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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,
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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 F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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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 M2A M21 O3A 113(10) . 4\_565 ?  
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 O1A M21 O3A 119(2) 2\_645 4\_565 ?  
 O2A M21 O3A 68.8(15) 4\_565 4\_565 ?  
 M2A M21 M1A 114(10) . 4\_566 ?  
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 O1A M21 M1A 43.9(9) 2\_645 4\_566 ?  
 O2A M21 M1A 130(2) 4\_565 4\_566 ?  
 O3A M21 M1A 132.9(8) 4\_565 4\_566 ?

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