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Evidence for differentiation in the iron-helicoidal chain in GdFe3(BO3)(4)

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# CIF-file generated for B2Fe1.50Gd0.50O6                    CP843C
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data_global
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 SHELXL97-2 & Manual Editing
;
_audit_update_record
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;

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# 1. SUBMISSION DETAILS

_publ_contact_author_name           # Name  of author for correspondence
;
   Drs. A. Meetsma
;
_publ_contact_author_address        # Address of author for correspondence
;
     Crystal Structure Center,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;
_publ_contact_author_email           A.Meetsma@fwn.rug.nl
_publ_contact_author_fax             '+31 50 3634441'
_publ_contact_author_phone           '+31 50 3634368'

_publ_requested_journal              'Acta Crystallographica B'
# Publication choise FI FM FO CI CM CO
_publ_requested_category             ?
_publ_requested_coeditor_name        ?

_publ_contact_letter                # Include date of submission
;
 Date of submission :  2005-01-27  13:10:20

 Consider this CIF submission for deposition of the low temperature
 X-ray structure of a manuscript to be submitted to : Acta Cryst B
  (Our Compound_Identification_Code : CP843C)
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# 2. PROCESSING SUMMARY (JOURNAL OFFICE ONLY)

_journal_date_recd_electronic        ?

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_journal_date_from_coeditor          ?
_journal_date_accepted               ?

_journal_date_printers_first         ?
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_journal_date_printers_final         ?
_journal_date_proofs_out             ?
_journal_date_proofs_in              ?

_journal_coeditor_name               ?
_journal_coeditor_code               ?
_journal_coeditor_notes
; ?
;

_journal_techeditor_code             ?
_journal_techeditor_notes
; ?
;

_journal_coden_ASTM                  ?
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_journal_year                        ?
_journal_volume                      ?
_journal_issue                       ?
_journal_page_first                  ?
_journal_page_last                   ?


_journal_suppl_publ_number           ?
_journal_suppl_publ_pages            ?


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# 3. TITLE AND AUTHOR LIST

_publ_section_title
;
 ?
;
_publ_section_title_footnote
;
 ?
;

# The loop structure below should contain the names and adresses of all
# authors, in the required order of publication. Repeat as necessary.


loop_
_publ_author_name
_publ_author_footnote
_publ_author_address

   'Meetsma, Auke'
;
 ? # author related footnote
;
;
     Crystal Structure Center,
     Inorganic Solid State Chemistry Laboratory
     Chemical Physics,
     Materials Science Center,
     Groningen University,
     Nijenborgh 4,
     NL-9747 AG Groningen,
     The Netherlands.
;

#=============================================================================
```

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# 4. TEXT

_publ_section_synopsis
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 ?
;
_publ_section_abstract
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 ?
;

# Insert blank lines between paragraphs

_publ_section_comment
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;
_publ_section_exptl_prep
;
 ?
;
_publ_section_exptl_refinement
;
 ?
;

# Insert blank lines between references

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;
 Altomare, A., Burla, M.C., Camalli, M., Cascarano, G.L., Giacovazzo, C.
   Guagliardi, A., Moliterni, A.G.G., Polidori, G. & Spagna, R.
   (1999). J. Appl. Cryst. 32, 115-119.


 Bruker, (2000). SMART, SAINT, SADABS, XPREP and  SHELXTL/NT.
  Software Reference Manual Bruker AXS Inc. Madison, Wisconsin, USA.

 Cremer, D. & Pople, J.A. (1975). J. Am. Chem. Soc. 97, 1354-1358.

 Flack, H.D. & Bernardinelli, G. (1999). Acta Cryst. A55, 908-915.

 Flack, H.D. & Bernardinelli, G. (2000). J. Appl. Cryst. 33, 1143-1148.

 Farrugia, L.J. (1997). J. Appl. Cryst. 30, 565.
  ORTEP-3 for Windows, Version 1.076. (2003)
  Department of Chemistry, Univ. of Glasgow, Scotland, UK

 International Tables for Crystallography (1983). Vol. A.
   Space-group symmetry, edited by T. Hahn. Dordrecht: Reidel.
   (Present distributor Kluwer Academic Publishers, Dordrecht).

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   Edited by A.J.C Wilson, Kluwer Academic Publishers,
   Dordrecht, The Netherlands.

 Le Page, Y. (1987). J. Appl. Cryst. 20, 264-269.

 Le Page, Y. (1988). J. Appl. Cryst. 21, 983-984.

 Meetsma, A. (2003). Extended version of the program PLUTO.
   Groningen University, The Netherlands. (unpublished).

 Sheldrick, G.M. SHELXL97. Program for Crystal Structure
   Refinement. University of G\"ottingen, Germany, 1997.
```

