Supporting Information

Electronic and structural properties of $Y_6Pt_{13}X_4$, the site occupancy variants of the $Ba_6Na_{16}N$ subnitride (X = Al, Ga)

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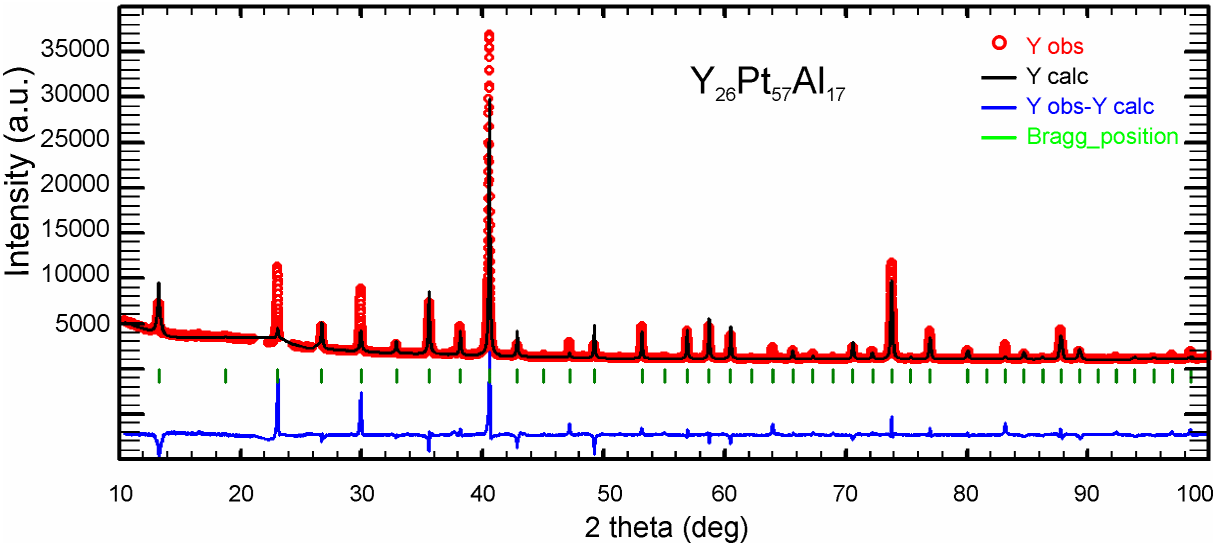

Figure S1. Powder X-ray diffraction intensity data of $Y_{26}Pt_{57}Al_{17}$ alloy refined on the basis of the $Ce_3Ni_6Si_2$ structure model (space group *Im*-3*m*, a=9.43052 Å, R_F=0.190, R_I=0.280).

