

data\_grie\_0m

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'x, x-y, z'
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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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O7 O 0.28476(8) 0.28479(7) 0.07841(15) 0.01155(19) Uani 1 1 d . . .
O8 O 0.20933(8) 0.26999(8) 0.44033(16) 0.0126(2) Uani 1 1 d . . .
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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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Na1 O4 2.823(2) 1_665 ?

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 Al2 O3 1.9898(9) . ?  
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Mg1 F1 Fe1 0.000(11) 2\_665 2\_665 ?  
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B1 O2 Mg1 119.34(8) . 2 ?  
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Si1 O4 Si1 143.76(11) 5 . ?  
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Si1 O5 Si1 132.04(11) 6 . ?  
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Si1 O6 Al2 130.48(7) 1\_556 . ?  
Si1 O6 Fe1 122.63(7) 1\_556 . ?  
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