Supporting Information :

- RKmax value, Exact SOC implementation details, and convergence tests:

The cutoff energy of the potential and the wavefunction was set to 196 Ry and 9 Ry, respectively. Additionally, self-consistent and spin-polarized including spin-orbit-coupling (SOC) calculations were carried out with a convergence criterion of 10^{-4} eV for the total energy. The SOC calculations was performed using the LAPWSO program implemented in Wien2k, it was activated for the 4f electrons of Gadolinium. As described by Singh and Nordström (2006) and Novák (1997) [1], the second variational procedure in LAPWSO computes eigenvectors and eigenvalues by building upon the scalar-relativistic wavefunctions from LAPW1. This specific implementation diagonalizes the SO coupling within the space of scalar-relativistic eigenstates.

References:

[1] **Singh, D. J. and Nordstrom, L. (2006). Planewaves, Pseudopotentials and the LAPW Method, 2nd ed. Springer, Berlin. 8, 11, 158**

- Cif file of the powder diffracted $GdPO_4$:

```
##############################################################################
###      FullProf-generated CIF output file  (version: May 2019)           ###
###      Template of CIF submission form for structure report              ###
##############################################################################

# This file has been generated using FullProf.2k taking one example of
# structure report provided by Acta Cryst. It is given as a 'template' with
# filled structural items. Many other items are left unfilled and it is the
# responsibility of the user to properly fill or suppress them. In principle
# all question marks '?' should be replaced by the appropriate text or
# numerical value depending on the kind of CIF item.
# See the document: cif_core.dic (URL: http://www.iucr.org) for details.

# Please notify any error or suggestion to:
#           Juan Rodriguez-Carvajal (jrc@ill.eu)
# Improvements will be progressively added as needed.
#      Date: 27/07/2025  Time: 00:40:20.317


#=============================================================================
 data_global
#=============================================================================

_audit_creation_date  27/07/2025
_audit_creation_method  "FullProf Suite"
# PROCESSING SUMMARY (IUCr Office Use Only)

_journal_data_validation_number      ?

_journal_date_recd_electronic        ?
_journal_date_to_coeditor            ?
_journal_date_from_coeditor          ?
_journal_date_accepted               ?
_journal_date_printers_first         ?
_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                  ?
_journal_name_full                   ?
_journal_year                        ?
_journal_volume                      ?
_journal_issue                       ?
_journal_page_first                  ?
_journal_page_last                   ?
_journal_paper_category              ?
_journal_suppl_publ_number           ?
_journal_suppl_publ_pages            ?

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

# 1. SUBMISSION DETAILS

_publ_contact_author_name            ?  # Name of author for correspondence
_publ_contact_author_address            # Address of author for correspondence
; ?
;
_publ_contact_author_email           ?
_publ_contact_author_fax             ?
_publ_contact_author_phone           ?

_publ_contact_letter
; ?
;

_publ_requested_journal              ?
_publ_requested_coeditor_name        ?
_publ_requested_category             ?   # Acta C: one of CI/CM/CO/FI/FM/FO


# Definition of non standard CIF items (Reliability indices used in FULLPROF)

loop_
_publ_manuscript_incl_extra_item
_publ_manuscript_incl_extra_info
_publ_manuscript_incl_extra_defn
#      Name                              Explanation                 Standard?
#     ------                             -----------                 ---------
 '_pd_proc_ls_prof_cR_factor'    'Prof. R-factor CORRECTED for background'   no
 '_pd_proc_ls_prof_cwR_factor'   'wProf.R-factor CORRECTED for background'   no
 '_pd_proc_ls_prof_cwR_expected' 'wProf.Expected CORRECTED for background'   no
 '_pd_proc_ls_prof_chi2'         'Chi-square for all considered points'      no
 '_pd_proc_ls_prof_echi2'        'Chi-2 for points with Bragg contribution'  no
#==============================================================================

# 3. TITLE AND AUTHOR LIST

_publ_section_title
; ' GdPO4'
;
_publ_section_title_footnote
;
;

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

loop_
    _publ_author_name
    _publ_author_footnote
```

```
    _publ_author_address
?                                   #<--'Last name, first name'
; ?
;
; ?
;

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

# 4. TEXT

_publ_section_synopsis
;  ?
;
_publ_section_abstract
; ?
;
_publ_section_comment
; ?
;
_publ_section_exptl_prep      # Details of the preparation of the sample(s)
                              # should be given here.
; ?
;
_publ_section_exptl_refinement
; ?
;
_publ_section_references
; ?
;
_publ_section_figure_captions
; ?
;
_publ_section_acknowledgements
; ?
;

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

#===============================================================================
# If more than one structure is reported, the remaining sections should be
# completed per structure. For each data set, replace the '?' in the
# data_? line below by a unique identifier.

data_GdPO4

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

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common             ?
