Electronic Supplementary Material (ESI) for RSC Advances.

Enhanced Electrochemical Performance of Ce-MOF/h-CeO_2 for high Capacitance Energy Storage Applications

Ruhani Baweja[a], Monika Verma[b,c], Sanjeev Gautam[*,b] , Shailesh Upreti[d], and Navdeep Goyal[a]

[a]Department of Physics, Panjab University, Chandigarh- 160014, India
[b]Advanced Functional Materials Lab, Dr. S.S.B. University Institute of Chemical Engineering & Technology, Panjab University, Chandigarh- 160014, India
[c]Energy Research Centre, Panjab University, Chandigarh- 160014, India
[d]Charge CCCV (C4V), Center of Excellence, Binghamton University, 45 Murray Hill Road, Vestal, NY 13850, USA

Ce-MOF and its composites with h-CeO_2 as potential electrode materials for enhanced electrochemical supercapacitor performance

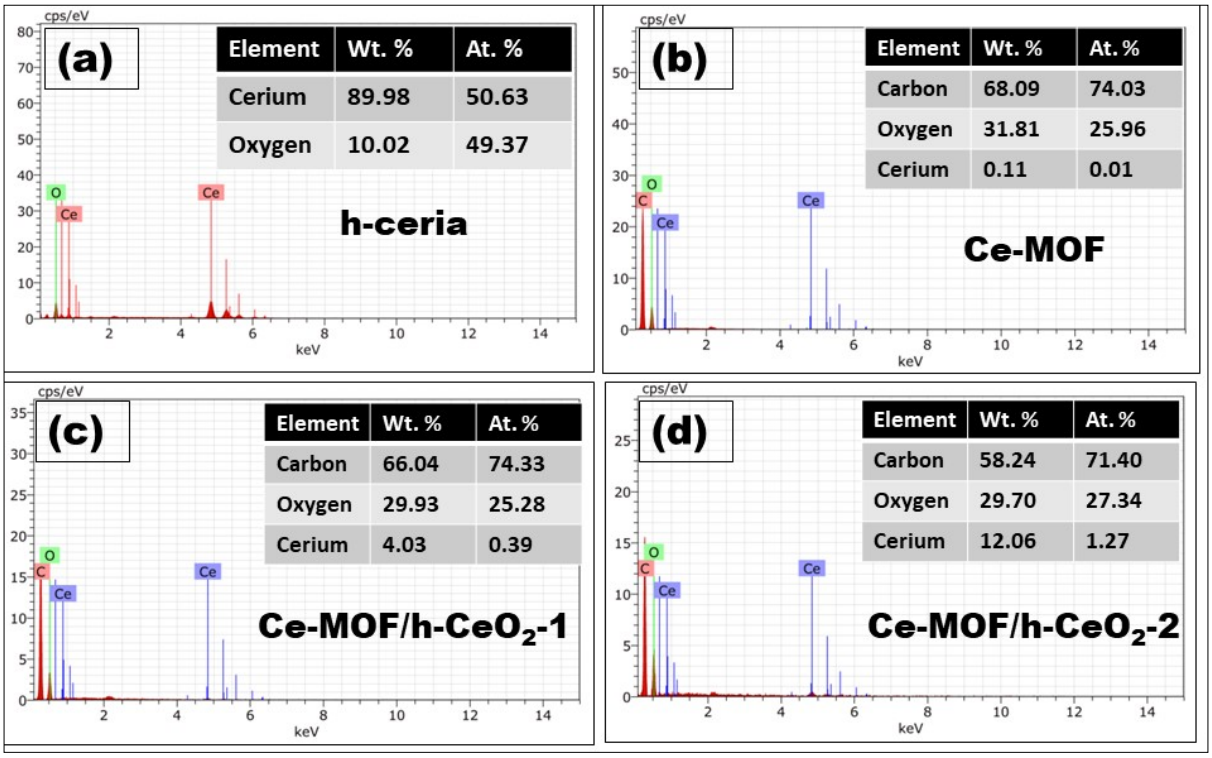

Figure S1: Elemental composition study of (a) h-CeO_2, (b) Ce-MOF, (c) Ce-MOF/h-CeO_2-1, and (d) Ce-MOF/h-CeO_2-2 using EDS analysis

