

data_gme-rt

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_chemical_name_systematic
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;
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_atom_type_scatter_source
'Si' 'Si' 0.0817 0.0704
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'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
'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'
'Na' 'Na' 0.0362 0.0249
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting          ?
_symmetry_space_group_name_H-M ?

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_symmetry_equiv_pos_as_xyz
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'x-y, x, z+1/2'
'-y, x-y, z'
'-x, -y, z+1/2'
'-x+y, -x, z'
'y, -x+y, z+1/2'
'-x+y, y, z'
'-x, -x+y, z+1/2'
'-y, -x, z'
'x-y, -y, z+1/2'
'x, x-y, z'
'y, x, z+1/2'
'-x, -y, -z'
'-x+y, -x, -z-1/2'
'y, -x+y, -z'
'x, y, -z-1/2'
'x-y, x, -z'
'-y, x-y, -z-1/2'
'x-y, -y, -z'
'x, x-y, -z-1/2'
'y, x, -z'
'-x+y, y, -z-1/2'
'-x, -x+y, -z'
'-y, -x, -z-1/2'

_cell_length_a                  13.7640(10)
_cell_length_b                  13.7640(10)
_cell_length_c                  10.0780(10)
_cell_angle_alpha               90.00

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4351_1_supp_69393_10k3z1.txt

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_cell_angle_gamma        120.00
_cell_volume             1653.5(2)
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_expt1_crystal_description ?
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_expt1_crystal_size_min   ?
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_expt1_crystal_density_method ?
_expt1_crystal_F_000      1061
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_expt1_absorpt_correction_type ?
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_diffn_ambient_temperature 293(2)
_diffn_radiation_wavelength 0.71073
_diffn_radiation_type      MoK\alpha
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_diffn_radiation_monochromator graphite
_diffn_measurement_device  ?
_diffn_measurement_method  ?
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_diffn_standards_interval_count ?
_diffn_standards_interval_time ?
_diffn_standards_decay_%   ?
_diffn_reflns_number       1165
_diffn_reflns_av_R_equivalents 0.0000
_diffn_reflns_av_sigmaI/netI 0.0224
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_diffn_reflns_limit_k_min   0
_diffn_reflns_limit_k_max   22
_diffn_reflns_limit_l_min   0
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_diffn_reflns_theta_min     3.42
_diffn_reflns_theta_max    35.62
_reflns_number_total        1165
_reflns_number_observed     1165
_reflns_observed_criterion  >2sigma(I)

_computing_data_collection ?
_computing_cell_refinement ?
_computing_data_reduction  ?
_computing_structure_solution 'SHELXS-86 (Sheldrick, 1990)'
_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 F2 for ALL reflections except for 0 with very negative F2
or flagged by the user for potential systematic errors. Weighted R-factors
wR and all goodnesses of fit S are based on F2, conventional R-factors R
are based on F, with F set to zero for negative F2. The observed criterion

