

data\_kss\_cry2\_p7

\_audit\_creation\_method SHELXL-97  
\_chemical\_name\_systematic  
;  
?  
;  
\_chemical\_name\_common ?  
\_chemical\_melting\_point ?  
\_chemical\_formula\_moiety ?  
\_chemical\_formula\_sum  
'Al2 K1.97 O8 Si2'  
\_chemical\_formula\_weight 315.17

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'  
'Al' 'Al' 0.0645 0.0514  
'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'  
'K' 'K' 0.2009 0.2494  
'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'  
'-y, x-y, z'  
'y, x, z+1/2'  
'-x+y, -x, z'  
'-x, -x+y, z+1/2'  
'x-y, -y, z+1/2'

\_cell\_length\_a 5.061(5)  
\_cell\_length\_b 5.061(5)  
\_cell\_length\_c 8.315(9)  
\_cell\_angle\_alpha 90.00  
\_cell\_angle\_beta 90.00  
\_cell\_angle\_gamma 120.00  
\_cell\_volume 184.4(3)  
\_cell\_formula\_units\_Z 1  
\_cell\_measurement\_temperature 295  
\_cell\_measurement\_pressure 4620000  
\_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   2.837
_exptl_crystal_density_method  'not measured'
_exptl_crystal_F_000           155
_exptl_absorpt_coefficient_mu   1.847
_exptl_absorpt_correction_type  ?
_exptl_absorpt_correction_T_min ?
_exptl_absorpt_correction_T_max ?
_exptl_absorpt_process_details  ?

_exptl_special_details
;
?
;

_diffrn_ambient_temperature     295
_diffrn_ambient_pressure        4620000
_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           1205
_diffrn_reflns_av_R_equivalents 0.1384
_diffrn_reflns_av_sigmaI/netI   0.2424
_diffrn_reflns_limit_h_min      -5
_diffrn_reflns_limit_h_max      6
_diffrn_reflns_limit_k_min      -9
_diffrn_reflns_limit_k_max      8
_diffrn_reflns_limit_l_min      -13
_diffrn_reflns_limit_l_max      10
_diffrn_reflns_theta_min        4.65
_diffrn_reflns_theta_max        40.54
_reflns_number_total             461
_reflns_number_gt                178
_reflns_threshold_expression     >2sigma(I)

_computing_data_collection      ?
_computing_cell_refinement      ?
_computing_data_reduction      ?

```

```

_computing_structure_solution    ?
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics   ?
_computing_publication_material ?

_refine_special_details
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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/[sigma2(Fo2)+(0.0100P)2+0.0000P] where P=(Fo2+2Fc2)/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       0.074(7)
_refine_ls_extinction_expression
'Fc*=kFc[1+0.001xFc2l3/sin(2q)]-1/4'
_refine_ls_abs_structure_details
'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack  0.8(4)
_refine_ls_number_reflns        461
_refine_ls_number_parameters     15
_refine_ls_number_restraints     8
_refine_ls_R_factor_all          0.2779
_refine_ls_R_factor_gt           0.1188
_refine_ls_wR_factor_ref         0.1440
_refine_ls_wR_factor_gt          0.1272
_refine_ls_goodness_of_fit_ref   1.689
_refine_ls_restrained_S_all      1.736
_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_symmetry_multiplicity

```

```

_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly
_atom_site_disorder_group
K K 0.0000 0.0000 0.2541 0.0276(6) Uani 1 3 d S . .
T2 Si 0.3333 0.6667 0.4556(4) 0.0343(12) Uiso 1 3 d SD . .
T1 Al 0.3333 0.6667 0.0697(5) 0.0105(8) Uiso 1 3 d SD . .
O1 O 0.3333 0.6667 0.2681(7) 0.096(3) Uiso 1 3 d SD . .
O2 O 0.6213(9) 0.0302(11) 1.0387(12) 0.068(2) Uiso 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
K 0.0271(8) 0.0271(8) 0.0288(14) 0.000 0.000 0.0135(4)

```

