QUESTIONNAIRE FOR the
STRUCTURE DETERMINATION BY POWDER DIFFRACTOMETRY ROUND ROBIN - 3

d
Please answer all questions as completely as possible. Provide one filled questionnaire for each data (samples 1 and 2).

Preferably, attach the results as one PDF file or as a MS Word document compressed by Winzip.

It is advised to complete the form as the structure determination progress.

O.0 Precise date of
- data download : Fri, 1 Feb 2008 afternoon
- results submission : Fri, 8 Feb 2008

0.1 Is the first sample structure solvable with this quality of data ? Yes [*] No [ ]
0.2 Is the second sample structure solvable with this quality of data ? Yes [*] No [ ]
0.3 If not, what data would be required ?

Then, for each sample :

1. Preliminary work

1.1 Did you obtained additional informations ? No.
(for instance from CSD or ICSD or ICDD databases)

1.2 Did you obtained additional informations from the powder pattern ? If yes, how and what information ? No.
(for instance using the JCPDS-ICDD database)

1.3 Did you extract the structure factors ? Yes [*] No [ ]

I extracted intensities using the Le Bail method with GSAS and used for input to Shelxs or Sir2002. Later on, I tried to perform whole pattern decomposition with EXPO, also without much success.

1.3.1 If yes, which program(s) did you use ?
1.3.2 Give the angular range: 8-50 in 2theta
1.3.3 Give the number of extracted structure factors: 180
1.3.4 Give the Rp and Rwp (conventional Rietveld, background subtracted): 0,0649 and 0,0658 with Manually determined background points
1.3.5 Give the Rp and Rwp (background not subtracted): 0,0279 and 0,0383

1.3.6 If not, did you use the whole pattern ?
1.3.7 Or a partial pattern (if yes, give the angular range):

1.3.8 If you use the whole or a partial pattern, did you keep fixed the
profile parameters, and if yes, how did you obtained them ?

2- Structure solution

2.1 Did you use direct methods ? Yes [*] No [ ]

2.1.1 If yes, was it on the whole dataset ? On the extracted reflections
2.1.2 Or on a partial dataset ?
2.1.3 Give the number of reflections: 180
2.1.4 Which program(s) did you use ? Shelxs, Sir2002
2.1.5 Did you modified intensities of closely neighbouring reflections ? If yes, explain how. No.

2.2 Did you use Patterson methods ? Yes [*] No [ ]

2.2.1 If yes, was it on the whole dataset ? On the same set of extracted intensities.
2.2.2 Or on a partial dataset ?
2.2.3 Give the number of reflections: 180
2.2.4 Which program(s) did you use ? Shelxs
2.2.5 Did you modified intensities of closely neighbouring reflections ? If yes, explain how. No.

2.3 Did you use another method ? Yes [*] No [ ]

2.3.1 If yes, which method(s) (give details : molecule location by direct space - genetic algorithm, Monte Carlo, Simulated annealing, scratch, charge flipping, other) ?
Paralell tempering

2.3.2 Which program(s) did you use (name and reference) ?
Fox, version 1.7.1.1 Dec 4 2007

2.3.3 If you used direct space methods, how many independent molecules did you use (give details on these molecules)? How many degrees of freedom (total) ? How many torsion angles ?

A few different attempts. (1) tartarate treated as a molecule, calcium and four oxygen atoms all treated independently of each other; dof: 24 torsions 3 . (2) only with two or three oxygen atoms bonded to calcium atom; dof: 18, torsions 3 (3) as 1 with more than four not bonded oxygen atoms dof: around 30, torsions 3.