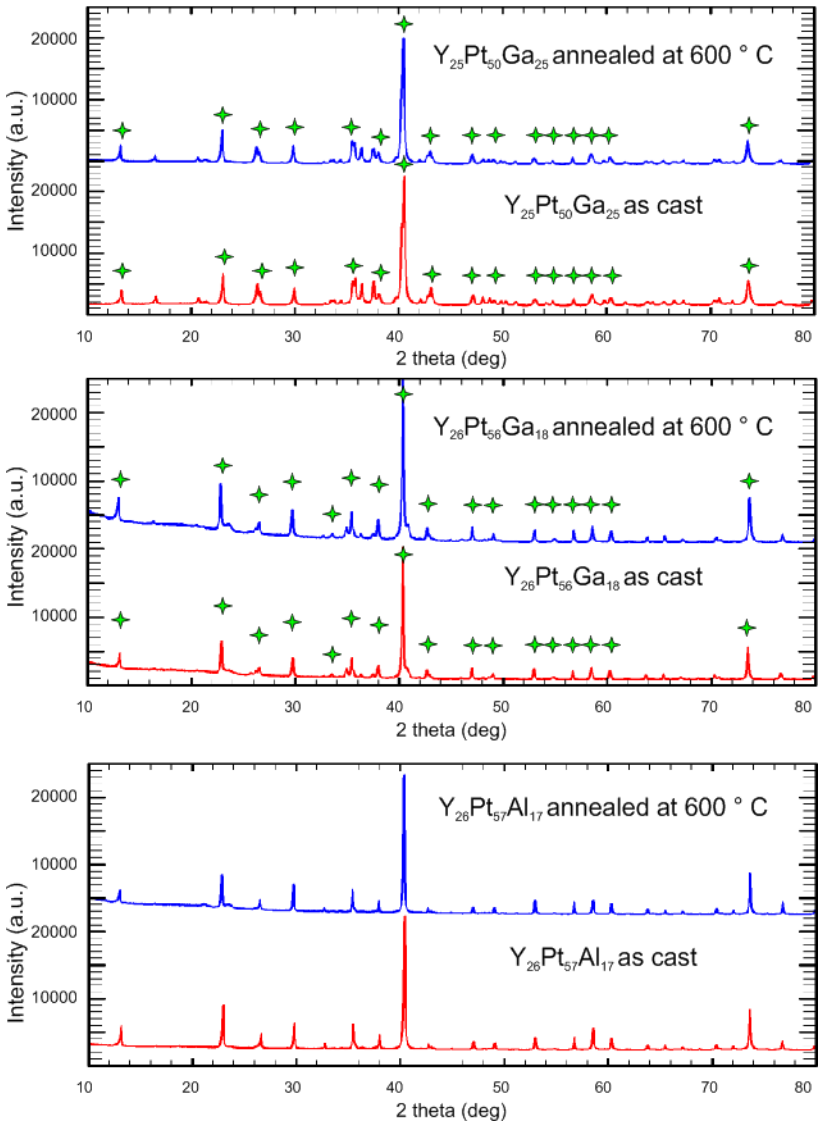

Figure S2. Powder X-ray diffraction intensity data of as cast and annealed multiphase Y-Pt-Ga alloys in comparison with single phase Y-Pt-Al alloy ($Y_6Pt_{13}Al_4$ compound). Reflections marked with green stars correspond to $Y_6Pt_{13}Ga_4$ phase.

$Y_6Pt_{13}Al_4$: Crystallographic Information File

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#  Using CIFtbx version 2.6.2 16 Jun 1998

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#  Dictionary vers : 2.2
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_cell_measurement_reflns_used	9166

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#------------------------------------------------------------------------#
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#------------------------------------------------------------------------#

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#------------------------------------------------------------------------#
#                REFINEMENT INFORMATION                                  #
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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^ > 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.
;
```

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Y1 Al1 Y1 107.01(2) . 81 ?
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Y1 Al1 Y1 72.99(2) . 9 ?
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Pt1 Al1 Y1 119.818(4) 9 77 ?
Pt1 Al1 Y1 120.449(14) 79 77 ?
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Pt1 Al1 Y1 60.182(4) 73 77 ?

Y1 Al1 Y1 107.01(2) . 77 ?
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$Y_6Pt_{13}Ga_4$: Crystallographic Information File

```
#\#CIF_1.1

#  CIF produced by WinGX routine CIF_UPDATE
#  Created on 2023-01-28 at 14:56:34
#  Using CIFtbx version 2.6.2 16 Jun 1998

#  Dictionary name : cif_core.dic
#  Dictionary vers : 2.2
#  Request file    : \wingx\files\archive.dat
#  CIF files read  : yptga1_5


data_yptga1_5

_audit_creation_date                2023-01-28T14:56:34-00:00
_audit_creation_method              'WinGX routine CIF_UPDATE'
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_audit_conform_dict_version         2.2
_audit_conform_dict_location        ftp://ftp.iucr.org/pub/cif_core.dic
_publ_requested_category            FI

#------------------------------------------------------------------------------#
#                 CHEMICAL INFORMATION                                         #
#------------------------------------------------------------------------------#

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;
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;
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_chemical_formula_weight            3348.51

#------------------------------------------------------------------------------#
#                 UNIT CELL INFORMATION                                        #
#------------------------------------------------------------------------------#

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_symmetry_space_group_name_Hall     '-I 4 2 3'
_symmetry_Int_Tables_number         229

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_cell_length_c	9.4465(10)
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_cell_volume	843.0(2)
_cell_formula_units_Z	2
_cell_measurement_temperature	293(2)
_cell_measurement_wavelength	0.71073
_cell_measurement_reflns_used	6167

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_cell_measurement_theta_min       3.05
_cell_measurement_theta_max       35.13

#------------------------------------------------------------------------#
#                CRYSTAL INFORMATION                                     #
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_exptl_crystal_colour             silver
_exptl_crystal_size_max           0.05
_exptl_crystal_size_mid           0.05
_exptl_crystal_size_min           0.05
_exptl_crystal_density_diffrn           13.192
_exptl_crystal_density_method           'not measured'
_exptl_crystal_F_000                    2744
_exptl_special_details
;
 ?
;