Spek, A.L. (1987). Acta Cryst. C43, 1233-1235.

Spek, A.L. (1988). J. Appl. Cryst. 21, 578-579.

Spek, A.L. (1990). Acta Cryst. A46, C-34.

Spek, A.L. (1994). Am. Crystallogr. Assoc.-Abstracts, 22, 66.
;

_publ_section_figure_captions
;
Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level.
;

#==

5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety
'B4 Fe3 Gd O12'
Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)3, (C6 N6 Cr 3-)2, 2(H2 O)'
_chemical_formula_structural ?
_chemical_formula_sum
'B4 Fe3 Gd O12'
_chemical_formula_iupac ?
_chemical_formula_weight 560.04
_chemical_compound_source 'see text'

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
O O 0.0106 0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Gd Gd -0.1653 3.9035
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Fe Fe 0.3463 0.8444
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
B B 0.0013 0.0007
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#==

6. CRYSTAL DATA

_symmetry_cell_setting Trigonal
_symmetry_space_group_name_Hall 'P 31 2"'
_symmetry_space_group_name_H-M 'P 31 2 1'
_symmetry_Int_Tables_number 152

```
loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -y,x-y,1/3+z
 -x+y,-x,2/3+z
 y,x,-z
 -x,-x+y,1/3-z
 x-y,-y,2/3-z

_cell_length_a                          9.5305(3)
_cell_length_b                          9.5305(3)
_cell_length_c                          7.5479(2)
_cell_angle_alpha                         90
_cell_angle_beta                          90
_cell_angle_gamma                        120
_cell_volume                            593.73(3)
_cell_formula_units_Z                 3

_cell_measurement_temperature    297(1)
_cell_measurement_reflns_used      5439
_cell_measurement_theta_min        3.66
_cell_measurement_theta_max       38.55
_cell_special_details
;
 The final unit cell was obtained from the xyz centroids of
   5439 reflections after integration using the SAINT software
   package (Bruker, 2000).
;

_exptl_crystal_description       'broken_block'
_exptl_crystal_colour            'light_green'
_exptl_crystal_size_max           0.22
_exptl_crystal_size_mid           0.15
_exptl_crystal_size_min           0.11
_exptl_crystal_size_rad           ?
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     4.699
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              774
_exptl_absorpt_coefficient_mu     13.737
_exptl_absorpt_correction_type    'Analytical'
_exptl_absorpt_process_details    'Bruker, 2000'
_exptl_absorpt_correction_T_min   0.0620
_exptl_absorpt_correction_T_max   0.2513

#===============================================================================

# 7. EXPERIMENTAL DATA

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; ?
;
_diffrn_ambient_temperature            90(1)
_diffrn_radiation_wavelength          0.71073
_diffrn_radiation_type               'MoK\a'
_diffrn_radiation_source             'fine focus sealed Siemens Mo tube '
_diffrn_radiation_monochromator      'parallel mounted graphite'
_diffrn_radiation_detector
;
  CCD area-detector
;
_diffrn_measurement_device_type
;
  Bruker Smart Apex
;
```

```
_diffrn_measurement_method           'phi and omega scans'
_diffrn_special_details
