```
##############################################################################
#####
###      FullProf-generated CIF output file  (version: May 2011)
###
###      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.

#==============================================================================
=====
 data_TON
#==============================================================================
=====

# PROCESSING SUMMARY (IUCr Office Use Only)


#==============================================================================
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# 1. SUBMISSION DETAILS


# 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

_journal_name_full               'The Journal of Physical Chemistry C'
_journal_year                    2017
_journal_volume                  ?
_journal_page                    ?
_publ_contact_author_name        ''Julien Haines'
_publ_contact_author_address
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
Universit\'e de Montpellier,
Montpellier,
France
;
_publ_contact_author_email       julien.haines@umontpellier.fr
_publ_section_title
;
High-pressure phase transition, pore collapse and amorphisation in the
siliceous 1D zeolite, TON
;
loop_
_publ_author_name
_publ_author_footnote
_publ_author_address
'Jean-Marc Thibaud' ?
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
Universit\'e de Montpellier,
Montpellier,
France
;
'Jerome Rouquette' ?
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
Universit\'e de Montpellier,
Montpellier,
France
;
'Patrick Hermet' ?
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
Universit\'e de Montpellier,
Montpellier,
France
;
'Kamil Dzuibek' ?
;European Laboratory  for non Linear Spectroscopy (LENS), Sesto
Fiorentino,
Firenze,
Italy
Dipartimento di Chimica dell'Universit\`a di Firenze,
Sesto Fiorentino,
Firenze,
```

Italy
;
'Federico A. Gorelli' ?
;European Laboratory for non Linear Spectroscopy (LENS), Sesto
Fiorentino,
Firenze,
Italy
INO-CNR,
Sesto Fiorentino,
Firenze,
Italy
;
'Mario Santoro' ?
;   INO-CNR,
Sesto Fiorentino,
Firenze,
Italy
European Laboratory for non Linear Spectroscopy (LENS), Sesto
Fiorentino,
Firenze,
Italy
;
'Gaston Garbarino' ?
;European Synchrotron Radiation Facility (ESRF),
Grenoble,
France
;
'Frederico G. Alabarse' ?
;Synchrotron SOLEIL,
Saint Aubin,
France
;
'Olivier Cambon' ?
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
Universit\'e de Montpellier,
Montpellier,
France
;
'Francesco Di Renzo' ?
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
ENSCM-Universit\'e de Montpellier,
Montpellier,
France
;
'Arie van der Lee' ?
;Institut Europ\'een des Membranes de Montpellier,
UMR-CNRS 5635,
Universit\'e de Montpellier,
Montpellier,
France
;
'Julien Haines' .
;Institut Charles Gerhardt Montpellier,
UMR 5253 CNRS,
Universit\'e de Montpellier,
Montpellier,

```
France
;

# The loop structure below should contain the names and addresses of all


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

# 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_TON

#=============================================================================
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# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
```

```
_chemical_name_common              TON
_chemical_formula_moiety           '     O24 Si12 C1.67'
_chemical_formula_structural       ?
_chemical_formula_analytical       ?
_chemical_formula_iupac            ?
_chemical_formula_sum              'C1.67 O24 Si12'
_chemical_formula_weight           741.15
_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
o      3.04850  13.27710   2.28680   5.70110   1.54630   0.32390
       0.86700  32.90890   0.25080   0.00300   0.00400

International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6
.1.1.5
si     6.29150   2.43860   3.03530  32.33370   1.98910   0.67850
       1.54100  81.69370   1.14070   0.04200   0.04300

International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6
.1.1.5
c      2.31000  20.84390   1.02000  10.20750   1.58860   0.56870
       0.86500  51.65120   0.21560   0.00000   0.00100

International_Tables_for_Crystallography_Vol.C(1991)_Tables_6.1.1.4_and_6
.1.1.5

#=============================================================================
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# 6. POWDER SPECIMEN AND CRYSTAL DATA

_symmetry_cell_setting               Orthorhombic
_symmetry_space_group_name_H-M       'C m c 21'
_symmetry_space_group_name_Hall      'C 2c -2'

loop_
    _symmetry_equiv_pos_as_xyz   #<--must include 'x,y,z'
'x,y,z'
'-x,y,z'
'x,-y,z+1/2'
'-x,-y,z+1/2'
'x+1/2,y+1/2,z'
'-x+1/2,y+1/2,z'
```

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

_cell_length_a                       13.7511(2)
_cell_length_b                       17.2725(4)
_cell_length_c                       4.99030(10)
_cell_angle_alpha                    90.00000
_cell_angle_beta                     90.00000
_cell_angle_gamma                    90.00000
_cell_volume                         1185.27(4)
_cell_formula_units_Z                2
_cell_measurement_temperature     293
_cell_measurement_pressure        420000
_cell_measurement_reflns_used    248
_cell_measurement_theta_min      2.05
_cell_measurement_theta_max      20.50
_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.
; 'mounted in a diamond-anvil cell '
;
_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      293
_diffrn_ambient_pressure      420000
_diffrn_source                   'ESRF synchrotron'
_diffrn_radiation_type           synchrotron
_diffrn_source_target            ? # Put here the chemical symbol of the
anode