*Corresponding Author: E-mail: sgautam@pu.ac.in; Tel: +91 97797 13212

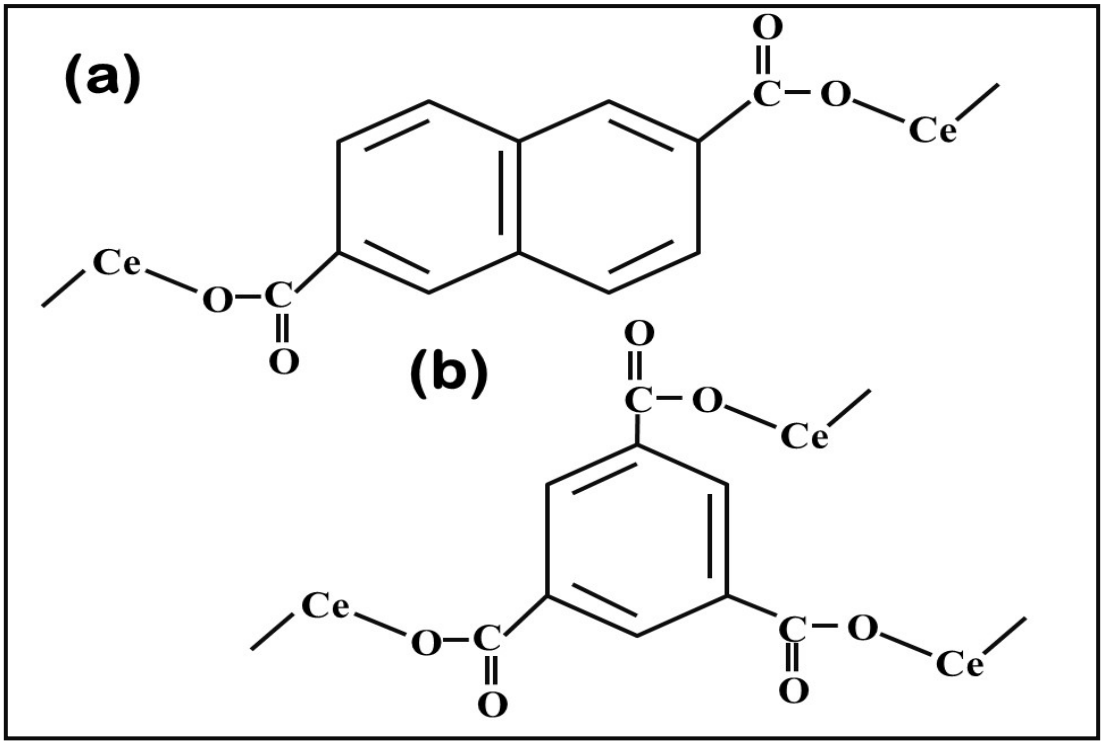

Figure S2: (a) 2,6-dinaphthalene dicarboxylic acid, (b) 1,3,5-tricarboxylic acid

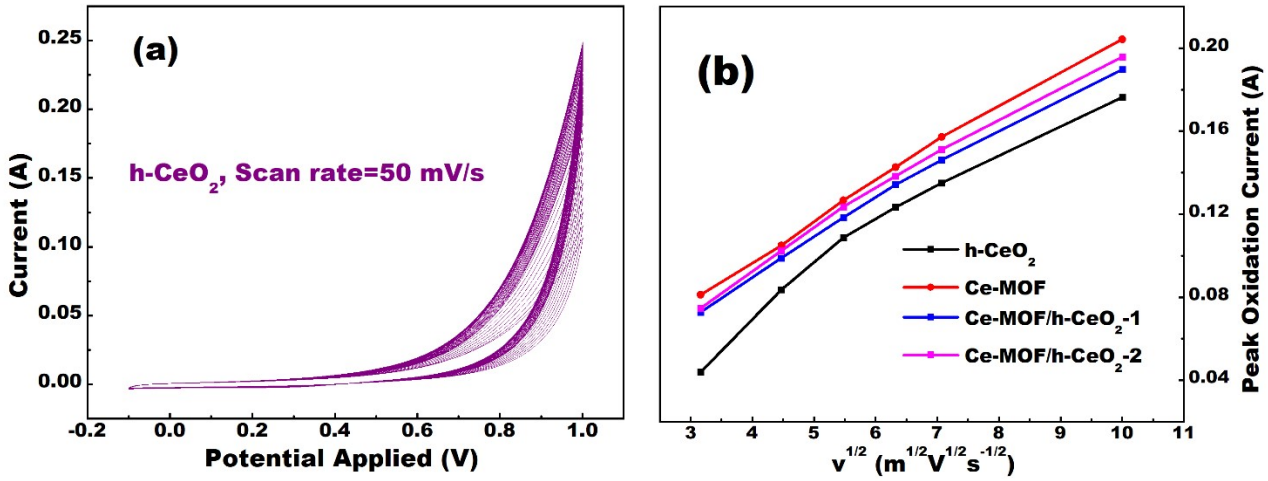

Figure S3: (a) CV curve for h-Ceria at a scan rate of 50 mV/s and 50 cycles, (b) Peak current vs. $v^{1/2}$ plot to understand the diffusivity of the samples in the electrolyte.

CIF FILE

```
##############################################################################
###
###      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: 28/05/2024  Time: 22:40:38.695


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

_audit_creation_date  28/05/2024
_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
; ' Ceria'
;
_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_Cubic

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

# 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
ce    21.16710   2.81219  19.76950   0.22684  11.85130  17.60830
      3.33049 127.11300   1.86264  -2.17000   9.64800
```

International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6.1.1.5
o 3.04850 13.27710 2.28680 5.70110 1.54630 0.32390
0.86700 32.90890 0.25080 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 Cubic
_symmetry_space_group_name_H-M 'F m -3 m'
_symmetry_space_group_name_Hall '-F 4 2 3'

loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'x,-y,-z'
'-x,y,-z'
'-x,-y,z'
'y,z,x'
'-y,-z,x'
'y,-z,-x'
'-y,z,-x'
'z,x,y'
'-z,x,-y'
'-z,-x,y'
'z,-x,-y'
'y,x,z'
'-y,x,-z'
'y,-x,-z'
'-y,-x,z'
'z,y,x'
'-z,-y,x'
'-z,y,-x'
'z,-y,-x'
'x,z,y'
'x,-z,-y'
'-x,-z,y'
'-x,z,-y'
'-x,-y,-z'
'-x,y,z'
'x,-y,z'
'x,y,-z'
'-y,-z,-x'
'y,z,-x'
'-y,z,x'
'y,-z,x'
'-z,-x,-y'
'z,-x,y'