;
 Crystal into the cold nitrogen stream of the low-temparature unit
   (KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean     '4096x4096 / 62x62 (binned 512)'

_diffrn_standards_number             ?
_diffrn_standards_interval_count     ?
_diffrn_standards_interval_time      ?

loop_
_diffrn_standard_refln_index_h
_diffrn_standard_refln_index_k
_diffrn_standard_refln_index_l
 ? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number              13868
_diffrn_reflns_av_R_equivalents    0.0338
_diffrn_reflns_av_sigmaI/netI      0.0189
_diffrn_reflns_limit_h_min         -16
_diffrn_reflns_limit_h_max         16
_diffrn_reflns_limit_k_min         -16
_diffrn_reflns_limit_k_max         16
_diffrn_reflns_limit_l_min         -13
_diffrn_reflns_limit_l_max         13
_diffrn_reflns_theta_min           2.47
_diffrn_reflns_theta_max           38.58
_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.999

_diffrn_reflns_reduction_process
;
 Intensity data were corrected for Lorentz and polarization
  effects, decay and absorption and reduced to F~o~^2^
  using SAINT (Bruker, 2000)
;

# number of unique reflections
_reflns_number_total               2217
_reflns_number_gt                  1956
_reflns_threshold_expression       I>2\s(I)


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_computing_data_reduction           'XPREP, Bruker Version 5.1/NT, 2000'
_computing_structure_solution
;
 SIR-97 (Altomare et al., 1997)
;
_computing_structure_refinement      'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
 PLUTO (Meetsma, 2003)
 ORTEP (Farrugia, 1997; Johnson et al., 2000)
 PLATON (Spek, 1994)
;
_computing_publication_material      'PLATON (Spek, 1990)'

#=============================================================================

# 8. REFINEMENT DATA
```

```
_refine_special_details
;
 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^ > 2sigma(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.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0312P)^2^+0.0P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      heavy
_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    ?
_refine_ls_hydrogen_treatment     ?
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0359(10)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_abs_structure_details
;
  Enantiomorph twin refinement resulted in 0.50(1) so ultimately set to 0.5
   Flack, H.D. & Bernardinelli, G. (1999, 2000)
;
_chemical_absolute_configuration  ad

_refine_ls_abs_structure_Flack    0.5
_refine_ls_number_reflns          2217
_refine_ls_number_parameters      95
_refine_ls_number_restraints      0
_refine_ls_number_constraints     ?
_refine_ls_R_factor_all           0.0187
_refine_ls_R_factor_gt            0.0167
_refine_ls_wR_factor_ref          0.0452
_refine_ls_wR_factor_gt           0.0443
_refine_ls_goodness_of_fit_ref    0.855
_refine_ls_restrained_S_all       0.855
_refine_ls_shift/su_max           0.003
_refine_ls_shift/su_mean          0.000

_refine_diff_density_max          0.816
_refine_diff_density_min         -0.512
_refine_diff_density_rms          0.101


_vrn_publ_code_squeezed_elec        0.0
_vrn_publ_code_void_volume          0.0
