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#####
#####
###      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)
```

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

```
# 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?
#      -----                               -----
```

Standard?	Name	Explanation
no	'_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'

```
'_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

#####

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;

```

```

_chemical_name_common          TON
_chemical_formula_moiety      '   O24 Si12 Cl.68'
_chemical_formula_structural  ?
_chemical_formula_analytical  ?
_chemical_formula_iupac       ?
_chemical_formula_sum         'Cl.68 O24 Si12'
_chemical_formula_weight      741.26
_chemical_melting_point       ?
_chemical_compound_source     ?          # for minerals and
                                   # natural products

```

```

loop_
  _atom_type_symbol
  _atom_type_scatter_Cromer_Mann_a1
  _atom_type_scatter_Cromer_Mann_b1
  _atom_type_scatter_Cromer_Mann_a2
  _atom_type_scatter_Cromer_Mann_b2
  _atom_type_scatter_Cromer_Mann_a3
  _atom_type_scatter_Cromer_Mann_b3
  _atom_type_scatter_Cromer_Mann_a4
  _atom_type_scatter_Cromer_Mann_b4
  _atom_type_scatter_Cromer_Mann_c
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_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

```

```

#=====
=====

```

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          13.8436(3)  
_cell_length_b          17.3835(7)  
_cell_length_c          5.03649(14)  
_cell_angle_alpha       90.00000  
_cell_angle_beta        90.00000  
_cell_angle_gamma       90.00000  
_cell_volume            1212.03(6)  
_cell_formula_units_Z   2  
_cell_measurement_temperature 293  
_cell_measurement_pressure 101  
_cell_measurement_reflns_used 254  
_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           101
_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           5548
_pd_meas_2theta_range_min           0.01585
_pd_meas_2theta_range_max           35.18017
_pd_meas_2theta_range_inc           0.006341

```

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

```
# 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          0.0837
_pd_proc_ls_prof_wR_factor         0.1421
_pd_proc_ls_prof_wR_expected       0.6195
```

```
# 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         12.0264
_pd_proc_ls_prof_cwR_factor         4.3457
_pd_proc_ls_prof_cwR_expected       18.9470
```

