

data\_la2n\_l\_tr

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\_chemical\_melting\_point ?  
\_chemical\_formula\_moiety ?  
\_chemical\_formula\_sum  
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\_chemical\_formula\_weight 275.10

loop\_  
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\_atom\_type\_description  
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'Li' 'Li' -0.0003 0.0001  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'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'  
'Ge' 'Ge' 0.1547 1.8001  
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'-x, -y, -z'  
'x-1/2, -y-1/2, z-1/2'

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 \_computing\_data\_reduction ?  
 \_computing\_structure\_solution ?  
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 \_computing\_publication\_material ?

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;
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 > 2σ(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.
;

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_refine_ls_weighting_details
'calc w=1/[σ^2(Fo^2)+(0.0287P)^2+0.6537P] where P=(Fo^2+2Fc^2)/3'
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_atom_sites_solution_secondary difmap
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment mixed
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_refine_ls_R_factor_gt 0.0218
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
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Al3 Al 0.49528(4) 0.08633(5) 0.24665(7) 0.00101(7) Uani 1 1 d . . .
Ge1 Ge 0.292643(17) 0.58272(2) 0.72762(3) 0.00647(5) Uani 1 1 d . . .

```

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 Al3 0.00036(16) 0.00064(15) 0.00205(17) -0.00004(11) 0.00043(12) 0.00005(12)  
 Ge1 0.00541(7) 0.00601(8) 0.00856(8) -0.00167(4) 0.00315(5) -0.00172(5)  
 Ge2 0.00499(7) 0.00609(7) 0.00620(7) 0.00024(4) 0.00209(5) 0.00109(5)  
 O1 0.0048(4) 0.0082(4) 0.0092(4) 0.0003(3) 0.0014(3) -0.0003(3)  
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 O3 0.0128(5) 0.0078(4) 0.0123(5) -0.0011(3) 0.0047(4) -0.0055(4)  
 O4 0.0088(4) 0.0116(5) 0.0064(4) -0.0010(3) 0.0014(3) 0.0031(4)  
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\_geom\_special\_details  
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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)  
 are estimated using the full covariance matrix. The cell s.u.'s are taken  
 into account individually in the estimation of s.u.'s in distances, angles  
 and torsion angles; correlations between s.u.'s in cell parameters are only  
 used when they are defined by crystal symmetry. An approximate (isotropic)  
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.  
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 Li1 O1 2.153(5) 2\_546 ?  
 Li1 O2 2.166(5) 3\_667 ?  
 Li1 Ge1 2.846(4) 3\_667 ?  
 Li1 Al3 2.953(4) 1\_556 ?  
 Li1 Al3 3.126(4) 3\_656 ?  
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Al3 O3 1.8259(12) 3\_666 ?  
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 Al3 O5 1.9449(12) 4\_666 ?  
 Al3 O5 2.0027(12) 2\_545 ?  
 Al3 O1 2.0067(12) 2\_545 ?  
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loop\_

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