#------------------------------------------------------------------------#
#                ABSORPTION CORRECTION                                   #
#------------------------------------------------------------------------#

_exptl_absorpt_coefficient_mu           133.955
_exptl_absorpt_correction_type          none

#------------------------------------------------------------------------#
#                DATA COLLECTION                                       #
#------------------------------------------------------------------------#

_diffrn_ambient_temperature             293(2)
_diffrn_radiation_wavelength            0.71073
_diffrn_radiation_type                  MoK\a
_diffrn_radiation_monochromator         graphite
_diffrn_measurement_device_type   'Bruker APEX II CCD area-detector'
_diffrn_reflns_av_R_equivalents         0.099
_diffrn_reflns_av_unetI/netI            0.0272
_diffrn_reflns_number                   6167
_diffrn_reflns_limit_h_min              -15
_diffrn_reflns_limit_h_max              14
_diffrn_reflns_limit_k_min              -15
_diffrn_reflns_limit_k_max              15
_diffrn_reflns_limit_l_min              -15
_diffrn_reflns_limit_l_max              14
_diffrn_reflns_theta_min                3.05
_diffrn_reflns_theta_max                35.13
_diffrn_reflns_theta_full               35.13
_diffrn_measured_fraction_theta_full
                                        0.995
_diffrn_measured_fraction_theta_max
                                        0.995
_reflns_number_total                    220
_reflns_number_gt                       192
_reflns_threshold_expression            >2sigma(I)

#------------------------------------------------------------------------#
#                COMPUTER PROGRAMS USED                                  #
#------------------------------------------------------------------------#

_computing_structure_refinement         'SHELXL-97 (Sheldrick, 1997)'

#------------------------------------------------------------------------#
#                REFINEMENT INFORMATION                                  #
#------------------------------------------------------------------------#

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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^ > 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^)+(0.0113P)^2^+2.4634P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary          direct
_atom_sites_solution_secondary        difmap
_atom_sites_solution_hydrogens        'none'
_refine_ls_hydrogen_treatment         'none'
_refine_ls_extinction_method          SHELXL
_refine_ls_extinction_expression
                                Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^
_refine_ls_extinction_coef            0.000042(12)
_refine_ls_number_reflns              220
_refine_ls_number_parameters          13
_refine_ls_number_restraints          0
_refine_ls_R_factor_all               0.0281
_refine_ls_R_factor_gt                0.0191
_refine_ls_wR_factor_ref              0.0353
_refine_ls_wR_factor_gt               0.0339
_refine_ls_goodness_of_fit_ref        1.052
_refine_ls_restrained_S_all           1.052
_refine_ls_shift/su_max               0
_refine_ls_shift/su_mean              0
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_refine_diff_density_min              -2.742
_refine_diff_density_rms              0.446

#----------------------------------------------------------------------------#
#                 ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS           #
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Pt Pt -1.7033 8.3905 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Y Y -2.7962 3.5667 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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    _atom_site_adp_type
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
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    _atom_site_refinement_flags
    _atom_site_disorder_assembly
    _atom_site_disorder_group
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Pt1 Pt 0 0.32427(3) 0.32427(3) 0.00560(10) Uani 1 4 d S . .
Y1 Y 0.30045(14) 0 0 0.0060(2) Uani 1 8 d S . .
Ga1 Ga 0.25 0.25 0.25 0.0076(3) Uani 1 12 d S . .

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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
Pt2 0.0074(2) 0.0074(2) 0.0074(2) 0 0 0
Pt1 0.00388(17) 0.00646(12) 0.00646(12) 0.00154(10) 0 0
Y1 0.0063(6) 0.0058(3) 0.0058(3) 0 0 0
Ga1 0.0076(3) 0.0076(3) 0.0076(3) 0.0029(4) 0.0029(4) 0.0029(4)


#----------------------------------------------------------------------------#
#                 MOLECULAR GEOMETRY                                         #
#----------------------------------------------------------------------------#
```