_chemical_formula_moiety          ?
_chemical_formula_structural      ?
_chemical_formula_analytical      ?
_chemical_formula_iupac           ?
_chemical_formula_sum             ?
_chemical_formula_weight          ?
_chemical_melting_point           ?
_chemical_compound_source         ?       # for minerals and
                                          # natural products

loop_
    _atom_type_symbol
    _atom_type_scat_Cromer_Mann_a1
    _atom_type_scat_Cromer_Mann_b1
```

```
    _atom_type_scat_Cromer_Mann_a2
    _atom_type_scat_Cromer_Mann_b2
    _atom_type_scat_Cromer_Mann_a3
    _atom_type_scat_Cromer_Mann_b3
    _atom_type_scat_Cromer_Mann_a4
    _atom_type_scat_Cromer_Mann_b4
    _atom_type_scat_Cromer_Mann_c
    _atom_type_scat_dispersion_real
    _atom_type_scat_dispersion_imag
    _atom_type_scat_source
gd+3  24.34660   2.13553  20.42080   0.15552  11.87080  10.57820
       3.71490  21.70290   0.64509  -9.24200  11.94600
 International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6.1.1.5
p      6.43450   1.90670   4.17910  27.15700   1.78000   0.52600
       1.49080  68.16450   1.11490   0.28300   0.43400
 International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6.1.1.5
o-2    4.75800   7.83100   3.63700  30.05000   0.00000   0.00000
       0.00000   0.00000   1.59400   0.04700   0.03200
 International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6.1.1.5

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

# 6. POWDER SPECIMEN AND CRYSTAL DATA

_symmetry_cell_setting               Monoclinic
_symmetry_space_group_name_H-M       'P 21/n'
_symmetry_space_group_name_Hall      '-P 2yn'

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

_cell_length_a                       6.6532(3)
_cell_length_b                       6.8491(3)
_cell_length_c                       6.3366(3)
_cell_angle_alpha                    90.0000
_cell_angle_beta                     104.0008(16)
_cell_angle_gamma                    90.0000
_cell_volume                         280.17(2)
_cell_formula_units_Z                ?
_cell_measurement_temperature        ?
_cell_special_details
; ?
;
# The next three fields give the specimen dimensions in mm.  The equatorial
# plane contains the incident and diffracted beam.

_pd_spec_size_axial              ?       # perpendicular to
                                         # equatorial plane
_pd_spec_size_equat              ?       # parallel to
                                         # scattering vector
                                         # in transmission
_pd_spec_size_thick              ?       # parallel to
                                         # scattering vector
                                         # in reflection

# The next five fields are character fields that describe the specimen.

_pd_spec_mounting                        # This field should be
                                         # used to give details of the
                                         # container.
; ?
;
_pd_spec_mount_mode              ?       # options are 'reflection'
                                         # or 'transmission'
```

```
_pd_spec_shape                    ?       # options are 'cylinder'
                                          # 'flat_sheet' or 'irregular'
_pd_char_particle_morphology      ?
_pd_char_colour                   ?       # use ICDD colour descriptions

# The following three fields describe the preparation of the specimen.
# The cooling rate is in K/min.  The pressure at which the sample was
# prepared is in kPa.  The temperature of preparation is in K.

_pd_prep_cool_rate                ?
_pd_prep_pressure                 ?
_pd_prep_temperature              ?

# The next four fields are normally only needed for transmission experiments.

_exptl_absorpt_coefficient_mu        ?
_exptl_absorpt_correction_type       ?
_exptl_absorpt_process_details       ?
_exptl_absorpt_correction_T_min      ?
_exptl_absorpt_correction_T_max      ?

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

# 7. EXPERIMENTAL DATA

_exptl_special_details
; ?
;

# The following item is used to identify the equipment used to record
# the powder pattern when the diffractogram was measured at a laboratory
# other than the authors' home institution, e.g. when neutron or synchrotron
# radiation is used.

_pd_instr_location
; ?
;
_pd_calibration_special_details           # description of the method used
                                          # to calibrate the instrument
; ?
;

_diffrn_ambient_temperature          ?
_diffrn_source              ? # Put here: 'rotating-anode X-ray tube' or similar
_diffrn_radiation_type     'X-ray'
_diffrn_source_target       ? # Put here the chemical symbol of the anode

_diffrn_radiation_monochromator      ?
_diffrn_measurement_device_type      ?
_diffrn_measurement_method           ?
_diffrn_detector_area_resol_mean     ?
_diffrn_detector                     ?
_diffrn_detector_type                ? # make or model of detector
_pd_meas_scan_method      ?   # options are 'step', 'cont',
                              # 'tof', 'fixed' or
                              # 'disp' (= dispersive)
_pd_meas_special_details
;  ?
;

#  The following four items give details of the measured (not processed)
#  powder pattern.  Angles are in degrees.

_pd_meas_number_of_points         3452
_pd_meas_2theta_range_min         10.00215
_pd_meas_2theta_range_max         79.99879
_pd_meas_2theta_range_inc         0.020283
```

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

# 8. REFINEMENT DATA

_refine_special_details
; ?
;