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

```
_pd_proc_ls_prof_chi2              0.0526
_pd_proc_ls_prof_echi2              0.0526
```

```
# Items related to LS refinement
```

```
_refine_ls_R_I_factor              4.9919
_refine_ls_number_reflns            1302
_refine_ls_number_parameters        86
_refine_ls_number_restraints        54
_refine_ls_goodness_of_fit_all      0.229
```

```
# 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          35.1802
_pd_proc_2theta_range_inc          0.006341
_pd_proc_wavelength                 0.414132

_pd_block_diffraction_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      2
_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                # Not in version 2.0.1
  _atom_site_type_symbol
O1  0.0937(18)  0.428(2)  0.70(2)  0.034(9)  1.00000  Uiso  O
O2  0.0910(16)  0.216(3)  0.22(2)  0.034(9)  1.00000  Uiso  O
O3  0.276(3)   0.3804(16)  0.69(3)  0.034(9)  1.00000  Uiso  O
O4  0.227(3)   0.495(4)   -0.013(12)  0.034(9)  1.00000  Uiso  O
O5  0.266(4)   0.265(3)   0.380(8)  0.034(9)  1.00000  Uiso  O
O6  0.00000    0.301(3)   0.560(8)  0.034(9)  1.00000  Uiso  O
O7  0.00000    0.347(3)   0.068(8)  0.034(9)  1.00000  Uiso  O
Si1 0.2945(16)  0.0489(13)  0.225(6)  0.040(5)  1.00000  Uiso  Si
Si2 0.2067(14)  0.2103(14)  0.181(6)  0.040(5)  1.00000  Uiso  Si
Si3 0.00000    0.2733(16)  0.25000  0.040(5)  1.00000  Uiso  Si
Si4 0.00000    0.3726(17)  0.761(6)  0.040(5)  1.00000  Uiso  Si
C1  0.50000    0.446(5)   0.11710  0.01(8)   0.42(3)  Uiso  C
C2  0.50000    0.446(5)   0.36710  0.01(8)   0.42(3)  Uiso  C

# 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_distance			
	_geom_bond_site_symmetry_2			
	_geom_bond_publ_flag			
01	01	2.59(4)	2_555	?
01	03	2.66(5)	1_555	?
01	04	2.62(8)	1_556	?
01	04	2.52(7)	3_565	?
01	06	2.66(6)	1_555	?
01	07	2.66(8)	1_556	?
01	Si1	1.60(3)	8_555	?
01	Si4	1.64(4)	1_555	?
02	02	2.52(3)	2_555	?
02	03	2.49(5)	8_554	?
02	05	2.69(7)	1_555	?
02	05	2.64(8)	8_554	?
02	06	2.59(8)	1_555	?
02	07	2.71(7)	1_555	?
02	Si2	1.62(3)	1_555	?
02	Si3	1.61(4)	1_555	?
03	01	2.66(5)	1_555	?
03	02	2.49(5)	8_555	?
03	04	2.58(11)	1_556	?
03	04	2.49(9)	3_565	?
03	05	2.55(11)	1_555	?
03	05	2.76(8)	8_555	?
03	Si1	1.58(4)	8_555	?
03	Si2	1.60(4)	8_555	?
04	01	2.62(8)	1_554	?
04	01	2.52(7)	3_564	?
04	03	2.58(11)	1_554	?
04	03	2.49(9)	3_564	?
04	04	2.52(9)	3_564	?
04	04	2.52(9)	3_565	?
04	Si1	1.55(7)	6_555	?
04	Si1	1.55(7)	8_554	?
05	02	2.69(7)	1_555	?
05	02	2.64(8)	8_555	?
05	03	2.55(11)	1_555	?
05	03	2.76(8)	8_554	?
05	05	2.61(6)	8_554	?
05	05	2.61(6)	8_555	?
05	Si2	1.61(6)	1_555	?
05	Si2	1.62(5)	8_555	?
06	01	2.66(6)	1_555	?
06	01	2.66(6)	2_555	?
06	02	2.59(8)	1_555	?
06	02	2.59(8)	2_555	?
06	07	2.60(6)	1_555	?
06	07	2.68(6)	1_556	?
06	Si3	1.63(4)	1_555	?
06	Si4	1.60(6)	1_555	?
07	01	2.66(8)	1_554	?

O7	O1	2.66(8)	2_554 ?
O7	O2	2.71(7)	1_555 ?
O7	O2	2.71(7)	2_555 ?
O7	O6	2.68(6)	1_554 ?
O7	O6	2.60(6)	1_555 ?
O7	Si3	1.58(5)	1_555 ?
O7	Si4	1.61(5)	1_554 ?
Si1	O1	1.60(3)	8_554 ?
Si1	O3	1.58(4)	8_554 ?
Si1	O4	1.55(7)	6_545 ?
Si1	O4	1.55(7)	8_555 ?
Si2	O2	1.62(3)	1_555 ?
Si2	O3	1.60(4)	8_554 ?
Si2	O5	1.61(6)	1_555 ?
Si2	O5	1.62(5)	8_554 ?
Si3	O2	1.61(4)	1_555 ?
Si3	O2	1.61(4)	2_555 ?
Si3	O6	1.63(4)	1_555 ?
Si3	O7	1.58(5)	1_555 ?
Si4	O1	1.64(4)	1_555 ?
Si4	O1	1.64(4)	2_555 ?
Si4	O6	1.60(6)	1_555 ?
Si4	O7	1.61(5)	1_556 ?
C1	C2	1.25912(4)	1_555 ?
C1	C2	2.26(10)	3_564 ?
C2	C1	1.25912(4)	1_555 ?
C2	C1	2.26(10)	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(3)	8_555	1_555 ?
Si2	O2	Si3	145(2)	1_555	1_555 ?
Si1	O3	Si2	150(3)	8_555	8_555 ?
Si1	O4	Si1	157(5)	6_555	8_554 ?
Si2	O5	Si2	149(4)	1_555	8_555 ?
Si3	O6	Si4	146(3)	1_555	1_555 ?
Si3	O7	Si4	142(4)	1_555	1_554 ?
O1	Si1	O3	113(4)	8_554	8_554 ?
O1	Si1	O4	106(5)	8_554	6_545 ?
O1	Si1	O4	112(6)	8_554	8_555 ?
O3	Si1	O4	105(6)	8_554	6_545 ?
O3	Si1	O4	111(7)	8_554	8_555 ?
O4	Si1	O4	109(6)	6_545	8_555 ?
O2	Si2	O3	102(3)	1_555	8_554 ?
O2	Si2	O5	113(5)	1_555	1_555 ?
O2	Si2	O5	109(5)	1_555	8_554 ?
O3	Si2	O5	119(5)	8_554	1_555 ?
O3	Si2	O5	105(6)	8_554	8_554 ?
O5	Si2	O5	108(4)	1_555	8_554 ?
O2	Si3	O2	103(3)	1_555	2_555 ?
O2	Si3	O6	106(5)	1_555	1_555 ?
O2	Si3	O7	117(5)	1_555	1_555 ?

O2	Si3	O6	106(5)	2_555	1_555	?
O2	Si3	O7	117(5)	2_555	1_555	?
O6	Si3	O7	108(4)	1_555	1_555	?
O1	Si4	O1	104(3)	1_555	2_555	?
O1	Si4	O6	110(4)	1_555	1_555	?
O1	Si4	O7	110(5)	1_555	1_556	?
O1	Si4	O6	110(4)	2_555	1_555	?
O1	Si4	O7	110(5)	2_555	1_556	?
O6	Si4	O7	113(4)	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
? ? ? ? ? ? ? ? ? ?

```

```

#=====
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```

```

#=====
=====

```

```

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

```