Supplementary information

Synthesis and magnetothermal properties of a ferromagnetically coupled Ni^{II}-Gd^{III}-Ni^{II} cluster

Apoorva Upadhyay,[a] Navatha Komatireddy,[a] Alberto Ghirri,[b] Floriana Tuna,[c] Stuart K. Langley,[d] Anant K. Srivastava,[e] E. Carolina Sañudo,[f] Boujemaa Moubaraki,[d] Keith S. Murray,[d] Eric J. L. McInnes,[c] Marco Affronte, *[b] and Maheswaran Shanmugam*[a]

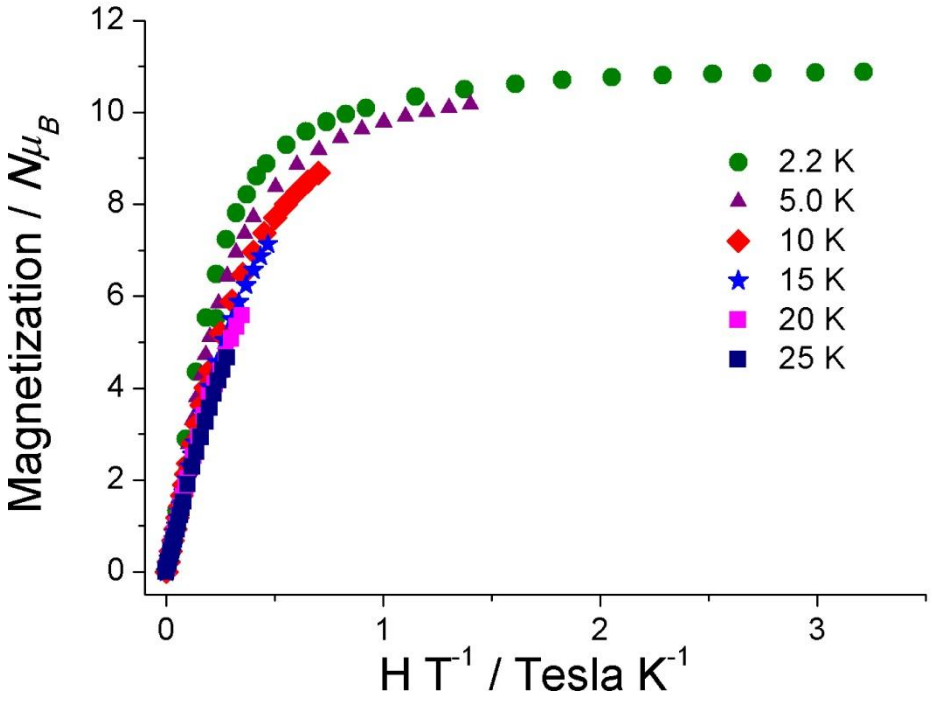

Figure S1. Reduced magnetization plot of **1** for the selected temperature sets indicated in the plot.

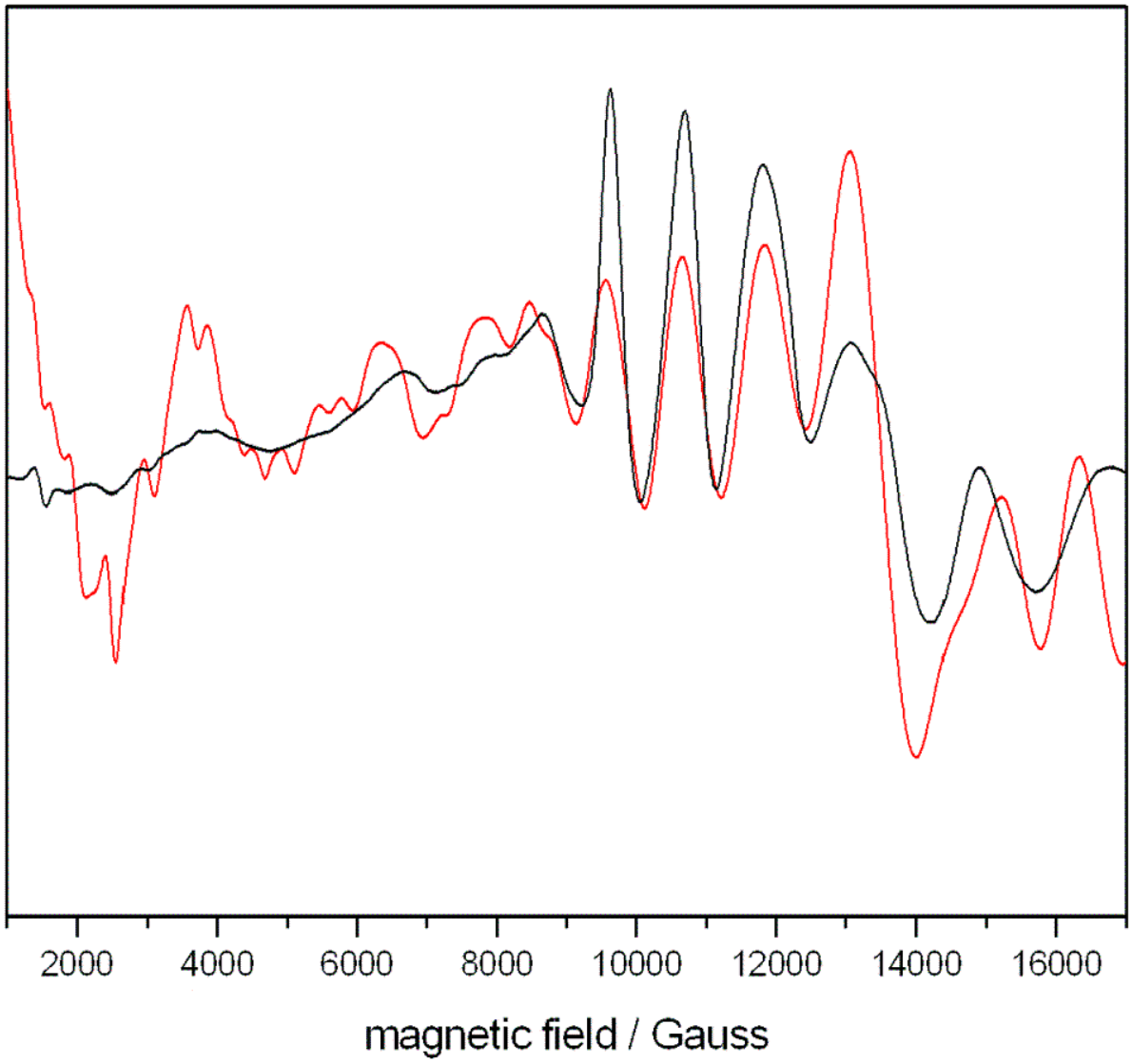

Figure S2. Frozen solution Q-band EPR spectrum of **1** in DCM (black) and the calculated spectrum (red) using the parameters given in the text recorded at 5.0 K.

Crystallographic information file

```
data_trial2_sq

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C84 H72 Gd N7 Ni2 O15'
_chemical_formula_weight          1694.16

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ni'  'Ni'   0.3393   1.1124
 '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'

_symmetry_cell_setting            Monoclinic
_symmetry_space_group_name_H-M    C2/c
```

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

_cell_length_a                 22.8250(18)
_cell_length_b                 23.4590(18)
_cell_length_c                 18.6760(14)
_cell_angle_alpha               90.00
_cell_angle_beta               120.296(2)
_cell_angle_gamma               90.00
_cell_volume                   8634.4(11)
_cell_formula_units_Z           4
_cell_measurement_temperature   100(2)
_cell_measurement_reflns_used   9914
_cell_measurement_theta_min     2.32
_cell_measurement_theta_max     28.34

_exptl_crystal_description      Needle
_exptl_crystal_colour           Green
_exptl_crystal_size_max         0.18
_exptl_crystal_size_mid         0.12
_exptl_crystal_size_min         0.09
_exptl_crystal_density_meas     ?
_exptl_crystal_density_diffrn   1.303
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000            3460
_exptl_absorpt_coefficient_mu   1.254
_exptl_absorpt_correction_type  'Multi-scan'
_exptl_absorpt_correction_T_min 0.8057
_exptl_absorpt_correction_T_max 0.8955
_exptl_absorpt_process_details  SADABS
```

```
_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature       100(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Bruker APEX-II CCD'
_diffrn_measurement_method        '\f and \w scans'
_diffrn_detector_area_resol_mean  ?
_diffrn_reflns_number             75627
_diffrn_reflns_av_R_equivalents   0.0555
_diffrn_reflns_av_sigmaI/netI     0.0347
_diffrn_reflns_limit_h_min        -30
_diffrn_reflns_limit_h_max        28
_diffrn_reflns_limit_k_min        -31
_diffrn_reflns_limit_k_max        31
_diffrn_reflns_limit_l_min        -15
_diffrn_reflns_limit_l_max        24
_diffrn_reflns_theta_min          1.35
_diffrn_reflns_theta_max          28.34
_reflns_number_total              10760
_reflns_number_gt                 8775
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Bruker APEX2'
_computing_cell_refinement        'Bruker SAINT'
_computing_data_reduction         'Bruker SAINT'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

_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.

Counter anion is disordered heavily which has been modelled using several restraints such as DFIX, FLAT, SIMU and DELU.

Disordered Solvent molecules could not be modelled, hence PLATON/SQUZEE routine was used and the SQUZEE void contains total of 594 electrons for four molecules.

