Supplementary Information

(1) Crystallographic information file for $Sr[Be(OH)_4]$

(2) Figure S1 Electron micrographs of $Sr[Be(OH)_4]$ crystals

(3) Profile fit to NPD data and crystallographic model with hydrogen positions alone refined against these data; extracted O-H distances from this model.

Cif for $Sr[Be(OH)_4]_2$

```
data_2009btl0118i41acd

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             'Strontium Tetrahydroxyberyllate'
_chemical_melting_point           'None'
_chemical_formula_moiety          '4O, 4H, Sr, Be'
_chemical_formula_sum
 'Be H4 O4 Sr'
_chemical_formula_weight          164.66

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'Be'  'Be'   0.0005   0.0002
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ge'  'Ge'   0.1547   1.8001
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Sr'  'Sr'  -1.5307   3.2498
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Si'  'Si'   0.0817   0.0704
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            tetragonal
_symmetry_space_group_name_H-M    I4(1)/acd

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x+1/2, -y, z+1/2'
 '-y+1/4, x+3/4, z+1/4'
 'y+1/4, -x+1/4, z+3/4'
 '-x+1/2, y, -z'
 'x, -y, -z+1/2'
 'y+1/4, x+3/4, -z+3/4'
 '-y+1/4, -x+1/4, -z+1/4'
 'x+1/2, y+1/2, z+1/2'
```

```
'-x+1, -y+1/2, z+1'
'-y+3/4, x+5/4, z+3/4'
'y+3/4, -x+3/4, z+5/4'
'-x+1, y+1/2, -z+1/2'
'x+1/2, -y+1/2, -z+1'
'y+3/4, x+5/4, -z+5/4'
'-y+3/4, -x+3/4, -z+3/4'
'-x, -y, -z'
'x-1/2, y, -z-1/2'
'y-1/4, -x-3/4, -z-1/4'
'-y-1/4, x-1/4, -z-3/4'
'x-1/2, -y, z'
'-x, y, z-1/2'
'-y-1/4, -x-3/4, z-3/4'
'y-1/4, x-1/4, z-1/4'
'-x+1/2, -y+1/2, -z+1/2'
'x, y+1/2, -z'
'y+1/4, -x-1/4, -z+1/4'
'-y+1/4, x+1/4, -z-1/4'
'x, -y+1/2, z+1/2'
'-x+1/2, y+1/2, z'
'-y+1/4, -x-1/4, z-1/4'
'y+1/4, x+1/4, z+1/4'

_cell_length_a                    9.5536(4)
_cell_length_b                    9.5536(4)
_cell_length_c                    17.1539(18)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      1565.66(19)
_cell_formula_units_Z             16
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     ?
_cell_measurement_theta_min       ?
_cell_measurement_theta_max       ?

_exptl_crystal_description        'Plate'
_exptl_crystal_colour             'Colourless'
_exptl_crystal_size_max           0.05
_exptl_crystal_size_mid           0.02
_exptl_crystal_size_min           0.01
_exptl_crystal_density_meas       'not measured'
_exptl_crystal_density_diffrn     2.803
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1440
_exptl_absorpt_coefficient_mu     13.661
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_correction_T_min   0.0838
_exptl_absorpt_correction_T_max   0.2684
_exptl_absorpt_process_details    'SORTAV'

_exptl_special_details
```

```
;
 ?
;

_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   'Kappa CCD'
_diffrn_measurement_method        None
_diffrn_detector_area_resol_mean  None
_diffrn_standards_number          None
_diffrn_standards_interval_count  None
_diffrn_standards_interval_time   None
_diffrn_standards_decay_%         None
_diffrn_reflns_number             8455
_diffrn_reflns_av_R_equivalents   0.0438
_diffrn_reflns_av_sigmaI/netI     0.0198
_diffrn_reflns_limit_h_min        -12
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        -11
_diffrn_reflns_limit_k_max        12
_diffrn_reflns_limit_l_min        -21
_diffrn_reflns_limit_l_max        22
_diffrn_reflns_theta_min          3.84
_diffrn_reflns_theta_max          27.80
_reflns_number_total              464
_reflns_number_gt                 308
_reflns_threshold_expression      >2\s(I)

_computing_data_collection        ?
_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     ?
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F, and
R-
 factors based on ALL data will be even larger.
