# Hexagonal YbMnO3 revisited

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_journal_volume     57
_journal_issue     10
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_publ_contact_author_name     'Dr A. Meetsma'
_publ_contact_author_address
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The Netherlands
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_publ_contact_author_email     a.meetsma@fwn.rug.nl
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The Netherlands.
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Unit cell parameters (Duisenberg, 1992) 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 not yield
extra symmetry elements (Spek, 1988; Le Page 1987, 1988)
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 Intensity data were corrected for Lorentz and polarisation effects, scale
 variation, for absorption and reduced to F~o~^2^
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    2 2 4
    2 0 2
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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\s(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.
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_refine_ls_weighting_scheme     calc
_refine_ls_weighting_details
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    Yb2  .33333  -.33333  .23061(3)  .00472(7) Uani 1.000 Yb
    Mn  .3333(5)  .00000  -.00194(14)  .0054(2) Uani 1.000 Mn
    O1  .3030(12)  .00000  .1617(6)  .0039(10) Uani 1.000 O
    O2  .3610(15)  .00000  -.1658(6)  .0074(11) Uani 1.000 O
    O3  .00000  .00000  -.0268(16)  .004(2) Uani 1.000 O
    O4  .33333  -.33333  .0192(9)  .0059(17) Uani 1.000 O
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    _atom_site_aniso_U_13
    _atom_site_aniso_U_23
    Yb1  .0047(2)  .0047(2)  .0035(2)  .00230(10)
                                                .0000  .0000
    Yb2  .00350(10)
                .00360(10)
                           .0071(2)  .00180(10)
                                                .0000  .0000
    Mn  .0069(4)  .0048(4)  .0039(2)  .0024(6)  .0002(3)  .0000
    O1  .0050(14)  .0017(18)  .0041(19)  .0009(9)  -.0019(15)  .0000
    O2  .014(2)  .0001(18)  .0033(17)  .0000(9)  .0002(19)  .0000
    O3  .003(2)  .003(2)  .005(6)  .0016(10)  .0000  .0000
    O4  .009(3)  .009(3)  .000(3)  .0047(13)  .0000  .0000
_geom_special_details
;
 Bond distances, angles etc. have been calculated using the rounded fractional
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 estimation of distances, angles and torsion angles
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    Yb1 Mn . 2_555 3.254(3) no
    Yb1 O2 . 2_555 2.294(8) yes
    Yb1 O3 . 2_555 2.269(18) yes
    Yb1 O3 . 1_555 3.409(18) yes
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    Yb1 O1 . 5_555 2.231(7) no
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    Yb1 Yb2 . 7_545 3.5313(4) no
    Yb1 Yb2 . 7_555 3.5313(4) no
    Yb1 Yb2 . 7_655 3.5313(4) no
    Yb2 O1 . . 2.257(5) yes
    Yb2 O4 . . 2.401(10) yes
    Yb2 O4 . 10_555 3.277(10) yes
    Yb2 O2 . 2_545 2.270(8) yes
    Yb2 O1 . 3_545 2.257(6) no
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```
    Mn O1 . . 1.867(7) yes
    Mn O2 . . 1.868(7) yes
    Mn O3 . . 2.039(4) yes
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    O1 Yb1 O2 . . 4_555 162.9(3) no
    O1 Yb1 O1 . . 5_555 90.9(2) no
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    O2 Yb1 O3 2_555 . 2_555 72.47(18) no
    O1 Yb1 O2 3_555 . 2_555 77.2(3) no
    O2 Yb1 O2 2_555 . 4_555 111.3(2) no
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    O2 Yb1 O2 2_555 . 6_555 111.3(3) no
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```

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O3 Mn O4 . . . 120.54(8) yes
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Yb1 O1 Yb2 . . . 103.8(2) no
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