```
##############################################################################
#####
###      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?
#     ------                               -----------                  ---
------
 '_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

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

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
```

```
_chemical_name_common              TON
_chemical_formula_moiety           '     O48 Si24 C3.26'
_chemical_formula_structural       ?
_chemical_formula_analytical       ?
_chemical_formula_iupac            ?
_chemical_formula_sum              'C3.26 O48 Si24'
_chemical_formula_weight           1481.22
_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

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

# 6. POWDER SPECIMEN AND CRYSTAL DATA

_symmetry_cell_setting               Orthorhombic
_symmetry_space_group_name_H-M       'P b n 21'
_symmetry_space_group_name_Hall      'P 2c -2ab'

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

_cell_length_a                       13.5365(3)
```

```
_cell_length_b                         16.8149(6)
_cell_length_c                         4.90294(9)
_cell_angle_alpha                      90.00000
_cell_angle_beta                       90.00000
_cell_angle_gamma                      90.00000
_cell_volume                           1115.98(5)
_cell_formula_units_Z                  1
_cell_measurement_temperature          293
_cell_measurement_pressure          1560000
_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      15600000
_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         5544
_pd_meas_2theta_range_min         0.04121
_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                0.1273
_pd_proc_ls_prof_wR_factor               0.2019
_pd_proc_ls_prof_wR_expected             0.4530

#  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               12.1583
_pd_proc_ls_prof_cwR_factor               4.6022
_pd_proc_ls_prof_cwR_expected            10.3256

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

_pd_proc_ls_prof_chi2                  0.1987
_pd_proc_ls_prof_echi2                 0.1987

#  Items related to LS refinement

_refine_ls_R_I_factor                  6.0252
_refine_ls_number_reflns                   2253
_refine_ls_number_parameters                 88
_refine_ls_number_restraints                 60
_refine_ls_goodness_of_fit_all   0.446


# 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                0.0412
_pd_proc_2theta_range_max               35.1802
_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    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  0.0742(20)  0.566(2)  0.183(11)  0.034(7)  1.00000 Uiso O
 O12  0.612(2)  0.079(2)  0.213(12)  0.034(7)  1.00000 Uiso O
 O2  0.0596(19)  0.797(2)  0.748(10)  0.034(7)  1.00000 Uiso O
 O22  0.6167(19)  0.267(3)  0.687(10)  0.034(7)  1.00000 Uiso O
 O3  0.238(3)  0.6436(17)  0.175(10)  0.034(7)  1.00000 Uiso O
 O32  0.798(3)  0.1045(18)  0.180(10)  0.034(7)  1.00000 Uiso O
 O4  0.233(3)  0.493(2)  0.339(7)  0.034(7)  1.00000 Uiso O
 O42  0.727(3)  0.971(2)  0.356(7)  0.034(7)  1.00000 Uiso O
 O5  0.202(3)  0.793(2)  1.081(6)  0.034(7)  1.00000 Uiso O
 O52  0.751(3)  0.244(2)  1.066(6)  0.034(7)  1.00000 Uiso O
 O6  0.483(4)  0.8046(20)  0.567(6)  0.034(7)  1.00000 Uiso O
 O7  0.503(4)  0.846(2)  0.046(6)  0.034(7)  1.00000 Uiso O
 S1  0.283(2)  0.9671(18)  0.661(8)  0.057(5)  1.00000 Uiso Si
 S12  0.8067(19)  0.4454(17)  0.690(9)  0.057(5)  1.00000 Uiso Si
 S2  0.1754(19)  0.8018(16)  0.720(9)  0.057(5)  1.00000 Uiso Si
 S22  0.7335(19)  0.2685(17)  0.745(9)  0.057(5)  1.00000 Uiso Si
 S3  0.487(2)  0.7775(16)  0.217(8)  0.057(5)  1.00000 Uiso Si
 S4  0.492(2)  0.8762(15)  0.75000  0.057(5)  1.00000 Uiso Si
 C1  1.050(4)  1.050(4)  0.11710  0.02(10)  0.20400 Uiso C
 C2  1.050(4)  1.050(4)  0.36710  0.02(10)  0.20400 Uiso C
 C12 -0.055(4) -0.055(4)  0.11710  0.02(10)  0.20400 Uiso C
 C22 -0.055(4) -0.055(4)  0.36710  0.02(10)  0.20400 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

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    O12   2.53(4)       2_555 ?