;
```

```
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0449P)^2^+10.1491P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          464
_refine_ls_number_parameters      37
_refine_ls_number_restraints      2
_refine_ls_R_factor_all           0.0514
_refine_ls_R_factor_gt            0.0314
_refine_ls_wR_factor_ref          0.1059
_refine_ls_wR_factor_gt           0.0865
_refine_ls_goodness_of_fit_ref    1.103
_refine_ls_restrained_S_all       1.102
_refine_ls_shift/su_max           0.035
_refine_ls_shift/su_mean          0.012

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Sr1 Sr 0.5000 0.2500 0.1250 0.0165(3) Uani 1 4 d S . .
O1 O 0.6060(3) 0.3731(3) -0.00439(17) 0.0203(7) Uani 1 1 d D . .
O4 O 0.2539(3) 0.3148(3) 0.07878(17) 0.0221(7) Uani 1 1 d D . .
Be Be 0.2500 0.2171(8) 0.0000 0.0163(14) Uani 1 2 d S . .
H1 H 0.612(6) 0.449(3) 0.015(3) 0.035(16) Uiso 1 1 d D . .
H2 H 0.260(6) 0.397(3) 0.069(3) 0.048(19) Uiso 1 1 d D . .
Sr2 Sr 0.0000 0.2500 0.1250 0.0145(3) Uani 1 4 d S . .

loop_
 _atom_site_aniso_label
 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
```

```
Sr1 0.0181(4) 0.0181(4) 0.0133(5) 0.000 0.000 0.000
O1 0.0200(15) 0.0185(15) 0.0224(15) -0.0064(13) -0.0030(13) 0.0016(14)
O4 0.0199(14) 0.0232(18) 0.0233(13) -0.0055(14) -0.0009(13) -0.0002(15)
Be 0.020(4) 0.014(4) 0.014(3) 0.000 0.002(3) 0.000
Sr2 0.0159(4) 0.0159(4) 0.0116(5) 0.000 0.000 0.0015(3)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are
taken
 into account individually in the estimation of s.u.'s in distances,
angles
 and torsion angles; correlations between s.u.'s in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

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
Sr1 O4 2.557(3) 27_565 ?
Sr1 O4 2.557(3) . ?
Sr1 O4 2.557(3) 20_656 ?
Sr1 O4 2.557(3) 10_554 ?
Sr1 O1 2.708(3) 10_554 ?
Sr1 O1 2.708(3) 20_656 ?
Sr1 O1 2.708(3) 27_565 ?
Sr1 O1 2.708(3) . ?
Sr1 Be 3.2250(8) 27_565 ?
Sr1 Be 3.2250(8) . ?
Sr1 Be 3.2250(8) 10_554 ?
Sr1 Be 3.2250(8) 20_656 ?
O1 Be 1.625(5) 10_554 ?
O1 Sr2 2.586(3) 11_544 ?
O4 Be 1.642(5) . ?
O4 Sr2 2.626(3) . ?
Be O1 1.625(5) 14_454 ?
Be O1 1.625(5) 10_554 ?
Be O4 1.642(5) 5 ?
Be Sr1 3.2250(8) 5 ?
Be Sr2 3.2250(8) 11_544 ?
Be Sr2 3.2250(8) . ?
Sr2 O1 2.586(3) 3_545 ?
Sr2 O1 2.586(3) 12_454 ?
Sr2 O1 2.586(3) 5 ?
```

```
Sr2 O1 2.586(3) 14_454 ?
Sr2 O4 2.626(3) 15_444 ?
Sr2 O4 2.626(3) 10_454 ?
Sr2 O4 2.626(3) 8 ?
Sr2 Be 3.2250(8) 12_454 ?
Sr2 Be 3.2250(8) 10_454 ?
Sr2 Be 3.2250(8) 3_545 ?

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
O4 Sr1 O4 95.52(4) 27_565 . ?
O4 Sr1 O4 143.87(13) 27_565 20_656 ?
O4 Sr1 O4 95.52(4) . 20_656 ?
O4 Sr1 O4 95.52(4) 27_565 10_554 ?
O4 Sr1 O4 143.87(13) . 10_554 ?
O4 Sr1 O4 95.52(4) 20_656 10_554 ?
O4 Sr1 O1 138.05(9) 27_565 10_554 ?
O4 Sr1 O1 60.47(9) . 10_554 ?
O4 Sr1 O1 76.38(9) 20_656 10_554 ?
O4 Sr1 O1 89.12(9) 10_554 10_554 ?
O4 Sr1 O1 60.47(9) 27_565 20_656 ?
O4 Sr1 O1 76.38(9) . 20_656 ?
O4 Sr1 O1 89.12(9) 20_656 20_656 ?
O4 Sr1 O1 138.05(9) 10_554 20_656 ?
O1 Sr1 O1 132.20(9) 10_554 20_656 ?
O4 Sr1 O1 89.12(9) 27_565 27_565 ?
O4 Sr1 O1 138.05(9) . 27_565 ?
O4 Sr1 O1 60.47(9) 20_656 27_565 ?
O4 Sr1 O1 76.38(9) 10_554 27_565 ?
O1 Sr1 O1 132.20(8) 10_554 27_565 ?
O1 Sr1 O1 69.92(13) 20_656 27_565 ?
O4 Sr1 O1 76.38(9) 27_565 . ?
O4 Sr1 O1 89.12(9) . . ?
O4 Sr1 O1 138.05(9) 20_656 . ?
O4 Sr1 O1 60.47(9) 10_554 . ?
O1 Sr1 O1 69.92(13) 10_554 . ?
O1 Sr1 O1 132.20(8) 20_656 . ?
O1 Sr1 O1 132.20(9) 27_565 . ?
O4 Sr1 Be 30.29(11) 27_565 27_565 ?
O4 Sr1 Be 86.41(14) . 27_565 ?
O4 Sr1 Be 116.82(8) 20_656 27_565 ?
O4 Sr1 Be 118.35(15) 10_554 27_565 ?
O1 Sr1 Be 146.10(13) 10_554 27_565 ?
O1 Sr1 Be 30.22(11) 20_656 27_565 ?
O1 Sr1 Be 76.96(9) 27_565 27_565 ?
O1 Sr1 Be 105.06(8) . 27_565 ?
O4 Sr1 Be 118.35(15) 27_565 . ?
```