_diffrn_radiation_monochromator  ?
_diffrn_measurement_device_type  ID09A
_diffrn_radiation_wavelength     0.414132
_diffrn_measurement_method       ?
_diffrn_detector_area_resol_mean ? # Not in version 2.0.1
_diffrn_detector                 ?
_diffrn_detector_type            'MAR555 flat panel 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         4369
_pd_meas_2theta_range_min         0.01585
_pd_meas_2theta_range_max         27.70609
_pd_meas_2theta_range_inc         0.006341
```

```
#=============================================================================
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# 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                0.1011
_pd_proc_ls_prof_wR_factor               0.1795
_pd_proc_ls_prof_wR_expected             0.6277

#  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               10.9464
_pd_proc_ls_prof_cwR_factor               4.0661
_pd_proc_ls_prof_cwR_expected            14.2204

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

_pd_proc_ls_prof_chi2                 0.0818
_pd_proc_ls_prof_echi2                0.0818

#  Items related to LS refinement

_refine_ls_R_I_factor                 4.3117
_refine_ls_number_reflns                   656
_refine_ls_number_parameters                84
_refine_ls_number_restraints                54
_refine_ls_goodness_of_fit_all   0.286

# 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                0.0158
```

```
_pd_proc_2theta_range_max               27.7061
_pd_proc_2theta_range_inc              0.006341
_pd_proc_wavelength                    0.414132

_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      ?

#=============================================================================
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# 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              # Not in version 2.0.1
    _atom_site_type_symbol
 O1  0.0951(14)  0.4276(19)  0.712(13)  0.048(7)  1.00000 Uiso O
 O2  0.0904(12)  0.2190(20)  0.246(16)  0.048(7)  1.00000 Uiso O
 O3  0.276(2)  0.3797(12)  0.723(19)  0.048(7)  1.00000 Uiso O
 O4  0.226(2)  0.489(3)  0.035(8)  0.048(7)  1.00000 Uiso O
 O5  0.274(3)  0.2682(20)  0.390(6)  0.048(7)  1.00000 Uiso O
 O6  0.00000  0.294(2)  0.578(6)  0.048(7)  1.00000 Uiso O
 O7  0.00000  0.356(2)  0.091(6)  0.048(7)  1.00000 Uiso O
 Si1  0.2924(13)  0.0492(12)  0.252(5)  0.054(4)  1.00000 Uiso Si
 Si2  0.2067(11)  0.2127(12)  0.207(5)  0.054(4)  1.00000 Uiso Si
 Si3  0.00000  0.2767(13)  0.25000  0.054(4)  1.00000 Uiso Si
 Si4  0.00000  0.3708(13)  0.763(5)  0.054(4)  1.00000 Uiso Si
 C1  0.50000  0.44598  0.11710  0.04(5)  0.41770 Uiso C
 C2  0.50000  0.44598  0.40167  0.04(5)  0.41770 Uiso C

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

#=============================================================================
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# 10. DISTANCES AND ANGLES / MOLECULAR GEOMETRY
```

```
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
O1    O1    2.62(3)       2_555 ?
O1    O3    2.62(3)       1_555 ?
O1    O4    2.64(6)       1_556 ?
O1    O4    2.47(5)       3_565 ?
O1    O6    2.74(4)       1_555 ?
O1    O7    2.61(6)       1_556 ?
O1    Si1   1.61(3)       8_555 ?
O1    Si4   1.65(3)       1_555 ?
O2    O2    2.49(2)       2_555 ?
O2    O3    2.51(4)       8_554 ?
O2    O5    2.76(5)       1_555 ?
O2    O5    2.58(7)       8_554 ?
O2    O6    2.44(6)       1_555 ?
O2    O7    2.78(5)       1_555 ?
O2    Si2   1.61(2)       1_555 ?
O2    Si3   1.59(3)       1_555 ?
O3    O1    2.62(3)       1_555 ?
O3    O2    2.51(4)       8_555 ?
O3    O4    2.54(8)       1_556 ?
O3    O4    2.55(6)       3_565 ?
O3    O5    2.54(7)       1_555 ?
O3    O5    2.77(5)       8_555 ?
O3    Si1   1.55(3)       8_555 ?
O3    Si2   1.62(3)       8_555 ?
O4    O1    2.64(6)       1_554 ?
O4    O1    2.47(5)       3_564 ?
O4    O3    2.54(8)       1_554 ?
O4    O3    2.55(6)       3_564 ?
O4    O4    2.52(6)       3_564 ?
O4    O4    2.52(6)       3_565 ?
O4    Si1   1.52(5)       6_555 ?
O4    Si1   1.58(5)       8_554 ?
O5    O2    2.76(5)       1_555 ?
O5    O2    2.58(7)       8_555 ?
O5    O3    2.54(7)       1_555 ?
O5    O3    2.77(5)       8_554 ?
O5    O5    2.66(4)       8_554 ?
O5    O5    2.66(4)       8_555 ?
O5    Si2   1.62(4)       1_555 ?
O5    Si2   1.64(4)       8_555 ?
O6    O1    2.74(4)       1_555 ?
O6    O1    2.74(4)       2_555 ?
O6    O2    2.44(6)       1_555 ?
O6    O2    2.44(6)       2_555 ?
O6    O7    2.66(4)       1_555 ?
O6    O7    2.77(4)       1_556 ?
O6    Si3   1.66(3)       1_555 ?
O6    Si4   1.62(4)       1_555 ?
O7    O1    2.61(6)       1_554 ?
O7    O1    2.61(6)       2_554 ?
O7    O2    2.78(5)       1_555 ?
O7    O2    2.78(5)       2_555 ?
```

