

data_vg3

_audit_creation_method SHELXL-97
_chemical_name_systematic
;
?
;
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety ?
_chemical_formula_sum
'Ca3 O12 Si3 V2'
_chemical_formula_weight 498.39

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
'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'
'V' 'V' 0.3005 0.5294
'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+1/2, -y, z+1/2'
'-x, y+1/2, -z+1/2'
'x+1/2, -y+1/2, -z'
'z, x, y'
'z+1/2, -x+1/2, -y'
'-z+1/2, -x, y+1/2'
'-z, x+1/2, -y+1/2'
'y, z, x'
'-y, z+1/2, -x+1/2'
'y+1/2, -z+1/2, -x'
'-y+1/2, -z, x+1/2'
'y+3/4, x+1/4, -z+1/4'
'-y+3/4, -x+3/4, -z+3/4'
'y+1/4, -x+1/4, z+3/4'
'-y+1/4, x+3/4, z+1/4'
'x+3/4, z+1/4, -y+1/4'
'-x+1/4, z+3/4, y+1/4'

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

'-x+1/2, -y+1/2, -z+1/2'
'x, y+1/2, -z'
'x+1/2, -y, z'
'-x, y, z+1/2'
'-z+1/2, -x+1/2, -y+1/2'
'-z, x, y+1/2'
'z, x+1/2, -y'
'z+1/2, -x, y'
'-y+1/2, -z+1/2, -x+1/2'
'y+1/2, -z, x'
'-y, z, x+1/2'
'y, z+1/2, -x'
'-y-1/4, -x+1/4, z+1/4'
'y-1/4, x-1/4, z-1/4'
'-y+1/4, x+1/4, -z-1/4'
'y+1/4, -x-1/4, -z+1/4'
'-x-1/4, -z+1/4, y+1/4'
'x+1/4, -z-1/4, -y+1/4'
'x-1/4, z-1/4, y-1/4'
'-x+1/4, z+1/4, -y-1/4'
'-z-1/4, -y+1/4, x+1/4'
'-z+1/4, y+1/4, -x-1/4'
'z+1/4, -y-1/4, -x+1/4'
'z-1/4, y-1/4, x-1/4'

_cell_length_a	12.0854(12)
_cell_length_b	12.0854(12)
_cell_length_c	12.0854(12)
_cell_angle_alpha	90.00
_cell_angle_beta	90.00
_cell_angle_gamma	90.00
_cell_volume	1765.2(3)
_cell_formula_units_Z	8
_cell_measurement_temperature	293(2)
_cell_measurement_reflns_used	?
_cell_measurement_theta_min	?
_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_diffn	3.751
_exptl_crystal_density_method	'not measured'
_exptl_crystal_F_000	1952
_exptl_absorpt_coefficient_mu	4.346
_exptl_absorpt_correction_type	?
_exptl_absorpt_correction_T_min	?
_exptl_absorpt_correction_T_max	?
_exptl_absorpt_process_details	?
_exptl_special_details	

```

;
?
;

_diffrn_ambient_temperature      293(2)
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_type           MoK\alpha
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
_diffrn_measurement_method       ?
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%       ?
_diffrn_reflns_number            2516
_diffrn_reflns_av_R_equivalents  0.0798
_diffrn_reflns_av_sigmaI/netI    0.0381
_diffrn_reflns_limit_h_min       -19
_diffrn_reflns_limit_h_max       0
_diffrn_reflns_limit_k_min       -12
_diffrn_reflns_limit_k_max       16
_diffrn_reflns_limit_l_min       -13
_diffrn_reflns_limit_l_max       13
_diffrn_reflns_theta_min         4.13
_diffrn_reflns_theta_max         34.87
_reflns_number_total             330
_reflns_number_gt                150
_reflns_threshold_expression      >2sigma(I)

