

data\_p12\_totale  
\_publ\_requested\_journal Am.Miner.  
\_publ\_section\_title 'High-pressure phase transition of a natural pigeonite'  
\_publ\_contact\_author\_name 'MATTEO ALVARO'  
\_publ\_contact\_author\_address  
;  
'Dipartimento di Scienze della Terra,  
Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'  
;  
loop\_  
\_publ\_author\_name  
\_publ\_author\_address  
'ALVARO, MATTEO'  
'Dipartimento di Scienze della Terra,  
Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'  
;  
'Nestola, Fabrizio'  
;'Dipartimento di Geoscienze, Universit\`a di Padova,  
Via Giotto 1, I-35137 Padova (Italy)'  
;  
'BOFFA BALLARAN, TIZIANA'  
;'Bayerisches Geoinstitut, Universit\"at Bayreuth,  
Universit\"atstrasse 37, D-95440 Bayreuth (Germany)'  
;  
'C\AMARA, FERNANDO'  
;'C.N.R. - Istituto di Geoscienze e Georisorse - Unit\`a di Pavia,  
Via Ferrata 1, I-27100 Pavia (Italy)'  
;  
'DOMENEGHETTI, CHIARA'  
;'Dipartimento di Scienze della Terra, Universit\`a di Pavia,  
Via Ferrata 1, I-27100 Pavia (Italy)'  
;  
'TAZZOLI, VITTORIO'  
;'Dipartimento di Scienze della Terra, Universit\`a di Pavia,  
Via Ferrata 1, I-27100 Pavia (Italy)'  
;  
\_audit\_creation\_method SHELXL-97  
\_chemical\_name\_systematic Pigeonite  
\_chemical\_name\_common ?  
\_chemical\_melting\_point ?  
\_chemical\_formula\_sum 'Ca0.48 Fe4 Mg3.48 O24 Si8'  
\_chemical\_formula\_weight 935.96  
  
loop\_  
\_atom\_type\_symbol  
\_atom\_type\_description  
\_atom\_type\_scat\_dispersion\_real  
\_atom\_type\_scat\_dispersion\_imag  
\_atom\_type\_scat\_source  
O O 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
O O-- 0.0080 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
Si Si 0.0817 0.0704 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
Si SiP4 0.0720 0.0710 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

Mg MgP2 0.0420 0.0360 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
Fe FeP2 0.3010 0.8450 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
Ca Ca+2 0.2030 0.3060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
Si Si+2 0.0720 0.0710 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting monoclinic  
\_symmetry\_space\_group\_name\_H-M 'P 21/c'  
\_symmetry\_int\_tables\_number 14

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'  
'-x, y+1/2, -z+1/2'  
'-x, -y, -z'  
'x, -y-1/2, z-1/2'

\_cell\_length\_a 9.622(14)  
\_cell\_length\_b 8.861(14)  
\_cell\_length\_c 5.181(7)  
\_cell\_angle\_alpha 90.00  
\_cell\_angle\_beta 107.92(13)  
\_cell\_angle\_gamma 90.00  
\_cell\_volume 420.3(11)  
\_cell\_formula\_units\_Z 4  
\_cell\_measurement\_temperature 293(2)  
\_cell\_measurement\_reflns\_used ?  
\_cell\_measurement\_theta\_min ?  
\_cell\_measurement\_theta\_max ?

\_exptl\_crystal\_description Irregular  
\_exptl\_crystal\_colour Green  
\_exptl\_crystal\_size\_max 0.120  
\_exptl\_crystal\_size\_mid 0.110  
\_exptl\_crystal\_size\_min 0.100  
\_exptl\_crystal\_density\_meas ?  
\_exptl\_crystal\_density\_diffrrn 3.585  
\_exptl\_crystal\_density\_method 'not measured'  
\_exptl\_crystal\_F\_000 460.0  
\_exptl\_absorpt\_coefficient\_mu 4.248  
\_exptl\_absorpt\_correction\_type numerical  
\_exptl\_absorpt\_correction\_T\_min ?  
\_exptl\_absorpt\_correction\_T\_max ?  
\_exptl\_absorpt\_process\_details ABSORB