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

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

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

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

_cell_length_a                  5.4180(6)
_cell_length_b                  5.4180(6)
_cell_length_c                  5.4180(6)
_cell_angle_alpha                90.0000
_cell_angle_beta                 90.0000
_cell_angle_gamma                   90.0000
_cell_volume                    159.04(3)
_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   1576
_pd_meas_2theta_range_min   23.01871
_pd_meas_2theta_range_max   74.99371
_pd_meas_2theta_range_inc   0.033000

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

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   9.3299
_pd_proc_ls_prof_wR_factor   12.0253
_pd_proc_ls_prof_wR_expected   8.9530

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   48.4323
_pd_proc_ls_prof_cwR_factor   31.9397
_pd_proc_ls_prof_cwR_expected   23.7795

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

_pd_proc_ls_prof_chi2               1.8041
_pd_proc_ls_prof_echi2              1.2533

#  Items related to LS refinement

_refine_ls_R_I_factor               3.3016
_refine_ls_number_reflns                 14
_refine_ls_number_parameters              7
_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            22.9413
_pd_proc_2theta_range_max            74.9163
_pd_proc_2theta_range_inc           0.033000
_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
 Ce  0.00000  0.00000  0.00000  0.00773  1.00000 Uiso Ce
 O  0.25000  0.25000  0.25000 -0.0172  1.09084 Uiso O

# 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
!@#$%^&*()_+{}:"~<>?|\-=[];'`,./