_vrn_publ_code_frame_time_sec      10.0
_vrn_publ_code_meas_time_hour      16.0

#===============================================================================

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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_atom_site_type_symbol
_atom_site_thermal_displace_type
_atom_site_fract_x
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_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_U_iso_or_equiv
_atom_site_calc_flag
_atom_site_refinement_flags
Gd1 Gd Uani -0.33342(1) -0.33342(1) 0.00000 1.000 0.0041(1) . .
Fe1 Fe Uani 0.11536(5) 0.11536(5) 0.00000 1.000 0.0036(1) . .
Fe2 Fe Uani -0.21410(6) -0.54975(4) 0.34154(2) 1.000 0.0037(1) . .
O1 O Uani 0.00000 -0.07819(15) 0.16667 1.000 0.0072(3) . .
O2 O Uani -0.5832(2) -0.27090(13) 0.13774(12) 1.000 0.0069(2) . .
O3 O Uani -0.1194(3) -0.30445(16) -0.17980(18) 1.000 0.0057(3) . .
O4 O Uani -0.1467(3) -0.36234(16) 0.18479(18) 1.000 0.0058(2) . .
O5 O Uani 0.4755(2) 0.1451(2) -0.15980(8) 1.000 0.0057(3) . .
O6 O Uani 0.1877(2) 0.00000 -0.16667 1.000 0.0053(3) . .
O7 O Uani -0.5235(3) -0.53811(17) -0.18533(18) 1.000 0.0056(2) . .
B1 B Uani 0.33204(14) 0.00000 -0.16667 1.000 0.0045(5) . .
B2 B Uani -0.4473(4) -0.1201(3) 0.15617(14) 1.000 0.0053(3) . .
B3 B Uani 0.00000 -0.2223(3) 0.16667 1.000 0.0049(4) . .

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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Gd1 0.0041(1) 0.0041(1) 0.0041(1) 0.0001(1) -0.0001(1) 0.0021(1)
Fe1 0.0036(1) 0.0036(1) 0.0036(1) 0.0001(1) -0.0001(1) 0.0017(1)
Fe2 0.0035(1) 0.0036(1) 0.0038(1) 0.0001(1) 0.0000(1) 0.0017(1)
O1 0.0081(6) 0.0054(4) 0.0089(4) 0.0012(2) 0.0024(4) 0.0040(3)
O2 0.0058(3) 0.0062(3) 0.0081(3) 0.0012(3) -0.0014(3) 0.0025(3)
O3 0.0062(4) 0.0040(5) 0.0065(4) 0.0006(3) 0.0007(3) 0.0023(4)
O4 0.0054(4) 0.0045(4) 0.0067(4) 0.0007(3) -0.0003(3) 0.0019(4)
O5 0.0051(4) 0.0050(4) 0.0063(5) 0.0007(3) -0.0003(3) 0.0019(5)
O6 0.0044(4) 0.0058(6) 0.0062(5) -0.0019(5) -0.0010(2) 0.0029(3)
O7 0.0047(4) 0.0063(4) 0.0064(4) -0.0008(3) -0.0001(3) 0.0033(4)
B1 0.0042(8) 0.0048(9) 0.0046(11) 0.0009(5) 0.0004(2) 0.0024(4)
B2 0.0050(6) 0.0067(7) 0.0055(5) 0.0004(5) 0.0001(4) 0.0040(4)
B3 0.0018(8) 0.0061(6) 0.0055(7) 0.0004(3) 0.0008(6) 0.0009(4)

#===============================================================================

# 10. MOLECULAR GEOMETRY

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

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_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
 Gd1     O3       2.3485(18)                    .       .                 yes
 Gd1     O4       2.3830(18)                    .       .                 yes
 Gd1     O7       2.3474(15)                    .       .                 yes
 Gd1     B2         2.985(3)                    .       .                 yes
```

```
 Gd1     O3       2.3485(16)                    .     4_555                yes
 Gd1     O4       2.3830(16)                    .     4_555                yes
 Gd1     O7       2.3474(16)                    .     4_555                yes
 Gd1     B2         2.985(3)                    .     4_555                yes
 Fe1     O1       2.0411(10)                    .       .                  yes