\_exptl\_special\_details

;  
Angel, R.J. (2004) Absorption corrections for diamond-anvil pressure cells  
implemented in the software package -- Absorb 6.0. Journal of Applied  
Crystallography, 37, 486-492.  
;

\_diffrn\_ambient\_temperature 293(2)  
\_diffrn\_radiation\_probe x-ray

`_diffrn_radiation_type MoK\alpha`  
`_diffrn_radiation_wavelength 0.71070`  
`_diffrn_source 'fine-focus sealed tube'`  
`_diffrn_radiation_monochromator graphite`  
`_diffrn_measurement_device_type ?`  
`_diffrn_measurement_method ?`  
`_diffrn_detector_area_resol_mean ?`  
`_diffrn_standards_number ?`  
`_diffrn_standards_interval_count ?`  
`_diffrn_standards_interval_time ?`  
`_diffrn_standards_decay_% ?`  
`_diffrn_reflns_number 959`  
`_diffrn_reflns_av_R_equivalents 0.0000`  
`_diffrn_reflns_av_sigmaI/netI 0.0696`  
`_diffrn_reflns_limit_h_min -12`  
`_diffrn_reflns_limit_h_max 11`  
`_diffrn_reflns_limit_k_min 0`  
`_diffrn_reflns_limit_k_max 11`  
`_diffrn_reflns_limit_l_min 0`  
`_diffrn_reflns_limit_l_max 7`  
`_diffrn_reflns_theta_min 3.20`  
`_diffrn_reflns_theta_max 29.90`  
`_reflns_number_total 959`  
`_reflns_number_gt 649`  
`_reflns_threshold_expression >2sigma(I)`  
  
`_computing_data_collection ?`  
`_computing_cell_refinement ?`  
`_computing_data_reduction ?`  
`_computing_structure_solution ?`  
`_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'`  
`_computing_molecular_graphics ?`  
`_computing_publication_material ?`  
  
`_refine_special_details`  
`;`  

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  $F^2 > 2\text{sigma}(F^2)$  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.

`;`  
`_refine_ls_structure_factor_coef Fsqd`  
`_refine_ls_matrix_type full`  
`_refine_ls_weighting_scheme calc`  
`_refine_ls_weighting_details`  
`'calc w=1/[s^2^(Fo^2)+(0.0817P)^2+0.0000P] where P=(Fo^2+2Fc^2)/3'`  
`_atom_sites_solution_primary direct`  
`_atom_sites_solution_secondary difmap`  
`_refine_ls_extinction_method none`  
`_refine_ls_extinction_coef ?`

\_refine\_ls\_number\_reflns 959  
\_refine\_ls\_number\_parameters 62  
\_refine\_ls\_number\_restraints 7  
\_refine\_ls\_R\_factor\_all 0.1349  
\_refine\_ls\_R\_factor\_gt 0.0766  
\_refine\_ls\_wR\_factor\_ref 0.1878  
\_refine\_ls\_wR\_factor\_gt 0.1579  
\_refine\_ls\_goodness\_of\_fit\_ref 1.181  
\_refine\_ls\_restrained\_S\_all 1.207  
\_refine\_ls\_shift/su\_max 0.000  
\_refine\_ls\_shift/su\_mean 0.000

loop\_

\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_U\_iso\_or\_equiv  
\_atom\_site\_adp\_type  
\_atom\_site\_occupancy  
\_atom\_site\_symmetry\_multiplicity  
\_atom\_site\_calc\_flag  
\_atom\_site\_refinement\_flags  
\_atom\_site\_disorder\_assembly  
\_atom\_site\_disorder\_group