2.4 Did you first locate the whole structure ? Yes [*] No [ ]

2.4.1 If not, how many atoms did you locate ?
2.4.2 Give their name and initial atomic coordinates

Atom	x	y	z
C1	0.5050	0.3701	0.8419

C2	0.3201	0.3840	0.7142
C3	0.0878	0.3767	0.7444
C4	-0.1148	0.3542	0.6100
O5	-0.2115	0.2242	0.5179
O6	-0.1985	0.4861	0.5947
O7	0.4499	0.2166	0.8786
O8	0.7007	0.4790	0.9012
O9	0.4197	0.5381	0.6720
O10	0.1210	0.5314	0.8256
H11	0.2846	0.2732	0.6370
H12	0.0252	0.2653	0.7966
Ca1	0.1592	0.3120	0.2280
O1	0.8055	0.1218	0.2725
O2	0.6237	0.8175	0.8893
O3	0.1132	0.8025	0.0111
O4	0.3191	0.1516	0.3977

_____atoms above: tartarate

2.4.3 Were the initial atomic coordinates taken from a known structure ? Not to me at least. Yes [ ] No [*]
If yes, which one (give reference) ?

3- Structure completion

3.1 Did you performed Fourier difference syntheses before refining the structure by the Rietveld method ? Yes [ ] No [*]
3.2 If yes, with what program ?
3.3 If yes, how many additional atoms did you obtained from Fourier difference syntheses ?
3.4 Give their name and atomic coordinates as they were obtained

Atom	x	y	z
.....			
.....			
.....			

3.5 Did you made first Rietveld refinements without preliminary Fourier difference syntheses ? Yes [*] No [ ]
3.5.1 If yes, with what program ? GSAS
3.5.2 What were the Rp and Rwp (background subtracted AND not subtracted) and RB and RF that you obtained at the first Rietveld application ?
Haven’t written it down. As I recall Rwp~0,11; Rwp(-bknd)~0,15

3.5.3 Did you get the structure factors from this result and performed a Fourier difference synthesis ? No.
3.5.4 Did you locate additional atoms at this stage ? No.
3.5.5 And which one ?

Atom	x	y	z
.....			
.....			
.....			

3.5.6 If you repeated Rietveld refinements and Fourier synthese several times before to complete the model, give the number of times and which atoms you locate and the Rp, Rwp RB, RF at each times.

Atom	x	y	z
.....			
.....			
.....			

4- Final refinement

- Give the final atomic coordinates, thermal parameters, standard deviations, Reliability factors.....

Atom	x	y	z	B
C1	0.4969(21)	0.3622(16)	0.8337(14)	1.0	0.0498(9)
C2	0.3004(28)	0.3898(16)	0.7160(13)	1.0	0.0498(9)
C3	0.0801(26)	0.3716(18)	0.7534(13)	1.0	0.0498(9)
C4	-0.0971(25)	0.3551(15)	0.6281(15)	1.0	0.0498(9)
O5	-0.2034(13)	0.2052(11)	0.5360(9)	1.0	0.0498(9)
O6	-0.1787(15)	0.4757(11)	0.5900(8)	1.0	0.0498(9)
O7	0.4271(14)	0.2031(12)	0.8697(8)	1.0	0.0498(9)
O8	0.6845(15)	0.4753(10)	0.9007(8)	1.0	0.0498(9)
O9	0.4214(15)	0.5354(11)	0.6732(8)	1.0	0.0498(9)
O10	0.1388(15)	0.5293(11)	0.8434(9)	1.0	0.0498(9)
H11	0.265(11)	0.277(7)	0.623(6)	1.0	0.0498(9)
H12	0.095(13)	0.255(7)	0.798(7)	1.0	0.0498(9)
CA13	0.1630(5)	0.3127(4)	0.22960(31)	1.0	0.0498(9)
O14	0.8067(13)	0.1226(9)	0.2715(8)	1.0	0.0498(9)
O15	0.6339(12)	0.8471(10)	0.8812(7)	1.0	0.0498(9)
O16	0.1216(14)	0.8148(10)	0.0100(9)	1.0	0.0498(9)
O17	0.3194(11)	0.1478(9)	0.3969(7)	1.0	0.0498(9)

- Give details about constraints, restraints

I used restraints on bond lengths and angles.