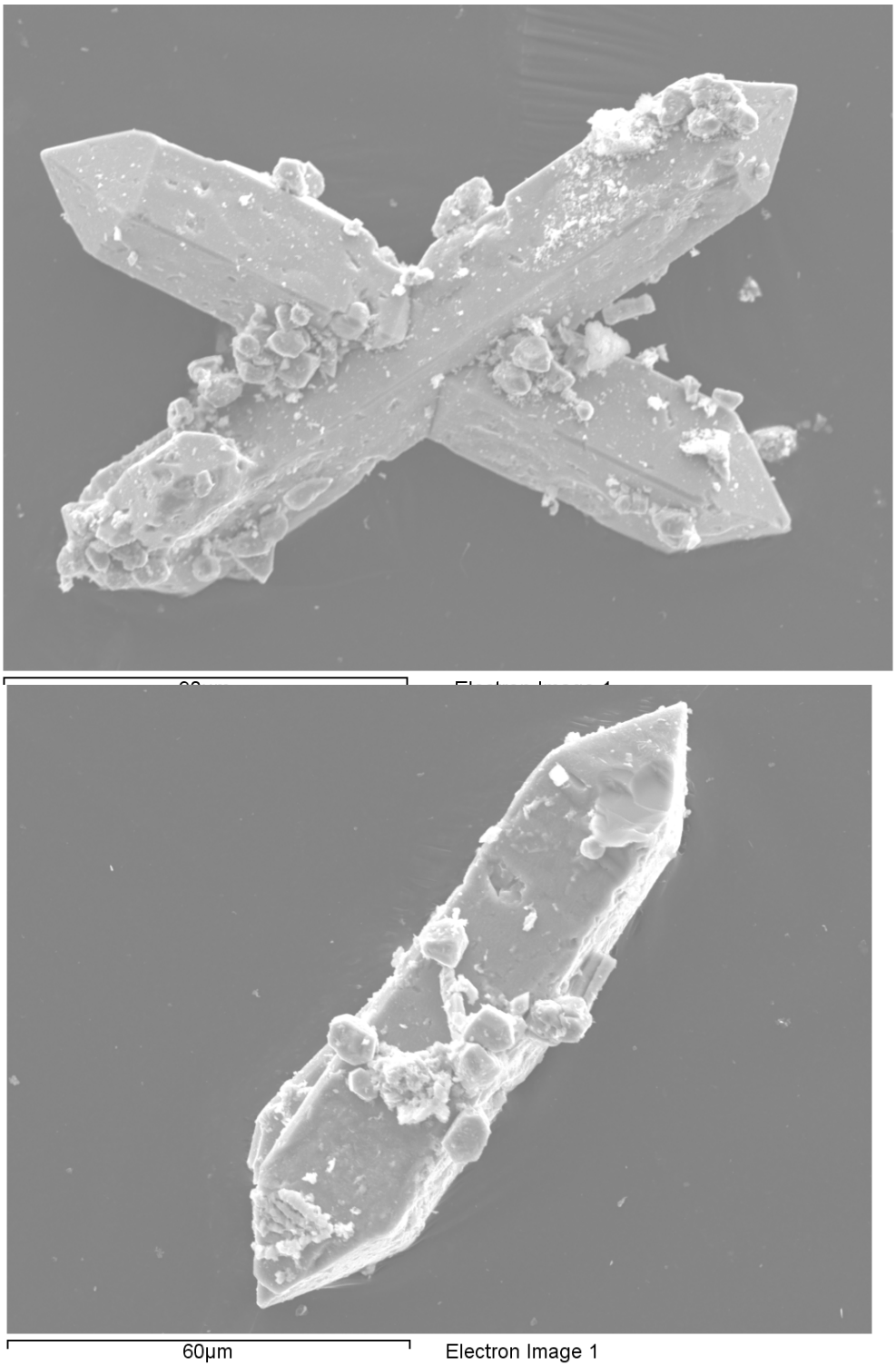
```
O4 Sr1 Be 30.29(11) . . ?
O4 Sr1 Be 86.41(14) 20_656 . ?
O4 Sr1 Be 116.82(8) 10_554 . ?
O1 Sr1 Be 30.22(11) 10_554 . ?
O1 Sr1 Be 105.06(8) 20_656 . ?
O1 Sr1 Be 146.10(13) 27_565 . ?
O1 Sr1 Be 76.96(9) . . ?
Be Sr1 Be 116.235(14) 27_565 . ?
O4 Sr1 Be 86.41(14) 27_565 10_554 ?
O4 Sr1 Be 116.82(8) . 10_554 ?
O4 Sr1 Be 118.35(15) 20_656 10_554 ?
O4 Sr1 Be 30.29(11) 10_554 10_554 ?
O1 Sr1 Be 76.96(9) 10_554 10_554 ?
O1 Sr1 Be 146.10(13) 20_656 10_554 ?
O1 Sr1 Be 105.06(8) 27_565 10_554 ?
O1 Sr1 Be 30.22(11) . 10_554 ?
Be Sr1 Be 116.235(14) 27_565 10_554 ?
Be Sr1 Be 96.66(2) . 10_554 ?
O4 Sr1 Be 116.82(8) 27_565 20_656 ?
O4 Sr1 Be 118.35(15) . 20_656 ?
O4 Sr1 Be 30.29(11) 20_656 20_656 ?
O4 Sr1 Be 86.41(14) 10_554 20_656 ?
O1 Sr1 Be 105.06(8) 10_554 20_656 ?
O1 Sr1 Be 76.96(9) 20_656 20_656 ?
O1 Sr1 Be 30.22(11) 27_565 20_656 ?
O1 Sr1 Be 146.10(13) . 20_656 ?
Be Sr1 Be 96.66(2) 27_565 20_656 ?
Be Sr1 Be 116.235(13) . 20_656 ?
Be Sr1 Be 116.235(14) 10_554 20_656 ?
Be O1 Sr2 97.33(19) 10_554 11_544 ?
Be O1 Sr1 92.78(18) 10_554 . ?
Sr2 O1 Sr1 108.17(12) 11_544 . ?
Be O4 Sr1 97.97(16) . . ?