```
O7    O6    2.77(4)       1_554 ?
O7    O6    2.66(4)       1_555 ?
O7    Si3   1.58(4)       1_555 ?
O7    Si4   1.66(4)       1_554 ?
Si1   O1    1.61(3)       8_554 ?
Si1   O3    1.55(3)       8_554 ?
Si1   O4    1.52(5)       6_545 ?
Si1   O4    1.58(5)       8_555 ?
Si2   O2    1.61(2)       1_555 ?
Si2   O3    1.62(3)       8_554 ?
Si2   O5    1.62(4)       1_555 ?
Si2   O5    1.64(4)       8_554 ?
Si3   O2    1.59(3)       1_555 ?
Si3   O2    1.59(3)       2_555 ?
Si3   O6    1.66(3)       1_555 ?
Si3   O7    1.58(4)       1_555 ?
Si3   Si4   2.92(3)       1_554 ?
Si4   O1    1.65(3)       1_555 ?
Si4   O1    1.65(3)       2_555 ?
Si4   O6    1.62(4)       1_555 ?
Si4   O7    1.66(4)       1_556 ?
Si4   Si3   2.92(3)       1_556 ?
C1    C2    1.42009(3)    1_555 ?
C1    C2    2.15364(4)    3_564 ?
C2    C1    1.42009(3)    1_555 ?
C2    C1    2.15364(4)    3_565 ?

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
 Si1  O1   Si4  153(2)         8_555    1_555 ?
 Si2  O2   Si3  144.7(18)      1_555    1_555 ?
 Si1  O3   Si2  151(3)         8_555    8_555 ?
 Si1  O4   Si1  153(4)         6_555    8_554 ?
 Si2  O5   Si2  139(3)         1_555    8_555 ?
 Si3  O6   Si4  135(2)         1_555    1_555 ?
 Si3  O7   Si4  129(3)         1_555    1_554 ?
 O1   Si1  O3   112(3)         8_554    8_554 ?
 O1   Si1  O4   104(4)         8_554    6_545 ?
 O1   Si1  O4   112(4)         8_554    8_555 ?
 O3   Si1  O4   112(5)         8_554    6_545 ?
 O3   Si1  O4   108(5)         8_554    8_555 ?
 O4   Si1  O4   109(4)         6_545    8_555 ?
 O2   Si2  O3   102(2)         1_555    8_554 ?
 O2   Si2  O5   117(3)         1_555    1_555 ?
 O2   Si2  O5   105(4)         1_555    8_554 ?
 O3   Si2  O5   118(3)         8_554    1_555 ?
 O3   Si2  O5   103(4)         8_554    8_554 ?
 O5   Si2  O5   109(3)         1_555    8_554 ?
 O2   Si3  O2   102.5(20)      1_555    2_555 ?
 O2   Si3  O6   97(4)          1_555    1_555 ?
 O2   Si3  O7   122(4)         1_555    1_555 ?
 O2   Si3  O6   97(4)          2_555    1_555 ?
```

```
 O2    Si3  O7    122(4)          2_555     1_555 ?
 O6    Si3  O7    110(3)          1_555     1_555 ?
 O1    Si4  O1    104(2)          1_555     2_555 ?
 O1    Si4  O6    114(3)          1_555     1_555 ?
 O1    Si4  O7    104(4)          1_555     1_556 ?
 O1    Si4  O6    114(3)          2_555     1_555 ?
 O1    Si4  O7    104(4)          2_555     1_556 ?
 O6    Si4  O7    116(3)          1_555     1_556 ?

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