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_publ_contact_author_name   'MATTEO ALVARO'
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;
'Dipartimento di Scienze della Terra,
Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'
;
loop_
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'ALVARO, MATTEO'
;'Dipartimento di Scienze della Terra,
Universit\`a di Pavia, Via Ferrata 1, I-27100 Pavia (Italy)'
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'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)'
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'-x, -y, -z'
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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^ > 2sigma(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
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 factors based on ALL data will be even larger.
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'calc w=1/[\s^2^(Fo^2^)+(0.0965P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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O2 O 0.3741(7) 0.2400(6) 0.3598(9) 0.0122(11) Uiso 1 1 d . . .
O3 O 0.3521(7) 0.0485(6) 0.9478(10) 0.0148(11) Uiso 1 1 d . . .
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Fe2A 0.0196(16) 0.0151(11) 0.0083(8) 0.000 -0.0006(8) 0.000
FE2B 0.0196(16) 0.0151(11) 0.0083(8) 0.000 -0.0006(8) 0.000
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 used when they are defined by crystal symmetry. An approximate (isotropic)
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O3 O3 2.669(4) 6 ?
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Si O3 O3 109.5(3) 6_556 6_556 ?
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