

data_gme-rt

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'Ca' 'Ca'	0.2262 0.3064
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'	
'Al' 'Al'	0.0645 0.0514
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'O' 'O'	0.0106 0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'	
'Na' 'Na'	0.0362 0.0249
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'	

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'-x, -y, z+1/2'	
'-x+y, -x, z'	
'y, -x+y, z+1/2'	
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'-x, -x+y, z+1/2'	
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_computing_data_reduction  ?
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_computing_structure_refinement 'SHELXL-93 (Sheldrick, 1993)'
_computing_molecular_graphics ?
_computing_publication_material ?

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_refine_special_details

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Refinement on F^2 for ALL reflections except for 0 with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion

of $F^2 > 2\sigma(F^2)$ is used only for calculating $R_{\text{factor_obs}}$ 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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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     ?
_refine_ls_extinction_method       SHELXL
_refine_ls_extinction_coef         0.0000(19)
_refine_ls_extinction_expression
'Fc^k=kFc[1+0.001xFc^2\l^3/sin(2\q)]^-1/4^'
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_refine_ls_wR_factor_obs           0.1154
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O2 O 0.85114(16) 0.42557(8) 0.06178(17) 0.0250(4) Uani 1 d S .
O3 O 0.41102(16) 0.06516(18) 0.2500 0.0275(4) Uani 1 d S .
O4 O 0.35569(14) 0.0000 0.0000 0.0288(4) Uani 1 d S .
Na1 Na 0.3333 0.6667 0.0747(2) 0.0364(7) Uani 1.020(10) d SP .
Na2 Na 0.1190(3) 0.2380(5) 0.0694(7) 0.082(3) Uani 0.299(1) d SP .
W1 O 0.1981(5) 0.5451(5) 0.2500 0.062(2) Uani 0.50 d SP .
W2 O 0.3388(6) 0.1694(3) -0.2500 0.134(3) Uani 1 d S .
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Si1 0.0139(2) 0.0115(2) 0.0105(2) -0.00195(12) -0.00158(12) 0.00709(14)
O1 0.0347(10) 0.0193(5) 0.0407(10) -0.0038(4) -0.0076(8) 0.0173(5)
O2 0.0323(9) 0.0224(5) 0.0237(7) -0.0023(4) -0.0047(7) 0.0161(5)
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Na1 0.0408(9) 0.0408(9) 0.0277(10) 0.000 0.000 0.0204(5)
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w2 0.092(5) 0.183(7) 0.097(5) 0.000 0.000 0.046(3)
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_geom_special_details

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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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All O1 1.6418(6) . ?
All O3 1.6469(7) . ?
All O2 1.6563(8) 5_665 ?
All Na2 3.327(5) 15 ?
All Na1 3.5553(11) 13_665 ?
All w3 3.693(6) . ?
All w1 3.727(2) 21 ?
All w2 4.003(2) . ?
All w1 4.025(5) 14_556 ?
All w2 4.0759(5) 15 ?
All w1 4.297(4) 2_654 ?
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Si1 O3 1.6469(7) . ?
Si1 O2 1.6563(8) 5_665 ?
Si1 Na2 3.327(5) 15 ?
Si1 w3 3.693(6) . ?
Si1 w1 3.727(2) 21 ?
Si1 w2 4.003(2) . ?
Si1 w1 4.025(5) 14_556 ?
Si1 w2 4.0759(5) 15 ?
Si1 w1 4.297(4) 2_654 ?
Si1 w1 4.514(4) 15 ?
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O1 All 1.6418(6) 11 ?
O1 Na2 2.503(6) 15 ?
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O1 w2 3.268(3) . ?
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