

data_gme-25r

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_chemical_name_systematic
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;
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_chemical_formula_weight        1978.21
_chemical_melting_point         ?
_chemical_compound_source       ?

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'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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'x-y, x, z+1/2'
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'-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                  13.6557(10)
_cell_length_b                  13.6557(10)
_cell_length_c                  10.0162(10)
_cell_angle_alpha               90.00

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4351_1_supp_69392_10k3z1.txt

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_cell_angle_beta          90.00
_cell_angle_gamma        120.00
_cell_volume             1617.6(2)
_cell_formula_units_Z    1
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_expt1_crystal_size_mid  ?
_expt1_crystal_size_min  ?
_expt1_crystal_density_meas ?
_expt1_crystal_density_diffn 2.031
_expt1_crystal_density_method ?
_expt1_crystal_F_000     981
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_expt1_absorpt_correction_T_max ?

_expt1_special_details
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_diffn_ambient_temperature 293(2)
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_diffn_radiation_type      MoK\alpha
_diffn_radiation_source    'fine-focus sealed tube'
_diffn_radiation_monochromator graphite
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_diffn_standards_interval_count ?
_diffn_standards_interval_time ?
_diffn_standards_decay_%  ?
_diffn_reflns_number       679
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_diffn_reflns_limit_h_min  -9
_diffn_reflns_limit_h_max   0
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_diffn_reflns_theta_min     2.98
_diffn_reflns_theta_max    34.61
_reflns_number_total        679
_reflns_number_observed     679
_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 ?

```

_refine_special_details

```

;
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

```

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)+(0.0779P)^2+1.0030P] 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 ?
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_number_reflns 679
_refine_ls_number_parameters 62
_refine_ls_number_restraints 0
_refine_ls_R_factor_all 0.0511
_refine_ls_R_factor_obs 0.0511
_refine_ls_wR_factor_all 0.1307
_refine_ls_wR_factor_obs 0.1307
_refine_ls_goodness_of_fit_all 1.119
_refine_ls_goodness_of_fit_obs 1.119
_refine_ls_restrained_S_all 1.119
_refine_ls_restrained_S_obs 1.119
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_atom_site_thermal_displace_type
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_group
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Si1 Si 0.44031(4) 0.10522(4) 0.09412(6) 0.01733(12) Uani 0.69 d P .
O1 O 0.41850(20) 0.20925(10) 0.06069(25) 0.0388(6) Uani 1 d S .
O2 O 0.85320(18) 0.42660(9) 0.06097(22) 0.0301(5) Uani 1 d S .
O3 O 0.41030(17) 0.06568(19) 0.2500 0.0354(6) Uani 1 d S .
O4 O 0.35437(16) 0.0000 0.0000 0.0360(6) Uani 1 d S .
Na1 Na 0.3333 0.6667 0.0698(3) 0.0508(9) Uani 0.993(7) d SP .
Na2 Na 0.1187(4) 0.2374(8) 0.0816(9) 0.133(4) Uani 0.325(6) d SP .
W1 O 0.2014(6) 0.5423(7) 0.2500 0.102(4) Uani 0.450(7) d SP .
W2 O 0.3336(8) 0.1668(4) -0.2500 0.148(5) Uani 0.795(14) d SP .
W3 O 0.1536(10) 0.0768(5) 0.1186(15) 0.365(13) Uani 0.65(2) d SP .
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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
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Si1 0.0192(2) 0.0165(2) 0.0175(2) -0.0026(2) -0.0020(2) 0.0099(2)
O1 0.0441(14) 0.0243(8) 0.055(2) -0.0055(6) -0.0110(12) 0.0220(7)
O2 0.0347(13) 0.0279(8) 0.0298(11) -0.0019(5) -0.0038(10) 0.0174(6)
O3 0.0326(11) 0.0449(12) 0.0216(11) 0.000 0.000 0.0141(10)
O4 0.0344(9) 0.0273(11) 0.0439(12) -0.0168(11) -0.0084(5) 0.0136(5)
```