 Fe1     O6       2.0061(12)                    .       .                  yes
 Fe1     O3         1.958(2)                    .     2_555                yes
 Fe1     O6        2.0061(9)                    .     2_555                yes
 Fe1     O1       2.0411(10)                    .     3_554                yes
 Fe1     O3       1.9583(14)                    .     6_554                yes
 Fe2     O4       1.9635(14)                    .       .                  yes
 Fe2     O5         2.025(2)                    .     2_545                yes
 Fe2     O7         1.971(3)                    .     3_545                yes
 Fe2     O5         2.017(2)                    .     3_555                yes
 Fe2     O2       2.0332(16)                    .     5_445                yes
 Fe2     O2       2.0490(10)                    .     6_545                yes
 O1      B3         1.373(3)                    .       .                  yes
 O2      B2         1.379(3)                    .       .                  yes
 O3      B2         1.370(3)                    .     4_555                yes
 O4      B3         1.374(3)                    .       .                  yes
 O5      B1       1.3761(19)                    .       .                  yes
 O6      B1         1.376(2)                    .       .                  yes
 O7      B2         1.360(5)                    .     3_444                yes

loop_
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_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
 O3      Gd1     O4         72.36(6)            .       .       .          yes
 O3      Gd1     O7         90.99(6)            .       .       .          yes
 O3      Gd1     B2        137.60(6)            .       .       .          yes
 O3      Gd1     O3        120.92(5)            .       .     4_555        yes
 O3      Gd1     O4         89.54(6)            .       .     4_555        yes
 O3      Gd1     O7        140.62(6)            .       .     4_555        yes
 O3      Gd1     B2         26.49(5)            .       .     4_555        yes
 O4      Gd1     O7        124.29(5)            .       .       .          yes
 O4      Gd1     B2        113.24(5)            .       .       .          yes
 O3      Gd1     O4         89.54(5)          4_555     .       .          yes
 O4      Gd1     O4        143.21(5)            .       .     4_555        yes
 O4      Gd1     O7         86.70(6)            .       .     4_555        yes
 O4      Gd1     B2         60.35(5)            .       .     4_555        yes
 O7      Gd1     B2        114.15(7)            .       .       .          yes
 O3      Gd1     O7        140.62(7)          4_555     .       .          yes
 O4      Gd1     O7         86.70(5)          4_555     .       .          yes
 O7      Gd1     O7         73.47(5)            .       .     4_555        yes
 O7      Gd1     B2         81.11(7)            .       .     4_555        yes
 O3      Gd1     B2         26.49(7)          4_555     .       .          yes
 O4      Gd1     B2         60.35(5)          4_555     .       .          yes
 O7      Gd1     B2         81.11(6)          4_555     .       .          yes