Be O4 Sr2 95.37(15) . . ?
Sr1 O4 Sr2 134.32(13) . . ?
O1 Be O1 116.0(5) 14_454 10_554 ?
O1 Be O4 106.40(16) 14_454 . ?
O1 Be O4 108.66(16) 10_554 . ?
O1 Be O4 108.66(16) 14_454 5 ?
O1 Be O4 106.40(16) 10_554 5 ?
O4 Be O4 110.8(5) . 5 ?
O1 Be Sr1 130.4(2) 14_454 . ?
O1 Be Sr1 57.00(12) 10_554 . ?
O4 Be Sr1 51.74(11) . . ?
O4 Be Sr1 120.6(2) 5 . ?
O1 Be Sr1 57.00(12) 14_454 5 ?
O1 Be Sr1 130.4(2) 10_554 5 ?
O4 Be Sr1 120.6(2) . 5 ?
O4 Be Sr1 51.74(11) 5 5 ?
Sr1 Be Sr1 168.8(3) . 5 ?
O1 Be Sr2 135.2(2) 14_454 11_544 ?
O1 Be Sr2 52.69(11) 10_554 11_544 ?
O4 Be Sr2 118.3(2) . 11_544 ?
```

```
O4 Be Sr2 54.16(11) 5 11_544 ?
Sr1 Be Sr2 83.34(2) . 11_544 ?
Sr1 Be Sr2 95.56(3) 5 11_544 ?
O1 Be Sr2 52.69(11) 14_454 . ?
O1 Be Sr2 135.2(2) 10_554 . ?
O4 Be Sr2 54.16(11) . . ?
O4 Be Sr2 118.3(2) 5 . ?
Sr1 Be Sr2 95.56(3) . . ?
Sr1 Be Sr2 83.34(2) 5 . ?
Sr2 Be Sr2 168.8(3) 11_544 . ?
O1 Sr2 O1 73.74(15) 3_545 12_454 ?
O1 Sr2 O1 106.50(15) 3_545 5 ?
O1 Sr2 O1 174.89(12) 12_454 5 ?
O1 Sr2 O1 174.89(12) 3_545 14_454 ?
O1 Sr2 O1 106.50(15) 12_454 14_454 ?
O1 Sr2 O1 73.74(15) 5 14_454 ?
O1 Sr2 O4 60.25(9) 3_545 15_444 ?
O1 Sr2 O4 90.75(9) 12_454 15_444 ?