```

_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
K O2 2.683(7) 2_544 ?
K O2 2.683(7) 1_454 ?
K O2 2.683(7) 4_664 ?
K O1 2.924(3) 1_545 ?
K O1 2.924(3) . ?
K O1 2.924(3) 1_445 ?
K O2 3.097(9) 5_664 ?
K O2 3.097(9) 6_454 ?
K O2 3.097(9) 3_544 ?
K T1 3.300(3) 1_545 ?
K T1 3.300(3) 1_445 ?
K T1 3.300(3) . ?
T2 O1 1.559(6) . ?
T2 O2 1.591(6) 6_564 ?
T2 O2 1.591(6) 3_554 ?
T2 O2 1.591(6) 5_664 ?
T2 K 3.368(3) 1_565 ?
T2 K 3.368(3) 1_665 ?

```

T2 K 3.834(4) 3\_665 ?  
 T2 K 3.834(4) 3\_565 ?  
 T2 K 3.834(4) 3 ?  
 T1 O1 1.650(6) . ?  
 T1 O2 1.701(5) 2\_554 ?  
 T1 O2 1.701(5) 1\_564 ?  
 T1 O2 1.701(5) 4\_664 ?  
 T1 K 3.300(3) 1\_565 ?  
 T1 K 3.300(3) 1\_665 ?  
 T1 K 3.928(4) 3\_554 ?  
 T1 K 3.928(4) 3\_564 ?  
 T1 K 3.928(4) 3\_664 ?  
 O1 K 2.924(3) 1\_565 ?  
 O1 K 2.924(3) 1\_665 ?  
 O2 T2 1.591(6) 3 ?  
 O2 T1 1.701(5) 1\_546 ?  
 O2 K 2.683(7) 1\_656 ?  
 O2 K 3.097(9) 3\_655 ?

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  
 O2 K O2 80.3(3) 2\_544 1\_454 ?  
 O2 K O2 80.3(3) 2\_544 4\_664 ?  
 O2 K O2 80.3(3) 1\_454 4\_664 ?  
 O2 K O1 53.74(17) 2\_544 1\_545 ?  
 O2 K O1 134.0(2) 1\_454 1\_545 ?  
 O2 K O1 88.70(13) 4\_664 1\_545 ?  
 O2 K O1 134.0(2) 2\_544 . ?  
 O2 K O1 88.70(13) 1\_454 . ?  
 O2 K O1 53.74(17) 4\_664 . ?  
 O1 K O1 119.842(16) 1\_545 . ?  
 O2 K O1 88.70(13) 2\_544 1\_445 ?  
 O2 K O1 53.74(17) 1\_454 1\_445 ?  
 O2 K O1 134.0(2) 4\_664 1\_445 ?  
 O1 K O1 119.842(16) 1\_545 1\_445 ?  
 O1 K O1 119.842(15) . 1\_445 ?  
 O2 K O2 143.44(18) 2\_544 5\_664 ?  
 O2 K O2 133.9(2) 1\_454 5\_664 ?  
 O2 K O2 91.96(17) 4\_664 5\_664 ?  
 O1 K O2 90.70(13) 1\_545 5\_664 ?  
 O1 K O2 52.50(16) . 5\_664 ?  
 O1 K O2 120.33(15) 1\_445 5\_664 ?  
 O2 K O2 133.9(2) 2\_544 6\_454 ?  
 O2 K O2 91.96(17) 1\_454 6\_454 ?  
 O2 K O2 143.44(18) 4\_664 6\_454 ?  
 O1 K O2 120.33(15) 1\_545 6\_454 ?  
 O1 K O2 90.70(13) . 6\_454 ?  
 O1 K O2 52.50(16) 1\_445 6\_454 ?

O2 K O2 67.9(2) 5\_664 6\_454 ?  
 O2 K O2 91.96(17) 2\_544 3\_544 ?  
 O2 K O2 143.44(18) 1\_454 3\_544 ?  
 O2 K O2 133.9(2) 4\_664 3\_544 ?  
 O1 K O2 52.50(16) 1\_545 3\_544 ?  
 O1 K O2 120.33(15) . 3\_544 ?  
 O1 K O2 90.70(13) 1\_445 3\_544 ?  
 O2 K O2 67.9(2) 5\_664 3\_544 ?  
 O2 K O2 67.9(2) 6\_454 3\_544 ?  
 O2 K T1 30.91(10) 2\_544 1\_545 ?  
 O2 K T1 106.3(2) 1\_454 1\_545 ?  
 O2 K T1 69.27(12) 4\_664 1\_545 ?  
