

data\_kss\_cry2\_p5

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\_chemical\_name\_systematic  
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\_chemical\_name\_common ?  
\_chemical\_melting\_point ?  
\_chemical\_formula\_moiety ?  
\_chemical\_formula\_sum  
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\_chemical\_formula\_weight 315.17

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\_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 5.079(4)  
\_cell\_length\_b 5.079(4)  
\_cell\_length\_c 8.587(5)  
\_cell\_angle\_alpha 90.00  
\_cell\_angle\_beta 90.00  
\_cell\_angle\_gamma 120.00  
\_cell\_volume 191.8(2)  
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\_cell\_measurement\_temperature 295  
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_exptl_crystal_size_mid        ?
_exptl_crystal_size_min        ?
_exptl_crystal_density_meas    ?
_exptl_crystal_density_diffn   2.728
_exptl_crystal_density_method  'not measured'
_exptl_crystal_F_000           155
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_exptl_absorpt_correction_T_max ?
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_exptl_special_details
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;

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_diffrn_radiation_type           MoK\alpha
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_diffrn_reflns_limit_l_min       -14
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_diffrn_reflns_theta_min         4.63
_diffrn_reflns_theta_max         38.91
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_reflns_number_gt                 184
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement       ?
_computing_data_reduction        ?

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

_refine_special_details
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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.
;

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_refine_ls_matrix_type          full
_refine_ls_weighting_scheme     calc
_refine_ls_weighting_details
'calc w=1/[sigma^2(Fo^2)+(0.0100P)^2+0.4000P] 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      0.005(12)
_refine_ls_extinction_expression
'Fc^*=kFc[1+0.001xFc^2/l^3/sin(2\q)]^-1/4'
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_number_restraints     8
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_refine_ls_R_factor_gt           0.1312
_refine_ls_wR_factor_ref         0.1458
_refine_ls_wR_factor_gt          0.1188
_refine_ls_goodness_of_fit_ref   1.230
_refine_ls_restrained_S_all      1.230
_refine_ls_shift/su_max          0.000
_refine_ls_shift/su_mean         0.000

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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

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T1 Al 0.3333 0.6667 0.0603(12) 0.016(3) Uiso 1 3 d SD . .
O1 O 0.3333 0.6667 0.2576(14) 0.060(3) Uiso 1 3 d SD . .
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```

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_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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K O2 2.863(16) 1_454 ?
K O2 2.863(16) 4_664 ?
K O1 2.933(2) 1_545 ?
K O1 2.933(2) . ?
K O1 2.933(2) 1_445 ?
K O2 2.938(18) 5_664 ?
K O2 2.938(18) 3_544 ?
K O2 2.938(18) 6_454 ?
K T2 3.354(5) 1_545 ?
K T2 3.354(5) . ?
K T2 3.354(5) 1_445 ?
T2 O1 1.597(7) . ?
T2 O2 1.605(8) 3_554 ?
T2 O2 1.605(8) 6_564 ?
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T2 K 3.354(5) 1_565 ?
T2 K 3.354(5) 1_665 ?

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T1 K 3.371(6) 1\_565 ?  
T1 K 3.371(6) 1\_665 ?  
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T1 K 3.939(7) 3\_564 ?  
T1 K 3.939(7) 3\_664 ?  
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O1 K 2.933(2) 1\_665 ?  
O2 T2 1.605(8) 3 ?  
O2 T1 1.718(7) 1\_546 ?  
O2 K 2.863(16) 1\_656 ?  
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loop\_

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