O1    O3    2.57(5)       1_555 ?
O1    O4    2.59(5)       1_555 ?
O1    O42   2.69(5)       3_464 ?
O1    O6    2.57(5)       3_464 ?
O1    O7    2.51(6)       3_465 ?
O1    S12   1.62(4)       4_664 ?
O1    S4    1.51(4)       3_464 ?
O12   O1    2.53(4)       2_545 ?
O12   O32   2.56(5)       1_555 ?
O12   O4    2.74(6)       3_554 ?
O12   O42   2.49(5)       1_545 ?
O12   O6    2.45(5)       4_664 ?
O12   O7    2.58(6)       4_665 ?
O12   S1    1.64(4)       4_664 ?
O12   S4    1.61(4)       4_664 ?
O2    O22   2.46(4)       2_555 ?
O2    O32   2.56(5)       4_665 ?
O2    O5    2.53(5)       1_555 ?
O2    O52   2.80(5)       4_664 ?
O2    O6    2.54(5)       3_465 ?
O2    O7    2.71(5)       3_465 ?
O2    S2    1.58(4)       1_555 ?
O2    S3    1.60(4)       3_465 ?
O22   O2    2.46(4)       2_545 ?
O22   O3    2.48(5)       4_665 ?
O22   O5    2.70(5)       4_664 ?
O22   O52   2.63(5)       1_555 ?
O22   O6    2.60(6)       4_665 ?
O22   O7    2.59(6)       4_665 ?
O22   S22   1.61(4)       1_555 ?
O22   S3    1.60(4)       4_665 ?
O3    O1    2.57(5)       1_555 ?
O3    O22   2.48(5)       4_664 ?
O3    O4    2.66(5)       1_555 ?
O3    O42   2.49(5)       3_464 ?
O3    O5    2.60(5)       1_554 ?
O3    O52   2.69(5)       4_664 ?
O3    S12   1.62(4)       4_664 ?
O3    S22   1.56(4)       4_664 ?
O32   O12   2.56(5)       1_555 ?
O32   O2    2.56(5)       4_664 ?
O32   O4    2.50(5)       3_554 ?
O32   O42   2.59(5)       1_545 ?
O32   O5    2.62(5)       4_664 ?
```

O32	O52	2.50(5)	1_554 ?
O32	S1	1.63(5)	4_664 ?
O32	S2	1.63(4)	4_664 ?
O4	O1	2.59(5)	1_555 ?
O4	O12	2.74(6)	3_455 ?
O4	O3	2.66(5)	1_555 ?
O4	O32	2.50(5)	3_455 ?
O4	O42	2.45(5)	3_464 ?
O4	O42	2.61(5)	3_465 ?
O4	S1	1.65(5)	2_545 ?
O4	S12	1.38(5)	4_664 ?
O42	O1	2.69(5)	3_565 ?
O42	O12	2.49(5)	1_565 ?
O42	O3	2.49(5)	3_565 ?
O42	O32	2.59(5)	1_565 ?
O42	O4	2.61(5)	3_564 ?
O42	O4	2.45(5)	3_565 ?
O42	S1	1.42(5)	4_674 ?
O42	S12	1.75(5)	2_655 ?
O42	C22	2.98(7)	1_665 ?
O5	O2	2.53(5)	1_555 ?
O5	O22	2.70(5)	4_665 ?
O5	O3	2.60(5)	1_556 ?
O5	O32	2.62(5)	4_665 ?
O5	O52	2.68(4)	4_664 ?
O5	O52	2.54(4)	4_665 ?
O5	S2	1.81(5)	1_555 ?
