 intensity decay: no decay, variation 2.8%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.065$
 $S = 1.05$
 833 reflections
 32 parameters
 1 restraint
 0 constraints

$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 2.0 (4) \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -5.6 (4) \text{ e } \text{Å}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 1997), $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0024 (2)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Lu1	0.00000	0.00000	0.27394 (6)	0.00438 (12)
Lu2	-0.66667	-0.33333	0.23038 (2)	0.00460 (1)
Mn	-0.3355 (10)	-0.3355 (10)	-0.00077 (13)	0.0048 (5)
O1	-0.3070 (18)	-0.3070 (18)	0.1642 (6)	0.0053 (16)
O2	-0.3614 (17)	-0.3614 (17)	-0.1638 (6)	0.0068 (16)
O3	0.00000	0.00000	-0.0285 (12)	0.0034 (19)
O4	-0.66667	-0.33333	0.0190 (9)	0.0077 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Lu1	0.0044 (2)	0.0044 (2)	0.0043 (2)	0.0022 (1)	0.0000	0.0000
Lu2	0.0041 (1)	0.0041 (1)	0.0056 (2)	0.0021 (1)	0.0000	0.0000

Mn	0.0053 (14)	0.0053 (6)	0.0023 (3)	0.0016 (7)	-0.0005	-0.0005 (3)
O1	0.007 (3)	0.007 (3)	0.004 (2)	0.005 (3)	0.0015 (17)	0.0015 (17)
O2	0.006 (3)	0.006 (3)	0.007 (2)	0.002 (3)	-0.0018 (17)	-0.0018 (17)
O3	0.004 (2)	0.004 (2)	0.002 (5)	0.0019 (12)	0.0000	0.0000
O4	0.009 (3)	0.009 (3)	0.005 (4)	0.0045 (14)	0.0000	0.0000

Geometric parameters (Å, °)

Lu1—O1	2.234 (9)	Lu2—O2 ^{vii}	2.277 (12)
Lu1—O2 ⁱ	2.294 (10)	Lu2—O1 ^{viii}	2.227 (15)
Lu1—O3 ⁱ	2.244 (14)	Lu2—O2 ^{ix}	2.277 (9)
Lu1—O3	3.436 (14)	Lu2—O1 ^x	2.227 (11)
Lu1—O1 ⁱⁱ	2.234 (12)	Lu2—O2 ^v	2.277 (10)
Lu1—O2 ⁱⁱⁱ	2.294 (9)	Mn—O1	1.882 (7)
Lu1—O1 ^{iv}	2.234 (11)	Mn—O2	1.859 (7)
Lu1—O2 ^v	2.294 (12)	Mn—O3	2.050 (6)
Lu2—O1	2.227 (12)	Mn—O4	2.019 (7)
Lu2—O4	2.401 (10)	Mn—O4 ^{xi}	2.019 (6)
Lu2—O4 ^{vi}	3.279 (10)		
O1—Lu1—O2 ⁱ	77.1 (4)	O1 ^{viii} —Lu2—O2 ^v	76.8 (4)
O1—Lu1—O3 ⁱ	123.9 (2)	O1 ^x —Lu2—O2 ^{ix}	77.6 (4)
O1—Lu1—O1 ⁱⁱ	91.9 (4)	O2 ^{ix} —Lu2—O2 ^v	94.7 (3)
O1—Lu1—O2 ⁱⁱⁱ	164.0 (3)	O1 ^x —Lu2—O2 ^v	167.8 (3)
O1—Lu1—O1 ^{iv}	91.9 (4)	O1—Mn—O2	179.6 (6)
O1—Lu1—O2 ^v	77.1 (4)	O1—Mn—O3	93.6 (5)
O2 ⁱ —Lu1—O3 ⁱ	72.04 (18)	O1—Mn—O4	86.2 (5)
O1 ⁱⁱ —Lu1—O2 ⁱ	77.1 (5)	O1—Mn—O4 ^{xi}	86.2 (5)
O2 ⁱ —Lu1—O2 ⁱⁱⁱ	110.9 (4)	O2—Mn—O3	86.0 (5)
O1 ^{iv} —Lu1—O2 ⁱ	164.0 (3)	O2—Mn—O4	94.0 (5)
O2 ⁱ —Lu1—O2 ^v	110.9 (4)	O2—Mn—O4 ^{xi}	94.0 (5)
O1 ⁱⁱ —Lu1—O3 ⁱ	123.9 (2)	O3—Mn—O4	120.2 (3)
O2 ⁱⁱⁱ —Lu1—O3 ⁱ	72.04 (18)	O3—Mn—O4 ^{xi}	120.2 (3)
O1 ^{iv} —Lu1—O3 ⁱ	123.9 (2)	O4—Mn—O4 ^{xi}	119.4 (3)
O2 ^v —Lu1—O3 ⁱ	72.04 (19)	Lu1—O1—Lu2	104.2 (4)
O1 ⁱⁱ —Lu1—O2 ⁱⁱⁱ	77.1 (4)	Lu1—O1—Mn	129.2 (5)
O1 ⁱⁱ —Lu1—O1 ^{iv}	91.9 (5)	Lu1—O1—Lu2 ^{xi}	104.2 (4)
O1 ⁱⁱ —Lu1—O2 ^v	164.0 (3)	Lu2—O1—Mn	106.8 (5)
O1 ^{iv} —Lu1—O2 ⁱⁱⁱ	77.1 (4)	Lu2—O1—Lu2 ^{xi}	103.0 (4)
O2 ⁱⁱⁱ —Lu1—O2 ^v	110.9 (4)	Lu2 ^{xi} —O1—Mn	106.8 (4)
O1 ^{iv} —Lu1—O2 ^v	77.1 (5)	Lu1 ^{xii} —O2—Mn	103.1 (4)
O1—Lu2—O4	70.3 (2)	Lu2 ^{xii} —O2—Mn	123.9 (5)
O1—Lu2—O2 ^{vii}	167.8 (3)	Lu2 ^{xiii} —O2—Mn	123.9 (6)
O1—Lu2—O1 ^{viii}	109.2 (4)	Lu1 ^{xii} —O2—Lu2 ^{xii}	100.8 (4)
O1—Lu2—O2 ^{ix}	76.8 (3)	Lu1 ^{xii} —O2—Lu2 ^{xiii}	100.8 (3)
O1—Lu2—O1 ^x	109.2 (5)	Lu2 ^{xii} —O2—Lu2 ^{xiii}	99.9 (3)
O1—Lu2—O2 ^v	77.6 (4)	Lu1 ^{xii} —O3—Mn	98.8 (4)
O2 ^{vii} —Lu2—O4	121.9 (2)	Mn—O3—Mn ⁱⁱ	117.7 (3)