Hence for one molecule it is 148.5 electron which is accounted for 8.25 molecules of MeOH. However, corresponding atom contents of this solvent was not added in atom site formula.
;

_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^)+(0.0585P)^2^+11.6241P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment mixed
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 10760
_refine_ls_number_parameters 544
_refine_ls_number_restraints 98
_refine_ls_R_factor_all 0.0463
_refine_ls_R_factor_gt 0.0365
_refine_ls_wR_factor_ref 0.1052
_refine_ls_wR_factor_gt 0.1009

_refine_ls_goodness_of_fit_ref 1.066
_refine_ls_restrained_S_all 1.091
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Gd1 Gd 0.5000 0.096861(7) 0.2500 0.01478(6) Uani 1 2 d S . .
Ni1 Ni 0.651787(15) 0.097189(13) 0.265851(19) 0.01221(8) Uani 1 1 d . . .
N1 N 0.7089(3) 0.1723(3) -0.0453(3) 0.102(3) Uani 0.50 1 d PDU . .
O3 O 0.6471(4) 0.1754(4) -0.0685(7) 0.051(3) Uani 0.25 1 d PDU A 1
O2 O 0.7320(6) 0.1286(5) -0.0609(11) 0.143(5) Uani 0.25 1 d PDU A 1
O1 O 0.7477(6) 0.2128(5) -0.0063(10) 0.136(5) Uani 0.25 1 d PDU . 1
O1A O 0.7671(5) 0.1788(8) -0.0350(14) 0.163(6) Uani 0.25 1 d PDU A 2
O3A O 0.6749(8) 0.2148(5) -0.0474(9) 0.097(4) Uani 0.25 1 d PDU A 2
O2A O 0.6847(9) 0.1232(4) -0.0534(14) 0.180(7) Uani 0.25 1 d PDU A 2
N11 N 0.71913(11) 0.02746(9) 0.31851(14) 0.0161(4) Uani 1 1 d . . .
N31 N 0.72356(11) 0.16080(9) 0.33651(14) 0.0165(4) Uani 1 1 d . . .
N51 N 0.66216(11) 0.10445(9) 0.15945(14) 0.0165(4) Uani 1 1 d . . .
O21 O 0.57415(9) 0.03968(7) 0.22214(11) 0.0147(3) Uani 1 1 d . . .
O22 O 0.45861(9) -0.00929(8) 0.15354(11) 0.0166(4) Uani 1 1 d . . .
O31 O 0.61920(9) 0.10297(7) 0.34981(11) 0.0142(3) Uani 1 1 d . . .
O32 O 0.55451(9) 0.09401(8) 0.42790(11) 0.0164(4) Uani 1 1 d . . .
O51 O 0.56754(9) 0.14792(7) 0.20547(11) 0.0147(3) Uani 1 1 d . . .
O52 O 0.46230(9) 0.20864(8) 0.16454(12) 0.0199(4) Uani 1 1 d . . .
C11 C 0.63530(13) -0.04803(11) 0.24322(16) 0.0164(5) Uani 1 1 d . . .

C12 C 0.62994(14) -0.10762(11) 0.22780(17) 0.0191(5) Uani 1 1 d . . .
H12 H 0.6701 -0.1296 0.2473 0.023 Uiso 1 1 calc R . .
C13 C 0.56807(15) -0.13418(11) 0.18538(17) 0.0212(6) Uani 1 1 d . . .
H13 H 0.5658 -0.1739 0.1746 0.025 Uiso 1 1 calc R . .
C14 C 0.50797(14) -0.10256(11) 0.15772(17) 0.0185(5) Uani 1 1 d . . .
H14 H 0.4650 -0.1208 0.1291 0.022 Uiso 1 1 calc R . .
C15 C 0.51227(13) -0.04487(11) 0.17267(15) 0.0149(5) Uani 1 1 d . . .
C16 C 0.57544(13) -0.01549(10) 0.21322(15) 0.0139(5) Uani 1 1 d . . .
C17 C 0.70227(13) -0.02474(11) 0.29513(16) 0.0167(5) Uani 1 1 d . . .
H17 H 0.7387 -0.0512 0.3146 0.020 Uiso 1 1 calc R . .
C18 C 0.79093(13) 0.03606(11) 0.37456(16) 0.0181(5) Uani 1 1 d . . .
C19 C 0.81299(14) 0.05308(12) 0.45552(17) 0.0213(6) Uani 1 1 d . . .
H19 H 0.7813 0.0580 0.4738 0.026 Uiso 1 1 calc R . .
C20 C 0.88171(15) 0.06295(14) 0.50966(18) 0.0270(6) Uani 1 1 d . . .
H20 H 0.8969 0.0750 0.5649 0.032 Uiso 1 1 calc R . .
C21 C 0.92831(15) 0.05512(15) 0.4829(2) 0.0311(7) Uani 1 1 d . . .
H21 H 0.9752 0.0619 0.5200 0.037 Uiso 1 1 calc R . .
C22 C 0.90620(15) 0.03757(15) 0.4027(2) 0.0304(7) Uani 1 1 d . . .
H22 H 0.9380 0.0322 0.3847 0.036 Uiso 1 1 calc R . .
C23 C 0.83762(14) 0.02768(13) 0.34815(18) 0.0233(6) Uani 1 1 d . . .
H23 H 0.8226 0.0153 0.2931 0.028 Uiso 1 1 calc R . .
C24 C 0.39212(13) -0.03010(12) 0.09526(17) 0.0225(6) Uani 1 1 d . . .
H24A H 0.3903 -0.0403 0.0433 0.034 Uiso 1 1 calc R . .
H24B H 0.3585 -0.0004 0.0845 0.034 Uiso 1 1 calc R . .
H24C H 0.3822 -0.0639 0.1182 0.034 Uiso 1 1 calc R . .
C31 C 0.71141(13) 0.15510(11) 0.45995(16) 0.0170(5) Uani 1 1 d . . .
C32 C 0.74012(14) 0.17580(12) 0.54217(17) 0.0215(6) Uani 1 1 d . . .
H32 H 0.7825 0.1951 0.5667 0.026 Uiso 1 1 calc R . .
C33 C 0.70818(15) 0.16867(12) 0.58720(17) 0.0227(6) Uani 1 1 d . . .
H33 H 0.7287 0.1823 0.6426 0.027 Uiso 1 1 calc R . .
C34 C 0.64485(14) 0.14102(11) 0.55098(16) 0.0196(5) Uani 1 1 d . . .
H34 H 0.6217 0.1370 0.5811 0.023 Uiso 1 1 calc R . .
C35 C 0.61666(12) 0.11980(11) 0.47172(16) 0.0148(5) Uani 1 1 d . . .
C36 C 0.64937(13) 0.12501(10) 0.42456(15) 0.0145(5) Uani 1 1 d . . .
C37 C 0.74316(13) 0.17216(11) 0.41300(17) 0.0192(5) Uani 1 1 d . . .
H37 H 0.7833 0.1944 0.4420 0.023 Uiso 1 1 calc R . .
C38 C 0.76180(14) 0.18920(12) 0.30541(17) 0.0197(5) Uani 1 1 d . . .
C39 C 0.72821(16) 0.22889(12) 0.24178(18) 0.0249(6) Uani 1 1 d . . .

H39 H 0.6818 0.2374 0.2215 0.030 Uiso 1 1 calc R . .
C40 C 0.76305(18) 0.25579(13) 0.20831(19) 0.0327(7) Uani 1 1 d . . .
H40 H 0.7403 0.2827 0.1649 0.039 Uiso 1 1 calc R . .
C41 C 0.83142(18) 0.24340(15) 0.2383(2) 0.0356(8) Uani 1 1 d . . .
H41 H 0.8548 0.2612 0.2143 0.043 Uiso 1 1 calc R . .
C42 C 0.86466(16) 0.20562(15) 0.3021(2) 0.0341(7) Uani 1 1 d . . .
H42 H 0.9114 0.1980 0.3231 0.041 Uiso 1 1 calc R . .
C43 C 0.83013(15) 0.17802(13) 0.33673(18) 0.0257(6) Uani 1 1 d . . .
H43 H 0.8534 0.1519 0.3812 0.031 Uiso 1 1 calc R . .
C44 C 0.52480(14) 0.07295(12) 0.47437(17) 0.0207(5) Uani 1 1 d . . .
H44A H 0.5549 0.0445 0.5144 0.031 Uiso 1 1 calc R . .
H44B H 0.4808 0.0554 0.4365 0.031 Uiso 1 1 calc R . .
H44C H 0.5183 0.1046 0.5039 0.031 Uiso 1 1 calc R . .
C51 C 0.58189(14) 0.18462(12) 0.09538(17) 0.0202(5) Uani 1 1 d . . .
C52 C 0.56139(16) 0.22621(14) 0.03188(19) 0.0287(7) Uani 1 1 d . . .
H52 H 0.5834 0.2280 0.0003 0.034 Uiso 1 1 calc R . .
C53 C 0.51035(16) 0.26369(14) 0.0157(2) 0.0310(7) Uani 1 1 d . . .
H53 H 0.4986 0.2923 -0.0253 0.037 Uiso 1 1 calc R . .
C54 C 0.47522(15) 0.26019(13) 0.05899(19) 0.0261(6) Uani 1 1 d . . .
H54 H 0.4389 0.2856 0.0466 0.031 Uiso 1 1 calc R . .
C55 C 0.49410(14) 0.21940(11) 0.11994(17) 0.0200(5) Uani 1 1 d . . .
C56 C 0.54985(13) 0.18259(11) 0.14241(16) 0.0168(5) Uani 1 1 d . . .
C57 C 0.63385(14) 0.14452(12) 0.10480(16) 0.0196(5) Uani 1 1 d . . .
C58 C 0.71212(13) 0.07294(12) 0.15028(16) 0.0179(5) Uani 1 1 d . . .
C59 C 0.70420(14) 0.01484(12) 0.13358(16) 0.0199(5) Uani 1 1 d . . .
H59 H 0.6657 -0.0045 0.1284 0.024 Uiso 1 1 calc R . .
C60 C 0.75256(15) -0.01492(13) 0.12440(18) 0.0264(6) Uani 1 1 d . . .
H60 H 0.7467 -0.0545 0.1123 0.032 Uiso 1 1 calc R . .
C61 C 0.80948(16) 0.01290(14) 0.13283(19) 0.0293(7) Uani 1 1 d . . .
H61 H 0.8430 -0.0078 0.1278 0.035 Uiso 1 1 calc R . .
C62 C 0.81723(16) 0.07129(14) 0.1487(2) 0.0298(7) Uani 1 1 d . . .
H62 H 0.8560 0.0905 0.1542 0.036 Uiso 1 1 calc R . .
C63 C 0.76818(16) 0.10161(12) 0.15657(19) 0.0241(6) Uani 1 1 d . . .
H63 H 0.7729 0.1416 0.1661 0.029 Uiso 1 1 calc R . .
C64 C 0.41397(15) 0.24971(13) 0.1583(2) 0.0268(6) Uani 1 1 d . . .
H64A H 0.4354 0.2874 0.1736 0.040 Uiso 1 1 calc R . .
H64B H 0.3974 0.2392 0.1958 0.040 Uiso 1 1 calc R . .
H64C H 0.3758 0.2508 0.1011 0.040 Uiso 1 1 calc R . .