# Use the next field to give any special details about the fitting of the
# powder pattern.

_pd_proc_ls_special_details
; ?
;

# The next three items are given as text.

_pd_proc_ls_profile_function      ?
_pd_proc_ls_background_function   ?
_pd_proc_ls_pref_orient_corr
; ?
;

#  The following profile R-factors are NOT CORRECTED for background
#  The sum is extended to all non-excluded points.
#  These are the current CIF standard

_pd_proc_ls_prof_R_factor               3.8909
_pd_proc_ls_prof_wR_factor              4.9237
_pd_proc_ls_prof_wR_expected            4.0678

#  The following profile R-factors are CORRECTED for background
#  The sum is extended to all non-excluded points.
#  These items are not in the current CIF standard, but are defined above

_pd_proc_ls_prof_cR_factor              34.4865
_pd_proc_ls_prof_cwR_factor             23.6001
_pd_proc_ls_prof_cwR_expected           19.4977

#  The following items are not in the CIF standard, but are defined above

_pd_proc_ls_prof_chi2                 1.4651
_pd_proc_ls_prof_echi2                1.3712

#  Items related to LS refinement

_refine_ls_R_I_factor               14.7744
_refine_ls_number_reflns                 374
_refine_ls_number_parameters              35
_refine_ls_number_restraints               0

# The following four items apply to angular dispersive measurements.
# 2theta minimum, maximum and increment (in degrees) are for the
# intensities used in the refinement.

_pd_proc_2theta_range_min               9.8356
_pd_proc_2theta_range_max              79.8322
_pd_proc_2theta_range_inc             0.020283
_pd_proc_wavelength                   1.540560

_pd_block_diffractogram_id        ?  # The id used for the block containing
                                     # the powder pattern profile (section 11)

# Give appropriate details in the next two text fields.

_pd_proc_info_excluded_regions    ?
_pd_proc_info_data_reduction      ?
```

```
# The following items are used to identify the programs used.

_computing_data_collection           ?
_computing_structure_solution        ?
_computing_structure_refinement      FULLPROF
_computing_molecular_graphics        ?
_computing_publication_material      ?

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

# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

loop_
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_adp_type
    _atom_site_type_symbol
 Gd  0.2798(5)  0.1553(6)  0.0959(6)  0.0103(14)  1.00000 Uiso Gd+3
 P  0.296(2)  0.163(2)  0.607(3)  0.008(4)  1.00000 Uiso P
 O1  0.252(4) -0.005(4)  0.418(6)  0.027(5)  1.00000 Uiso O-2
 O2  0.369(3)  0.325(4)  0.508(5)  0.027(5)  1.00000 Uiso O-2
 O3  0.467(4)  0.119(4)  0.816(4)  0.027(5)  1.00000 Uiso O-2
 O4  0.114(4)  0.223(4)  0.714(4)  0.027(5)  1.00000 Uiso O-2

# Note: if the displacement parameters were refined anisotropically
# the U matrices should be given as for single-crystal studies.

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

# 10. DISTANCES AND ANGLES / MOLECULAR GEOMETRY

_geom_special_details                ?

loop_
    _geom_bond_atom_site_label_1
    _geom_bond_atom_site_label_2
    _geom_bond_site_symmetry_1
    _geom_bond_site_symmetry_2
    _geom_bond_distance
    _geom_bond_publ_flag
    ?   ?   ?   ?   ?   ?

loop_
    _geom_contact_atom_site_label_1
    _geom_contact_atom_site_label_2
    _geom_contact_distance
    _geom_contact_site_symmetry_1
    _geom_contact_site_symmetry_2
    _geom_contact_publ_flag
    ?   ?   ?   ?   ?   ?

loop_
_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_2
_geom_angle_site_symmetry_3
_geom_angle
_geom_angle_publ_flag
?   ?   ?   ?   ?   ?   ?   ?

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_site_symmetry_1
_geom_torsion_site_symmetry_2
_geom_torsion_site_symmetry_3
_geom_torsion_site_symmetry_4
_geom_torsion
_geom_torsion_publ_flag
?   ?   ?   ?   ?   ?   ?   ?   ?   ?

loop_
_geom_hbond_atom_site_label_D
_geom_hbond_atom_site_label_H
_geom_hbond_atom_site_label_A
_geom_hbond_site_symmetry_D
_geom_hbond_site_symmetry_H
_geom_hbond_site_symmetry_A
_geom_hbond_distance_DH
_geom_hbond_distance_HA
_geom_hbond_distance_DA
_geom_hbond_angle_DHA
_geom_hbond_publ_flag
?   ?   ?   ?   ?   ?   ?   ?   ?   ?   ?

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

#===============================================================================
# Additional structures (last six sections and associated data_? identifiers)
# may be added at this point.
#===============================================================================

# The following lines are used to test the character set of files sent by
# network email or other means. They are not part of the CIF data set.
# abcdefghijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789
# !@#$%^&*()_+{}:"~<>?|\-=[];'`,./
```