5- Feel free to add any intermediate results (list of extracted structure factors, software decisive input and output data...) or comments you might consider as essential (details on hardware, time for solving the structure, number of moves by Monte Carlo or molecule position trial, any picture...).

I strongly believe that this is the correct structure. I had a few doubts as it is stated on the website that this is a polymorph of enantiomerically pure calcium tartarate. This structure I got to is a racemate. I have tried to find initial model using all of the above named methods in P1 space group but with no meaningful results. And I would be very surprised to find that I could get a Rietveld fit this good and chemically very sensible structure with a wrong structure. Additionally, this structure model didn’t show a hint of divergence in least squares.

I hope I’ve answered all questions. I will be happy to answer if I left something that needs clarification.

With kind regards,

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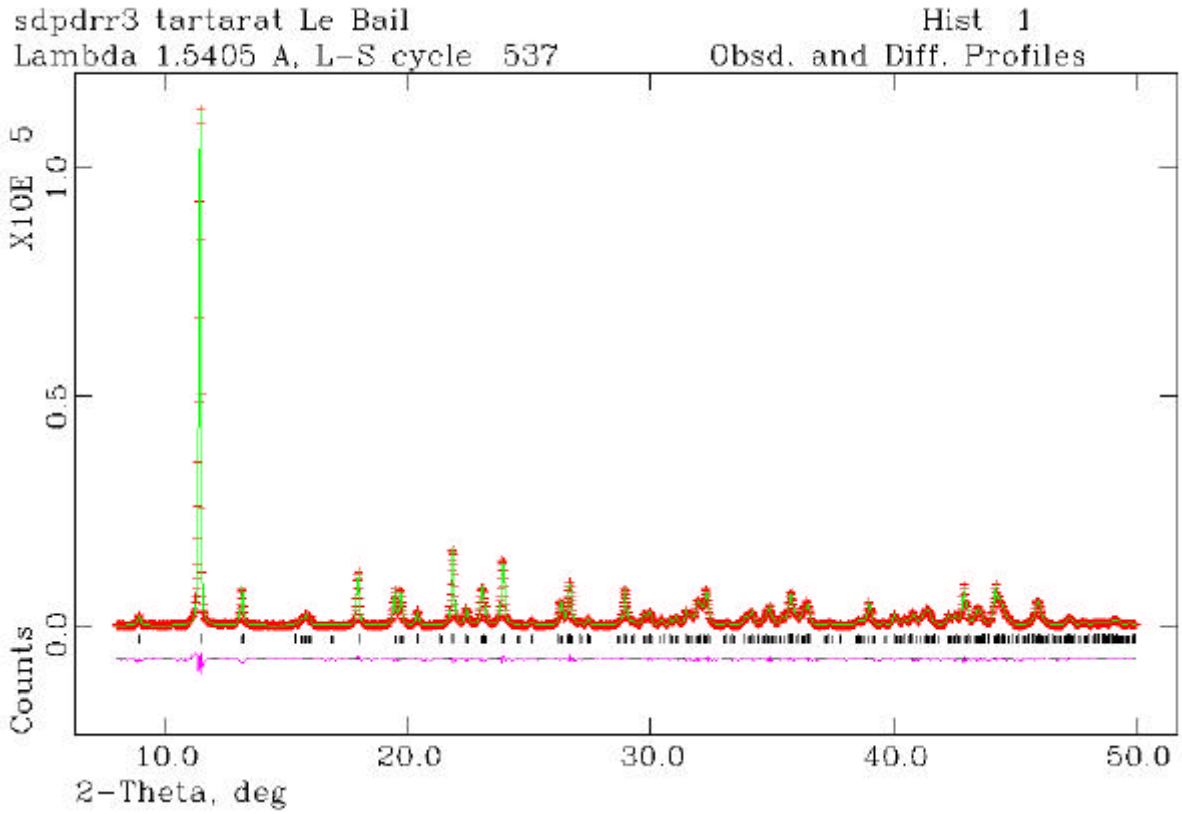
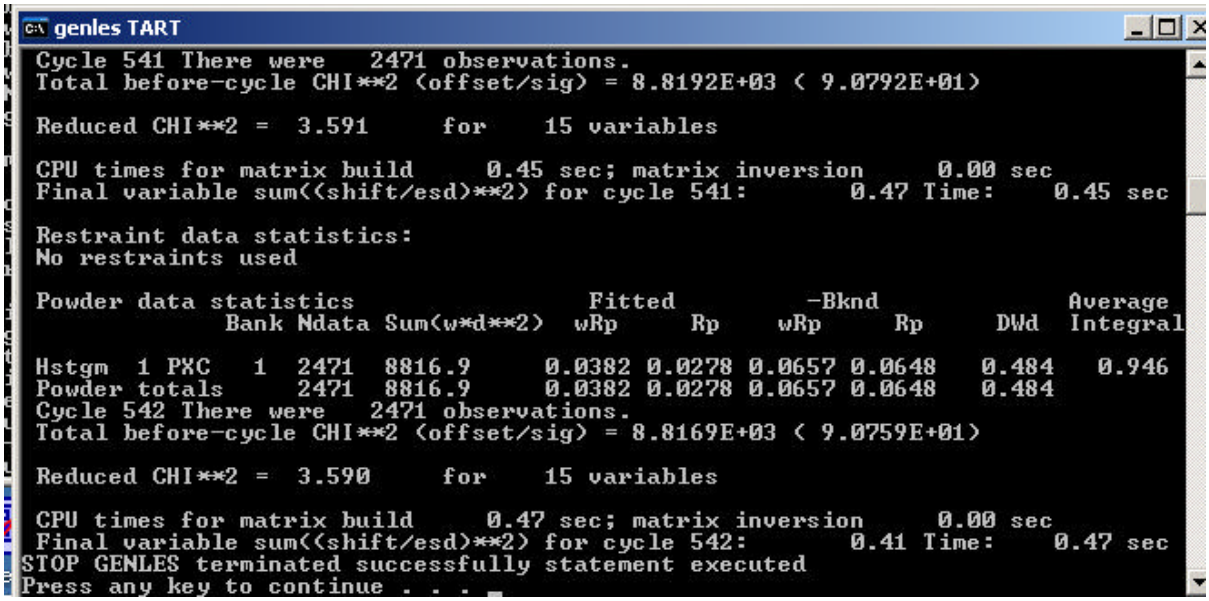
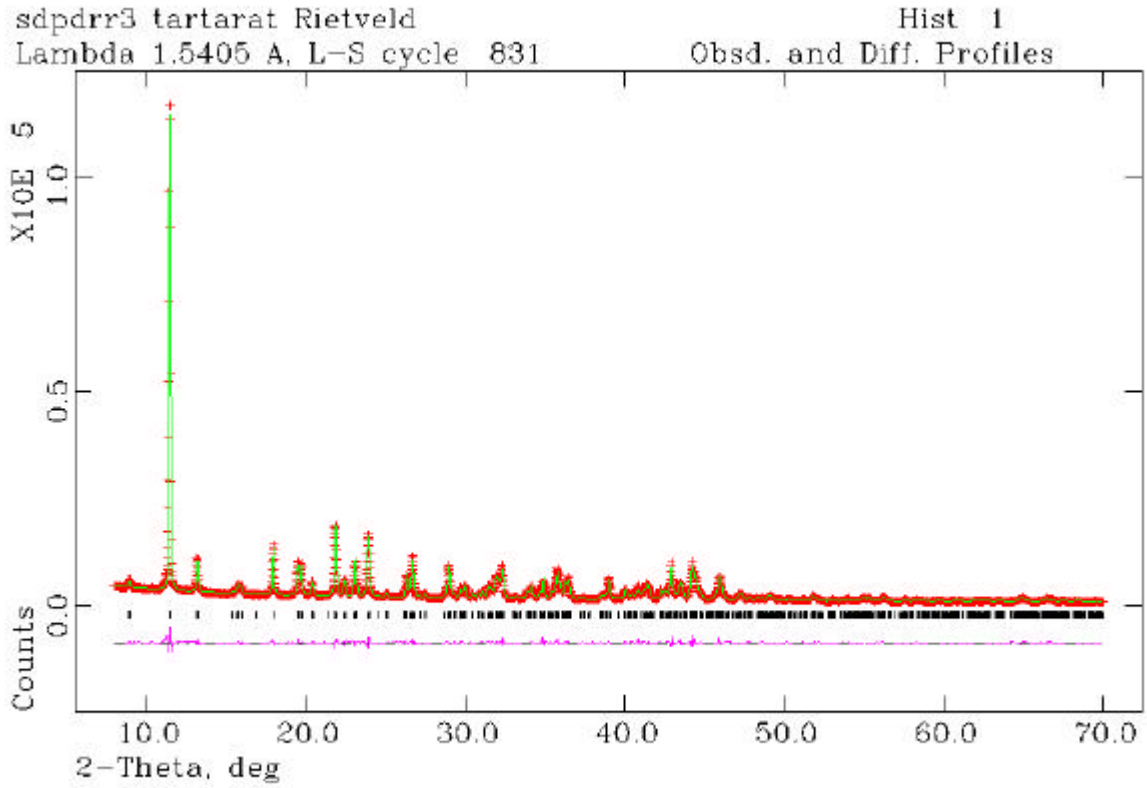