H57 H 0.6478(14) 0.1491(12) 0.0608(18) 0.011(7) Uiso 1 1 d . . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _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 0.01094(9) 0.01527(9) 0.01887(10) 0.000 0.00806(7) 0.000
Ni1 0.01078(15) 0.01250(16) 0.01373(16) 0.00022(11) 0.00646(13) -0.00040(11)
N1 0.156(8) 0.110(7) 0.069(5) 0.014(5) 0.078(6) -0.043(6)
O3 0.074(7) 0.036(5) 0.078(7) -0.018(5) 0.064(6) -0.009(5)
O2 0.116(10) 0.174(12) 0.152(11) -0.013(10) 0.078(9) -0.068(9)
O1 0.194(10) 0.129(10) 0.083(8) -0.005(8) 0.068(8) -0.030(9)
O1A 0.169(11) 0.167(13) 0.154(11) 0.005(11) 0.083(10) -0.001(10)
O3A 0.124(9) 0.144(10) 0.072(7) 0.010(8) 0.085(7) 0.041(8)
O2A 0.171(12) 0.180(11) 0.147(11) -0.011(11) 0.048(11) -0.041(10)
N11 0.0130(10) 0.0185(11) 0.0181(10) 0.0017(8) 0.0087(9) 0.0007(8)
N31 0.0155(10) 0.0152(10) 0.0198(11) 0.0000(8) 0.0098(9) -0.0037(8)
N51 0.0145(10) 0.0183(11) 0.0179(11) -0.0021(8) 0.0090(9) -0.0024(8)
O21 0.0133(8) 0.0112(8) 0.0183(9) -0.0012(7) 0.0070(7) -0.0007(6)
O22 0.0124(8) 0.0157(9) 0.0198(9) -0.0027(7) 0.0067(7) -0.0007(7)
O31 0.0136(8) 0.0161(9) 0.0133(8) -0.0016(6) 0.0069(7) -0.0016(6)
O32 0.0137(8) 0.0217(9) 0.0146(9) -0.0008(7) 0.0076(7) -0.0030(7)
O51 0.0138(8) 0.0139(8) 0.0162(8) 0.0046(7) 0.0075(7) 0.0023(6)
O52 0.0166(9) 0.0172(9) 0.0273(10) 0.0042(8) 0.0120(8) 0.0042(7)
C11 0.0175(12) 0.0144(12) 0.0192(12) 0.0010(9) 0.0107(10) 0.0021(9)
C12 0.0220(13) 0.0151(12) 0.0232(13) 0.0011(10) 0.0136(11) 0.0045(10)
C13 0.0276(14) 0.0132(12) 0.0254(14) -0.0021(10) 0.0152(12) -0.0001(10)
C14 0.0191(13) 0.0192(13) 0.0195(13) -0.0027(10) 0.0113(11) -0.0030(10)
C15 0.0146(11) 0.0167(12) 0.0160(12) 0.0006(9) 0.0097(10) 0.0011(9)
C16 0.0171(12) 0.0129(11) 0.0132(11) -0.0010(9) 0.0087(10) -0.0003(9)
C17 0.0169(12) 0.0171(12) 0.0179(12) 0.0033(9) 0.0101(10) 0.0054(9)
C18 0.0127(11) 0.0203(13) 0.0189(12) 0.0040(10) 0.0061(10) 0.0026(10)
C19 0.0185(13) 0.0246(14) 0.0211(13) 0.0038(11) 0.0102(11) 0.0036(11)
C20 0.0221(14) 0.0348(17) 0.0165(13) 0.0012(11) 0.0043(11) -0.0007(12)

C21 0.0143(13) 0.0433(18) 0.0280(15) 0.0025(13) 0.0050(12) -0.0020(12)
C22 0.0163(13) 0.0442(19) 0.0308(16) 0.0022(14) 0.0120(13) 0.0019(12)
C23 0.0174(13) 0.0312(15) 0.0217(13) 0.0006(11) 0.0101(11) 0.0017(11)
C24 0.0140(12) 0.0268(14) 0.0224(13) -0.0046(11) 0.0059(11) -0.0033(10)
C31 0.0171(12) 0.0166(12) 0.0172(12) -0.0010(9) 0.0086(10) -0.0029(9)
C32 0.0212(13) 0.0201(13) 0.0199(13) -0.0034(10) 0.0081(11) -0.0069(10)
C33 0.0263(14) 0.0203(13) 0.0177(13) -0.0053(10) 0.0083(11) -0.0062(11)
C34 0.0222(13) 0.0210(13) 0.0175(12) 0.0014(10) 0.0115(11) 0.0004(10)
C35 0.0132(11) 0.0135(11) 0.0162(12) 0.0014(9) 0.0063(10) -0.0005(9)
C36 0.0152(11) 0.0119(11) 0.0146(11) 0.0001(9) 0.0063(10) 0.0003(9)
C37 0.0153(12) 0.0181(12) 0.0211(13) 0.0009(10) 0.0070(10) -0.0041(10)
C38 0.0208(13) 0.0197(13) 0.0205(13) -0.0049(10) 0.0118(11) -0.0088(10)
C39 0.0296(15) 0.0208(14) 0.0223(14) -0.0032(11) 0.0115(12) -0.0083(11)
C40 0.048(2) 0.0254(15) 0.0237(15) -0.0025(12) 0.0174(15) -0.0156(14)
C41 0.047(2) 0.0382(18) 0.0277(16) -0.0106(13) 0.0234(15) -0.0270(16)
C42 0.0258(15) 0.047(2) 0.0346(17) -0.0142(15) 0.0188(14) -0.0186(14)
C43 0.0208(14) 0.0316(16) 0.0251(14) -0.0027(12) 0.0118(12) -0.0082(12)
C44 0.0188(13) 0.0263(14) 0.0191(13) 0.0029(11) 0.0111(11) -0.0019(11)
C51 0.0190(13) 0.0213(13) 0.0190(13) 0.0056(10) 0.0086(11) 0.0006(10)
C52 0.0285(15) 0.0352(17) 0.0238(15) 0.0118(12) 0.0142(13) 0.0043(13)
C53 0.0296(16) 0.0309(16) 0.0294(16) 0.0166(13) 0.0127(13) 0.0061(13)
C54 0.0211(14) 0.0224(14) 0.0299(15) 0.0103(12) 0.0093(12) 0.0046(11)
C55 0.0187(13) 0.0169(12) 0.0231(13) 0.0026(10) 0.0095(11) 0.0007(10)
C56 0.0147(12) 0.0150(12) 0.0177(12) 0.0018(9) 0.0059(10) -0.0015(9)
C57 0.0199(13) 0.0244(14) 0.0155(12) -0.0008(10) 0.0097(11) -0.0031(10)
C58 0.0173(12) 0.0222(13) 0.0153(12) -0.0006(10) 0.0089(10) -0.0025(10)
C59 0.0200(13) 0.0232(13) 0.0153(12) -0.0017(10) 0.0080(11) -0.0030(10)
C60 0.0304(15) 0.0260(15) 0.0221(14) -0.0072(11) 0.0129(12) 0.0013(12)
C61 0.0272(15) 0.0369(17) 0.0303(16) -0.0050(13) 0.0193(13) 0.0047(13)
C62 0.0251(15) 0.0381(18) 0.0343(17) -0.0040(14) 0.0210(14) -0.0039(13)
C63 0.0284(15) 0.0243(14) 0.0256(15) -0.0031(11) 0.0180(13) -0.0049(11)
C64 0.0241(14) 0.0223(14) 0.0373(17) 0.0032(12) 0.0180(13) 0.0076(11)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles

