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  _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)'
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  _publ_author_name
  _publ_author_address
  'ALVARO, MATTEO'
; 'Dipartimento di Scienze della Terra,
Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'
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'Nestola, Fabrizio'
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'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)'
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Si Si 0.0817 0.0704 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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Mg MgP2 0.0420 0.0360 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
Ca CaP2 0.2030 0.3060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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

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_cell_length_c 5.060(3)
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_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.

;

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_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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_atom_site_occupancy
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O2 O 0.3732(8) 0.2395(7) 0.3595(11) 0.0116(13) Uiso 1 1 d ...
O3 O 0.3517(8) 0.0496(7) 0.9446(11) 0.0152(13) Uiso 1 1 d ...
Si Si 0.2956(3) 0.0905(2) 0.2237(4) 0.0081(7) Uiso 1 1 d ...
Fe1A FeP2 0.0000 0.9064(3) 0.2500 0.0098(8) Uani 0.25 2 d SP ..
FE1B MgP2 0.0000 0.9064(3) 0.2500 0.0098(8) Uani 0.75 2 d SP ..
Fe2A FeP2 0.0000 0.2779(2) 0.2500 0.0157(8) Uani 0.75 2 d SP ..
FE2B MgP2 0.0000 0.2779(2) 0.2500 0.0157(8) Uani 0.12 2 d SP ..
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Fe1A 0.015(2) 0.0058(16) 0.0080(12) 0.000 0.0012(13) 0.000
FE1B 0.015(2) 0.0058(16) 0.0080(12) 0.000 0.0012(13) 0.000
Fe2A 0.0216(18) 0.0149(13) 0.0086(9) 0.000 0.0000(9) 0.000
FE2B 0.0216(18) 0.0149(13) 0.0086(9) 0.000 0.0000(9) 0.000
FE2C 0.0216(18) 0.0149(13) 0.0086(9) 0.000 0.0000(9) 0.000

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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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O2 Si 1.580(6) . ?

O2 FE2C 2.054(6) 7_556 ?

O2 Fe2A 2.054(6) 7_556 ?

O2 Fe1A 2.061(7) 3_545 ?

O3 Si 1.664(6) 6_556 ?

O3 Si 1.666(6) 1_556 ?

O3 O3 2.677(4) 6 ?

O3 O3 2.677(4) 6_556 ?

Si O3 1.664(6) 6 ?

Si O3 1.666(6) 1_554 ?

Fe1A O1 2.041(6) 6_566 ?

Fe1A O1 2.041(6) 5_565 ?

Fe1A O2 2.061(7) 4 ?

Fe1A O2 2.061(7) 3_455 ?

Fe1A O1 2.129(6) 1_565 ?

Fe1A O1 2.129(6) 2_565 ?

Fe2A O2 2.054(6) 7_556 ?

Fe2A O2 2.054(6) 8_455 ?

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 Si O2 FE2C 117.3(3) . 7_556 ?
 Si O2 Fe2A 117.3(3) . 7_556 ?
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 FE2C O2 Fe1A 93.9(3) 7_556 3_545 ?
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 Si O3 Si 127.9(4) 6_556 1_556 ?
 Si O3 O3 161.0(3) 1_556 6 ?
 Si O3 O3 108.6(4) 6_556 6_556 ?
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 O1 Fe1A O1 177.9(3) 6_566 5_565 ?
 O1 Fe1A O2 92.6(3) 6_566 4 ?
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 O2 Fe1A O1 176.3(2) 3_455 1_565 ?
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 O2 Fe2A O1 85.7(3) 7_556 2 ?
 O2 Fe2A O1 87.7(3) 8_455 2 ?
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 O2 Fe2A O3 85.3(2) 7_556 8_455 ?
 O2 Fe2A O3 100.0(2) 8_455 8_455 ?
 O1 Fe2A O3 89.0(2) 2 8_455 ?
 O1 Fe2A O3 167.2(2) . 8_455 ?
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