 O1 K T1 29.98(12) 1\_545 1\_545 ?  
 O1 K T1 117.45(6) . 1\_545 ?  
 O1 K T1 117.45(6) 1\_445 1\_545 ?  
 O2 K T1 113.14(10) 5\_664 1\_545 ?  
 O2 K T1 146.06(11) 6\_454 1\_545 ?  
 O2 K T1 80.94(15) 3\_544 1\_545 ?  
 O2 K T1 69.27(12) 2\_544 1\_445 ?  
 O2 K T1 30.91(10) 1\_454 1\_445 ?  
 O2 K T1 106.3(2) 4\_664 1\_445 ?  
 O1 K T1 117.45(6) 1\_545 1\_445 ?  
 O1 K T1 117.45(6) . 1\_445 ?  
 O1 K T1 29.98(12) 1\_445 1\_445 ?  
 O2 K T1 146.06(11) 5\_664 1\_445 ?  
 O2 K T1 80.94(15) 6\_454 1\_445 ?  
 O2 K T1 113.14(11) 3\_544 1\_445 ?  
 T1 K T1 100.15(9) 1\_545 1\_445 ?  
 O2 K T1 106.3(2) 2\_544 . ?  
 O2 K T1 69.27(12) 1\_454 . ?  
 O2 K T1 30.91(10) 4\_664 . ?  
 O1 K T1 117.45(6) 1\_545 . ?  
 O1 K T1 29.98(12) . . ?  
 O1 K T1 117.45(6) 1\_445 . ?  
 O2 K T1 80.94(15) 5\_664 . ?  
 O2 K T1 113.14(10) 6\_454 . ?  
 O2 K T1 146.06(11) 3\_544 . ?  
 T1 K T1 100.15(9) 1\_545 . ?  
 T1 K T1 100.15(9) 1\_445 . ?  
 O1 T2 O2 115.7(4) . 6\_564 ?  
 O1 T2 O2 115.7(4) . 3\_554 ?  
 O2 T2 O2 102.5(5) 6\_564 3\_554 ?  
 O1 T2 O2 115.7(4) . 5\_664 ?  
 O2 T2 O2 102.5(5) 6\_564 5\_664 ?  
 O2 T2 O2 102.5(5) 3\_554 5\_664 ?  
 O1 T2 K 60.16(7) . 1\_565 ?  
 O2 T2 K 96.2(2) 6\_564 1\_565 ?  
 O2 T2 K 66.4(3) 3\_554 1\_565 ?  
 O2 T2 K 160.1(2) 5\_664 1\_565 ?  
 O1 T2 K 60.16(7) . . ?  
 O2 T2 K 160.1(2) 6\_564 . ?  
 O2 T2 K 96.2(2) 3\_554 . ?  
 O2 T2 K 66.4(3) 5\_664 . ?  
 K T2 K 97.39(9) 1\_565 . ?

O1 T2 K 60.16(7) . 1\_665 ?  
 O2 T2 K 66.4(3) 6\_564 1\_665 ?  
 O2 T2 K 160.1(2) 3\_554 1\_665 ?  
 O2 T2 K 96.2(2) 5\_664 1\_665 ?  
 K T2 K 97.39(9) 1\_565 1\_665 ?  
 K T2 K 97.39(9) . 1\_665 ?  
 O1 T2 K 130.34(6) . 3\_665 ?  
 O2 T2 K 34.7(2) 6\_564 3\_665 ?  
 O2 T2 K 110.8(4) 3\_554 3\_665 ?  
 O2 T2 K 67.9(3) 5\_664 3\_665 ?  
 K T2 K 130.74(3) 1\_565 3\_665 ?  
 K T2 K 130.74(3) . 3\_665 ?  
 K T2 K 70.18(8) 1\_665 3\_665 ?  
 O1 T2 K 130.34(6) . 3\_565 ?  
 O2 T2 K 67.9(3) 6\_564 3\_565 ?  
 O2 T2 K 34.7(2) 3\_554 3\_565 ?  
 O2 T2 K 110.8(4) 5\_664 3\_565 ?  
 K T2 K 70.18(8) 1\_565 3\_565 ?  
 K T2 K 130.74(3) . 3\_565 ?  
 K T2 K 130.74(3) 1\_665 3\_565 ?  
 K T2 K 82.61(9) 3\_665 3\_565 ?  
 O1 T2 K 130.34(6) . 3 ?  
 O2 T2 K 110.8(4) 6\_564 3 ?  
 O2 T2 K 67.9(3) 3\_554 3 ?  
 O2 T2 K 34.7(2) 5\_664 3 ?  
 K T2 K 130.74(3) 1\_565 3 ?  
 K T2 K 70.18(8) . 3 ?  
 K T2 K 130.74(3) 1\_665 3 ?  