and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
Gd1 O31 2.4043(18) . ?
Gd1 O31 2.4043(18) 2_655 ?
Gd1 O51 2.4075(17) . ?
Gd1 O51 2.4076(17) 2_655 ?
Gd1 O21 2.4130(18) . ?
Gd1 O21 2.4131(18) 2_655 ?
Gd1 O32 2.9019(18) 2_655 ?
Gd1 O32 2.9019(18) . ?
Gd1 O22 2.9363(18) . ?
Gd1 O22 2.9364(18) 2_655 ?
Gd1 Ni1 3.3249(4) 2_655 ?
Gd1 Ni1 3.3250(4) . ?
Ni1 O21 2.0413(17) . ?
Ni1 O51 2.0488(17) . ?
Ni1 O31 2.0511(18) . ?
Ni1 N31 2.114(2) . ?
Ni1 N11 2.117(2) . ?
Ni1 N51 2.123(2) . ?
N1 O3 1.2516(9) . ?
N1 O2 1.2519(9) . ?
N1 O2A 1.2521(9) . ?
N1 O1A 1.2521(9) . ?
N1 O3A 1.2521(9) . ?
N1 O1 1.2527(9) . ?
O1 O1 1.76(2) 7_655 ?
N11 C17 1.292(3) . ?
N11 C18 1.446(3) . ?

N31 C37 1.291(3) . ?
N31 C38 1.433(3) . ?
N51 C57 1.295(3) . ?
N51 C58 1.440(3) . ?
O21 C16 1.307(3) . ?
O22 C15 1.372(3) . ?
O22 C24 1.435(3) . ?
O31 C36 1.312(3) . ?
O32 C35 1.370(3) . ?
O32 C44 1.432(3) . ?
O51 C56 1.316(3) . ?
O52 C55 1.376(3) . ?
O52 C64 1.424(3) . ?
C11 C16 1.411(3) . ?
C11 C12 1.420(3) . ?
C11 C17 1.442(4) . ?
C12 C13 1.372(4) . ?
C12 H12 0.9500 . ?
C13 C14 1.408(4) . ?
C13 H13 0.9500 . ?
C14 C15 1.375(3) . ?
C14 H14 0.9500 . ?
C15 C16 1.423(3) . ?
C17 H17 0.9500 . ?
C18 C19 1.390(4) . ?
C18 C23 1.396(4) . ?
C19 C20 1.392(4) . ?
C19 H19 0.9500 . ?
C20 C21 1.396(4) . ?
C20 H20 0.9500 . ?
C21 C22 1.380(5) . ?
C21 H21 0.9500 . ?
C22 C23 1.390(4) . ?
C22 H22 0.9500 . ?
C23 H23 0.9500 . ?
C24 H24A 0.9800 . ?
C24 H24B 0.9800 . ?
C24 H24C 0.9800 . ?

C31 C36 1.413(3) . ?
C31 C32 1.417(4) . ?
C31 C37 1.448(4) . ?
C32 C33 1.373(4) . ?
C32 H32 0.9500 . ?
C33 C34 1.408(4) . ?
C33 H33 0.9500 . ?
C34 C35 1.376(4) . ?
C34 H34 0.9500 . ?
C35 C36 1.418(4) . ?
C37 H37 0.9500 . ?
C38 C43 1.387(4) . ?
C38 C39 1.396(4) . ?
C39 C40 1.387(4) . ?
C39 H39 0.9500 . ?
C40 C41 1.397(5) . ?
C40 H40 0.9500 . ?
C41 C42 1.367(5) . ?
C41 H41 0.9500 . ?
C42 C43 1.405(4) . ?
C42 H42 0.9500 . ?
C43 H43 0.9500 . ?
C44 H44A 0.9800 . ?
C44 H44B 0.9800 . ?
C44 H44C 0.9800 . ?
C51 C56 1.399(4) . ?
C51 C52 1.420(4) . ?
C51 C57 1.453(4) . ?
C52 C53 1.366(4) . ?
C52 H52 0.9500 . ?
C53 C54 1.400(4) . ?
C53 H53 0.9500 . ?
C54 C55 1.379(4) . ?
C54 H54 0.9500 . ?
C55 C56 1.415(4) . ?
C57 H57 1.03(3) . ?
C58 C59 1.390(4) . ?
C58 C63 1.397(4) . ?

C59 C60 1.388(4) . ?
C59 H59 0.9500 . ?
C60 C61 1.390(4) . ?
C60 H60 0.9500 . ?
C61 C62 1.394(5) . ?
C61 H61 0.9500 . ?
C62 C63 1.395(4) . ?
C62 H62 0.9500 . ?
C63 H63 0.9500 . ?
C64 H64A 0.9800 . ?
C64 H64B 0.9800 . ?
C64 H64C 0.9800 . ?

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
O31 Gd1 O31 173.16(8) . 2_655 ?
O31 Gd1 O51 64.33(6) . . ?
O31 Gd1 O51 111.96(6) 2_655 . ?
O31 Gd1 O51 111.96(6) . 2_655 ?
O31 Gd1 O51 64.33(6) 2_655 2_655 ?
O51 Gd1 O51 120.33(8) . 2_655 ?
O31 Gd1 O21 63.76(6) . . ?
O31 Gd1 O21 120.56(6) 2_655 . ?
O51 Gd1 O21 63.96(6) . . ?
O51 Gd1 O21 172.75(6) 2_655 . ?
O31 Gd1 O21 120.56(6) . 2_655 ?
O31 Gd1 O21 63.76(6) 2_655 2_655 ?
O51 Gd1 O21 172.75(6) . 2_655 ?
O51 Gd1 O21 63.96(6) 2_655 2_655 ?
O21 Gd1 O21 112.46(8) . 2_655 ?
O31 Gd1 O32 123.57(6) . 2_655 ?
O31 Gd1 O32 56.62(6) 2_655 2_655 ?

O51 Gd1 O32 66.14(6) . 2_655 ?
O51 Gd1 O32 115.31(5) 2_655 2_655 ?
O21 Gd1 O32 71.49(5) . 2_655 ?
O21 Gd1 O32 106.96(6) 2_655 2_655 ?
O31 Gd1 O32 56.62(6) . . ?
O31 Gd1 O32 123.57(6) 2_655 . ?
O51 Gd1 O32 115.31(5) . . ?
O51 Gd1 O32 66.13(6) 2_655 . ?
O21 Gd1 O32 106.96(6) . . ?
O21 Gd1 O32 71.49(5) 2_655 . ?
O32 Gd1 O32 177.36(7) 2_655 . ?
O31 Gd1 O22 114.47(5) . . ?
O31 Gd1 O22 71.75(5) 2_655 . ?
O51 Gd1 O22 105.89(6) . . ?
O51 Gd1 O22 124.74(5) 2_655 . ?
O21 Gd1 O22 55.94(5) . . ?
O21 Gd1 O22 67.50(5) 2_655 . ?
O32 Gd1 O22 57.22(5) 2_655 . ?
O32 Gd1 O22 120.15(5) . . ?
O31 Gd1 O22 71.76(5) . 2_655 ?
O31 Gd1 O22 114.47(5) 2_655 2_655 ?
O51 Gd1 O22 124.75(5) . 2_655 ?
O51 Gd1 O22 105.89(6) 2_655 2_655 ?
O21 Gd1 O22 67.50(5) . 2_655 ?
O21 Gd1 O22 55.94(5) 2_655 2_655 ?
O32 Gd1 O22 120.15(5) 2_655 2_655 ?
O32 Gd1 O22 57.22(5) . 2_655 ?
O22 Gd1 O22 63.99(7) . 2_655 ?
O31 Gd1 Ni1 142.15(4) . 2_655 ?
O31 Gd1 Ni1 37.82(4) 2_655 2_655 ?
O51 Gd1 Ni1 142.01(4) . 2_655 ?
O51 Gd1 Ni1 37.78(4) 2_655 2_655 ?
O21 Gd1 Ni1 142.63(4) . 2_655 ?
O21 Gd1 Ni1 37.61(4) 2_655 2_655 ?
O32 Gd1 Ni1 94.15(4) 2_655 2_655 ?
O32 Gd1 Ni1 85.85(4) . 2_655 ?
O22 Gd1 Ni1 87.08(3) . 2_655 ?
O22 Gd1 Ni1 93.15(3) 2_655 2_655 ?