 B2      Gd1     B2        161.73(7)            .       .     4_555        yes
 O3      Gd1     O4         72.36(5)          4_555     .     4_555        yes
 O3      Gd1     O7         90.99(5)          4_555     .     4_555        yes
 O3      Gd1     B2        137.60(6)          4_555     .     4_555        yes
 O4      Gd1     O7        124.29(6)          4_555     .     4_555        yes
 O4      Gd1     B2        113.24(5)          4_555     .     4_555        yes
 O7      Gd1     B2        114.15(6)          4_555     .     4_555        yes
 O1      Fe1     O6         93.94(3)            .       .       .          yes
 O1      Fe1     O3         86.00(7)            .       .     2_555        yes
 O1      Fe1     O6         77.53(5)            .       .     2_555        yes
 O1      Fe1     O1         87.69(3)            .       .     3_554        yes
 O1      Fe1     O3        167.95(9)            .       .     6_554        yes
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O3	Fe1	O6	92.67(7)	2_555	.	.	yes
O6	Fe1	O6	168.27(6)	.	.	2_555	yes
O1	Fe1	O6	77.53(5)	3_554	.	.	yes
O3	Fe1	O6	94.71(6)	6_554	.	.	yes
O3	Fe1	O6	94.71(6)	2_555	.	2_555	yes
O1	Fe1	O3	167.95(8)	3_554	.	2_555	yes
O3	Fe1	O3	101.96(10)	2_555	.	6_554	yes
O1	Fe1	O6	93.94(5)	3_554	.	2_555	yes
O3	Fe1	O6	92.67(8)	6_554	.	2_555	yes
O1	Fe1	O3	86.00(6)	3_554	.	6_554	yes
O4	Fe2	O5	94.90(7)	.	.	2_545	yes
O4	Fe2	O7	100.45(7)	.	.	3_545	yes
O4	Fe2	O5	92.35(7)	.	.	3_555	yes
O2	Fe2	O4	91.99(6)	5_445	.	.	yes
O2	Fe2	O4	168.53(8)	6_545	.	.	yes
O5	Fe2	O7	90.43(9)	2_545	.	3_545	yes
O5	Fe2	O5	167.41(9)	2_545	.	3_555	yes
O2	Fe2	O5	76.55(8)	5_445	.	2_545	yes
O2	Fe2	O5	95.92(7)	6_545	.	2_545	yes
O5	Fe2	O7	98.38(9)	3_555	.	3_545	yes
O2	Fe2	O7	162.76(8)	5_445	.	3_545	yes
O2	Fe2	O7	83.30(7)	6_545	.	3_545	yes
O2	Fe2	O5	92.94(8)	5_445	.	3_555	yes
O2	Fe2	O5	76.33(6)	6_545	.	3_555	yes
O2	Fe2	O2	86.82(6)	5_445	.	6_545	yes
Fe1	O1	B3	129.38(5)	.	.	.	yes
Fe1	O1	Fe1	101.24(5)	.	.	2_555	yes
Fe1	O1	B3	129.38(7)	2_555	.	.	yes
Fe2	O2	B2	128.74(13)	5_455	.	.	yes
Fe2	O2	B2	124.47(10)	6_445	.	.	yes
Fe2	O2	Fe2	102.46(6)	5_455	.	6_445	yes
Gd1	O3	Fe1	121.40(8)	.	.	3_554	yes
Gd1	O3	B2	103.63(13)	.	.	4_555	yes
Fe1	O3	B2	134.71(15)	3_554	.	4_555	yes
Gd1	O4	Fe2	122.30(8)	.	.	.	yes
Gd1	O4	B3	106.58(10)	.	.	.	yes
Fe2	O4	B3	130.89(13)	.	.	.	yes
Fe2	O5	B1	127.32(10)	2_554	.	.	yes
Fe2	O5	B1	128.71(9)	3_654	.	.	yes
Fe2	O5	Fe2	103.91(8)	2_554	.	3_654	yes
Fe1	O6	B1	128.15(4)	.	.	.	yes
Fe1	O6	Fe1	103.71(9)	.	.	3_554	yes
Fe1	O6	B1	128.15(5)	3_554	.	.	yes
Gd1	O7	Fe2	117.67(9)	.	.	2_444	yes
Gd1	O7	B2	113.03(12)	.	.	3_444	yes
Fe2	O7	B2	129.29(13)	2_444	.	3_444	yes
O5	B1	O6	119.41(10)	.	.	.	yes
O5	B1	O5	121.21(17)	.	.	6_554	yes
O5	B1	O6	119.38(12)	6_554	.	.	yes
Gd1	B2	O2	73.87(12)	.	.	.	yes
Gd1	B2	O7	150.31(12)	.	.	2_455	yes
Gd1	B2	O3	49.88(10)	.	.	4_555	yes
O2	B2	O7	119.6(3)	.	.	2_455	yes
O2	B2	O3	115.6(2)	.	.	4_555	yes
O3	B2	O7	124.9(2)	4_555	.	2_455	yes
O1	B3	O4	117.55(13)	.	.	.	yes
O1	B3	O4	117.6(2)	.	.	5_555	yes
O4	B3	O4	124.9(2)	.	.	5_555	yes

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_geom_torsion_atom_site_label_1
_geom_torsion_atom_site_label_2
_geom_torsion_atom_site_label_3
_geom_torsion_atom_site_label_4
