data_vmx1_130k_abs

_audit_creation_method          SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common            ?
_chemical_melting_point        ?
_chemical_formula_moiety         ?
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 'H B Ca O5 Si'
_chemical_formula_weight        159.99

loop_
 _atom_type_symbol
 _atom_type_description
 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'H' 'H'  0.0000  0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'B' 'B'  0.0013  0.0007
 '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'
 'Si' 'Si'  0.0817  0.0704
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ca' 'Ca'  0.2262  0.3064
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting           ?
_symmetry_space_group_name_H-M    ?

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

_cell_length_a              4.82980(10)
_cell_length_b              7.60020(10)
_cell_length_c              9.6321(2)
_cell_angle_alpha            90.00
_cell_angle_beta            90.183(2)
_cell_angle_gamma            90.00
_cell_volume             353.568(11)
_cell_formula_units_Z         4
_cell_measurement_temperature    403(2)
_cell_measurement_reflns_used    ?
_cell_measurement_theta_min      ?

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_cell_measurement_theta_max        ?

_exptl_crystal_description         ?
_exptl_crystal_colour              ?
_exptl_crystal_size_max            ?
_exptl_crystal_size_mid            ?
_exptl_crystal_size_min            ?
_exptl_crystal_density_meas        ?
_exptl_crystal_density_diffrn      3.006
_exptl_crystal_density_method      'not measured'
_exptl_crystal_F_000               320
_exptl_absorpt_coefficient_mu      2.002
_exptl_absorpt_correction_type     ?
_exptl_absorpt_correction_T_min    ?
_exptl_absorpt_correction_T_max    ?
_exptl_absorpt_process_details     ?

_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature        130(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    ?
_diffrn_measurement_method         ?
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_diffrn_standards_interval_time    ?
_diffrn_standards_decay_%          ?
_diffrn_reflns_number              8549
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_diffrn_reflns_av_sigmaI/netI      0.0248
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_diffrn_reflns_limit_h_max         8
_diffrn_reflns_limit_k_min         -13
_diffrn_reflns_limit_k_max         13
_diffrn_reflns_limit_l_min         -16
_diffrn_reflns_limit_l_max         17
_diffrn_reflns_theta_min           4.22
_diffrn_reflns_theta_max           40.11
_reflns_number_total               2200
_reflns_number_gt                  1942
_reflns_threshold_expression       >2sigma(I)

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_computing_cell_refinement         ?
_computing_data_reduction          ?
_computing_structure_solution      ?
_computing_structure_refinement    'SHELXL-97 (Sheldrick, 1997)'
```

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_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
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 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^ > 2sigma(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^)+(0.0100P)^2^+0.0000P] 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     SHELXL
_refine_ls_extinction_coef       0.036(2)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns         2200
_refine_ls_number_parameters      78
_refine_ls_number_restraints      0
_refine_ls_R_factor_all          0.0256
_refine_ls_R_factor_gt           0.0203
_refine_ls_wR_factor_ref          0.0433
_refine_ls_wR_factor_gt           0.0426
_refine_ls_goodness_of_fit_ref   1.428
_refine_ls_restrained_S_all       1.428
_refine_ls_shift/su_max          0.000
_refine_ls_shift/su_mean          0.000

loop_
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 _atom_site_type_symbol
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 _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
Ca Ca 0.99179(3) 0.106284(18) 0.336025(16) 0.00352(4) Uani 1 1 d . . .
```

Si Si 0.46966(4) 0.26660(3) 0.08426(2) 0.00261(5) Uani 1 1 d . . .
B B 0.56930(17) 0.41066(10) 0.34092(9) 0.00352(12) Uani 1 1 d . . .
O1 O 0.24102(12) 0.40192(7) 0.03711(6) 0.00432(9) Uani 1 1 d . . .
O2 O 0.67129(11) 0.30110(7) 0.45762(6) 0.00399(9) Uani 1 1 d . . .
O3 O 0.67642(11) 0.33458(7) 0.21062(6) 0.00382(9) Uani 1 1 d . . .
O4 O 0.31455(11) 0.08837(7) 0.14577(6) 0.00418(9) Uani 1 1 d . . .
O5 O 0.25886(12) 0.41322(7) 0.33656(6) 0.00454(9) Uani 1 1 d . . .
H H 0.203(3) 0.4486(17) 0.4117(17) 0.025(4) Uiso 1 1 d . . .