O31 Gd1 Ni1 37.82(4) . . ?
O31 Gd1 Ni1 142.15(4) 2_655 . ?
O51 Gd1 Ni1 37.78(4) . . ?
O51 Gd1 Ni1 142.01(4) 2_655 . ?
O21 Gd1 Ni1 37.61(4) . . ?
O21 Gd1 Ni1 142.63(4) 2_655 . ?
O32 Gd1 Ni1 85.85(4) 2_655 . ?
O32 Gd1 Ni1 94.15(4) . . ?
O22 Gd1 Ni1 93.14(3) . . ?
O22 Gd1 Ni1 87.08(3) 2_655 . ?
Ni1 Gd1 Ni1 179.735(12) 2_655 . ?
O21 Ni1 O51 77.25(7) . . ?
O21 Ni1 O31 76.88(7) . . ?
O51 Ni1 O31 77.33(7) . . ?
O21 Ni1 N31 163.52(8) . . ?
O51 Ni1 N31 98.63(8) . . ?
O31 Ni1 N31 86.66(8) . . ?
O21 Ni1 N11 87.45(8) . . ?
O51 Ni1 N11 164.70(8) . . ?
O31 Ni1 N11 98.88(8) . . ?
N31 Ni1 N11 95.91(9) . . ?
O21 Ni1 N51 99.38(8) . . ?
O51 Ni1 N51 87.43(8) . . ?
O31 Ni1 N51 164.75(8) . . ?
N31 Ni1 N51 96.34(8) . . ?
N11 Ni1 N51 95.69(9) . . ?
O21 Ni1 Gd1 46.17(5) . . ?
O51 Ni1 Gd1 46.04(5) . . ?
O31 Ni1 Gd1 45.96(5) . . ?
N31 Ni1 Gd1 120.11(6) . . ?
N11 Ni1 Gd1 121.29(6) . . ?
N51 Ni1 Gd1 121.33(6) . . ?
O3 N1 O2 120.07(10) . . ?
O3 N1 O2A 70.2(8) . . ?
O2 N1 O2A 55.4(8) . . ?
O3 N1 O1A 165.7(10) . . ?
O2 N1 O1A 66.2(7) . . ?
O2A N1 O1A 120.02(10) . . ?

O3 N1 O3A 50.9(7) . . ?
O2 N1 O3A 166.3(10) . . ?
O2A N1 O3A 119.98(10) . . ?
O1A N1 O3A 120.00(10) . . ?
O3 N1 O1 119.95(10) . . ?
O2 N1 O1 119.98(10) . . ?
O2A N1 O1 155.2(13) . . ?
O1A N1 O1 55.5(8) . . ?
O3A N1 O1 70.0(8) . . ?
N1 O1 O1 144.0(14) . 7_655 ?
C17 N11 C18 114.4(2) . . ?
C17 N11 Ni1 123.56(18) . . ?
C18 N11 Ni1 121.38(17) . . ?
C37 N31 C38 114.2(2) . . ?
C37 N31 Ni1 124.27(18) . . ?
C38 N31 Ni1 120.90(17) . . ?
C57 N51 C58 112.9(2) . . ?
C57 N51 Ni1 123.29(19) . . ?
C58 N51 Ni1 122.62(17) . . ?
C16 O21 Ni1 129.38(16) . . ?
C16 O21 Gd1 129.88(16) . . ?
Ni1 O21 Gd1 96.21(7) . . ?
C15 O22 C24 117.0(2) . . ?
C15 O22 Gd1 112.79(14) . . ?
C24 O22 Gd1 130.07(15) . . ?
C36 O31 Ni1 129.91(16) . . ?
C36 O31 Gd1 129.04(16) . . ?
Ni1 O31 Gd1 96.22(7) . . ?
C35 O32 C44 117.0(2) . . ?
C35 O32 Gd1 112.98(14) . . ?
C44 O32 Gd1 129.88(15) . . ?
C56 O51 Ni1 129.09(16) . . ?
C56 O51 Gd1 130.98(16) . . ?
Ni1 O51 Gd1 96.18(7) . . ?
C55 O52 C64 116.7(2) . . ?
C16 C11 C12 119.0(2) . . ?
C16 C11 C17 123.2(2) . . ?
C12 C11 C17 117.6(2) . . ?

C13 C12 C11 121.5(2) . . ?
C13 C12 H12 119.2 . . ?
C11 C12 H12 119.2 . . ?
C12 C13 C14 120.1(2) . . ?
C12 C13 H13 120.0 . . ?
C14 C13 H13 120.0 . . ?
C15 C14 C13 119.2(2) . . ?
C15 C14 H14 120.4 . . ?
C13 C14 H14 120.4 . . ?
O22 C15 C14 125.6(2) . . ?
O22 C15 C16 112.1(2) . . ?
C14 C15 C16 122.3(2) . . ?
O21 C16 C11 124.4(2) . . ?
O21 C16 C15 117.7(2) . . ?
C11 C16 C15 117.9(2) . . ?
N11 C17 C11 128.3(2) . . ?
N11 C17 H17 115.8 . . ?
C11 C17 H17 115.8 . . ?
C19 C18 C23 120.2(2) . . ?
C19 C18 N11 118.9(2) . . ?
C23 C18 N11 120.9(2) . . ?
C18 C19 C20 119.7(3) . . ?
C18 C19 H19 120.2 . . ?
C20 C19 H19 120.2 . . ?
C19 C20 C21 120.1(3) . . ?
C19 C20 H20 120.0 . . ?
C21 C20 H20 120.0 . . ?
C22 C21 C20 120.0(3) . . ?
C22 C21 H21 120.0 . . ?
C20 C21 H21 120.0 . . ?
C21 C22 C23 120.4(3) . . ?
C21 C22 H22 119.8 . . ?
C23 C22 H22 119.8 . . ?
C22 C23 C18 119.7(3) . . ?
C22 C23 H23 120.2 . . ?
C18 C23 H23 120.2 . . ?
O22 C24 H24A 109.5 . . ?
O22 C24 H24B 109.5 . . ?

H24A C24 H24B 109.5 . . ?
O22 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
C36 C31 C32 119.0(2) . . ?
C36 C31 C37 123.0(2) . . ?
C32 C31 C37 117.5(2) . . ?
C33 C32 C31 121.6(2) . . ?
C33 C32 H32 119.2 . . ?
C31 C32 H32 119.2 . . ?
C32 C33 C34 119.7(3) . . ?
C32 C33 H33 120.1 . . ?
C34 C33 H33 120.1 . . ?
C35 C34 C33 119.6(3) . . ?
C35 C34 H34 120.2 . . ?
C33 C34 H34 120.2 . . ?
O32 C35 C34 125.7(2) . . ?
O32 C35 C36 112.2(2) . . ?
C34 C35 C36 122.0(2) . . ?
O31 C36 C31 124.0(2) . . ?
O31 C36 C35 118.0(2) . . ?
C31 C36 C35 118.0(2) . . ?
N31 C37 C31 127.8(2) . . ?
N31 C37 H37 116.1 . . ?
C31 C37 H37 116.1 . . ?
C43 C38 C39 120.2(3) . . ?
C43 C38 N31 121.8(3) . . ?
C39 C38 N31 118.0(3) . . ?
C40 C39 C38 119.6(3) . . ?
C40 C39 H39 120.2 . . ?
C38 C39 H39 120.2 . . ?
C39 C40 C41 120.2(3) . . ?
C39 C40 H40 119.9 . . ?
C41 C40 H40 119.9 . . ?
C42 C41 C40 120.0(3) . . ?
C42 C41 H41 120.0 . . ?
C40 C41 H41 120.0 . . ?
C41 C42 C43 120.5(3) . . ?

C41 C42 H42 119.8 . . ?
C43 C42 H42 119.8 . . ?
C38 C43 C42 119.4(3) . . ?
C38 C43 H43 120.3 . . ?
C42 C43 H43 120.3 . . ?
O32 C44 H44A 109.5 . . ?
O32 C44 H44B 109.5 . . ?
H44A C44 H44B 109.5 . . ?
O32 C44 H44C 109.5 . . ?
H44A C44 H44C 109.5 . . ?
H44B C44 H44C 109.5 . . ?
C56 C51 C52 119.4(3) . . ?
C56 C51 C57 123.7(2) . . ?
C52 C51 C57 116.8(3) . . ?
C53 C52 C51 120.8(3) . . ?
C53 C52 H52 119.6 . . ?
C51 C52 H52 119.6 . . ?
C52 C53 C54 120.5(3) . . ?
C52 C53 H53 119.8 . . ?
C54 C53 H53 119.8 . . ?
C55 C54 C53 119.1(3) . . ?
C55 C54 H54 120.5 . . ?
C53 C54 H54 120.5 . . ?
O52 C55 C54 125.9(3) . . ?
O52 C55 C56 112.2(2) . . ?
C54 C55 C56 121.9(3) . . ?
O51 C56 C51 124.1(2) . . ?
O51 C56 C55 117.8(2) . . ?
C51 C56 C55 118.0(2) . . ?
N51 C57 C51 128.1(3) . . ?
N51 C57 H57 118.3(16) . . ?
C51 C57 H57 113.5(16) . . ?
C59 C58 C63 120.1(3) . . ?
C59 C58 N51 120.6(2) . . ?
C63 C58 N51 119.3(2) . . ?
C60 C59 C58 120.0(3) . . ?
C60 C59 H59 120.0 . . ?
C58 C59 H59 120.0 . . ?

C59 C60 C61 120.4(3) . . ?
C59 C60 H60 119.8 . . ?
C61 C60 H60 119.8 . . ?
C60 C61 C62 119.8(3) . . ?
C60 C61 H61 120.1 . . ?
C62 C61 H61 120.1 . . ?
C61 C62 C63 120.1(3) . . ?
C61 C62 H62 120.0 . . ?
C63 C62 H62 120.0 . . ?
C62 C63 C58 119.7(3) . . ?
C62 C63 H63 120.2 . . ?
C58 C63 H63 120.2 . . ?
O52 C64 H64A 109.5 . . ?
O52 C64 H64B 109.5 . . ?
H64A C64 H64B 109.5 . . ?
O52 C64 H64C 109.5 . . ?
H64A C64 H64C 109.5 . . ?
H64B C64 H64C 109.5 . . ?

loop_
 _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
O31 Gd1 Ni1 O21 119.37(10) . . . . ?
O31 Gd1 Ni1 O21 -71.78(10) 2_655 . . . ?
O51 Gd1 Ni1 O21 -120.05(10) . . . . ?
O51 Gd1 Ni1 O21 168.17(10) 2_655 . . . ?
O21 Gd1 Ni1 O21 48.07(14) 2_655 . . . ?
O32 Gd1 Ni1 O21 -64.70(8) 2_655 . . . ?
O32 Gd1 Ni1 O21 112.65(8) . . . . ?
O22 Gd1 Ni1 O21 -7.91(8) . . . . ?