O1 Sr2 O4 85.06(9) 5 15_444 ?
O1 Sr2 O4 124.70(9) 14_454 15_444 ?
O1 Sr2 O4 85.06(9) 3_545 10_454 ?
O1 Sr2 O4 124.70(9) 12_454 10_454 ?
O1 Sr2 O4 60.25(9) 5 10_454 ?
O1 Sr2 O4 90.75(9) 14_454 10_454 ?
O4 Sr2 O4 121.76(14) 15_444 10_454 ?
O1 Sr2 O4 124.70(9) 3_545 . ?
O1 Sr2 O4 85.06(9) 12_454 . ?
O1 Sr2 O4 90.75(9) 5 . ?
O1 Sr2 O4 60.25(9) 14_454 . ?
O4 Sr2 O4 69.87(14) 15_444 . ?
O4 Sr2 O4 144.85(12) 10_454 . ?
O1 Sr2 O4 90.75(9) 3_545 8 ?
O1 Sr2 O4 60.25(9) 12_454 8 ?
O1 Sr2 O4 124.70(9) 5 8 ?
O1 Sr2 O4 85.06(9) 14_454 8 ?
O4 Sr2 O4 144.85(12) 15_444 8 ?
O4 Sr2 O4 69.87(14) 10_454 8 ?
O4 Sr2 O4 121.76(14) . 8 ?
O1 Sr2 Be 29.98(12) 3_545 12_454 ?
O1 Sr2 Be 78.60(10) 12_454 12_454 ?
O1 Sr2 Be 99.04(9) 5 12_454 ?
O1 Sr2 Be 155.05(12) 14_454 12_454 ?
O4 Sr2 Be 30.47(11) 15_444 12_454 ?
O4 Sr2 Be 106.57(16) 10_454 12_454 ?
O4 Sr2 Be 96.68(14) . 12_454 ?
O4 Sr2 Be 117.41(8) 8 12_454 ?
O1 Sr2 Be 99.04(9) 3_545 10_454 ?
O1 Sr2 Be 155.05(12) 12_454 10_454 ?
O1 Sr2 Be 29.98(12) 5 10_454 ?
O1 Sr2 Be 78.60(10) 14_454 10_454 ?
O4 Sr2 Be 106.57(16) 15_444 10_454 ?
O4 Sr2 Be 30.47(11) 10_454 10_454 ?
O4 Sr2 Be 117.41(8) . 10_454 ?
```