genles TART
Cycle 541 There were 2471 observations.
Total before-cycle CHI**2 (offset/sig) = 8.8192E+03 (9.0792E+01)
Reduced CHI**2 = 3.591 for 15 variables
CPU times for matrix build 0.45 sec; matrix inversion 0.00 sec
Final variable sum((shift/esd)**2) for cycle 541: 0.47 Time: 0.45 sec
Restraint data statistics:
No restraints used
Powder data statistics Fitted -Bknd Average
Bank Ndata Sum(w*d**2) wRp Rp wRp Rp DWd Integral
Hstgm 1 PXC 1 2471 8816.9 0.0382 0.0278 0.0657 0.0648 0.484 0.946
Powder totals 2471 8816.9 0.0382 0.0278 0.0657 0.0648 0.484
Cycle 542 There were 2471 observations.
Total before-cycle CHI**2 (offset/sig) = 8.8169E+03 (9.0759E+01)
Reduced CHI**2 = 3.590 for 15 variables
CPU times for matrix build 0.47 sec; matrix inversion 0.00 sec
Final variable sum((shift/esd)**2) for cycle 542: 0.41 Time: 0.47 sec
STOP GENLES terminated successfully statement executed
Press any key to continue . . .




```
data_TART_publ

_pd_block_id
  2008-02-08T12:31|TART|Ivan_Halasz|Overall

_audit_creation_method  "from EXP file using GSAS2CIF"
_audit_creation_date                    2008-02-08T12:31
_audit_author_name                      "Ivan Halasz"
_audit_update_record
; 2008-02-08T12:31  Initial CIF as created by GSAS2CIF
;

#=============================================================================
# this information describes the project, paper etc. for the CIF             #
# Acta Cryst. Section C papers and editorial correspondence is generated     #
# from the information in this section                                       #
#                                                                            #
#   (from)   CIF submission form for Rietveld refinements (Acta Cryst. C)    #
#                                                 Version 14 December 1998   #
#=============================================================================
# 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

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

# 2. 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            ?

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

# 3. TITLE AND AUTHOR LIST

_publ_section_title
; ?
;
_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
; ?
;

#===============================================================================
# 5. OVERALL REFINEMENT & COMPUTING DETAILS

_refine_special_details
; ?
;
_pd_proc_ls_special_details
; ?
;

# The following items are used to identify the programs used.
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_ls_weighting_scheme       ?
_refine_ls_weighting_details      ?
_refine_ls_hydrogen_treatment     ?
_refine_ls_extinction_method      ?
_refine_ls_extinction_coef        ?
_refine_ls_number_constraints     ?

_refine_ls_restrained_S_all       ?
```

```
_refine_ls_restrained_S_obs       ?

#===============================================================================
# 6. SAMPLE PREPARATION DATA

# (In the unusual case where multiple samples are used in a single
#  Rietveld study, this information should be moved into the phase
#  blocks)

# The following three fields describe the preparation of the material.
# 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             ?

_pd_char_colour                  ?       # use ICDD colour descriptions
data_TART_overall

_refine_ls_shift/su_max               0.00
_refine_ls_shift/su_mean              0.00
_computing_structure_refinement       GSAS
_refine_ls_number_parameters          1
_refine_ls_goodness_of_fit_all        5.30
_refine_ls_number_restraints          35
