

data_kss_cry2_air

_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 5.1552(16)
_cell_length_b 5.1552(16)
_cell_length_c 8.7096(19)
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 120.00
_cell_volume 200.46(10)
_cell_formula_units_Z 1
_cell_measurement_temperature 295
_cell_measurement_pressure 100
_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   2.611
_exptl_crystal_density_method  'not measured'
_exptl_crystal_F_000           155
_exptl_absorpt_coefficient_mu   1.699
_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        100
_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           5686
_diffrn_reflns_av_R_equivalents 0.0425
_diffrn_reflns_av_sigmaI/netI   0.0403
_diffrn_reflns_limit_h_min      -7
_diffrn_reflns_limit_h_max      7
_diffrn_reflns_limit_k_min      -8
_diffrn_reflns_limit_k_max      8
_diffrn_reflns_limit_l_min      -14
_diffrn_reflns_limit_l_max      14
_diffrn_reflns_theta_min        4.57
_diffrn_reflns_theta_max        36.01
_reflns_number_total            626
_reflns_number_gt               473
_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/[sigma^2(Fo^2)+(0.0250P)^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     none
_refine_ls_extinction_coef      ?
_refine_ls_abs_structure_details
'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack  0.50(11)
_refine_ls_number_reflns        626
_refine_ls_number_parameters     24
_refine_ls_number_restraints     9
_refine_ls_R_factor_all          0.0623
_refine_ls_R_factor_gt           0.0371
_refine_ls_wR_factor_ref         0.0760
_refine_ls_wR_factor_gt         0.0730
_refine_ls_goodness_of_fit_ref   1.511
_refine_ls_restrained_S_all      1.519
_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 0.2539(5) 0.0184(3) Uani 0.981(4) 3 d SP . .
T2 Si 0.3333 0.6667 0.44372(10) 0.0069(5) Uani 1 3 d SD . .
T1 Al 0.3333 0.6667 0.06192(11) 0.0105(7) Uani 1 3 d SD . .
O1 O 0.3333 0.6667 0.2588(5) 0.0315(8) Uani 1 3 d SD . .
O2 O 0.6175(6) 0.0161(9) 1.0052(11) 0.0211(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
K 0.0173(3) 0.0173(3) 0.0205(4) 0.000 0.000 0.00867(16)
T2 0.0068(9) 0.0068(9) 0.0072(7) 0.000 0.000 0.0034(4)
T1 0.0089(11) 0.0089(11) 0.0138(11) 0.000 0.000 0.0044(6)
O1 0.0403(12) 0.0403(12) 0.0138(14) 0.000 0.000 0.0202(6)
O2 0.0105(17) 0.0128(12) 0.0354(11) 0.0037(13) -0.006(3) 0.0025(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.

```

;

```

```

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 2.958(8) 2_544 ?
K O2 2.958(8) 1_454 ?
K O2 2.958(8) 4_664 ?
K O1 2.9767(9) 1_545 ?
K O1 2.9767(9) . ?
K O1 2.9767(9) 1_445 ?
K O2 2.975(8) 5_664 ?
K O2 2.975(8) 6_454 ?
K O2 2.975(8) 3_544 ?
K T2 3.405(2) 1_545 ?
K T2 3.405(2) . ?
K T2 3.405(2) 1_445 ?
T2 O1 1.611(4) . ?
T2 O2 1.616(3) 3_554 ?
T2 O2 1.616(3) 6_564 ?
T2 O2 1.616(2) 5_664 ?