 K T2 K 82.61(9) 3\_665 3 ?  
 K T2 K 82.61(9) 3\_565 3 ?  
 O1 T1 O2 98.7(3) . 2\_554 ?  
 O1 T1 O2 98.7(3) . 1\_564 ?  
 O2 T1 O2 117.75(17) 2\_554 1\_564 ?  
 O1 T1 O2 98.7(3) . 4\_664 ?  
 O2 T1 O2 117.75(17) 2\_554 4\_664 ?  
 O2 T1 O2 117.75(17) 1\_564 4\_664 ?  
 O1 T1 K 62.32(7) . 1\_565 ?  
 O2 T1 K 54.1(2) 2\_554 1\_565 ?  
 O2 T1 K 84.1(3) 1\_564 1\_565 ?  
 O2 T1 K 154.1(3) 4\_664 1\_565 ?  
 O1 T1 K 62.32(7) . 1\_665 ?  
 O2 T1 K 154.1(3) 2\_554 1\_665 ?  
 O2 T1 K 54.1(2) 1\_564 1\_665 ?  
 O2 T1 K 84.1(3) 4\_664 1\_665 ?  
 K T1 K 100.15(8) 1\_565 1\_665 ?  
 O1 T1 K 62.32(7) . . ?  
 O2 T1 K 84.1(3) 2\_554 . ?  
 O2 T1 K 154.1(3) 1\_564 . ?  
 O2 T1 K 54.1(2) 4\_664 . ?  
 K T1 K 100.15(8) 1\_565 . ?  
 K T1 K 100.15(9) 1\_665 . ?  
 O1 T1 K 131.93(6) . 3\_554 ?  
 O2 T1 K 75.8(2) 2\_554 3\_554 ?  
 O2 T1 K 126.6(4) 1\_564 3\_554 ?

O2 T1 K 49.2(3) 4\_664 3\_554 ?  
 K T1 K 129.78(4) 1\_565 3\_554 ?  
 K T1 K 129.78(4) 1\_665 3\_554 ?  
 K T1 K 69.61(8) . 3\_554 ?  
 O1 T1 K 131.93(6) . 3\_564 ?  
 O2 T1 K 49.2(3) 2\_554 3\_564 ?  
 O2 T1 K 75.8(2) 1\_564 3\_564 ?  
 O2 T1 K 126.6(4) 4\_664 3\_564 ?  
 K T1 K 69.61(8) 1\_565 3\_564 ?  
 K T1 K 129.78(4) 1\_665 3\_564 ?  
 K T1 K 129.78(4) . 3\_564 ?  
 K T1 K 80.23(9) 3\_554 3\_564 ?  
 O1 T1 K 131.93(6) . 3\_664 ?  
 O2 T1 K 126.6(4) 2\_554 3\_664 ?  
 O2 T1 K 49.2(3) 1\_564 3\_664 ?  
 O2 T1 K 75.8(2) 4\_664 3\_664 ?  
 K T1 K 129.78(4) 1\_565 3\_664 ?  
 K T1 K 69.61(8) 1\_665 3\_664 ?  
 K T1 K 129.78(4) . 3\_664 ?  
 K T1 K 80.23(9) 3\_554 3\_664 ?  
 K T1 K 80.23(9) 3\_564 3\_664 ?  
 T2 O1 T1 180.000(1) . . ?  
 T2 O1 K 92.29(11) . 1\_565 ?  
 T1 O1 K 87.71(11) . 1\_565 ?  
 T2 O1 K 92.29(11) . . ?  
 T1 O1 K 87.71(11) . . ?  
 K O1 K 119.842(15) 1\_565 . ?  
 T2 O1 K 92.29(11) . 1\_665 ?  
 T1 O1 K 87.71(11) . 1\_665 ?  
 K O1 K 119.842(15) 1\_565 1\_665 ?  
 K O1 K 119.842(15) . 1\_665 ?  
 T2 O2 T1 137.8(3) 3 1\_546 ?  
 T2 O2 K 125.6(3) 3 1\_656 ?  
 T1 O2 K 95.0(3) 1\_546 1\_656 ?  
 T2 O2 K 85.5(4) 3 3\_655 ?  
 T1 O2 K 106.2(4) 1\_546 3\_655 ?  
 K O2 K 91.72(17) 1\_656 3\_655 ?

\_diffn\_measured\_fraction\_theta\_max 0.756  
 \_diffn\_reflns\_theta\_full 40.54  
 \_diffn\_measured\_fraction\_theta\_full 0.756  
 \_refine\_diff\_density\_max 1.266  
 \_refine\_diff\_density\_min -1.387  
 \_refine\_diff\_density\_rms 0.280