```

```

_computing_data_collection       ?
_computing_cell_refinement       ?
_computing_data_reduction        ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement  'SHELXL-97 (Sheldrick, 1997)'
_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  $F^2 > 2\sigma(F^2)$  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^)+(0.0215P)^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 0.00021(13)
_refine_ls_extinction_expression
'Fc^*=kFc[1+0.001xFc^2^/l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns 330
_refine_ls_number_parameters 20
_refine_ls_number_restraints 0
_refine_ls_R_factor_all 0.0835
_refine_ls_R_factor_gt 0.0269
_refine_ls_wR_factor_ref 0.0644
_refine_ls_wR_factor_gt 0.0498
_refine_ls_goodness_of_fit_ref 0.966
_refine_ls_restrained_S_all 0.966
_refine_ls_shift/su_max 0.000
_refine_ls_shift/su_mean 0.000

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_symetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
Ca Ca 0.1250 0.0000 0.2500 0.0078(3) Uani 0.954(7) 4 d SP . .
V V 0.0000 0.0000 0.0000 0.0057(3) Uani 0.951(6) 6 d SP . .
Si Si 0.3750 0.0000 0.2500 0.0055(4) Uani 1 4 d S . .
O O 0.03925(17) 0.04767(16) 0.65498(16) 0.0118(5) Uani 1 1 d . . .

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
Ca 0.0056(6) 0.0089(4) 0.0089(4) 0.0008(4) 0.000 0.000
V 0.0057(3) 0.0057(3) 0.0057(3) 0.0006(3) 0.0006(3) 0.0006(3)
Si 0.0043(7) 0.0061(5) 0.0061(5) 0.000 0.000 0.000
O 0.0140(10) 0.0107(10) 0.0107(11) 0.0002(8) -0.0015(8) -0.0004(8)

_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.
;

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
Ca O 2.365(2) 90_565 ?
Ca O 2.365(2) 76_554 ?
Ca O 2.365(2) 67_656 ?
Ca O 2.365(2) 49_556 ?
Ca O 2.517(2) 70_656 ?
Ca O 2.517(2) 55_556 ?
Ca O 2.517(2) 93_655 ?
Ca O 2.517(2) 80_455 ?
Ca Si 3.0213(3) . ?
Ca Si 3.0213(3) 50_556 ?
Ca V 3.3780(3) . ?
Ca V 3.3780(3) 38_444 ?
V O 2.0162(19) 84_545 ?
V O 2.0162(19) 76_554 ?
V O 2.0162(19) 28_445 ?
V O 2.0162(19) 80_455 ?
V O 2.0162(19) 32_544 ?
V O 2.0162(19) 36_454 ?
V Ca 3.3780(3) 5 ?
V Ca 3.3780(3) 49 ?
V Ca 3.3780(3) 9 ?
V Ca 3.3780(3) 53 ?
V Ca 3.3780(3) 57 ?
Si O 1.651(2) 27_545 ?
Si O 1.651(2) 67_656 ?
Si O 1.651(2) 2_554 ?
Si O 1.651(2) 90_565 ?
Si Ca 3.0213(3) 50_656 ?
O Si 1.651(2) 2 ?
O V 2.0162(19) 28_445 ?
O Ca 2.365(2) 49_556 ?
O Ca 2.517(2) 58_566 ?

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
 O Ca O 117.91(9) 90_565 76_554 ?