O22 Gd1 Ni1 O21 55.83(8) 2_655 . . . ?
Ni1 Gd1 Ni1 O21 -155.77(8) 2_655 . . . ?
O31 Gd1 Ni1 O51 -120.58(10) . . . . ?
O31 Gd1 Ni1 O51 48.26(10) 2_655 . . . ?
O51 Gd1 Ni1 O51 -71.78(14) 2_655 . . . ?
O21 Gd1 Ni1 O51 120.05(10) . . . . ?
O21 Gd1 Ni1 O51 168.12(10) 2_655 . . . ?
O32 Gd1 Ni1 O51 55.35(8) 2_655 . . . ?
O32 Gd1 Ni1 O51 -127.30(8) . . . . ?
O22 Gd1 Ni1 O51 112.14(8) . . . . ?
O22 Gd1 Ni1 O51 175.88(8) 2_655 . . . ?
Ni1 Gd1 Ni1 O51 -35.73(8) 2_655 . . . ?
O31 Gd1 Ni1 O31 168.84(13) 2_655 . . . ?
O51 Gd1 Ni1 O31 120.58(10) . . . . ?
O51 Gd1 Ni1 O31 48.80(10) 2_655 . . . ?
O21 Gd1 Ni1 O31 -119.37(10) . . . . ?
O21 Gd1 Ni1 O31 -71.30(10) 2_655 . . . ?
O32 Gd1 Ni1 O31 175.93(8) 2_655 . . . ?
O32 Gd1 Ni1 O31 -6.73(8) . . . . ?
O22 Gd1 Ni1 O31 -127.28(8) . . . . ?
O22 Gd1 Ni1 O31 -63.55(8) 2_655 . . . ?
Ni1 Gd1 Ni1 O31 84.85(7) 2_655 . . . ?
O31 Gd1 Ni1 N31 -49.12(10) . . . . ?
O31 Gd1 Ni1 N31 119.72(10) 2_655 . . . ?
O51 Gd1 Ni1 N31 71.45(10) . . . . ?
O51 Gd1 Ni1 N31 -0.33(10) 2_655 . . . ?
O21 Gd1 Ni1 N31 -168.50(10) . . . . ?
O21 Gd1 Ni1 N31 -120.43(10) 2_655 . . . ?
O32 Gd1 Ni1 N31 126.80(8) 2_655 . . . ?
O32 Gd1 Ni1 N31 -55.85(8) . . . . ?
O22 Gd1 Ni1 N31 -176.41(8) . . . . ?
O22 Gd1 Ni1 N31 -112.67(8) 2_655 . . . ?
Ni1 Gd1 Ni1 N31 35.73(7) 2_655 . . . ?
O31 Gd1 Ni1 N11 70.33(10) . . . . ?
O31 Gd1 Ni1 N11 -120.82(10) 2_655 . . . ?
O51 Gd1 Ni1 N11 -169.09(10) . . . . ?
O51 Gd1 Ni1 N11 119.13(10) 2_655 . . . ?
O21 Gd1 Ni1 N11 -49.04(10) . . . . ?

O21 Gd1 Ni1 N11 -0.97(10) 2_655 . . . ?
O32 Gd1 Ni1 N11 -113.74(8) 2_655 . . . ?
O32 Gd1 Ni1 N11 63.61(8) . . . . ?
O22 Gd1 Ni1 N11 -56.95(8) . . . . ?
O22 Gd1 Ni1 N11 6.79(8) 2_655 . . . ?
Ni1 Gd1 Ni1 N11 155.18(8) 2_655 . . . ?
O31 Gd1 Ni1 N51 -169.28(10) . . . . ?
O31 Gd1 Ni1 N51 -0.44(10) 2_655 . . . ?
O51 Gd1 Ni1 N51 -48.70(10) . . . . ?
O51 Gd1 Ni1 N51 -120.49(10) 2_655 . . . ?
O21 Gd1 Ni1 N51 71.34(10) . . . . ?
O21 Gd1 Ni1 N51 119.41(10) 2_655 . . . ?
O32 Gd1 Ni1 N51 6.64(8) 2_655 . . . ?
O32 Gd1 Ni1 N51 -176.01(8) . . . . ?
O22 Gd1 Ni1 N51 63.43(8) . . . . ?
O22 Gd1 Ni1 N51 127.17(8) 2_655 . . . ?
Ni1 Gd1 Ni1 N51 -84.43(8) 2_655 . . . ?
O3 N1 O1 O1 -31(3) . . . 7_655 ?
O2 N1 O1 O1 149(3) . . . 7_655 ?
O2A N1 O1 O1 -139(3) . . . 7_655 ?
O1A N1 O1 O1 133(3) . . . 7_655 ?
O3A N1 O1 O1 -21(3) . . . 7_655 ?
O21 Ni1 N11 C17 18.9(2) . . . . ?
O51 Ni1 N11 C17 20.9(4) . . . . ?
O31 Ni1 N11 C17 95.2(2) . . . . ?
N31 Ni1 N11 C17 -177.3(2) . . . . ?
N51 Ni1 N11 C17 -80.3(2) . . . . ?
Gd1 Ni1 N11 C17 52.0(2) . . . . ?
O21 Ni1 N11 C18 -171.2(2) . . . . ?
O51 Ni1 N11 C18 -169.3(2) . . . . ?
O31 Ni1 N11 C18 -94.94(19) . . . . ?
N31 Ni1 N11 C18 -7.4(2) . . . . ?
N51 Ni1 N11 C18 89.6(2) . . . . ?
Gd1 Ni1 N11 C18 -138.18(17) . . . . ?
O21 Ni1 N31 C37 23.6(4) . . . . ?
O51 Ni1 N31 C37 97.7(2) . . . . ?
O31 Ni1 N31 C37 21.1(2) . . . . ?
N11 Ni1 N31 C37 -77.5(2) . . . . ?

N51 Ni1 N31 C37 -173.9(2) . . . . ?
Gd1 Ni1 N31 C37 54.1(2) . . . . ?
O21 Ni1 N31 C38 -165.8(2) . . . . ?
O51 Ni1 N31 C38 -91.6(2) . . . . ?
O31 Ni1 N31 C38 -168.3(2) . . . . ?
N11 Ni1 N31 C38 93.1(2) . . . . ?
N51 Ni1 N31 C38 -3.3(2) . . . . ?
Gd1 Ni1 N31 C38 -135.29(18) . . . . ?
O21 Ni1 N51 C57 96.1(2) . . . . ?
O51 Ni1 N51 C57 19.5(2) . . . . ?
O31 Ni1 N51 C57 21.7(4) . . . . ?
N31 Ni1 N51 C57 -78.9(2) . . . . ?
N11 Ni1 N51 C57 -175.5(2) . . . . ?
Gd1 Ni1 N51 C57 52.3(2) . . . . ?
O21 Ni1 N51 C58 -97.27(19) . . . . ?
O51 Ni1 N51 C58 -173.90(19) . . . . ?
O31 Ni1 N51 C58 -171.7(2) . . . . ?
N31 Ni1 N51 C58 87.7(2) . . . . ?
N11 Ni1 N51 C58 -8.9(2) . . . . ?
Gd1 Ni1 N51 C58 -141.12(17) . . . . ?
O51 Ni1 O21 C16 162.8(2) . . . . ?
O31 Ni1 O21 C16 -117.5(2) . . . . ?
N31 Ni1 O21 C16 -120.0(3) . . . . ?
N11 Ni1 O21 C16 -17.7(2) . . . . ?
N51 Ni1 O21 C16 77.6(2) . . . . ?
Gd1 Ni1 O21 C16 -157.5(2) . . . . ?
O51 Ni1 O21 Gd1 -39.71(7) . . . . ?
O31 Ni1 O21 Gd1 40.03(6) . . . . ?
N31 Ni1 O21 Gd1 37.5(3) . . . . ?
N11 Ni1 O21 Gd1 139.76(8) . . . . ?
N51 Ni1 O21 Gd1 -124.89(8) . . . . ?
O31 Gd1 O21 C16 120.8(2) . . . . ?
O31 Gd1 O21 C16 -65.3(2) 2_655 . . . ?
O51 Gd1 O21 C16 -166.5(2) . . . . ?
O51 Gd1 O21 C16 65.6(5) 2_655 . . . ?
O21 Gd1 O21 C16 6.57(18) 2_655 . . . ?
O32 Gd1 O21 C16 -94.6(2) 2_655 . . . ?
O32 Gd1 O21 C16 83.1(2) . . . . ?

