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  _publ_section_title 'High-pressure phase transition of a natural pigeonite'
  _publ_contact_author_name    'MATTEO ALVARO'
  _publ_contact_author_address
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'Dipartimento di Scienze della Terra,
Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'
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  'ALVARO, MATTEO'
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Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'
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'Nestola, Fabrizio'
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;
'DOMENEGHETTI, CHIARA'
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;
'TAZZOLI, VITTORIO'
; 'Dipartimento di Scienze della Terra, Universit\`a di Pavia,
Via Ferrata 1, I-27100 Pavia (Italy)'
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;
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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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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O3 O 0.3518(10) 0.0523(8) 0.9349(13) 0.0134(17) Uiso 1 1 d . . .
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Fe2A FeP2 0.0000 0.2805(3) 0.2500 0.0142(10) Uani 0.75 2 d SP . .
FE2B MgP2 0.0000 0.2805(3) 0.2500 0.0142(10) Uani 0.12 2 d SP . .
FE2C CaP2 0.0000 0.2805(3) 0.2500 0.0142(10) Uani 0.12 2 d SP . .

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FE1B 0.017(3) 0.003(2) 0.0119(16) 0.000 0.0037(17) 0.000
Fe2A 0.019(2) 0.0125(16) 0.0118(12) 0.000 0.0042(11) 0.000
FE2B 0.019(2) 0.0125(16) 0.0118(12) 0.000 0.0042(11) 0.000
FE2C 0.019(2) 0.0125(16) 0.0118(12) 0.000 0.0042(11) 0.000

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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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O1 Fe2A 2.157(8) . ?

O2 Si 1.592(8) . ?

O2 Fe1A 2.018(8) 3_545 ?

O2 FE2C 2.037(8) 7_556 ?

O2 Fe2A 2.037(8) 7_556 ?

O3 Si 1.650(8) 1_556 ?

O3 Si 1.651(8) 6_556 ?

O3 Fe2A 2.337(8) 7_556 ?

O3 O3 2.648(6) 6 ?

O3 O3 2.648(6) 6_556 ?

Si O3 1.650(8) 1_554 ?

Si O3 1.651(8) 6 ?

Fe1A O1 2.012(8) 6_566 ?

Fe1A O1 2.012(8) 5_565 ?

Fe1A O2 2.018(8) 3_455 ?

Fe1A O2 2.018(8) 4 ?

Fe1A O1 2.087(8) 1_565 ?

Fe1A O1 2.087(8) 2_565 ?

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Fe1A Fe2A 2.977(4) 5_565 ?

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Fe2A O2 2.037(8) 8_455 ?

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Fe2A O1 2.157(8) 2 ?

Fe2A O3 2.337(8) 7_556 ?

Fe2A O3 2.337(8) 8_455 ?

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O1 Fe1A Fe2A 134.7(2) 6_566 5_565 ?
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