```
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;
 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.
;
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   _geom_bond_site_symmetry_2
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Pt2 Y1 2.8382(13) 53 ?
Pt2 Y1 2.8382(13) 9 ?
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Pt1 Ga1 2.5616(3) . ?
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Pt1 Pt1 2.7350(3) 77_455 ?
Pt1 Pt1 2.7350(3) 35_455 ?
Pt1 Y1 3.0108(9) 73 ?
Pt1 Y1 3.0108(9) 25_455 ?
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Pt1 Y1 3.0715(4) 9 ?
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Y1 Pt1 3.0108(9) 75_545 ?
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Y1 Pt1 3.0108(9) 25_544 ?
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Y1 Ga1 3.3737(4) . ?
Y1 Ga1 3.3737(4) 28_545 ?
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Ga1 Pt1 2.5616(3) 9 ?
Ga1 Pt1 2.5616(3) 73 ?
Ga1 Pt1 2.5616(3) 7 ?
Ga1 Pt1 2.5616(3) 79 ?
Ga1 Y1 3.3737(4) 81 ?
Ga1 Y1 3.3737(4) 73 ?
Ga1 Y1 3.3737(4) 5 ?
Ga1 Y1 3.3737(4) 77 ?
Ga1 Y1 3.3737(4) 9 ?

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Ga1 Pt1 Y1 151.55(2) . 25_455 ?
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Pt1 Pt1 Y1 109.162(12) 79 25_455 ?
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Ga1 Pt1 Y1 72.949(8) . 9 ?
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Pt2 Y1 Pt1 128.763(19) . 25_544 ?
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Pt1 Y1 Pt1 53.434(8) 73 9 ?
Pt1 Y1 Pt1 120.27(3) 75_545 9 ?
Pt1 Y1 Pt1 53.434(8) 27_554 9 ?
Pt1 Y1 Pt1 120.27(3) 25_544 9 ?
Pt2 Y1 Pt1 94.20(2) . 7 ?
Pt1 Y1 Pt1 53.434(8) 73 7 ?
Pt1 Y1 Pt1 53.434(8) 75_545 7 ?
Pt1 Y1 Pt1 120.27(3) 27_554 7 ?
Pt1 Y1 Pt1 120.27(3) 25_544 7 ?
Pt1 Y1 Pt1 89.692(3) 9 7 ?
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Pt1 Y1 Pt1 120.27(3) 73 11 ?
Pt1 Y1 Pt1 53.434(8) 75_545 11 ?
Pt1 Y1 Pt1 120.27(3) 27_554 11 ?
Pt1 Y1 Pt1 53.434(8) 25_544 11 ?
Pt1 Y1 Pt1 171.60(5) 9 11 ?
Pt1 Y1 Pt1 89.692(3) 7 11 ?
Pt2 Y1 Pt1 94.20(2) . 53 ?
Pt1 Y1 Pt1 120.27(3) 73 53 ?
Pt1 Y1 Pt1 120.27(3) 75_545 53 ?
Pt1 Y1 Pt1 53.434(8) 27_554 53 ?

