

```

data_nabimusaite
#=====

# 5. CHEMICAL DATA

_chemical_name_systematic
; ?
;
_chemical_name_common                ?
_chemical_name_mineral               nabimusaite
_chemical_formula_structural         ?
_chemical_formula_analytical         ?
_chemical_formula_iupac              ?
_chemical_formula_sum                'Ba0.036 Ca12 F1 K0.964 O26 S2
Si4'
_chemical_formula_weight             1135
_chemical_melting_point              ?
_chemical_compound_source            'Bellerberg vulcano, Germany'
_chemical_absolute_configuration     .

#=====

# 6. CRYSTAL DATA

_symmetry_cell_setting               trigonal
_symmetry_space_group_name_H-M      'R -3 m'
_symmetry_Int_Tables_number         166

loop_
  _space_group_symop_id
  _space_group_symop_operation_xyz
1    x,y,z
2    -y,x-y,z
3    -x+y,-x,z
4    y,x,-z
5    x-y,-y,-z
6    -x,-x+y,-z
7    -x,-y,-z
8    y,-x+y,-z
9    x-y,x,-z
10   -y,-x,z
11   -x+y,y,z
12   x,x-y,z
13   x+2/3,y+1/3,z+1/3
14   -y+2/3,x-y+1/3,z+1/3
15   -x+y+2/3,-x+1/3,z+1/3
16   y+2/3,x+1/3,-z+1/3
17   x-y+2/3,-y+1/3,-z+1/3
18   -x+2/3,-x+y+1/3,-z+1/3
19   -x+2/3,-y+1/3,-z+1/3
20   y+2/3,-x+y+1/3,-z+1/3
21   x-y+2/3,x+1/3,-z+1/3
22   -y+2/3,-x+1/3,z+1/3
23   -x+y+2/3,y+1/3,z+1/3
24   x+2/3,x-y+1/3,z+1/3
25   x+1/3,y+2/3,z+2/3
26   -y+1/3,x-y+2/3,z+2/3
27   -x+y+1/3,-x+2/3,z+2/3

```

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28  y+1/3,x+2/3,-z+2/3
29  x-y+1/3,-y+2/3,-z+2/3
30  -x+1/3,-x+y+2/3,-z+2/3
31  -x+1/3,-y+2/3,-z+2/3
32  y+1/3,-x+y+2/3,-z+2/3
33  x-y+1/3,x+2/3,-z+2/3
34  -y+1/3,-x+2/3,z+2/3
35  -x+y+1/3,y+2/3,z+2/3
36  x+1/3,x-y+2/3,z+2/3

```

```

_cell_length_a      7.19660(10)
_cell_length_b      7.19660(10)
_cell_length_c      41.2146(5)
_cell_angle_alpha    90
_cell_angle_beta     90
_cell_angle_gamma    120
_cell_volume         1848.57(4)
_cell_formula_units_Z 3

```

```

_cell_measurement_reflns_used  5953
_cell_measurement_theta_min    2.93
_cell_measurement_theta_max    34.65
_cell_measurement_temperature  293
_cell_special_details
; ?
;

```

```

_exptl_crystal_density_diffrn  3.0587
_exptl_crystal_density_meas    ?
_exptl_crystal_density_method  ?
_exptl_crystal_F_000          1696

```

```

_exptl_absorpt_coefficient_mu  3.157
_exptl_crystal_description     prism
_exptl_crystal_size_max        0.3
_exptl_crystal_size_mid        0.2
_exptl_crystal_size_min        0.3
_exptl_crystal_size_rad        ?
_exptl_crystal_colour          colorless
_exptl_absorpt_correction_type  'multi-scan'
_exptl_absorpt_process_details
;

```

CrysAlisPro 1.171.40.67a (Rigaku Oxford Diffraction, 2019)
 Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.

```

;
_exptl_absorpt_correction_T_min  0.877
_exptl_absorpt_correction_T_max  1

```

```

#=====

```

7. EXPERIMENTAL DATA

```

_diffrn_radiation_type  synchrotron
_diffrn_radiation_probe x-ray
_diffrn_radiation_source 'SLS super-bending magnet 2.9T, X06DA'
_diffrn_ambient_temperature 293(2)

```