O1 ^{viii} —Lu2—O4	70.3 (2)	Mn—O3—Mn ^{iv}	117.7 (3)
O2 ^{ix} —Lu2—O4	121.87 (19)	Lu1 ^{xii} —O3—Mn ⁱⁱ	98.8 (4)
O1 ^x —Lu2—O4	70.27 (19)	Lu1 ^{xii} —O3—Mn ^{iv}	98.8 (4)
O2 ^v —Lu2—O4	121.9 (2)	Mn ⁱⁱ —O3—Mn ^{iv}	117.7 (4)
O1 ^{viii} —Lu2—O2 ^{vii}	77.6 (4)	Lu2—O4—Mn	96.4 (3)
O2 ^{vii} —Lu2—O2 ^{ix}	94.7 (3)	Lu2—O4—Mn ^{viii}	96.4 (3)
O1 ^x —Lu2—O2 ^{vii}	76.8 (4)	Lu2—O4—Mn ^x	96.4 (3)
O2 ^{vii} —Lu2—O2 ^v	94.7 (3)	Mn—O4—Mn ^{viii}	118.8 (3)
O1 ^{viii} —Lu2—O2 ^{ix}	167.8 (3)	Mn—O4—Mn ^x	118.8 (3)
O1 ^{viii} —Lu2—O1 ^x	109.2 (5)	Mn ^{viii} —O4—Mn ^x	118.8 (3)

Symmetry codes: (i) $x-y, x, z+1/2$; (ii) $-y, x-y, z$; (iii) $-x, -y, z+1/2$; (iv) $-x+y, -x, z$; (v) $y, -x+y, z+1/2$; (vi) $-x+y-1, y, z+1/2$; (vii) $x-y-1, x, z+1/2$; (viii) $-y-1, x-y, z$; (ix) $-x-1, -y-1, z+1/2$; (x) $-x+y-1, -x-1, z$; (xi) y, x, z ; (xii) $x-y, x, z-1/2$; (xiii) $-x+y-1, y, z-1/2$.