Pt1 Y1 Pt1 53.434(8) 25_544 53 ?
Pt1 Y1 Pt1 89.692(3) 9 53 ?
Pt1 Y1 Pt1 171.60(5) 7 53 ?
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Pt1 Y1 Ga1 95.074(11) 27_554 2 ?
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Pt1 Y1 Ga1 46.545(2) 53 2 ?
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Pt1 Y1 Ga1 46.545(2) 9 . ?
Pt1 Y1 Ga1 46.545(2) 7 . ?
Pt1 Y1 Ga1 135.112(4) 11 . ?
Pt1 Y1 Ga1 135.112(4) 53 . ?
Ga1 Y1 Ga1 163.76(4) 2 . ?
Pt2 Y1 Ga1 81.88(2) . 28_545 ?
Pt1 Y1 Ga1 95.074(11) 73 28_545 ?
Pt1 Y1 Ga1 46.884(5) 75_545 28_545 ?
Pt1 Y1 Ga1 149.36(4) 27_554 28_545 ?
Pt1 Y1 Ga1 95.074(11) 25_544 28_545 ?
Pt1 Y1 Ga1 135.112(4) 9 28_545 ?
Pt1 Y1 Ga1 46.545(2) 7 28_545 ?
Pt1 Y1 Ga1 46.545(2) 11 28_545 ?
Pt1 Y1 Ga1 135.112(4) 53 28_545 ?
Ga1 Y1 Ga1 88.857(6) 2 28_545 ?
Ga1 Y1 Ga1 88.857(6) . 28_545 ?
Pt1 Ga1 Pt1 64.532(5) . 81 ?
Pt1 Ga1 Pt1 115.468(5) . 9 ?
Pt1 Ga1 Pt1 180 81 9 ?
Pt1 Ga1 Pt1 180 . 73 ?
Pt1 Ga1 Pt1 115.468(5) 81 73 ?
Pt1 Ga1 Pt1 64.532(5) 9 73 ?
Pt1 Ga1 Pt1 115.468(5) . 7 ?
Pt1 Ga1 Pt1 64.532(5) 81 7 ?
Pt1 Ga1 Pt1 115.468(5) 9 7 ?
Pt1 Ga1 Pt1 64.532(5) 73 7 ?
Pt1 Ga1 Pt1 64.532(5) . 79 ?
Pt1 Ga1 Pt1 115.468(5) 81 79 ?
Pt1 Ga1 Pt1 64.532(5) 9 79 ?
Pt1 Ga1 Pt1 115.468(5) 73 79 ?
Pt1 Ga1 Pt1 180 7 79 ?
Pt1 Ga1 Y1 120.91(2) . . ?
Pt1 Ga1 Y1 119.494(7) 81 . ?
Pt1 Ga1 Y1 60.506(7) 9 . ?
Pt1 Ga1 Y1 59.09(2) 73 . ?
Pt1 Ga1 Y1 60.506(7) 7 . ?
Pt1 Ga1 Y1 119.494(7) 79 . ?
Pt1 Ga1 Y1 119.494(7) . 81 ?
Pt1 Ga1 Y1 120.91(2) 81 81 ?
Pt1 Ga1 Y1 59.09(2) 9 81 ?
Pt1 Ga1 Y1 60.506(7) 73 81 ?
Pt1 Ga1 Y1 119.494(7) 7 81 ?
Pt1 Ga1 Y1 60.506(7) 79 81 ?
Y1 Ga1 Y1 106.99(3) . 81 ?
Pt1 Ga1 Y1 59.09(2) . 73 ?
Pt1 Ga1 Y1 60.506(7) 81 73 ?
Pt1 Ga1 Y1 119.494(7) 9 73 ?
Pt1 Ga1 Y1 120.91(2) 73 73 ?
Pt1 Ga1 Y1 119.494(7) 7 73 ?
Pt1 Ga1 Y1 60.506(7) 79 73 ?
Y1 Ga1 Y1 180.00(4) . 73 ?
Y1 Ga1 Y1 73.01(3) 81 73 ?
Pt1 Ga1 Y1 60.506(7) . 5 ?
Pt1 Ga1 Y1 119.494(7) 81 5 ?
Pt1 Ga1 Y1 60.506(7) 9 5 ?
Pt1 Ga1 Y1 119.494(7) 73 5 ?
Pt1 Ga1 Y1 120.91(2) 7 5 ?
Pt1 Ga1 Y1 59.09(2) 79 5 ?
Y1 Ga1 Y1 73.01(3) . 5 ?

Y1 Ga1 Y1 106.99(3) 81 5 ?
Y1 Ga1 Y1 106.99(3) 73 5 ?
Pt1 Ga1 Y1 119.494(7) . 77 ?
Pt1 Ga1 Y1 60.506(7) 81 77 ?
Pt1 Ga1 Y1 119.494(7) 9 77 ?
Pt1 Ga1 Y1 60.506(7) 73 77 ?
Pt1 Ga1 Y1 59.09(2) 7 77 ?
Pt1 Ga1 Y1 120.91(2) 79 77 ?
Y1 Ga1 Y1 106.99(3) . 77 ?
Y1 Ga1 Y1 73.01(3) 81 77 ?
Y1 Ga1 Y1 73.01(3) 73 77 ?
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Pt1 Ga1 Y1 60.506(7) . 9 ?
Pt1 Ga1 Y1 59.09(2) 81 9 ?
Pt1 Ga1 Y1 120.91(2) 9 9 ?
Pt1 Ga1 Y1 119.494(7) 73 9 ?
Pt1 Ga1 Y1 60.506(7) 7 9 ?
Pt1 Ga1 Y1 119.494(7) 79 9 ?
Y1 Ga1 Y1 73.01(3) . 9 ?
Y1 Ga1 Y1 180 81 9 ?
Y1 Ga1 Y1 106.99(3) 73 9 ?
Y1 Ga1 Y1 73.01(3) 5 9 ?
Y1 Ga1 Y1 106.99(3) 77 9 ?