```

_diffrn_radiation_wavelength      0.70848
_diffrn_radiation_monochromator
;Bartels Monochromator with dual channel cut crystals (DCCM)
  in (+--+) geometry
;
_diffrn_measurement_device          'multi-axis goniometer'
_diffrn_measurement_device_type     PRIGo
_diffrn_detector                    'hybrid pixel CMOS'
_diffrn_detector_type                PILATUS2M-F
_diffrn_detector_area_resol_mean     5.81
_diffrn_measurement_method           '\w scans'
_diffrn_measurement_specimen_support 'litho-loop'
_diffrn_measurement_details
;
  Swiss Light Source, Paul Scherrer Insitute, Villigen, Switzerland
  Beamline X06DA (PXIII)
  single omega-scan
  3600 frames, detector distance = 90 mm
  Detector threshold setting 8750 eV
  oscillation 0.1 deg, 0.1 sec exposure
  vertical detector offset 55 mm
;

```

```

_diffrn_reflns_number              8246
_diffrn_reflns_theta_min           2.96
_diffrn_reflns_theta_max           34.64
_diffrn_reflns_theta_full          34.36
_diffrn_measured_fraction_theta_max 0.97
_diffrn_measured_fraction_theta_full 0.98
_diffrn_reflns_av_R_equivalents     0.0368
_diffrn_reflns_av_unetI/netI        0.0144
_diffrn_reflns_limit_h_min          -11
_diffrn_reflns_limit_h_max          11
_diffrn_reflns_limit_k_min          -9
_diffrn_reflns_limit_k_max          9
_diffrn_reflns_limit_l_min          -65
_diffrn_reflns_limit_l_max          65
_diffrn_reflns_reduction_process     ?

```

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```

``` # 8. REFINEMENT DATA ```

```

_refine_special_details
; ?
;

```

```

_reflns_number_total              1036
_reflns_number_gt                  932
_reflns_threshold_expression       'I>3\s(I) '

_refine_ls_structure_factor_coef   F
_refine_ls_R_factor_gt              0.0197
_refine_ls_wR_factor_gt             0.0271
_refine_ls_R_factor_all             0.0216
_refine_ls_wR_factor_ref            0.0279
_refine_ls_goodness_of_fit_ref      1.64

```

```

_refine_ls_goodness_of_fit_gt      1.68
_refine_ls_restrained_S_gt         ?
_refine_ls_restrained_S_all        ?
_refine_ls_number_reflns           1036
_refine_ls_number_parameters        57
_refine_ls_number_restraints        0
_refine_ls_number_constraints       5
_refine_ls_weighting_scheme         sigma
_refine_ls_weighting_details        'w=1/(\s^2^(F)+0.0001F^2^)'
_refine_ls_hydrogen_treatment       ?
_refine_ls_shift/su_max             0.1676
_refine_ls_shift/su_mean            0.0139
_refine_diff_density_max            0.66
_refine_diff_density_min            -0.36
_refine_ls_extinction_method        'none'
_refine_ls_extinction_coef          ?
_refine_ls_extinction_expression    ?
_refine_ls_abs_structure_details    ?
_refine_ls_abs_structure_Flack      ?
_refine_ls_abs_structure_Rogers     ?

```

```

loop_
  _atom_type_symbol
  _atom_type_scatter_dispersion_real
  _atom_type_scatter_dispersion_imag
  _atom_type_scatter_source
Ba  -0.2823  2.2981
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
Ca   0.2282  0.3092
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
F    0.0178  0.0106
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
K    0.2016  0.2519
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
O    0.0113  0.0062
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
S    0.1258  0.1248
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'
Si   0.0833  0.0715
'International Tables Vol C tables 4.2.6.8 and 6.1.1.1'

```

```

_computing_data_collection
'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_cell_refinement
'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_data_reduction
'CrysAlisPro 1.171.40.67a (Rigaku OD, 2019)'
_computing_structure_solution      ?
_computing_structure_refinement
;

```

```

Jana2006
Petricek, V., Dusek, M. & Palatinus L. (2014). Z. Kristallogr. 229(5),
345-352
;

```

```

_computing_molecular_graphics      ?
_computing_publication_material    ?