O22 Gd1 O21 C16 -32.22(18) . . . . ?
O22 Gd1 O21 C16 40.75(19) 2_655 . . . ?
Ni1 Gd1 O21 C16 -22.9(2) 2_655 . . . ?
Ni1 Gd1 O21 C16 157.3(2) . . . . ?
O31 Gd1 O21 Ni1 -36.57(6) . . . . ?
O31 Gd1 O21 Ni1 137.40(6) 2_655 . . . ?
O51 Gd1 O21 Ni1 36.17(6) . . . . ?
O51 Gd1 O21 Ni1 -91.7(4) 2_655 . . . ?
O21 Gd1 O21 Ni1 -150.75(8) 2_655 . . . ?
O32 Gd1 O21 Ni1 108.03(7) 2_655 . . . ?
O32 Gd1 O21 Ni1 -74.23(7) . . . . ?
O22 Gd1 O21 Ni1 170.45(9) . . . . ?
O22 Gd1 O21 Ni1 -116.57(7) 2_655 . . . ?
Ni1 Gd1 O21 Ni1 179.821(8) 2_655 . . . ?
O31 Gd1 O22 C15 -2.28(17) . . . . ?
O31 Gd1 O22 C15 174.68(16) 2_655 . . . ?
O51 Gd1 O22 C15 66.29(16) . . . . ?
O51 Gd1 O22 C15 -146.93(15) 2_655 . . . ?
O21 Gd1 O22 C15 24.32(15) . . . . ?
O21 Gd1 O22 C15 -116.87(16) 2_655 . . . ?
O32 Gd1 O22 C15 113.16(16) 2_655 . . . ?
O32 Gd1 O22 C15 -66.51(16) . . . . ?
O22 Gd1 O22 C15 -55.07(14) 2_655 . . . ?
Ni1 Gd1 O22 C15 -150.00(15) 2_655 . . . ?
Ni1 Gd1 O22 C15 30.14(15) . . . . ?
O31 Gd1 O22 C24 173.3(2) . . . . ?
O31 Gd1 O22 C24 -9.8(2) 2_655 . . . ?
O51 Gd1 O22 C24 -118.2(2) . . . . ?
O51 Gd1 O22 C24 28.6(2) 2_655 . . . ?
O21 Gd1 O22 C24 -160.1(2) . . . . ?
O21 Gd1 O22 C24 58.7(2) 2_655 . . . ?
O32 Gd1 O22 C24 -71.3(2) 2_655 . . . ?
O32 Gd1 O22 C24 109.0(2) . . . . ?
O22 Gd1 O22 C24 120.5(2) 2_655 . . . ?
Ni1 Gd1 O22 C24 25.5(2) 2_655 . . . ?
Ni1 Gd1 O22 C24 -154.3(2) . . . . ?
O21 Ni1 O31 C36 163.3(2) . . . . ?
O51 Ni1 O31 C36 -117.1(2) . . . . ?

N31 Ni1 O31 C36 -17.5(2) . . . . ?
N11 Ni1 O31 C36 78.0(2) . . . . ?
N51 Ni1 O31 C36 -119.4(3) . . . . ?
Gd1 Ni1 O31 C36 -156.5(2) . . . . ?
O21 Ni1 O31 Gd1 -40.21(6) . . . . ?
O51 Ni1 O31 Gd1 39.43(6) . . . . ?
N31 Ni1 O31 Gd1 139.06(8) . . . . ?
N11 Ni1 O31 Gd1 -125.47(7) . . . . ?
N51 Ni1 O31 Gd1 37.1(3) . . . . ?
O31 Gd1 O31 C36 62.62(19) 2_655 . . . ?
O51 Gd1 O31 C36 121.0(2) . . . . ?
O51 Gd1 O31 C36 6.8(2) 2_655 . . . ?
O21 Gd1 O31 C36 -166.8(2) . . . . ?
O21 Gd1 O31 C36 -65.1(2) 2_655 . . . ?
O32 Gd1 O31 C36 151.95(18) 2_655 . . . ?
O32 Gd1 O31 C36 -31.22(18) . . . . ?
O22 Gd1 O31 C36 -142.38(18) . . . . ?
O22 Gd1 O31 C36 -93.47(19) 2_655 . . . ?
Ni1 Gd1 O31 C36 -22.7(2) 2_655 . . . ?
Ni1 Gd1 O31 C36 156.8(2) . . . . ?
O31 Gd1 O31 Ni1 -94.20(5) 2_655 . . . ?
O51 Gd1 O31 Ni1 -35.81(6) . . . . ?
O51 Gd1 O31 Ni1 -150.04(6) 2_655 . . . ?
O21 Gd1 O31 Ni1 36.37(6) . . . . ?
O21 Gd1 O31 Ni1 138.11(6) 2_655 . . . ?
O32 Gd1 O31 Ni1 -4.88(9) 2_655 . . . ?
O32 Gd1 O31 Ni1 171.96(9) . . . . ?
O22 Gd1 O31 Ni1 60.79(8) . . . . ?
O22 Gd1 O31 Ni1 109.70(7) 2_655 . . . ?
Ni1 Gd1 O31 Ni1 -179.57(2) 2_655 . . . ?
O31 Gd1 O32 C35 24.34(15) . . . . ?
O31 Gd1 O32 C35 -147.46(15) 2_655 . . . ?
O51 Gd1 O32 C35 -3.34(17) . . . . ?
O51 Gd1 O32 C35 -117.02(16) 2_655 . . . ?
O21 Gd1 O32 C35 65.35(16) . . . . ?
O21 Gd1 O32 C35 173.96(16) 2_655 . . . ?
O32 Gd1 O32 C35 119.33(15) 2_655 . . . ?
O22 Gd1 O32 C35 125.35(15) . . . . ?

O22 Gd1 O32 C35 113.11(16) 2_655 . . . ?
Ni1 Gd1 O32 C35 -150.46(15) 2_655 . . . ?
Ni1 Gd1 O32 C35 29.28(15) . . . . ?
O31 Gd1 O32 C44 -159.5(2) . . . . ?
O31 Gd1 O32 C44 28.7(2) 2_655 . . . ?
O51 Gd1 O32 C44 172.84(19) . . . . ?
O51 Gd1 O32 C44 59.2(2) 2_655 . . . ?
O21 Gd1 O32 C44 -118.5(2) . . . . ?
O21 Gd1 O32 C44 -9.9(2) 2_655 . . . ?
O32 Gd1 O32 C44 -64.5(2) 2_655 . . . ?
O22 Gd1 O32 C44 -58.5(2) . . . . ?
O22 Gd1 O32 C44 -70.7(2) 2_655 . . . ?
Ni1 Gd1 O32 C44 25.7(2) 2_655 . . . ?
Ni1 Gd1 O32 C44 -154.5(2) . . . . ?
O21 Ni1 O51 C56 -119.9(2) . . . . ?
O31 Ni1 O51 C56 160.9(2) . . . . ?
N31 Ni1 O51 C56 76.4(2) . . . . ?
N11 Ni1 O51 C56 -121.9(3) . . . . ?
N51 Ni1 O51 C56 -19.7(2) . . . . ?
Gd1 Ni1 O51 C56 -159.7(2) . . . . ?
O21 Ni1 O51 Gd1 39.81(7) . . . . ?
O31 Ni1 O51 Gd1 -39.37(6) . . . . ?
N31 Ni1 O51 Gd1 -123.95(8) . . . . ?
N11 Ni1 O51 Gd1 37.8(3) . . . . ?
N51 Ni1 O51 Gd1 140.03(8) . . . . ?
O31 Gd1 O51 C56 -165.0(2) . . . . ?
O31 Gd1 O51 C56 8.7(2) 2_655 . . . ?
O51 Gd1 O51 C56 -63.5(2) 2_655 . . . ?
O21 Gd1 O51 C56 123.1(2) . . . . ?
O21 Gd1 O51 C56 61.2(5) 2_655 . . . ?
O32 Gd1 O51 C56 42.9(2) 2_655 . . . ?
O32 Gd1 O51 C56 -139.5(2) . . . . ?
O22 Gd1 O51 C56 85.0(2) . . . . ?
O22 Gd1 O51 C56 154.09(19) 2_655 . . . ?
Ni1 Gd1 O51 C56 -21.1(2) 2_655 . . . ?
Ni1 Gd1 O51 C56 159.1(2) . . . . ?
O31 Gd1 O51 Ni1 35.86(6) . . . . ?
O31 Gd1 O51 Ni1 -150.42(6) 2_655 . . . ?