_geom_torsion
_geom_torsion_site_symmetry_1

_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion_publ_flag

O4	Gd1	O3	Fe1	-126.76(9)	.	.	.	3_554	no
O4	Gd1	O3	B2	58.28(12)	.	.	.	4_555	no
O7	Gd1	O3	Fe1	107.39(9)	.	.	.	3_554	no
O7	Gd1	O3	B2	-67.57(12)	.	.	.	4_555	no
B2	Gd1	O3	Fe1	-21.35(13)	.	.	.	3_554	no
B2	Gd1	O3	B2	163.69(11)	.	.	.	4_555	no
O3	Gd1	O4	Fe2	-127.20(9)	.	.	.	.	no
O3	Gd1	O4	B3	57.76(10)	.	.	.	.	no
O7	Gd1	O4	Fe2	-48.43(11)	.	.	.	.	no
O7	Gd1	O4	B3	136.53(9)	.	.	.	.	no
B2	Gd1	O4	Fe2	97.83(9)	.	.	.	.	no
B2	Gd1	O4	B3	-77.21(11)	.	.	.	.	no
O3	Gd1	O4	Fe2	110.00(9)	4_555	.	.	.	no
O3	Gd1	O4	B3	-65.04(10)	4_555	.	.	.	no
O4	Gd1	O4	Fe2	168.87(7)	4_555	.	.	.	no
O4	Gd1	O4	B3	-6.17(15)	4_555	.	.	.	no
O7	Gd1	O4	Fe2	18.98(8)	4_555	.	.	.	no
O7	Gd1	O4	B3	-156.07(10)	4_555	.	.	.	no
B2	Gd1	O4	Fe2	-101.31(10)	4_555	.	.	.	no
B2	Gd1	O4	B3	83.65(11)	4_555	.	.	.	no
O3	Gd1	O7	Fe2	25.80(7)	.	.	.	2_444	no
O3	Gd1	O7	B2	-155.03(12)	.	.	.	3_444	no
O4	Gd1	O7	Fe2	-43.40(9)	.	.	.	2_444	no
O4	Gd1	O7	B2	135.77(12)	.	.	.	3_444	no
B2	Gd1	O7	Fe2	170.60(6)	.	.	.	2_444	no
B2	Gd1	O7	B2	-10.22(13)	.	.	.	3_444	no
O3	Gd1	B2	O2	153.06(8)	.	.	.	.	no
O3	Gd1	B2	O7	31.1(4)	.	.	.	2_455	no
O3	Gd1	B2	O3	-60.72(13)	.	.	.	4_555	no
O4	Gd1	B2	O2	-118.03(8)	.	.	.	.	no
O4	Gd1	B2	O7	120.0(3)	.	.	.	2_455	no
O4	Gd1	B2	O3	28.20(13)	.	.	.	4_555	no
O7	Gd1	B2	O2	31.78(9)	.	.	.	.	no
O7	Gd1	B2	O7	-90.2(4)	.	.	.	2_455	no
O7	Gd1	B2	O3	178.01(10)	.	.	.	4_555	no
O3	Gd1	B2	O2	-146.23(14)	4_555	.	.	.	no
O4	Gd1	B2	O2	102.65(10)	4_555	.	.	.	no
O7	Gd1	B2	O2	-35.53(8)	4_555	.	.	.	no
O3	Gd1	O3	B2	136.72(11)	.	.	4_555	.	no
O4	Gd1	O3	B2	-154.27(11)	.	.	4_555	.	no
O7	Gd1	O3	B2	-2.87(15)	.	.	4_555	.	no
O4	Gd1	B2	O3	-111.13(14)	.	.	4_555	.	no
O7	Gd1	B2	O3	110.69(12)	.	.	4_555	.	no
O6	Fe1	O1	B3	8.13(11)	.	.	.	.	no
O1	Fe1	O6	B1	-93.24(3)	.	.	.	.	no
O5	Fe2	O4	Gd1	98.55(10)	2_545	.	.	.	no
O5	Fe2	O4	B3	-87.73(16)	2_545	.	.	.	no
O7	Fe2	O4	Gd1	-170.11(9)	3_545	.	.	.	no
O7	Fe2	O4	B3	3.61(17)	3_545	.	.	.	no
O5	Fe2	O4	Gd1	-71.13(10)	3_555	.	.	.	no
O5	Fe2	O4	B3	102.58(16)	3_555	.	.	.	no
O2	Fe2	O4	Gd1	21.89(9)	5_445	.	.	.	no
O2	Fe2	O4	B3	-164.40(15)	5_445	.	.	.	no
O4	Fe2	O7	B2	10.8(2)	.	.	3_545	2_555	no
O4	Fe2	O2	B2	-69.01(16)	.	.	5_445	5_445	no
Fe1	O1	B3	O4	-133.57(9)	.	.	.	.	no
Fe2	O2	B2	Gd1	-119.34(12)	5_455	.	.	.	no
Fe2	O2	B2	O7	31.78(19)	5_455	.	.	2_455	no
Fe2	O2	B2	O3	-147.46(11)	5_455	.	.	4_555	no
Fe2	O2	B2	Gd1	88.25(12)	6_445	.	.	.	no
Fe2	O2	B2	O7	-120.64(14)	6_445	.	.	2_455	no
Fe2	O2	B2	O3	60.13(18)	6_445	.	.	4_555	no

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 Gd1     O4      B3      O1         43.05(8)     .       .       .       .   no
 Gd1     O4      B3      O4       -136.96(9)     .       .       .     5_555 no
 Fe2     O4      B3      O1       -131.41(12)    .       .       .       .   no
 Fe2     O4      B3      O4         48.59(17)    .       .       .     5_555 no
 Fe2     O5      B1      O6       -55.03(12)   2_554     .       .       .   no
 Fe2     O5      B1      O6       128.13(12)   3_654     .       .       .   no
 Fe1     O6      B1      O5        -50.40(3)     .       .       .       .   no

#===END of Crystallographic Information File
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