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 _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
Ca 0.00365(6) 0.00388(6) 0.00304(6) -0.00006(4) 0.00029(4) -0.00017(4)
Si 0.00302(8) 0.00266(8) 0.00214(9) -0.00010(6) 0.00017(6) 0.00014(6)
B 0.0036(3) 0.0041(3) 0.0029(3) 0.0000(2) 0.0002(2) 0.0001(2)
O1 0.0045(2) 0.0042(2) 0.0042(2) -0.00018(17) -0.00037(17) 0.00106(16)
O2 0.0043(2) 0.0045(2) 0.0032(2) 0.00088(16) 0.00047(17) 0.00022(16)
O3 0.0042(2) 0.0048(2) 0.0025(2) -0.00090(16) 0.00027(16) 0.00008(16)
O4 0.0046(2) 0.0031(2) 0.0048(2) 0.00037(16) 0.00133(17) 0.00012(16)
O5 0.0033(2) 0.0063(2) 0.0041(2) -0.00092(17) 0.00066(17) 0.00050(16)

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

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 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
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Ca O1 2.2757(6) 2_645 ?
Ca O1 2.2781(6) 4_666 ?
Ca O4 2.4135(6) 1_655 ?
Ca O2 2.4437(6) . ?
Ca O5 2.5237(6) 2_645 ?
Ca O3 2.6035(6) . ?
Ca O3 2.6530(6) 2_745 ?
Ca O5 2.6656(6) 1_655 ?
Si O1 1.5748(6) . ?
Si O2 1.6458(6) 4_565 ?
Si O3 1.6546(6) . ?
Si O4 1.6583(6) . ?

B O4 1.4679(10) 2_655 ?
B O3 1.4770(10) . ?
B O2 1.4819(10) . ?
B O5 1.5000(10) . ?
O1 Ca 2.2757(6) 2_655 ?
O1 Ca 2.2781(6) 4_465 ?
O2 Si 1.6458(6) 4_566 ?
O3 Ca 2.6530(6) 2_755 ?
O4 B 1.4679(10) 2_645 ?
O4 Ca 2.4135(6) 1_455 ?
O5 Ca 2.5237(6) 2_655 ?
O5 Ca 2.6656(6) 1_455 ?


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 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O1 Ca O1 77.61(2) 2_645 4_666 ?
O1 Ca O4 133.68(2) 2_645 1_655 ?
O1 Ca O4 107.65(2) 4_666 1_655 ?
O1 Ca O2 80.87(2) 2_645 . ?
O1 Ca O2 86.73(2) 4_666 . ?
O4 Ca O2 144.072(19) 1_655 . ?
O1 Ca O5 73.74(2) 2_645 2_645 ?
O1 Ca O5 142.673(19) 4_666 2_645 ?
O4 Ca O5 77.10(2) 1_655 2_645 ?
O2 Ca O5 111.389(19) . 2_645 ?
O1 Ca O3 114.498(19) 2_645 . ?
O1 Ca O3 136.013(19) 4_666 . ?
O4 Ca O3 93.650(19) 1_655 . ?
O2 Ca O3 56.497(18) . . ?
O5 Ca O3 78.649(18) 2_645 . ?
O1 Ca O3 81.920(19) 2_645 2_745 ?
O1 Ca O3 78.748(19) 4_666 2_745 ?
O4 Ca O3 55.637(18) 1_655 2_745 ?
O2 Ca O3 159.494(19) . 2_745 ?
O5 Ca O3 74.017(18) 2_645 2_745 ?
O3 Ca O3 142.465(9) . 2_745 ?
O1 Ca O5 146.74(2) 2_645 1_655 ?
O1 Ca O5 76.582(19) 4_666 1_655 ?
O4 Ca O5 74.759(19) 1_655 1_655 ?
O2 Ca O5 77.063(19) . 1_655 ?
O5 Ca O5 137.832(13) 2_645 1_655 ?
O3 Ca O5 72.544(17) . 1_655 ?
O3 Ca O5 112.889(18) 2_745 1_655 ?
O1 Si O2 113.98(3) . 4_565 ?
O1 Si O3 115.41(3) . . ?
O2 Si O3 106.60(3) 4_565 . ?
O1 Si O4 108.62(3) . . ?
O2 Si O4 106.17(3) 4_565 . ?

O3 Si O4 105.34(3) . . ?
O4 B O3 107.43(6) 2_655 . ?
O4 B O2 108.95(6) 2_655 . ?
O3 B O2 107.95(6) . . ?
O4 B O5 111.85(6) 2_655 . ?
O3 B O5 109.52(6) . . ?
O2 B O5 111.00(6) . . ?
Si O1 Ca 129.65(3) . 2_655 ?
Si O1 Ca 126.54(3) . 4_465 ?
Ca O1 Ca 102.39(2) 2_655 4_465 ?
B O2 Si 122.81(5) . 4_566 ?
B O2 Ca 100.75(4) . . ?
Si O2 Ca 122.89(3) 4_566 . ?
B O3 Si 122.35(5) . . ?
B O3 Ca 94.17(4) . . ?
Si O3 Ca 118.95(3) . . ?
B O3 Ca 93.02(4) . 2_755 ?
Si O3 Ca 118.81(3) . 2_755 ?
Ca O3 Ca 104.153(18) . 2_755 ?
B O4 Si 127.57(5) 2_645 . ?
B O4 Ca 103.49(4) 2_645 1_455 ?
Si O4 Ca 121.25(3) . 1_455 ?
B O5 Ca 120.22(4) . 2_655 ?
B O5 Ca 118.19(4) . 1_455 ?
Ca O5 Ca 106.05(2) 2_655 1_455 ?

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_diffrn_reflns_theta_full          40.00
_diffrn_measured_fraction_theta_full   0.994
_refine_diff_density_max    0.460
_refine_diff_density_min   -0.398
_refine_diff_density_rms    0.105