

data_manganoquadratite

_audit_creation_method SHELXL-97

_chemical_name_systematic

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?

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_chemical_name_common ?

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_chemical_formula_moiety ?

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'Ag8 As6 Cu0 Mn8 S24 Sb2'

_chemical_formula_weight 2764.94

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

_atom_type_scatter_dispersion_imag

_atom_type_scatter_source

'Ag' 'Ag' -0.8971 1.1015

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'As' 'As' 0.0499 2.0058

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Mn' 'Mn' 0.3368 0.7283

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'S' 'S' 0.1246 0.1234

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Sb' 'Sb' -0.5866 1.5461

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Cu' 'Cu' 0.3201 1.2651

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting ?

_symmetry_space_group_name_H-M ?

loop_

_symmetry_equiv_pos_as_xyz

'x, y, z'

'-y, x, z+3/4'

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

'y, -x, z+1/4'

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

'y, x, -z+1/4'

'-x, y, -z'

'-y, -x, -z+3/4'

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_cell_length_b 5.4496(5)

_cell_length_c 32.9490(10)

_cell_angle_alpha 90.00

_cell_angle_beta 90.00

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_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 4.692
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000       1260
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_diffrn_reflns_limit_l_min   -46
_diffrn_reflns_limit_l_max    38
_diffrn_reflns_theta_min     4.17
_diffrn_reflns_theta_max     31.75
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_computing_data_reduction       ?
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_computing_molecular_graphics    ?
_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 $F^2 > 2\sigma(F^2)$ 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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'calc w=1/[\s^2*(Fo^2)+(0.0618P)^2+3.0204P] where P=(Fo^2+2Fc^2)/3'
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_wR_factor_gt           0.1869
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loop_
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_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type

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Ag1 Ag 0.7366(3) 0.2344(3) 0.03501(4) 0.0354(5) Uani 1.000(9) 1 d . . .
Mn1 Mn 0.2153(6) 0.2153(6) 0.1250 0.0222(11) Uani 1 2 d S . .
Mn2 Mn 0.7105(6) 0.7105(6) 0.1250 0.0268(12) Uani 1 2 d S . .
As1 As 0.2381(3) 0.7380(3) 0.04809(4) 0.0210(5) Uani 0.799(19) 1 d P . .
Sb1 Sb 0.2381(3) 0.7380(3) 0.04809(4) 0.0210(5) Uani 0.201(19) 1 d P . .
S1 S 0.1959(8) 0.7001(9) 0.11962(9) 0.0249(9) Uani 1 1 d . . .
S2 S 0.6670(9) 0.7092(11) 0.04912(12) 0.0300(12) Uani 1 1 d . . .
S3 S 0.2106(10) 0.1632(9) 0.04775(12) 0.0285(12) Uani 1 1 d . . .

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loop_

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_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
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Mn1 0.0272(16) 0.0272(16) 0.0123(13) -0.0016(8) 0.0016(8) 0.006(2)
Mn2 0.0324(18) 0.0324(18) 0.0156(14) 0.0010(10) -0.0010(10) -0.002(3)
As1 0.0173(9) 0.0249(10) 0.0207(6) -0.0014(6) 0.0037(6) -0.0047(7)
Sb1 0.0173(9) 0.0249(10) 0.0207(6) -0.0014(6) 0.0037(6) -0.0047(7)
S1 0.026(3) 0.034(3) 0.0143(14) 0.0016(17) 0.0055(16) -0.0068(18)
S2 0.025(2) 0.046(3) 0.0184(17) 0.001(2) 0.0004(17) -0.006(2)
S3 0.042(3) 0.024(2) 0.0197(17) 0.0005(16) -0.001(2) -0.005(2)

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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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loop_

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Ag1 S2 2.656(6) . ?
Ag1 S3 2.769(4) 7_655 ?
Ag1 S3 2.923(6) . ?
Ag1 S2 2.924(6) 1_545 ?
Mn1 S3 2.561(4) . ?

```

Mn1 S3 2.561(4) 6 ?
 Mn1 S1 2.650(6) 6 ?
 Mn1 S1 2.650(6) . ?
 Mn1 S1 2.815(6) 1_545 ?
 Mn1 S1 2.815(6) 6_455 ?
 Mn2 S2 2.511(4) . ?
 Mn2 S2 2.511(4) 6 ?
 Mn2 S1 2.652(5) 6_565 ?
 Mn2 S1 2.652(5) 1_655 ?
 Mn2 S1 2.810(5) . ?
 Mn2 S1 2.810(5) 6 ?
 As1 S3 2.322(5) 1_565 ?
 As1 S2 2.343(5) . ?
 As1 S1 2.377(3) . ?
 S1 Mn2 2.652(5) 1_455 ?
 S1 Mn1 2.815(6) 1_565 ?
 S2 Ag1 2.924(6) 1_565 ?
 S3 Sb1 2.322(5) 1_545 ?
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 S3 Ag1 2.769(4) 7_655 ?

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 S2 Ag1 S3 87.94(16) . . ?
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 S3 Ag1 S2 87.59(16) 1_655 1_545 ?
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 S3 Ag1 S2 91.88(14) 7_655 1_545 ?
 S3 Ag1 S2 73.74(12) . 1_545 ?
 S3 Mn1 S3 170.2(3) . 6 ?
 S3 Mn1 S1 94.13(16) . 6 ?
 S3 Mn1 S1 92.50(14) 6 6 ?
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S1 Mn1 S1 85.9(2) 1_545 6_455 ?
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 S2 As1 S1 94.37(17) . . ?
 As1 S1 Mn1 98.57(15) . . ?
 As1 S1 Mn2 99.25(16) . 1_455 ?
 Mn1 S1 Mn2 93.24(15) . 1_455 ?
 As1 S1 Mn2 87.96(12) . . ?
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 Mn2 S1 Mn1 86.48(13) . 1_565 ?
 As1 S2 Mn2 96.22(17) . . ?
 As1 S2 Ag1 101.8(2) . . ?
 Mn2 S2 Ag1 99.4(2) . . ?
 As1 S2 Ag1 93.53(19) . 1_565 ?
 Mn2 S2 Ag1 98.23(19) . 1_565 ?
 Ag1 S2 Ag1 155.11(18) . 1_565 ?
 Sb1 S3 As1 0.00(6) 1_545 1_545 ?
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 Sb1 S3 Ag1 102.1(2) 1_545 1_455 ?
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 Mn1 S3 Ag1 164.2(2) . 7_655 ?
 Ag1 S3 Ag1 85.68(14) 1_455 7_655 ?
 Sb1 S3 Ag1 94.01(18) 1_545 . ?
 As1 S3 Ag1 94.01(18) 1_545 . ?
 Mn1 S3 Ag1 96.78(18) . . ?
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