```

T2 K 3.405(2) 1_565 ?
T2 K 3.405(2) 1_665 ?
T1 O1 1.715(4) . ?
T1 O2 1.731(3) 2_554 ?
T1 O2 1.731(3) 1_564 ?
T1 O2 1.731(3) 4_664 ?
T1 K 3.414(3) 1_565 ?
T1 K 3.414(3) 1_665 ?
T1 K 4.007(3) 3_554 ?
T1 K 4.007(3) 3_564 ?
T1 K 4.007(3) 3_664 ?
O1 K 2.9767(9) 1_565 ?
O1 K 2.9767(9) 1_665 ?
O2 T2 1.616(2) 3 ?
O2 T1 1.731(3) 1_546 ?
O2 K 2.958(8) 1_656 ?
O2 K 2.975(8) 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 72.3(2) 2_544 1_454 ?
O2 K O2 72.3(2) 2_544 4_664 ?
O2 K O2 72.3(2) 1_454 4_664 ?
O2 K O1 55.47(12) 2_544 1_545 ?
O2 K O1 127.7(2) 1_454 1_545 ?
O2 K O1 89.21(13) 4_664 1_545 ?
O2 K O1 127.7(2) 2_544 . ?
O2 K O1 89.21(13) 1_454 . ?
O2 K O1 55.47(12) 4_664 . ?
O1 K O1 119.980(6) 1_545 . ?
O2 K O1 89.21(13) 2_544 1_445 ?
O2 K O1 55.47(12) 1_454 1_445 ?
O2 K O1 127.7(2) 4_664 1_445 ?
O1 K O1 119.980(6) 1_545 1_445 ?
O1 K O1 119.980(6) . 1_445 ?
O2 K O2 142.86(14) 2_544 5_664 ?
O2 K O2 137.76(14) 1_454 5_664 ?
O2 K O2 94.51(6) 4_664 5_664 ?
O1 K O2 90.78(12) 1_545 5_664 ?
O1 K O2 52.51(12) . 5_664 ?
O1 K O2 124.31(19) 1_445 5_664 ?
O2 K O2 137.76(14) 2_544 6_454 ?
O2 K O2 94.51(6) 1_454 6_454 ?
O2 K O2 142.86(14) 4_664 6_454 ?
O1 K O2 124.31(19) 1_545 6_454 ?
O1 K O2 90.78(12) . 6_454 ?
O1 K O2 52.51(12) 1_445 6_454 ?
O2 K O2 71.8(2) 5_664 6_454 ?

O2 K O2 94.51(6) 2_544 3_544 ?
 O2 K O2 142.86(14) 1_454 3_544 ?
 O2 K O2 137.76(14) 4_664 3_544 ?
 O1 K O2 52.51(12) 1_545 3_544 ?
 O1 K O2 124.31(19) . 3_544 ?
 O1 K O2 90.78(12) 1_445 3_544 ?
 O2 K O2 71.8(2) 5_664 3_544 ?
 O2 K O2 71.8(2) 6_454 3_544 ?
 O2 K T2 81.42(10) 2_544 1_545 ?
 O2 K T2 151.81(14) 1_454 1_545 ?
 O2 K T2 109.53(12) 4_664 1_545 ?
 O1 K T2 28.23(9) 1_545 1_545 ?
 O1 K T2 115.48(8) . 1_545 ?
 O1 K T2 115.48(8) 1_445 1_545 ?
 O2 K T2 70.36(9) 5_664 1_545 ?
 O2 K T2 98.32(18) 6_454 1_545 ?
 O2 K T2 28.33(5) 3_544 1_545 ?
 O2 K T2 151.81(14) 2_544 . ?
 O2 K T2 109.53(12) 1_454 . ?
 O2 K T2 81.42(10) 4_664 . ?
 O1 K T2 115.48(8) 1_545 . ?
 O1 K T2 28.23(9) . . ?
 O1 K T2 115.48(8) 1_445 . ?
 O2 K T2 28.33(5) 5_664 . ?
 O2 K T2 70.36(9) 6_454 . ?
 O2 K T2 98.32(18) 3_544 . ?
 T2 K T2 98.42(9) 1_545 . ?
 O2 K T2 109.53(12) 2_544 1_445 ?
 O2 K T2 81.42(10) 1_454 1_445 ?
 O2 K T2 151.81(14) 4_664 1_445 ?
 O1 K T2 115.48(8) 1_545 1_445 ?
 O1 K T2 115.48(8) . 1_445 ?
 O1 K T2 28.23(9) 1_445 1_445 ?
 O2 K T2 98.32(18) 5_664 1_445 ?
 O2 K T2 28.33(5) 6_454 1_445 ?
 O2 K T2 70.36(9) 3_544 1_445 ?
 T2 K T2 98.42(9) 1_545 1_445 ?
 T2 K T2 98.42(9) . 1_445 ?
 O1 T2 O2 109.3(4) . 3_554 ?
 O1 T2 O2 109.3(4) . 6_564 ?
 O2 T2 O2 109.6(4) 3_554 6_564 ?
 O1 T2 O2 109.3(4) . 5_664 ?
 O2 T2 O2 109.6(4) 3_554 5_664 ?
 O2 T2 O2 109.6(4) 6_564 5_664 ?
 O1 T2 K 60.95(7) . 1_565 ?
 O2 T2 K 60.9(3) 3_554 1_565 ?
 O2 T2 K 92.4(2) 6_564 1_565 ?
 O2 T2 K 158.00(17) 5_664 1_565 ?
 O1 T2 K 60.95(7) . . ?
 O2 T2 K 92.4(2) 3_554 . ?
 O2 T2 K 158.00(17) 6_564 . ?
 O2 T2 K 60.9(3) 5_664 . ?
 K T2 K 98.42(9) 1_565 . ?
 O1 T2 K 60.95(7) . 1_665 ?