```

```

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```

9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_site_symmetry_multiplicity
  _atom_site_occupancy
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
K1 K 0 0 0 Uani 0.0303(3) 3 0.964(2) d . . .
Ba1 Ba 0 0 0 Uani 0.0303(3) 3 0.036(2) d . . .
Ca1 Ca 0.15861(2) 0.84139(2) 0.398007(7) Uani 0.01155(10) 18 1 d . . .
Ca2 Ca 0.15321(2) 0.84679(2) 0.532565(7) Uani 0.01074(9) 18 1 d . . .
S1 S 0 0 0.675649(13) Uani 0.01023(13) 6 1 d . . .
Si1 Si 0 0 0.206204(15) Uani 0.00730(14) 6 1 d . . .
Si2 Si 0 0 0.082799(15) Uani 0.00820(14) 6 1 d . . .
O1 O 0.55601(9) 0.44399(9) 0.64537(3) Uani 0.0207(4) 18 1 d . . .
O2 O 0.12482(8) 0.87518(8) 0.19425(3) Uani 0.0157(3) 18 1 d . . .
O3 O 0.12552(9) 0.87448(9) 0.07243(3) Uani 0.0158(3) 18 1 d . . .
O4 O 0 0 0.36042(4) Uani 0.0138(4) 6 1 d . . .
O5 O 0 0 0.75354(4) Uani 0.0161(4) 6 1 d . . .
O6 O 0 0 0.12298(4) Uani 0.0117(4) 6 1 d . . .
F7 F 0 0 0.43054(4) Uani 0.0128(4) 6 0.5 d . . .
O7 O 0 0 0.43054(4) Uani 0.0128(4) 6 0.5 d . . .
O8 O 0 0 0.5 Uani 0.0058(5) 3 1 d . . .
```

```
loop_
  _atom_site_aniso_label
  _atom_site_aniso_type_symbol
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
K1 K 0.0299(4) 0.0299(4) 0.0311(5) 0.01494(19) 0 0
Ba1 Ba 0.0299(4) 0.0299(4) 0.0311(5) 0.01494(19) 0 0
Ca1 Ca 0.00931(11) 0.00931(11) 0.01562(14) 0.00436(10) 0.00092(5) -
0.00092(5)
Ca2 Ca 0.00819(10) 0.00819(10) 0.01504(13) 0.00351(10) -0.00110(4)
0.00110(4)
S1 S 0.01051(16) 0.01051(16) 0.0097(2) 0.00525(8) 0 0
Si1 Si 0.00544(17) 0.00544(17) 0.0110(3) 0.00272(8) 0 0
Si2 Si 0.00613(17) 0.00613(17) 0.0124(3) 0.00307(9) 0 0
O1 O 0.0279(5) 0.0279(5) 0.0174(5) 0.0221(5) -0.0013(2) 0.0013(2)
O2 O 0.0105(3) 0.0105(3) 0.0280(5) 0.0068(4) 0.0012(2) -0.0012(2)
O3 O 0.0114(3) 0.0114(3) 0.0259(5) 0.0067(4) 0.0024(2) -0.0024(2)
O4 O 0.0161(5) 0.0161(5) 0.0093(7) 0.0080(3) 0 0
O5 O 0.0180(5) 0.0180(5) 0.0123(7) 0.0090(3) 0 0
O6 O 0.0109(5) 0.0109(5) 0.0134(7) 0.0054(2) 0 0
```

F7 F 0.0122(5) 0.0122(5) 0.0139(7) 0.0061(2) 0 0
O7 O 0.0122(5) 0.0122(5) 0.0139(7) 0.0061(2) 0 0
O8 O 0.0047(5) 0.0047(5) 0.0080(9) 0.0024(3) 0 0

#=====

10. MOLECULAR GEOMETRY

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
K1 Ba1 . . 0 ?
K1 Si2 . . 3.4125(6) ?
K1 Si2 . 4_555 3.4125(6) ?
K1 O1 . 13_444 2.9111(8) ?
K1 O1 . 14_554 2.9111(8) ?
K1 O1 . 15_454 2.9111(8) ?
K1 O1 . 28_445 2.9111(8) ?
K1 O1 . 29_555 2.9111(8) ?
K1 O1 . 30_545 2.9111(8) ?
K1 O3 . 1_545 3.3703(10) ?
K1 O3 . 2_665 3.3703(10) ?
K1 O3 . 3_455 3.3703(10) ?
K1 O3 . 4_455 3.3703(10) ?
K1 O3 . 5_665 3.3703(10) ?
K1 O3 . 6_545 3.3703(10) ?
Ba1 Si2 . . 3.4125(6) ?
Ba1 Si2 . 4_555 3.4125(6) ?
Ba1 O1 . 13_444 2.9111(8) ?
Ba1 O1 . 14_554 2.9111(8) ?
Ba1 O1 . 15_454 2.9111(8) ?
Ba1 O1 . 28_445 2.9111(8) ?
Ba1 O1 . 29_555 2.9111(8) ?
Ba1 O1 . 30_545 2.9111(8) ?
Ba1 O3 . 1_545 3.3703(10) ?
Ba1 O3 . 2_665 3.3703(10) ?
Ba1 O3 . 3_455 3.3703(10) ?
Ba1 O3 . 4_455 3.3703(10) ?
Ba1 O3 . 5_665 3.3703(10) ?
Ba1 O3 . 6_545 3.3703(10) ?
Ca1 Ca1 . 2_675 3.4245(3) ?
Ca1 Ca1 . 3_465 3.4245(3) ?
Ca1 Ca2 . 5_676 3.4595(4) ?
Ca1 Ca2 . 6_556 3.4595(4) ?
Ca1 S1 . 25_554 3.1641(5) ?
Ca1 Si1 . 28_555 3.3718(5) ?
Ca1 O1 . 5_566 2.6150(10) ?
Ca1 O1 . 6_666 2.6150(10) ?
Ca1 O2 . 28_455 3.1293(12) ?
Ca1 O3 . 14_565 2.3663(5) ?
Ca1 O3 . 15_465 2.3663(5) ?
Ca1 O4 . 1_565 2.5119(11) ?
Ca1 O5 . 25_554 2.3622(7) ?

