

data\_kss\_cry2\_p4

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\_chemical\_name\_common ?  
\_chemical\_melting\_point ?  
\_chemical\_formula\_moiety ?  
\_chemical\_formula\_sum  
'Al2 K1.97 O8 Si2'  
\_chemical\_formula\_weight 315.17

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\_atom\_type\_symbol  
\_atom\_type\_description  
\_atom\_type\_scatter\_dispersion\_real  
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\_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 5.099(3)  
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\_cell\_length\_c 8.637(6)  
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\_cell\_angle\_gamma 120.00  
\_cell\_volume 194.5(2)  
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\_cell\_measurement\_reflns\_used ?

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_exptl_crystal_density_meas    ?
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_exptl_special_details
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_diffrn_reflns_limit_k_max      8
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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_weighting_details
'calc w=1/[sigma2(Fo2)+(0.0100P)2+0.8000P] where P=(Fo2+2Fc2)/3'
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_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens  geom
_refine_ls_hydrogen_treatment   mixed
_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef      0.077(10)
_refine_ls_extinction_expression
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_R_factor_gt           0.0918
_refine_ls_wR_factor_ref         0.1282
_refine_ls_wR_factor_gt         0.1000
_refine_ls_goodness_of_fit_ref   1.093
_refine_ls_restrained_S_all      1.089
_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 0.0620(11) 0.015(2) Uiso 1 3 d SD . .
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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 2.864(19) 6_454 ?
K O1 2.9441(17) 1_545 ?
K O1 2.9441(17) . ?
K O1 2.9441(17) 1_445 ?
K O2 2.955(19) 2_544 ?
K O2 2.955(19) 1_454 ?
K O2 2.955(19) 4_664 ?
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K T2 3.367(4) . ?
K T2 3.367(4) 1_445 ?
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T2 K 3.367(4) 1_665 ?

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T1 K 3.968(7) 3\_564 ?  
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loop\_

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