_refine_ls_matrix_type                full

# pointers to the phase blocks
loop_   _pd_phase_block_id
      2008-02-08T12:31|TART_phase1|Ivan_Halasz||
# pointers to the diffraction patterns
loop_   _pd_block_diffractogram_id
      ?

# Information for phase 1
data_TART_phase_1

_pd_block_id
  2008-02-08T12:31|TART_phase1|Ivan_Halasz||

#===============================================================================
# 7. CHEMICAL, STRUCTURAL AND CRYSTAL DATA

_pd_char_particle_morphology     ?

_chemical_name_systematic
; ?
;
_chemical_name_common            ?
_chemical_formula_moiety         ?
_chemical_formula_structural     ?
_chemical_formula_analytical     ?
_chemical_melting_point          ?
_chemical_compound_source        ?       # for minerals and
                                         # natural products
_symmetry_space_group_name_Hall  ?

_exptl_crystal_F_000              ?
_exptl_crystal_density_diffrn     ?
_exptl_crystal_density_meas       ?
```

```
_exptl_crystal_density_method      ?

_cell_measurement_temperature     ?

_cell_special_details
; ?
;

_geom_special_details             ?

# The following item identifies the program(s) used (if appropriate).
_computing_structure_solution     ?

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

# 8. Phase information from GSAS

_pd_phase_name                          tart
_cell_length_a                          6.25092(15)
_cell_length_b                          8.22598(23)
_cell_length_c                          10.43844(20)
_cell_angle_alpha                       94.9368(15)
_cell_angle_beta                        105.9512(16)
_cell_angle_gamma                       107.5183(17)
_cell_volume                            483.732(20)
_symmetry_cell_setting                  triclinic
_symmetry_space_group_name_H-M          "P -1"
loop_ _symmetry_equiv_pos_site_id _symmetry_equiv_pos_as_xyz
       1 +x,+y,+z
      -1 -x,-y,-z

# ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS


loop_
      _atom_site_type_symbol
      _atom_site_label
      _atom_site_fract_x
      _atom_site_fract_y
      _atom_site_fract_z
      _atom_site_occupancy
      _atom_site_thermal_displace_type
      _atom_site_U_iso_or_equiv
      _atom_site_symmetry_multiplicity
C
C1      0.505        0.3701       0.8419       1.0        Uiso   0.025         2
C
C2      0.3201       0.384        0.7142       1.0        Uiso   0.025         2
C
C3      0.0878       0.3767       0.7444       1.0        Uiso   0.025         2
C
C4     -0.1148       0.3542       0.61         1.0        Uiso   0.025         2
O
O5     -0.2115       0.2242       0.5179       1.0        Uiso   0.025         2
O
O6     -0.1985       0.4861       0.5947       1.0        Uiso   0.025         2
O
O7      0.4499       0.2166       0.8786       1.0        Uiso   0.025         2
O
O8      0.7007       0.479        0.9012       1.0        Uiso   0.025         2
O
```

```
O9      0.4197      0.5381      0.672       1.0       Uiso   0.025         2
O
O10     0.121       0.5314      0.8256      1.0       Uiso   0.025         2
H
H11     0.2846      0.2732      0.637       1.0       Uiso   0.025         2
H
H12     0.0252      0.2653      0.7966      1.0       Uiso   0.025         2
Ca
CA13    0.1592      0.312       0.228       1.0       Uiso   0.025         2
O
O14     0.8055      0.1218      0.2725      1.0       Uiso   0.025         2
O
O15     0.6237      0.8175      0.8893      1.0       Uiso   0.025         2
O
O16     0.1132      0.8025      0.0111      1.0       Uiso   0.025         2
O
O17     0.3191      0.1516      0.3977      1.0       Uiso   0.025         2