 O Ca O 65.83(9) 90_565 67_656 ?
 O Ca O 160.29(10) 76_554 67_656 ?
 O Ca O 160.29(10) 90_565 49_556 ?
 O Ca O 65.83(9) 76_554 49_556 ?
 O Ca O 117.91(9) 67_656 49_556 ?
 O Ca O 123.14(4) 90_565 70_656 ?
 O Ca O 91.39(5) 76_554 70_656 ?
 O Ca O 72.24(9) 67_656 70_656 ?
 O Ca O 74.57(8) 49_556 70_656 ?
 O Ca O 91.39(5) 90_565 55_556 ?
 O Ca O 123.14(4) 76_554 55_556 ?
 O Ca O 74.57(8) 67_656 55_556 ?
 O Ca O 72.24(9) 49_556 55_556 ?
 O Ca O 112.76(9) 70_656 55_556 ?
 O Ca O 72.24(9) 90_565 93_655 ?
 O Ca O 74.57(8) 76_554 93_655 ?
 O Ca O 123.14(4) 67_656 93_655 ?
 O Ca O 91.39(5) 49_556 93_655 ?
 O Ca O 163.45(9) 70_656 93_655 ?
 O Ca O 69.79(9) 55_556 93_655 ?
 O Ca O 74.57(8) 90_565 80_455 ?
 O Ca O 72.24(9) 76_554 80_455 ?
 O Ca O 91.39(5) 67_656 80_455 ?
 O Ca O 123.14(4) 49_556 80_455 ?
 O Ca O 69.79(9) 70_656 80_455 ?
 O Ca O 163.45(9) 55_556 80_455 ?
 O Ca O 112.76(9) 93_655 80_455 ?
 O Ca Si 32.91(5) 90_565 . ?
 O Ca Si 147.09(5) 76_554 . ?
 O Ca Si 32.91(5) 67_656 . ?
 O Ca Si 147.09(5) 49_556 . ?
 O Ca Si 98.28(4) 70_656 . ?
 O Ca Si 81.72(4) 55_556 . ?
 O Ca Si 98.28(4) 93_655 . ?
 O Ca Si 81.72(4) 80_455 . ?
 O Ca Si 147.09(5) 90_565 50_556 ?
 O Ca Si 32.91(5) 76_554 50_556 ?
 O Ca Si 147.09(5) 67_656 50_556 ?
 O Ca Si 32.91(5) 49_556 50_556 ?
 O Ca Si 81.72(4) 70_656 50_556 ?
 O Ca Si 98.28(4) 55_556 50_556 ?
 O Ca Si 81.72(4) 93_655 50_556 ?
 O Ca Si 98.28(4) 80_455 50_556 ?
 Si Ca Si 180.0 . 50_556 ?
 O Ca V 99.06(5) 90_565 . ?
 O Ca V 35.92(5) 76_554 . ?
 O Ca V 126.40(5) 67_656 . ?
 O Ca V 93.38(5) 49_556 . ?
 O Ca V 76.53(5) 70_656 . ?
 O Ca V 158.95(4) 55_556 . ?
 O Ca V 95.98(5) 93_655 . ?

O Ca V 36.43(4) 80_455 . ?
 Si Ca V 116.6 . . ?
 Si Ca V 63.4 50_556 . ?
 O Ca V 35.92(5) 90_565 38_444 ?
 O Ca V 99.06(5) 76_554 38_444 ?
 O Ca V 93.38(5) 67_656 38_444 ?
 O Ca V 126.40(5) 49_556 38_444 ?
 O Ca V 158.95(4) 70_656 38_444 ?
 O Ca V 76.53(5) 55_556 38_444 ?
 O Ca V 36.43(4) 93_655 38_444 ?
 O Ca V 95.98(5) 80_455 38_444 ?
 Si Ca V 63.4 . 38_444 ?
 Si Ca V 116.6 50_556 38_444 ?
 V Ca V 101.5 . 38_444 ?
 O V O 91.16(8) 84_545 76_554 ?
 O V O 88.84(8) 84_545 28_445 ?
 O V O 180.00(12) 76_554 28_445 ?
 O V O 91.16(8) 84_545 80_455 ?
 O V O 91.16(8) 76_554 80_455 ?
 O V O 88.84(8) 28_445 80_455 ?
 O V O 88.84(8) 84_545 32_544 ?
 O V O 88.84(8) 76_554 32_544 ?
 O V O 91.16(8) 28_445 32_544 ?
 O V O 180.00(16) 80_455 32_544 ?