O1A O 0.8668(9) 0.3381(7) 0.1713(12) 0.0083(14) Uiso 1 1 d ...  
O1B O 0.3741(9) 0.8374(7) 0.1307(12) 0.0083(13) Uiso 1 1 d ...  
O2A O 0.1187(9) 0.5021(8) 0.3293(11) 0.0119(14) Uiso 1 1 d ...  
O2B O 0.6276(10) 0.9878(7) 0.3708(12) 0.0131(14) Uiso 1 1 d ...  
O3A O 0.1032(11) 0.2616(8) 0.5748(14) 0.0203(17) Uiso 1 1 d ...  
O3B O 0.6065(10) 0.7055(8) 0.4714(13) 0.0134(16) Uiso 1 1 d ...  
SiA Si+2 0.0418(4) 0.3417(3) 0.2740(5) 0.0086(6) Uiso 1 1 d ...  
SiB Si+2 0.5497(4) 0.8380(3) 0.2334(5) 0.0079(6) Uiso 1 1 d ...  
M1A MgP2 0.2505(4) 0.6563(3) 0.2284(4) 0.0100(6) Uani 0.75 1 d P ..  
M1B FeP2 0.2505(4) 0.6563(3) 0.2284(4) 0.0100(6) Uani 0.25 1 d P ..  
M2A MgP2 0.2562(5) 0.0218(3) 0.2234(4) 0.0111(6) Uani 0.12 1 d PDU ..  
M2B FeP2 0.2562(5) 0.0218(3) 0.2234(4) 0.0111(6) Uani 0.75 1 d P ..  
M21 Ca+2 0.251(7) 0.028(5) 0.277(6) 0.030 Uiso 0.12 1 d PDU ..

loop\_

\_atom\_site\_aniso\_label  
\_atom\_site\_aniso\_U\_11  
\_atom\_site\_aniso\_U\_22  
\_atom\_site\_aniso\_U\_33  
\_atom\_site\_aniso\_U\_23  
\_atom\_site\_aniso\_U\_13  
\_atom\_site\_aniso\_U\_12

M1A 0.0122(19) 0.0079(13) 0.0103(10) 0.0006(9) 0.0038(11) 0.0039(12)  
M1B 0.0122(19) 0.0079(13) 0.0103(10) 0.0006(9) 0.0038(11) 0.0039(12)  
M2A 0.0104(15) 0.0151(11) 0.0065(10) 0.0042(9) 0.0006(11) 0.0021(9)  
M2B 0.0104(15) 0.0151(11) 0.0065(10) 0.0042(9) 0.0006(11) 0.0021(9)

\_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.

;

loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

O1A SiA 1.603(9) 1\_655 ?

O1A M1A 2.032(8) 3\_665 ?

O1A M21 2.09(5) 2\_655 ?

O1A M1A 2.121(7) 2\_645 ?

O1A M2A 2.179(8) 2\_655 ?

O1B SiB 1.608(9) . ?

O1B M1A 2.058(8) 4\_575 ?

O1B M2A 2.127(7) 1\_565 ?

O1B M1A 2.149(7) . ?

O2A SiA 1.587(8) . ?

O2A M1A 2.039(8) . ?

O2A M2A 2.074(8) 4\_566 ?

O2B SiB 1.581(7) . ?

O2B M21 1.84(4) 3\_666 ?

O2B M2A 2.057(8) 3\_666 ?

O2B M1A 2.059(8) 2\_655 ?

O3A SiA 1.621(8) 4\_566 ?

O3A SiA 1.647(8) . ?

O3A M2A 2.397(9) 4\_566 ?

O3A O3A 2.599(4) 4\_565 ?

O3A O3A 2.599(4) 4\_566 ?

O3A M2A 3.413(8) . ?

O3B SiB 1.657(7) 4\_576 ?

O3B SiB 1.668(7) . ?

O3B M2A 2.497(8) 2\_655 ?

O3B O3B 2.708(5) 4\_576 ?

O3B O3B 2.708(5) 4\_575 ?

O3B M2A 2.966(8) 3\_666 ?

SiA O1A 1.603(9) 1\_455 ?

SiA O3A 1.621(8) 4\_565 ?

SiB O3B 1.657(7) 4\_575 ?