Ca1 F7 . 1_565 2.3889(9) ?
 Ca1 O7 . 1_565 2.3889(9) ?
 Ca2 Ca2 . 2_675 3.3078(3) ?
 Ca2 Ca2 . 3_465 3.3078(3) ?
 Ca2 Ca2 . 5_676 3.2943(4) ?
 Ca2 Ca2 . 6_556 3.2943(4) ?
 Ca2 Si2 . 28_555 3.0841(5) ?
 Ca2 O2 . 14_565 2.3412(5) ?
 Ca2 O2 . 15_465 2.3412(5) ?
 Ca2 O2 . 28_455 2.5730(12) ?
 Ca2 O3 . 28_455 2.6314(11) ?
 Ca2 O6 . 28_555 2.2916(4) ?
 Ca2 F7 . 4_566 2.4411(10) ?
 Ca2 O7 . 4_566 2.4411(10) ?
 Ca2 O8 . 1_565 2.3342(2) ?
 S1 O1 . 16_446 1.4697(9) ?
 S1 O1 . 17_456 1.4697(9) ?
 S1 O1 . 18_556 1.4697(9) ?
 S1 O4 . 4_556 1.4864(18) ?
 S1 O5 . . 3.2101(19) ?
 Si1 O2 . 1_545 1.6320(8) ?
 Si1 O2 . 2_665 1.6320(8) ?
 Si1 O2 . 3_455 1.6320(8) ?
 Si1 O5 . 4_556 1.6593(19) ?
 Si1 O6 . . 3.4301(18) ?
 Si2 O3 . 1_545 1.6220(8) ?
 Si2 O3 . 2_665 1.6220(8) ?
 Si2 O3 . 3_455 1.6220(8) ?
 Si2 O6 . . 1.6560(18) ?
 O1 O1 . 2_655 2.3891(12) ?
 O1 O1 . 3_665 2.3891(12) ?
 O1 O1 . 17_566 3.2840(11) ?
 O1 O1 . 18_556 3.2840(11) ?
 O1 O3 . 29_665 3.2017(13) ?
 O1 O3 . 30_545 3.2017(13) ?
 O1 O4 . 13_555 2.4244(18) ?
 O1 O5 . 16_556 3.0343(19) ?
 O2 O2 . 2_675 2.6948(11) ?
 O2 O2 . 3_465 2.6948(11) ?
 O2 O2 . 17_565 3.4532(12) ?
 O2 O2 . 18_555 3.4532(12) ?
 O2 O5 . 4_566 2.6555(18) ?
 O2 O6 . 1_565 3.3240(18) ?
 O2 F7 . 28_555 3.1200(12) ?
 O2 O7 . 28_555 3.1200(12) ?
 O2 O8 . 25_554 2.8369(8) ?
 O3 O3 . 2_675 2.7100(11) ?
 O3 O3 . 3_465 2.7100(11) ?
 O3 O4 . 25_554 3.1942(13) ?
 O3 O6 . 1_565 2.6055(17) ?
 O3 F7 . 25_554 2.7844(10) ?
 O3 O7 . 25_554 2.7844(10) ?
 O4 F7 . . 2.890(2) ?
 O4 O7 . . 2.890(2) ?
 F7 O7 . . 0 ?
 F7 O8 . . 2.8627(16) ?
 O7 O8 . . 2.8627(16) ?