4351_1_supp_69392_10k3z1.txt

Na1 0.0526(11) 0.0526(11) 0.047(2) 0.000 0.000 0.0263(6)
Na2 0.182(8) 0.116(7) 0.079(6) 0.027(5) 0.013(2) 0.058(4)
w1 0.077(5) 0.116(7) 0.044(4) 0.000 0.000 -0.003(5)
w2 0.147(10) 0.166(8) 0.123(7) 0.000 0.000 0.074(5)
w3 0.137(12) 0.438(24) 0.420(24) 0.044(5) 0.088(10) 0.069(6)

_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_site_symmetry_2
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A11 O4 1.6261(8) . ?
A11 O3 1.6358(8) . ?
A11 O2 1.6443(10) 5_665 ?
A11 Na2 3.364(7) 15 ?
A11 Na1 3.5106(14) 13_665 ?
A11 w1 3.703(3) 21 ?
A11 w3 3.744(11) . ?
A11 w2 3.992(3) . ?
A11 w1 4.016(6) 14_556 ?
A11 w2 4.0388(5) 15 ?
A11 w1 4.313(6) 2_654 ?
S11 O1 1.6254(9) . ?
S11 O4 1.6261(8) . ?
S11 O3 1.6358(8) . ?
S11 O2 1.6443(10) 5_665 ?
S11 Na2 3.364(7) 15 ?
S11 Na1 3.5106(14) 13_665 ?
S11 w1 3.703(3) 21 ?
S11 w3 3.744(11) . ?
S11 w2 3.992(3) . ?
S11 w1 4.016(6) 14_556 ?
S11 w2 4.0388(5) 15 ?
S11 w1 4.313(6) 2_654 ?
O1 S11 1.6254(9) 11 ?
O1 A11 1.6254(9) 11 ?
O1 Na2 2.572(9) 15 ?
O1 w3 3.186(12) . ?
O1 w2 3.270(4) . ?
O1 w1 3.569(5) 15 ?
O1 w1 3.569(5) 21 ?
O2 S11 1.6443(9) 9_665 ?
O2 A11 1.6443(9) 9_665 ?
O2 A11 1.6443(9) 3_655 ?
O2 S11 1.6443(9) 3_655 ?
O2 Na1 2.565(3) 13_665 ?
O2 w1 3.279(4) 13_665 ?
O2 w1 3.279(4) 8_654 ?
O2 w1 4.247(6) 19_665 ?
O2 w1 4.247(6) 2_654 ?
O3 S11 1.6358(9) 16_556 ?
O3 A11 1.6358(9) 16_556 ?
O3 w2 3.252(2) 15 ?
O3 w1 3.278(7) 14_556 ?
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O3 w3 3.817(11) 16_556 ?

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 04 Na2 2.904(5) 5 ?
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 04 W3 3.592(9) 15 ?
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 W1 O2 3.279(4) 4_665 ?
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 W2 O4 3.4907(11) 16 ?
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02 A11 Na2 132.4(2) 5_665 15 ?
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Na2 A11 Na1 95.20(14) 15 13_665 ?
01 A11 w1 72.5(2) . 21 ?
04 A11 w1 75.59(10) . 21 ?
03 A11 w1 173.2(2) . 21 ?
02 A11 w1 62.3(2) 5_665 21 ?
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01 A11 w1 88.33(13) . 2_654 ?
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Na1 A11 w1 35.68(10) 13_665 2_654 ?
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w3 A11 w1 127.8(2) . 2_654 ?
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 01 s1l w3 57.66(13) . . ?
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 Na2 s1l w1 113.7(2) 15 14_556 ?
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 04 s1l w1 83.67(11) . 2_654 ?
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 Na2 s1l w1 91.7(2) 15 2_654 ?
 Na1 s1l w1 35.68(10) 13_665 2_654 ?
 w1 s1l w1 21.2(2) 21 2_654 ?
 w3 s1l w1 127.8(2) . 2_654 ?
 w2 s1l w1 61.1(2) . 2_654 ?
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 Si1 01 W3 96.80(11) 11 . ?
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 Si1 01 W2 104.17(9) 11 . ?
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 W3 01 W2 82.6(3) . . ?
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