M1A O1A 2.032(8) 3\_665 ?

M1A O1B 2.058(8) 4\_576 ?

M1A O2B 2.059(8) 2\_645 ?

M1A O1A 2.121(7) 2\_655 ?

M1A M21 2.85(3) 4\_565 ?

M1A M2A 2.997(4) 4\_566 ?

M1A M2A 3.071(5) 4\_565 ?

M2A M21 0.303(18) . ?  
M2A O2B 2.057(8) 3\_666 ?  
M2A O2A 2.074(8) 4\_565 ?  
M2A O1B 2.127(7) 1\_545 ?  
M2A O1A 2.179(8) 2\_645 ?  
M2A O3A 2.397(9) 4\_565 ?  
M2A O3B 2.497(8) 2\_645 ?  
M2A SiA 2.861(6) 4\_565 ?  
M2A O3B 2.966(8) 3\_666 ?  
M21 O2B 1.84(4) 3\_666 ?  
M21 O1A 2.09(5) 2\_645 ?  
M21 M1A 2.85(3) 4\_566 ?

loop\_

\_geom\_angle\_atom\_site\_label\_1  
\_geom\_angle\_atom\_site\_label\_2  
\_geom\_angle\_atom\_site\_label\_3  
\_geom\_angle  
\_geom\_angle\_site\_symmetry\_1  
\_geom\_angle\_site\_symmetry\_3  
\_geom\_angle\_publ\_flag  
SiA O1A M1A 122.4(4) 1\_655 3\_665 ?  
SiA O1A M21 119.9(16) 1\_655 2\_655 ?  
M1A O1A M21 87.5(11) 3\_665 2\_655 ?  
SiA O1A M1A 121.2(4) 1\_655 2\_645 ?  
M1A O1A M1A 95.6(3) 3\_665 2\_645 ?  
M21 O1A M1A 103.3(12) 2\_655 2\_645 ?  
SiA O1A M2A 119.9(4) 1\_655 2\_655 ?  
M1A O1A M2A 93.6(3) 3\_665 2\_655 ?  
M1A O1A M2A 97.8(3) 2\_645 2\_655 ?  
SiB O1B M1A 123.8(4) . 4\_575 ?  
SiB O1B M2A 120.1(4) . 1\_565 ?  
M1A O1B M2A 91.5(3) 4\_575 1\_565 ?  
SiB O1B M1A 121.7(4) .. ?  
M1A O1B M1A 94.0(3) 4\_575 . ?  
M2A O1B M1A 98.5(3) 1\_565 . ?  
SiA O2A M1A 147.7(4) .. ?  
SiA O2A M2A 101.9(3) . 4\_566 ?  
M1A O2A M2A 93.6(4) . 4\_566 ?  
SiB O2B M21 116.6(15) . 3\_666 ?  
SiB O2B M2A 117.3(4) . 3\_666 ?  
SiB O2B M1A 136.3(4) . 2\_655 ?  
M21 O2B M1A 93.9(16) 3\_666 2\_655 ?  
M2A O2B M1A 96.5(4) 3\_666 2\_655 ?  
SiA O3A SiA 138.6(7) 4\_566 . ?  
SiA O3A M2A 123.8(4) 4\_566 4\_566 ?  
SiA O3A M2A 88.0(3) . 4\_566 ?  
SiA O3A O3A 134.6(5) 4\_566 4\_565 ?  
M2A O3A O3A 101.3(3) 4\_566 4\_565 ?  
SiA O3A O3A 150.1(4) . 4\_566 ?  
M2A O3A O3A 86.1(3) 4\_566 4\_566 ?  
O3A O3A O3A 170.9(6) 4\_565 4\_566 ?  
SiA O3A M2A 106.8(3) 4\_566 . ?  
SiA O3A M2A 81.5(3) .. ?