O2 T2 K 158.00(17) 3_554 1_665 ?
O2 T2 K 60.9(3) 6_564 1_665 ?
O2 T2 K 92.4(2) 5_664 1_665 ?
K T2 K 98.42(9) 1_565 1_665 ?
K T2 K 98.42(9) . 1_665 ?
O1 T1 O2 106.6(3) . 2_554 ?
O1 T1 O2 106.6(3) . 1_564 ?
O2 T1 O2 112.2(3) 2_554 1_564 ?
O1 T1 O2 106.6(3) . 4_664 ?
O2 T1 O2 112.2(3) 2_554 4_664 ?
O2 T1 O2 112.2(3) 1_564 4_664 ?
O1 T1 K 60.67(7) . 1_565 ?
O2 T1 K 60.1(2) 2_554 1_565 ?
O2 T1 K 89.6(2) 1_564 1_565 ?
O2 T1 K 157.75(19) 4_664 1_565 ?
O1 T1 K 60.67(7) . 1_665 ?
O2 T1 K 157.75(19) 2_554 1_665 ?
O2 T1 K 60.1(2) 1_564 1_665 ?
O2 T1 K 89.6(2) 4_664 1_665 ?
K T1 K 98.05(9) 1_565 1_665 ?
O1 T1 K 60.67(7) . . ?
O2 T1 K 89.6(2) 2_554 . ?
O2 T1 K 157.75(19) 1_564 . ?
O2 T1 K 60.1(2) 4_664 . ?
K T1 K 98.05(9) 1_565 . ?
K T1 K 98.05(9) 1_665 . ?
O1 T1 K 132.03(5) . 3_554 ?
O2 T1 K 71.57(19) 2_554 3_554 ?
O2 T1 K 118.6(3) 1_564 3_554 ?
O2 T1 K 42.6(3) 4_664 3_554 ?
K T1 K 130.67(3) 1_565 3_554 ?
K T1 K 130.67(3) 1_665 3_554 ?
K T1 K 71.36(3) . 3_554 ?
O1 T1 K 132.03(5) . 3_564 ?
O2 T1 K 42.6(3) 2_554 3_564 ?
O2 T1 K 71.57(19) 1_564 3_564 ?
O2 T1 K 118.6(3) 4_664 3_564 ?
K T1 K 71.36(3) 1_565 3_564 ?
K T1 K 130.67(3) 1_665 3_564 ?
K T1 K 130.67(3) . 3_564 ?
K T1 K 80.08(8) 3_554 3_564 ?
O1 T1 K 132.03(5) . 3_664 ?
O2 T1 K 118.6(3) 2_554 3_664 ?
O2 T1 K 42.6(3) 1_564 3_664 ?
O2 T1 K 71.57(19) 4_664 3_664 ?
K T1 K 130.67(3) 1_565 3_664 ?
K T1 K 71.36(3) 1_665 3_664 ?
K T1 K 130.67(3) . 3_664 ?
K T1 K 80.08(8) 3_554 3_664 ?
K T1 K 80.08(8) 3_564 3_664 ?
T2 O1 T1 180.0 . . ?
T2 O1 K 90.81(12) . 1_565 ?
T1 O1 K 89.19(12) . 1_565 ?
T2 O1 K 90.81(12) . 1_665 ?

T1 O1 K 89.19(12) . 1_665 ?
K O1 K 119.980(7) 1_565 1_665 ?
T2 O1 K 90.81(12) . . ?
T1 O1 K 89.19(12) . . ?
K O1 K 119.980(7) 1_565 . ?
K O1 K 119.980(6) 1_665 . ?
T2 O2 T1 140.42(14) 3 1_546 ?
T2 O2 K 120.1(3) 3 1_656 ?
T1 O2 K 89.5(2) 1_546 1_656 ?
T2 O2 K 90.8(3) 3 3_655 ?
T1 O2 K 114.1(3) 1_546 3_655 ?
K O2 K 94.44(6) 1_656 3_655 ?

_diffn_measured_fraction_theta_max 0.964
_diffn_reflns_theta_full 36.01
_diffn_measured_fraction_theta_full 0.964
_refine_diff_density_max 0.787
_refine_diff_density_min -0.627
_refine_diff_density_rms 0.130