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\_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  
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\_publ\_author\_name  
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'ALVARO, MATTEO'  
'Dipartimento di Scienze della Terra,  
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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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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'  
Fe FeP2 0.3010 0.8450 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
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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  $F^2 > 2\text{sigma}(F^2)$  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.

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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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O1B SiB 1.629(10) . ?

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\_diffrn\_measured\_fraction\_theta\_max 0.630

\_diffrn\_reflns\_theta\_full 29.68  
\_diffrn\_measured\_fraction\_theta\_full 0.630  
\_refine\_diff\_density\_max 1.152  
\_refine\_diff\_density\_min -0.995  
\_refine\_diff\_density\_rms 0.284  
\_diffrn\_ambient\_pressure 984000  
\_chemical\_formula\_moiety 'Ca0.48 Fe4 Mg3.48 O24 Si8'