loop_ _atom_type_symbol
      _atom_type_number_in_cell
                  C   8.0
                  O  20.0
                  H   4.0
                  Ca  2.0

# If you change Z, be sure to change all 3 of the following
_chemical_formula_sum                 "C4 H2 Ca O10"
_chemical_formula_weight              250.13
_cell_formula_units_Z                 2

# MOLECULAR GEOMETRY

loop_
      _geom_bond_atom_site_label_1
      _geom_bond_atom_site_label_2
      _geom_bond_distance
      _geom_bond_site_symmetry_1
      _geom_bond_site_symmetry_2
      _geom_bond_publ_flag
  C1        C2             1.54427(4)  .      1_555  N
  C1        O7           1.324280(30)  .      1_555  N
  C1        O8             1.22913(4)  .      1_555  N
  C1        CA13           3.10524(8)  .     -1_666  N
  C2        C1             1.54427(4)  .      1_555  N
  C2        C3             1.55368(4)  .      1_555  N
  C2        O9           1.400090(30)  .      1_555  N
  C2        H11          1.087610(30)  .      1_555  N
  C3        C2             1.55368(4)  .      1_555  N
  C3        C4             1.56332(4)  .      1_555  N
  C3        O10            1.39269(4)  .      1_555  N
  C3        H12          1.130050(30)  .      1_555  N
  C4        C3             1.56332(4)  .      1_555  N
  C4        O5             1.24407(4)  .      1_555  N
  C4        O6           1.342440(30)  .      1_555  N
  C4        CA13           3.22394(8)  .     -1_566  N
  O5        C4             1.24407(4)  .      1_555  N
  O6        C4           1.342440(30)  .      1_555  N
  O6        CA13           2.28459(5)  .     -1_566  N
  O7        C1           1.324280(30)  .      1_555  N
  O8        C1             1.22913(4)  .      1_555  N
  O8        CA13           2.38398(5)  .     -1_666  N
```

```
  O9        C2            1.400090(30)  .      1_555  N
  O9        H11             2.04463(6)  .      1_555  N
  O9        CA13            2.41932(7)  .     -1_666  N
  O10       C3              1.39269(4)  .      1_555  N
  O10       H12             2.05885(6)  .      1_555  N
  O10       CA13            2.44622(5)  .     -1_566  N
  H11       C2            1.087610(30)  .      1_555  N
  H11       O9              2.04463(6)  .      1_555  N
  H12       C3            1.130050(30)  .      1_555  N
  H12       O10             2.05885(6)  .      1_555  N
  CA13      C1              3.10524(8)  .     -1_666  N
  CA13      C4              3.22394(8)  .     -1_566  N
  CA13      O6              2.28459(5)  .     -1_566  N
  CA13      O8              2.38398(5)  .     -1_666  N
  CA13      O9              2.41932(7)  .     -1_666  N
  CA13      O10             2.44622(5)  .     -1_566  N
  CA13      O14             2.48174(6)  .      1_455  N
  CA13      O15             2.45658(5)  .     -1_666  N
  CA13      O16             2.51192(7)  .     -1_565  N
  CA13      O17             2.47000(5)  .      1_555  N
  O14       CA13            2.48174(6)  .      1_655  N
  O15       CA13            2.45658(5)  .     -1_666  N
  O16       CA13            2.51192(7)  .     -1_565  N
  O17       CA13            2.47000(5)  .      1_555  N

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_2
     _geom_angle_site_symmetry_3
     _geom_angle_publ_flag
  C2        C1        O7          114.1749(20)     1_555  .      1_555  N
  C2        C1        O8          126.3713(18)     1_555  .      1_555  N
  O7        C1        O8          119.0339(17)     1_555  .      1_555  N
  C1        C2        C3          110.4558(17)     1_555  .      1_555  N