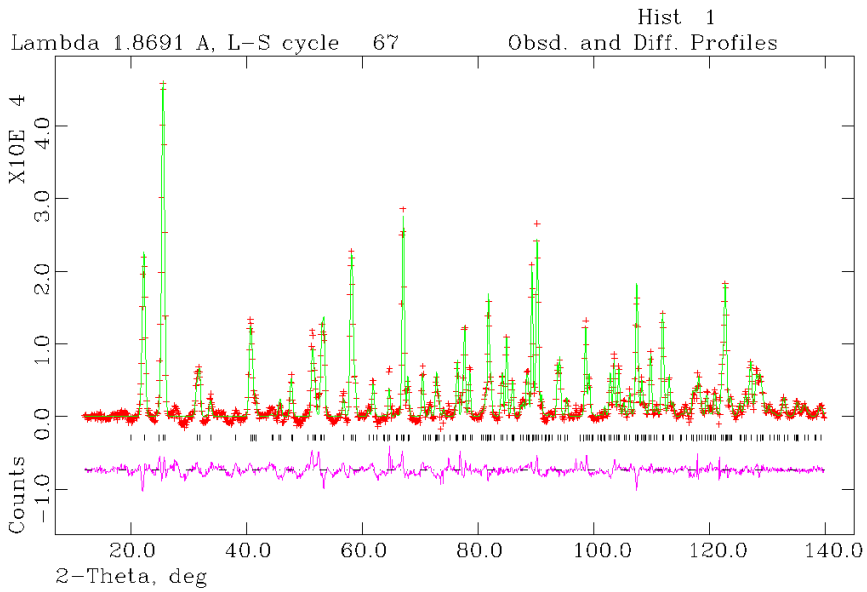
```
O4 Sr2 Be 96.68(14) 8 10_454 ?
Be Sr2 Be 107.3(2) 12_454 10_454 ?
O1 Sr2 Be 78.60(10) 3_545 3_545 ?
O1 Sr2 Be 29.98(12) 12_454 3_545 ?
O1 Sr2 Be 155.05(12) 5 3_545 ?
O1 Sr2 Be 99.04(9) 14_454 3_545 ?
O4 Sr2 Be 117.41(8) 15_444 3_545 ?
O4 Sr2 Be 96.68(14) 10_454 3_545 ?
O4 Sr2 Be 106.57(16) . 3_545 ?
O4 Sr2 Be 30.47(11) 8 3_545 ?
Be Sr2 Be 96.66(2) 12_454 3_545 ?
Be Sr2 Be 125.9(2) 10_454 3_545 ?
O1 Sr2 Be 155.05(12) 3_545 . ?
O1 Sr2 Be 99.04(9) 12_454 . ?
O1 Sr2 Be 78.60(10) 5 . ?
O1 Sr2 Be 29.98(12) 14_454 . ?
O4 Sr2 Be 96.68(14) 15_444 . ?
O4 Sr2 Be 117.41(8) 10_454 . ?
O4 Sr2 Be 30.47(11) . . ?
O4 Sr2 Be 106.57(16) 8 . ?
Be Sr2 Be 125.9(2) 12_454 . ?
Be Sr2 Be 96.66(2) 10_454 . ?
Be Sr2 Be 107.3(2) 3_545 . ?

_diffrn_measured_fraction_theta_max    0.987
_diffrn_reflns_theta_full              27.80
_diffrn_measured_fraction_theta_full   0.987
_refine_diff_density_max    0.417
_refine_diff_density_min   -0.527
_refine_diff_density_rms    0.132
```

Figure S1 Electron micrograph images of Sr[Be(OH)4] crystals



3. NPD data analysis



Profile fit to NPD collected from $SrBe(OH)_4$ at 250 K on D20, ILL Grenoble for 2 hours. Crystallographic model was that obtained at 298 K from SXD data (see cif above) with refinement of hydrogen atomic positions and ADPs only – see below. Red crosses are experimental data, green continuous line the calculated profile and the magneta lower continuous line the difference. Tick marks show reflection positions.

Refined hydrogen positions – crystallographic coordinates and esds. Labelling as in cif above.

H1	0.6018(9)	0.4680(10)	0.0117(7)
H2	0.2493(18)	0.4154(8)	0.0714(5)

Extracted bond lengths

O1_H1	0.948(9)
O4_H2	0.969(8)