O51 Gd1 O51 Ni1 137.36(7) 2_655 . . . ?
O21 Gd1 O51 Ni1 -36.01(6) . . . . ?
O21 Gd1 O51 Ni1 -97.9(4) 2_655 . . . ?
O32 Gd1 O51 Ni1 -116.21(8) 2_655 . . . ?
O32 Gd1 O51 Ni1 61.35(8) . . . . ?
O22 Gd1 O51 Ni1 -74.08(7) . . . . ?
O22 Gd1 O51 Ni1 -5.02(9) 2_655 . . . ?
Ni1 Gd1 O51 Ni1 179.748(12) 2_655 . . . ?
C16 C11 C12 C13 -0.8(4) . . . . ?
C17 C11 C12 C13 174.1(3) . . . . ?
C11 C12 C13 C14 -1.5(4) . . . . ?
C12 C13 C14 C15 1.0(4) . . . . ?
C24 O22 C15 C14 -16.8(4) . . . . ?
Gd1 O22 C15 C14 159.4(2) . . . . ?
C24 O22 C15 C16 165.0(2) . . . . ?
Gd1 O22 C15 C16 -18.8(2) . . . . ?
C13 C14 C15 O22 -176.2(2) . . . . ?
C13 C14 C15 C16 1.8(4) . . . . ?
Ni1 O21 C16 C11 8.6(4) . . . . ?
Gd1 O21 C16 C11 -141.7(2) . . . . ?
Ni1 O21 C16 C15 -173.37(16) . . . . ?
Gd1 O21 C16 C15 36.4(3) . . . . ?
C12 C11 C16 O21 -178.5(2) . . . . ?
C17 C11 C16 O21 6.9(4) . . . . ?
C12 C11 C16 C15 3.4(4) . . . . ?
C17 C11 C16 C15 -171.1(2) . . . . ?
O22 C15 C16 O21 -3.9(3) . . . . ?
C14 C15 C16 O21 177.8(2) . . . . ?
O22 C15 C16 C11 174.3(2) . . . . ?
C14 C15 C16 C11 -4.0(4) . . . . ?
C18 N11 C17 C11 176.8(3) . . . . ?
Ni1 N11 C17 C11 -12.7(4) . . . . ?
C16 C11 C17 N11 -4.0(4) . . . . ?
C12 C11 C17 N11 -178.7(3) . . . . ?
C17 N11 C18 C19 -113.9(3) . . . . ?
Ni1 N11 C18 C19 75.4(3) . . . . ?
C17 N11 C18 C23 66.3(3) . . . . ?
Ni1 N11 C18 C23 -104.4(3) . . . . ?

C23 C18 C19 C20 1.4(4) . . . . ?
N11 C18 C19 C20 -178.4(3) . . . . ?
C18 C19 C20 C21 -0.8(5) . . . . ?
C19 C20 C21 C22 0.0(5) . . . . ?
C20 C21 C22 C23 0.1(5) . . . . ?
C21 C22 C23 C18 0.6(5) . . . . ?
C19 C18 C23 C22 -1.3(4) . . . . ?
N11 C18 C23 C22 178.5(3) . . . . ?
C36 C31 C32 C33 -1.8(4) . . . . ?
C37 C31 C32 C33 170.6(3) . . . . ?
C31 C32 C33 C34 -1.1(4) . . . . ?
C32 C33 C34 C35 2.1(4) . . . . ?
C44 O32 C35 C34 -18.6(4) . . . . ?
Gd1 O32 C35 C34 158.1(2) . . . . ?
C44 O32 C35 C36 164.0(2) . . . . ?
Gd1 O32 C35 C36 -19.3(2) . . . . ?
C33 C34 C35 O32 -177.3(2) . . . . ?
C33 C34 C35 C36 -0.2(4) . . . . ?
Ni1 O31 C36 C31 6.2(4) . . . . ?
Gd1 O31 C36 C31 -143.2(2) . . . . ?
Ni1 O31 C36 C35 -175.86(16) . . . . ?
Gd1 O31 C36 C35 34.8(3) . . . . ?
C32 C31 C36 O31 -178.4(2) . . . . ?
C37 C31 C36 O31 9.5(4) . . . . ?
C32 C31 C36 C35 3.6(4) . . . . ?
C37 C31 C36 C35 -168.5(2) . . . . ?
O32 C35 C36 O31 -3.3(3) . . . . ?
C34 C35 C36 O31 179.3(2) . . . . ?
O32 C35 C36 C31 174.8(2) . . . . ?
C34 C35 C36 C31 -2.6(4) . . . . ?
C38 N31 C37 C31 173.4(3) . . . . ?
Ni1 N31 C37 C31 -15.4(4) . . . . ?
C36 C31 C37 N31 -4.0(4) . . . . ?
C32 C31 C37 N31 -176.2(3) . . . . ?
C37 N31 C38 C43 64.6(3) . . . . ?
Ni1 N31 C38 C43 -106.9(3) . . . . ?
C37 N31 C38 C39 -115.5(3) . . . . ?
Ni1 N31 C38 C39 73.0(3) . . . . ?

C43 C38 C39 C40 2.0(4) . . . . ?
N31 C38 C39 C40 -177.9(3) . . . . ?
C38 C39 C40 C41 -0.2(4) . . . . ?
C39 C40 C41 C42 -1.5(5) . . . . ?
C40 C41 C42 C43 1.5(5) . . . . ?
C39 C38 C43 C42 -2.0(4) . . . . ?
N31 C38 C43 C42 177.8(3) . . . . ?
C41 C42 C43 C38 0.3(5) . . . . ?
C56 C51 C52 C53 -0.8(5) . . . . ?
C57 C51 C52 C53 176.5(3) . . . . ?
C51 C52 C53 C54 -2.8(5) . . . . ?
C52 C53 C54 C55 1.8(5) . . . . ?
C64 O52 C55 C54 -12.4(4) . . . . ?
C64 O52 C55 C56 168.5(2) . . . . ?
C53 C54 C55 O52 -176.2(3) . . . . ?
C53 C54 C55 C56 2.8(4) . . . . ?
Ni1 O51 C56 C51 10.5(4) . . . . ?
Gd1 O51 C56 C51 -142.3(2) . . . . ?
Ni1 O51 C56 C55 -170.68(17) . . . . ?
Gd1 O51 C56 C55 36.5(3) . . . . ?
C52 C51 C56 O51 -176.1(3) . . . . ?
C57 C51 C56 O51 6.9(4) . . . . ?
C52 C51 C56 C55 5.1(4) . . . . ?
C57 C51 C56 C55 -172.0(3) . . . . ?
O52 C55 C56 O51 -6.0(3) . . . . ?
C54 C55 C56 O51 174.9(3) . . . . ?
O52 C55 C56 C51 172.9(2) . . . . ?
C54 C55 C56 C51 -6.2(4) . . . . ?
C58 N51 C57 C51 -179.8(3) . . . . ?
Ni1 N51 C57 C51 -12.0(4) . . . . ?
C56 C51 C57 N51 -5.4(5) . . . . ?
C52 C51 C57 N51 177.4(3) . . . . ?
C57 N51 C58 C59 -118.7(3) . . . . ?
Ni1 N51 C58 C59 73.5(3) . . . . ?
C57 N51 C58 C63 60.0(3) . . . . ?
Ni1 N51 C58 C63 -107.9(3) . . . . ?
C63 C58 C59 C60 1.0(4) . . . . ?
N51 C58 C59 C60 179.6(2) . . . . ?

C58 C59 C60 C61 0.8(4) . . . . ?
C59 C60 C61 C62 -1.5(5) . . . . ?
C60 C61 C62 C63 0.3(5) . . . . ?
C61 C62 C63 C58 1.5(5) . . . . ?
C59 C58 C63 C62 -2.1(4) . . . . ?
N51 C58 C63 C62 179.3(3) . . . . ?

loop_
 _geom_hbond_atom_site_label_D
 _geom_hbond_atom_site_label_H
 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
 _geom_hbond_distance_HA
 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
C14 H14 O3 0.95 2.56 3.504(8) 173.2 5_655
C24 H24C O2A 0.98 1.97 2.659(8) 125.6 5_655
C40 H40 O1A 0.95 2.51 3.33(2) 143.7 7_655
loop_
  _platon_squeeze_void_nr
  _platon_squeeze_void_average_x
  _platon_squeeze_void_average_y
  _platon_squeeze_void_average_z
  _platon_squeeze_void_volume
  _platon_squeeze_void_count_electrons
  _platon_squeeze_void_content
   1 0.000 1.000 -0.033   903   297 ' '
   2 0.500 0.500 0.040   903   297 ' '
_platon_squeeze_details   ?

_diffrn_measured_fraction_theta_max   0.998
_diffrn_reflns_theta_full   28.34
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max   2.834
_refine_diff_density_min   -0.915
_refine_diff_density_rms   0.118

CHECK CIF INFORMATION

checkCIF/PLATON (standard)

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: trial2_sq

Bond precision: C-C = 0.0046 A Wavelength=0.71073

Cell: a=22.8250(18) b=23.4590(18) c=18.6760(14)
alpha=90 beta=120.296(2) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	8634.4(12)	8634.4(11)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C84 H72 Gd N6 Ni2 O12, N O3	?
Sum formula	C84 H72 Gd N7 Ni2 O15	C84 H72 Gd N7 Ni2 O15
Mr	1694.12	1694.16
Dx,g cm-3	1.303	1.303
Z	4	4
Mu (mm-1)	1.254	1.254
F000	3460.0	3460.0
F000'	3463.36	
h,k,lmax	30,31,24	30,31,24
Nref	10774	10760
Tmin,Tmax	0.835,0.893	0.806,0.896
Tmin'	0.798	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 28.340

R(reflections)= 0.0365(8775) wR2(reflections)= 0.1052(10760)

S = 1.066 Npar= 544

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.10

PLAT395_ALERT_2_C Deviating X-O-Y Angle from 120 Deg for <O1 144.0 Deg.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 7

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ? Do !

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.
11.62
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.
1
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =
3
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of
N1
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder .....
100 %
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .
882 A**3
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #
10
NI1 -GD1 -NI1 -O21 -155.77 0.08 2.655 1.555 1.555
1.555
And 13 other PLAT710 Alerts
More ...
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .....
98
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed
! Info

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
20 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta*

Crystallographica Section C or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 01/06/2013; check.def file version of 24/05/2013

Datablock trial2_sq - ellipsoid plot