  C1        C2        O9          108.0528(20)     1_555  .      1_555  N
  C1        C2        H11         106.7168(20)     1_555  .      1_555  N
  C3        C2        O9          112.1487(16)     1_555  .      1_555  N
  C3        C2        H11         109.3994(19)     1_555  .      1_555  N
  O9        C2        H11         109.9149(19)     1_555  .      1_555  N
  C2        C3        C4          110.5267(18)     1_555  .      1_555  N
  C2        C3        O10         109.9851(18)     1_555  .      1_555  N
  C2        C3        H12         112.3067(15)     1_555  .      1_555  N
  C4        C3        O10         107.3331(20)     1_555  .      1_555  N
  C4        C3        H12         107.5796(20)     1_555  .      1_555  N
  O10       C3        H12         108.9514(19)     1_555  .      1_555  N
  C3        C4        O5          126.5707(17)     1_555  .      1_555  N
  C3        C4        O6          116.6538(17)     1_555  .      1_555  N
  O5        C4        O6          116.7299(18)     1_555  .      1_555  N
  C4        O6        CA13        123.3521(15)     1_555  .     -1_566  N
  C1        O8        CA13        114.6948(18)     1_555  .     -1_666  N
  C2        O9        CA13        117.7954(17)     1_555  .     -1_666  N
  C3        O10       CA13        121.8789(18)     1_555  .     -1_566  N
  O6        CA13      O8           94.4849(20)    -1_566  .     -1_666  N
  O6        CA13      O9           74.6355(21)    -1_566  .     -1_666  N
  O6        CA13      O10          66.1752(17)    -1_566  .     -1_566  N
  O6        CA13      O14          87.8266(21)    -1_566  .      1_455  N
  O6        CA13      O15         144.4202(11)    -1_566  .     -1_666  N
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  O6        CA13      O16          136.1651(13)     -1_566  .     -1_565  N
  O6        CA13      O17           87.3647(19)     -1_566  .      1_555  N
  O8        CA13      O9            69.2527(17)     -1_666  .     -1_666  N
  O8        CA13      O10           72.8463(17)     -1_666  .     -1_566  N
  O8        CA13      O14          145.5281(10)     -1_666  .      1_455  N
  O8        CA13      O15           75.7452(18)     -1_666  .     -1_666  N
  O8        CA13      O16           74.3590(20)     -1_666  .     -1_565  N
  O8        CA13      O17          138.6830(13)     -1_666  .      1_555  N
  O9        CA13      O10          121.8813(19)     -1_666  .     -1_566  N
  O9        CA13      O14          143.3066(12)     -1_666  .      1_455  N
  O9        CA13      O15           69.8952(20)     -1_666  .     -1_666  N
  O9        CA13      O16          134.0727(15)     -1_666  .     -1_565  N
  O9        CA13      O17           71.5624(19)     -1_666  .      1_555  N
  O10       CA13      O14           76.7993(20)     -1_566  .      1_455  N
  O10       CA13      O15          137.7502(11)     -1_566  .     -1_666  N
  O10       CA13      O16           70.0426(17)     -1_566  .     -1_565  N
  O10       CA13      O17           142.2617(9)     -1_566  .      1_555  N
  O14       CA13      O15          119.6049(19)      1_455  .     -1_666  N
  O14       CA13      O16           80.2779(21)      1_455  .     -1_565  N
  O14       CA13      O17           75.7401(19)      1_455  .      1_555  N
  O15       CA13      O16           74.8075(18)     -1_666  .     -1_565  N
  O15       CA13      O17           79.0598(16)     -1_666  .      1_555  N
  O16       CA13      O17          128.9280(16)     -1_565  .      1_555  N
#--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--eof--#
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