O5	S22	1.57(5)	4_665 ?
O52	O2	2.80(5)	4_665 ?
O52	O22	2.63(5)	1_555 ?
O52	O3	2.69(5)	4_665 ?
O52	O32	2.50(5)	1_556 ?
O52	O5	2.54(4)	4_664 ?
O52	O5	2.68(4)	4_665 ?
O52	S2	1.47(5)	4_665 ?
O52	S22	1.64(5)	1_555 ?
O6	O1	2.57(5)	3_565 ?
O6	O12	2.45(5)	4_665 ?
O6	O2	2.54(5)	3_564 ?
O6	O22	2.60(6)	4_664 ?
O6	O7	2.66(4)	1_555 ?
O6	O7	2.46(4)	1_556 ?
O6	S3	1.78(5)	1_555 ?
O6	S4	1.51(4)	1_555 ?
O7	O1	2.51(6)	3_564 ?
O7	O12	2.58(6)	4_664 ?
O7	O2	2.71(5)	3_564 ?
O7	O22	2.59(6)	4_664 ?
O7	O6	2.46(4)	1_554 ?
O7	O6	2.66(4)	1_555 ?
O7	S3	1.44(5)	1_555 ?
O7	S4	1.54(3)	1_554 ?
S1	O12	1.64(4)	4_665 ?
S1	O32	1.63(5)	4_665 ?
S1	O4	1.65(5)	2_555 ?
S1	O42	1.42(5)	4_675 ?
S1	S12	2.76(5)	3_464 ?
S1	S12	3.00(6)	3_465 ?

S12	O1	1.62(4)	4_665 ?
S12	O3	1.62(4)	4_665 ?
S12	O4	1.38(5)	4_665 ?
S12	O42	1.75(5)	2_645 ?
S12	S1	3.00(6)	3_564 ?
S12	S1	2.76(5)	3_565 ?
S12	S4	2.98(4)	2_645 ?
S2	O2	1.58(4)	1_555 ?
S2	O32	1.63(4)	4_665 ?
S2	O5	1.81(5)	1_555 ?
S2	O52	1.47(5)	4_664 ?
S2	S22	2.89(6)	4_664 ?
S2	S3	2.88(4)	3_465 ?
S22	O22	1.61(4)	1_555 ?
S22	O3	1.56(4)	4_665 ?
S22	O5	1.57(5)	4_664 ?
S22	O52	1.64(5)	1_555 ?
S22	S2	2.89(6)	4_665 ?
S3	O2	1.60(4)	3_564 ?
S3	O22	1.60(4)	4_664 ?
S3	O6	1.78(5)	1_555 ?
S3	O7	1.44(5)	1_555 ?
S3	S2	2.88(4)	3_564 ?
S3	S4	2.83(4)	1_554 ?
S4	O1	1.51(4)	3_565 ?
S4	O12	1.61(4)	4_665 ?
S4	O6	1.51(4)	1_555 ?
S4	O7	1.54(3)	1_556 ?
S4	S12	2.98(4)	2_655 ?
S4	S3	2.83(4)	1_556 ?
C1	C2	1.22573(2)	1_555 ?
C1	C2	2.48(8)	4_774 ?
C1	C12	2.27(9)	1_665 ?
C1	C12	2.454(4)	4_664 ?
C1	C12	2.454(4)	4_665 ?
C1	C22	2.58(8)	1_665 ?
C1	C22	1.230(8)	4_664 ?
C2	C1	1.22573(2)	1_555 ?
C2	C1	2.48(8)	4_775 ?
C2	C12	2.58(8)	1_665 ?
C2	C12	1.230(8)	4_665 ?
C2	C22	2.27(9)	1_665 ?
C2	C22	2.454(4)	4_664 ?
C2	C22	2.454(4)	4_665 ?
C12	C1	2.27(9)	1_445 ?
C12	C1	2.454(4)	4_664 ?
C12	C1	2.454(4)	4_665 ?
C12	C2	2.58(8)	1_445 ?