 O V O 180.00(12) 84_545 36_454 ?
 O V O 88.84(8) 76_554 36_454 ?
 O V O 91.16(8) 28_445 36_454 ?
 O V O 88.84(8) 80_455 36_454 ?
 O V O 91.16(8) 32_544 36_454 ?
 O V Ca 94.74(6) 84_545 . ?
 O V Ca 43.47(6) 76_554 . ?
 O V Ca 136.53(6) 28_445 . ?
 O V Ca 47.85(6) 80_455 . ?
 O V Ca 132.15(6) 32_544 . ?
 O V Ca 85.26(6) 36_454 . ?
 O V Ca 47.85(6) 84_545 5 ?
 O V Ca 94.74(6) 76_554 5 ?
 O V Ca 85.26(6) 28_445 5 ?
 O V Ca 43.47(6) 80_455 5 ?
 O V Ca 136.53(6) 32_544 5 ?
 O V Ca 132.15(6) 36_454 5 ?
 Ca V Ca 66.4 . 5 ?
 O V Ca 85.26(6) 84_545 49 ?
 O V Ca 136.53(6) 76_554 49 ?
 O V Ca 43.47(6) 28_445 49 ?
 O V Ca 132.15(6) 80_455 49 ?
 O V Ca 47.85(6) 32_544 49 ?
 O V Ca 94.74(6) 36_454 49 ?
 Ca V Ca 180.0 . 49 ?
 Ca V Ca 113.6 5 49 ?
 O V Ca 43.47(6) 84_545 9 ?
 O V Ca 47.85(6) 76_554 9 ?
 O V Ca 132.15(6) 28_445 9 ?
 O V Ca 94.74(6) 80_455 9 ?

O V Ca 85.26(6) 32_544 9 ?
 O V Ca 136.53(6) 36_454 9 ?
 Ca V Ca 66.4 . 9 ?
 Ca V Ca 66.4 5 9 ?
 Ca V Ca 113.6 49 9 ?
 O V Ca 132.15(6) 84_545 53 ?
 O V Ca 85.26(6) 76_554 53 ?
 O V Ca 94.74(6) 28_445 53 ?
 O V Ca 136.53(6) 80_455 53 ?
 O V Ca 43.47(6) 32_544 53 ?
 O V Ca 47.85(6) 36_454 53 ?
 Ca V Ca 113.6 . 53 ?
 Ca V Ca 180.0 5 53 ?
 Ca V Ca 66.4 49 53 ?
 Ca V Ca 113.6 9 53 ?
 O V Ca 136.53(6) 84_545 57 ?
 O V Ca 132.15(6) 76_554 57 ?
 O V Ca 47.85(6) 28_445 57 ?
 O V Ca 85.26(6) 80_455 57 ?
 O V Ca 94.74(6) 32_544 57 ?
 O V Ca 43.47(6) 36_454 57 ?
 Ca V Ca 113.6 . 57 ?
 Ca V Ca 113.6 5 57 ?
 Ca V Ca 66.4 49 57 ?
 Ca V Ca 180.0 9 57 ?
 Ca V Ca 66.4 53 57 ?
 O Si O 113.21(7) 27_545 67_656 ?
 O Si O 102.22(14) 27_545 2_554 ?
 O Si O 113.21(7) 67_656 2_554 ?
 O Si O 113.21(7) 27_545 90_565 ?
 O Si O 102.22(14) 67_656 90_565 ?
 O Si O 113.21(7) 2_554 90_565 ?
 O Si Ca 51.11(7) 27_545 50_656 ?
 O Si Ca 128.89(7) 67_656 50_656 ?
 O Si Ca 51.11(7) 2_554 50_656 ?
 O Si Ca 128.89(7) 90_565 50_656 ?
 O Si Ca 128.89(7) 27_545 . ?
 O Si Ca 51.11(7) 67_656 . ?
 O Si Ca 128.89(7) 2_554 . ?
 O Si Ca 51.11(7) 90_565 . ?
 Ca Si Ca 180.0 50_656 . ?
 Si O V 133.97(12) 2 28_445 ?
 Si O Ca 95.98(8) 2 49_556 ?
 V O Ca 100.61(8) 28_445 49_556 ?
 Si O Ca 123.88(10) 2 58_566 ?
 V O Ca 95.71(7) 28_445 58_566 ?
 Ca O Ca 98.53(7) 49_556 58_566 ?

_diffn_measured_fraction_theta_max 0.997
 _diffn_reflns_theta_full 34.87
 _diffn_measured_fraction_theta_full 0.997
 _refine_diff_density_max 0.441
 _refine_diff_density_min -0.489
 _refine_diff_density_rms 0.118