M2A O3A M2A 110.3(3) 4\_566 . ?  
O3A O3A M2A 127.9(3) 4\_566 . ?  
SiB O3B SiB 130.8(5) 4\_576 . ?  
SiB O3B M2A 121.9(4) 4\_576 2\_655 ?  
SiB O3B M2A 104.7(3) . 2\_655 ?  
SiB O3B O3B 113.9(4) . 4\_576 ?  
M2A O3B O3B 137.1(3) 2\_655 4\_576 ?  
SiB O3B O3B 161.5(3) 4\_576 4\_575 ?  
M2A O3B O3B 69.3(2) 2\_655 4\_575 ?  
O3B O3B O3B 146.1(5) 4\_576 4\_575 ?  
SiB O3B M2A 87.6(3) 4\_576 3\_666 ?  
SiB O3B M2A 79.1(3) . 3\_666 ?  
M2A O3B M2A 122.8(4) 2\_655 3\_666 ?  
O3B O3B M2A 52.0(2) 4\_576 3\_666 ?  
O3B O3B M2A 98.1(3) 4\_575 3\_666 ?  
O2A SiA O1A 117.5(4) . 1\_455 ?  
O2A SiA O3A 112.3(4) . 4\_565 ?  
O1A SiA O3A 109.2(4) 1\_455 4\_565 ?  
O2A SiA O3A 101.7(4) . . ?  
O1A SiA O3A 109.9(4) 1\_455 . ?  
O3A SiA O3A 105.3(4) 4\_565 . ?  
O2B SiB O1B 117.1(4) . . ?  
O2B SiB O3B 109.5(4) . 4\_575 ?  
O1B SiB O3B 107.8(4) . 4\_575 ?  
O2B SiB O3B 104.8(4) . . ?  
O1B SiB O3B 108.3(4) . . ?  
O3B SiB O3B 109.0(4) 4\_575 . ?  
O1A M1A O2A 94.8(3) 3\_665 . ?  
O1A M1A O1B 176.7(3) 3\_665 4\_576 ?  
O2A M1A O1B 88.3(3) . 4\_576 ?  
O1A M1A O2B 86.8(3) 3\_665 2\_645 ?  
O2A M1A O2B 91.5(3) . 2\_645 ?  
O1B M1A O2B 94.4(3) 4\_576 2\_645 ?  
O1A M1A O1A 93.5(3) 3\_665 2\_655 ?  
O2A M1A O1A 91.5(3) . 2\_655 ?  
O1B M1A O1A 85.2(3) 4\_576 2\_655 ?  
O2B M1A O1A 177.0(3) 2\_645 2\_655 ?  
O1A M1A O1B 85.2(3) 3\_665 . ?  
O2A M1A O1B 173.7(3) . . ?  
O1B M1A O1B 91.7(3) 4\_576 . ?  
O2B M1A O1B 94.8(3) 2\_645 . ?  
O1A M1A O1B 82.2(3) 2\_655 . ?  
O1A M1A M21 47.2(11) 3\_665 4\_565 ?  
O2A M1A M21 89.1(9) . 4\_565 ?  
O1B M1A M21 134.3(11) 4\_576 4\_565 ?  
O2B M1A M21 40.1(12) 2\_645 4\_565 ?  
O1A M1A M21 140.5(11) 2\_655 4\_565 ?  
O1B M1A M21 95.4(8) . 4\_565 ?  
O1A M1A M2A 138.0(3) 3\_665 4\_566 ?  
O2A M1A M2A 43.7(2) . 4\_566 ?  
O1B M1A M2A 45.2(2) 4\_576 4\_566 ?  
O2B M1A M2A 88.3(2) 2\_645 4\_566 ?  
O1A M1A M2A 93.5(2) 2\_655 4\_566 ?  
O1B M1A M2A 136.8(2) . 4\_566 ?