C12	C2	1.230(8)	4_664 ?
C12	C22	1.22573(2)	1_555 ?
C12	C22	2.67(8)	4_554 ?
C22	O42	2.98(7)	1_445 ?
C22	C1	2.58(8)	1_445 ?
C22	C1	1.230(8)	4_665 ?
C22	C2	2.27(9)	1_445 ?
C22	C2	2.454(4)	4_664 ?
C22	C2	2.454(4)	4_665 ?
C22	C12	1.22573(2)	1_555 ?

```
C22   C12   2.67(8)       4_555 ?

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
 S12  O1   S4    143(3)         4_664    3_464 ?
 S1   O12  S4    177(3)         4_664    4_664 ?
 S2   O2   S3    130(3)         1_555    3_465 ?
 S22  O22  S3    149(3)         1_555    4_665 ?
 S12  O3   S22   163(4)         4_664    4_664 ?
 S1   O32  S2    150(3)         4_664    4_664 ?
 S1   O4   S12   131(5)         2_545    4_664 ?
 S1   O42  S12   142(5)         4_674    2_655 ?
 S2   O5   S22   132(4)         1_555    4_665 ?
 S2   O52  S22   136(5)         4_665    1_555 ?
 S3   O6   S4    141(3)         1_555    1_555 ?
 S3   O7   S4    143(4)         1_555    1_554 ?
 O12  S1   O32   103(3)         4_665    4_665 ?
 O12  S1   O4    113(4)         4_665    2_555 ?
 O12  S1   O42   109(4)         4_665    4_675 ?
 O32  S1   O4    99(4)          4_665    2_555 ?
 O32  S1   O42   116(4)         4_665    4_675 ?
 O4   S1   O42   116(4)         2_555    4_675 ?
 O1   S12  O3    105(3)         4_665    4_665 ?
 O1   S12  O4    119(4)         4_665    4_665 ?
 O1   S12  O42   106(4)         4_665    2_645 ?
 O3   S12  O4    125(4)         4_665    4_665 ?
 O3   S12  O42   95(3)          4_665    2_645 ?
 O4   S12  O42   102(4)         4_665    2_645 ?
 O2   S2   O32   106(3)         1_555    4_665 ?
 O2   S2   O5    96(3)          1_555    1_555 ?
 O2   S2   O52   134(4)         1_555    4_664 ?
 O32  S2   O5    99(3)          4_665    1_555 ?
 O32  S2   O52   107(4)         4_665    4_664 ?
 O5   S2   O52   109(4)         1_555    4_664 ?
 O22  S22  O3    103(4)         1_555    4_665 ?
 O22  S22  O5    116(4)         1_555    4_664 ?
 O22  S22  O52   108(4)         1_555    1_555 ?
 O3   S22  O5    112(4)         4_665    4_664 ?
 O3   S22  O52   114(4)         4_665    1_555 ?
 O5   S22  O52   104(3)         4_664    1_555 ?
 O2   S3   O22   100(3)         3_564    4_664 ?
 O2   S3   O6    97(3)          3_564    1_555 ?
 O2   S3   O7    126(4)         3_564    1_555 ?
 O22  S3   O6    101(4)         4_664    1_555 ?
 O22  S3   O7    117(5)         4_664    1_555 ?
 O6   S3   O7    111(3)         1_555    1_555 ?
 O1   S4   O12   109(3)         3_565    4_665 ?
 O1   S4   O6    116(4)         3_565    1_555 ?
 O1   S4   O7    110(4)         3_565    1_556 ?
 O12  S4   O6    104(4)         4_665    1_555 ?
 O12  S4   O7    110(4)         4_665    1_556 ?
 O6   S4   O7    108(3)         1_555    1_556 ?
```

```
 C2   C1   C22   175.0(5)       1_555    4_664 ?
 C1   C2   C12   175.0(5)       1_555    4_665 ?
 C2   C12  C22   175.0(5)       4_664    1_555 ?
 C1   C22  C12   175.0(5)       4_665    1_555 ?

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