

MEJILLONESITE

_audit_creation_method SHELXL-97

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_chemical_name_common ?

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_atom_type_scatter_source

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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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'Na' 'Na' 0.0362 0.0249

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'Mg' 'Mg' 0.0486 0.0363

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'P' 'P' 0.1023 0.0942

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_computing_data_reduction       ?
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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_sites_solution_secondary  difmap
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H5 H 0.141(4) 0.209(4) -0.047(8) 0.052 Uiso 1 1 d . . .
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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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Mg1 O11 2.026(4) 2_565 ?
Mg1 O21 2.059(4) 1_556 ?
Mg1 O13 2.081(5) 1_565 ?
Mg1 OZ1 2.146(5) 7_665 ?
Mg1 OZ2 2.197(5) 7_666 ?
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 P1 O14 Na1 99.0(2) 1_565 5_576 ?
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 P2 O24 Na1 111.1(2) 8_575 1_554 ?
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 Mg1 OZ1 Mg2 116.03(18) 7_655 2_565 ?

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