M21 M1A M2A 113.3(7) 4\_565 4\_566 ?  
O1A M1A M2A 45.1(2) 3\_665 4\_565 ?  
O2A M1A M2A 92.9(2) . 4\_565 ?  
O1B M1A M2A 136.1(2) 4\_576 4\_565 ?  
O2B M1A M2A 41.7(2) 2\_645 4\_565 ?  
O1A M1A M2A 138.5(2) 2\_655 4\_565 ?  
O1B M1A M2A 91.5(2) . 4\_565 ?  
M21 M1A M2A 4.1(7) 4\_565 4\_565 ?  
M2A M1A M2A 117.26(16) 4\_566 4\_565 ?  
M21 M2A O2B 42(10) . 3\_666 ?  
M21 M2A O2A 134(10) . 4\_565 ?  
O2B M2A O2A 169.5(3) 3\_666 4\_565 ?  
M21 M2A O1B 127(10) . 1\_545 ?  
O2B M2A O1B 92.2(3) 3\_666 1\_545 ?  
O2A M2A O1B 85.5(3) 4\_565 1\_545 ?  
M21 M2A O1A 70(10) . 2\_645 ?  
O2B M2A O1A 83.1(3) 3\_666 2\_645 ?  
O2A M2A O1A 86.5(3) 4\_565 2\_645 ?  
O1B M2A O1A 81.4(3) 1\_545 2\_645 ?  
M21 M2A O3A 84(10) . 4\_565 ?  
O2B M2A O3A 116.7(3) 3\_666 4\_565 ?  
O2A M2A O3A 67.8(3) 4\_565 4\_565 ?  
O1B M2A O3A 149.3(2) 1\_545 4\_565 ?  
O1A M2A O3A 110.6(4) 2\_645 4\_565 ?  
M21 M2A O3B 120(10) . 2\_645 ?  
O2B M2A O3B 104.6(3) 3\_666 2\_645 ?  
O2A M2A O3B 85.7(3) 4\_565 2\_645 ?  
O1B M2A O3B 91.4(3) 1\_545 2\_645 ?  
O1A M2A O3B 169.8(2) 2\_645 2\_645 ?  
O3A M2A O3B 72.4(3) 4\_565 2\_645 ?  
M21 M2A SiA 113(10) . 4\_565 ?  
O2B M2A SiA 151.5(2) 3\_666 4\_565 ?  
O2A M2A SiA 32.9(2) 4\_565 4\_565 ?  
O1B M2A SiA 116.2(2) 1\_545 4\_565 ?  
O1A M2A SiA 102.0(3) 2\_645 4\_565 ?  
O3A M2A SiA 35.13(19) 4\_565 4\_565 ?  
O3B M2A SiA 74.6(2) 2\_645 4\_565 ?  
M21 M2A O3B 62(10) . 3\_666 ?  
O2B M2A O3B 58.4(2) 3\_666 3\_666 ?  
O2A M2A O3B 130.8(3) 4\_565 3\_666 ?  
O1B M2A O3B 124.4(3) 1\_545 3\_666 ?  
O1A M2A O3B 131.5(2) 2\_645 3\_666 ?  
O3A M2A O3B 69.4(3) 4\_565 3\_666 ?  
O3B M2A O3B 58.68(16) 2\_645 3\_666 ?  
SiA M2A O3B 100.4(2) 4\_565 3\_666 ?  
M2A M21 O2B 132(10) . 3\_666 ?  
M2A M21 O1A 102(10) . 2\_645 ?  
O2B M21 O1A 90.9(16) 3\_666 2\_645 ?  
M2A M21 M1A 134(10) . 4\_566 ?  
O2B M21 M1A 46.1(8) 3\_666 4\_566 ?  
O1A M21 M1A 45.3(7) 2\_645 4\_566 ?

\_diffrn\_measured\_fraction\_theta\_max 0.640  
\_diffrn\_reflns\_theta\_full 29.90

\_diffrn\_measured\_fraction\_theta\_full 0.640  
\_refine\_diff\_density\_max 0.876  
\_refine\_diff\_density\_min -1.108  
\_refine\_diff\_density\_rms 0.230  
\_diffrn\_ambient\_pressure 3172000  
\_chemical\_formula\_moiety 'Ca0.48 Fe4 Mg3.48 O24 Si8'