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of $F^2 > 2\sigma(F^2)$ is used only for calculating $_R$ _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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_refine_ls_matrix_type full
_refine_ls_weighting_scheme
'calc w=1/[\s^2^(Fo^2)+(0.0662P)^2+1.4421P] 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 ?
_refine_ls_extinction_method SHELXL
_refine_ls_extinction_coef 0.0000(19)
_refine_ls_extinction_expression
'Fc^2=kFc[1+0.001xFc^2\l^3/sin(2\q)]^-1/4^'
_refine_ls_number_reflns 1165
_refine_ls_number_parameters 62
_refine_ls_number_restraints 0
_refine_ls_R_factor_all 0.0412
_refine_ls_R_factor_obs 0.0412
_refine_ls_wR_factor_all 0.1154
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_refine_ls_goodness_of_fit_obs 1.090
_refine_ls_restrained_S_all 1.090
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_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_thermal_displace_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_group
Al1 Al 0.44096(3) 0.10562(3) 0.09431(3) 0.01164(14) Uani 0.31 d P .
Si1 Si 0.44096(3) 0.10562(3) 0.09431(3) 0.01164(14) Uani 0.69 d P .
O1 O 0.41690(16) 0.20845(8) 0.06081(21) 0.0298(4) Uani 1 d S .
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 .
W3 O 0.1618(6) 0.0809(3) 0.1196(11) 0.250(8) Uani 0.849(2) d SP .
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loop_
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_atom_site_aniso_U_33
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_atom_site_aniso_U_13
_atom_site_aniso_U_12
Al1 0.0139(2) 0.0115(2) 0.0105(2) -0.00195(12) -0.00158(12) 0.00709(14)
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)
```

4351_1_supp_69393_10k3z1.txt

o3 0.0256(8) 0.0380(10) 0.0130(6) 0.000 0.000 0.0114(8)
 o4 0.0307(6) 0.0211(7) 0.0314(9) -0.0129(7) -0.0065(3) 0.0105(4)
 Na1 0.0408(9) 0.0408(9) 0.0277(10) 0.000 0.000 0.0204(5)
 Na2 0.113(5) 0.052(4) 0.061(4) 0.019(3) 0.009(2) 0.026(2)
 w1 0.048(3) 0.066(3) 0.040(2) 0.000 0.000 0.005(3)
 w2 0.092(5) 0.183(7) 0.097(5) 0.000 0.000 0.046(3)
 w3 0.073(6) 0.279(11) 0.330(13) 0.014(3) 0.028(6) 0.036(3)

_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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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
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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 ?
 Si1 o4 1.6395(6) . ?
 Si1 o1 1.6418(6) . ?
 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 ?
 O1 Si1 1.6418(6) 11 ?
 O1 All 1.6418(6) 11 ?
 O1 Na2 2.503(6) 15 ?
 O1 w3 3.098(7) . ?
 O1 w2 3.268(3) . ?
 O1 w1 3.633(4) 21 ?
 O1 w1 3.633(4) 15 ?
 O2 Si1 1.6563(8) 9_665 ?
 O2 All 1.6563(8) 9_665 ?
 O2 All 1.6563(8) 3_655 ?
 O2 Si1 1.6563(8) 3_655 ?
 O2 Na1 2.594(2) 13_665 ?
 O2 w1 3.281(3) 13_665 ?
 O2 w1 3.281(3) 8_654 ?
 O2 w1 4.310(5) 19_665 ?
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 O3 All 1.6469(7) 16_556 ?
 O3 w2 3.278(2) 15 ?
 O3 w1 3.273(6) 14_556 ?

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04 Al1 1.6395(6) 19 ?
04 Na2 2.906(4) 5 ?
04 Na2 2.906(4) 15 ?
04 W2 3.5186(9) 15 ?
04 W2 3.5186(9) . ?
04 W3 3.576(6) 15 ?
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04 W1 3.670(4) 21 ?
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Na2 W2 2.181(8) 2 ?
Na2 O1 2.503(6) 17 ?
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Na2 O4 2.906(4) 3 ?
Na2 O4 2.906(4) 17 ?
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03 A11 O2 110.80(9) . 5_665 ?
04 A11 Na2 60.87(8) . 15 ?
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01 A11 Na1 66.76(7) . 13_665 ?
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03 A11 w3 80.2(2) . . ?
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03 A11 w1 51.78(8) . 14_556 ?
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w2 A11 w1 59.73(12) . 2_654 ?

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 W2 Al1 w1 139.25(10) 15 2_654 ?
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 O1 Si1 O2 108.37(9) . 5_665 ?
 O3 Si1 O2 110.80(9) . 5_665 ?
 O4 Si1 Na2 60.87(8) . 15 ?
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 O4 Si1 w3 73.00(13) . . ?
 O1 Si1 w3 56.26(10) . . ?
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 Na2 Si1 w3 34.5(2) 15 . ?
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 O3 Si1 w1 172.28(12) . 21 ?
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 O2 Si1 w1 99.95(11) 5_665 14_556 ?
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 W3 Si1 w2 57.26(12) . 15 ?
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 W2 Si1 w2 106.13(14) . 15 ?
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 O2 Si1 w1 42.84(9) 5_665 2_654 ?
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 Si1 01 W2 104.29(7) 11 . ?
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 Na2 01 W2 41.8(2) 15 . ?
 W3 01 W2 84.5(2) . . ?
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 Si1 01 W1 80.34(12) 11 15 ?
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