

data_cix1dc_abs

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;
_chemical_name_common ?
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'H B Ca O5 Si'
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_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
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'H' 'H' 0.0000 0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'B' 'B' 0.0013 0.0007
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'O' 'O' 0.0106 0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Si' 'Si' 0.0817 0.0704
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Ca' 'Ca' 0.2262 0.3064
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'
'-x, y+1/2, -z+1/2'
'-x, -y, -z'
'x, -y-1/2, z-1/2'

_cell_length_a 4.83610(10)
_cell_length_b 7.6155(2)
_cell_length_c 9.6392(2)
_cell_angle_alpha 90.00
_cell_angle_beta 90.134(2)
_cell_angle_gamma 90.00
_cell_volume 355.004(14)
_cell_formula_units_Z 4
_cell_measurement_temperature 293(2)
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_diffn_reflns_av_sigmaI/netI    0.0320
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_computing_cell_refinement      ?
_computing_data_reduction       ?
_computing_structure_solution   ?
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'

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_computing_molecular_graphics ?
_computing_publication_material ?

_refine_special_details

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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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'calc w=1/[\s^2^(Fo^2^)+(0.0250P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'
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loop_

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_atom_site_occupancy
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Ca Ca 0.99162(4) 0.10613(2) 0.336144(18) 0.00701(5) Uani 1 1 d . . .
Si Si 0.46897(5) 0.26613(3) 0.08442(3) 0.00484(6) Uani 1 1 d . . .
B B 0.5685(2) 0.41057(13) 0.34094(11) 0.00587(15) Uani 1 1 d . . .

O1 O 0.24048(16) 0.40086(9) 0.03762(8) 0.00813(12) Uani 1 1 d . . .
 O2 O 0.67002(15) 0.30090(9) 0.45741(7) 0.00697(11) Uani 1 1 d . . .
 O3 O 0.67496(15) 0.33448(10) 0.21036(7) 0.00693(11) Uani 1 1 d . . .
 O4 O 0.31472(16) 0.08787(9) 0.14591(8) 0.00773(12) Uani 1 1 d . . .
 O5 O 0.25896(15) 0.41351(10) 0.33667(8) 0.00794(12) Uani 1 1 d . . .
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 Si 0.00572(11) 0.00435(11) 0.00446(11) -0.00022(8) -0.00004(8) 0.00028(7)
 B 0.0067(4) 0.0061(4) 0.0049(3) -0.0003(3) 0.0004(3) 0.0000(3)
 O1 0.0090(3) 0.0075(3) 0.0079(3) -0.0003(2) -0.0010(2) 0.0025(2)
 O2 0.0074(3) 0.0077(3) 0.0058(2) 0.0020(2) 0.0012(2) 0.0013(2)
 O3 0.0073(3) 0.0084(3) 0.0051(2) -0.0015(2) -0.0004(2) 0.0001(2)
 O4 0.0083(3) 0.0049(3) 0.0100(3) 0.0010(2) 0.0024(2) 0.0001(2)
 O5 0.0061(3) 0.0102(3) 0.0075(3) -0.0009(2) 0.0008(2) 0.0006(2)

_geom_special_details
 ;
 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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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
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 Ca O1 2.2830(8) 4_666 ?
 Ca O4 2.4159(8) 1_655 ?
 Ca O2 2.4482(7) . ?
 Ca O5 2.5270(8) 2_645 ?
 Ca O3 2.6135(7) . ?
 Ca O3 2.6616(8) 2_745 ?
 Ca O5 2.6742(8) 1_655 ?
 Si O1 1.5732(8) . ?
 Si O2 1.6463(7) 4_565 ?
 Si O3 1.6527(7) . ?
 Si O4 1.6591(7) . ?
 B O4 1.4690(13) 2_655 ?
 B O3 1.4793(12) . ?

B O2 1.4821(12) . ?
B O5 1.4974(13) . ?
O1 Ca 2.2783(7) 2_655 ?
O1 Ca 2.2830(8) 4_465 ?
O2 Si 1.6463(7) 4_566 ?
O3 Ca 2.6616(8) 2_755 ?
O4 B 1.4690(13) 2_645 ?
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O5 Ca 2.6742(8) 1_455 ?

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_geom_angle_atom_site_label_3
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O1 Ca O4 133.33(3) 2_645 1_655 ?
O1 Ca O4 107.68(3) 4_666 1_655 ?
O1 Ca O2 81.16(3) 2_645 . ?
O1 Ca O2 86.69(3) 4_666 . ?
O4 Ca O2 144.09(2) 1_655 . ?
O1 Ca O5 73.60(3) 2_645 2_645 ?
O1 Ca O5 142.96(3) 4_666 2_645 ?
O4 Ca O5 77.07(3) 1_655 2_645 ?
O2 Ca O5 111.24(3) . 2_645 ?
O1 Ca O3 114.55(3) 2_645 . ?
O1 Ca O3 135.83(3) 4_666 . ?
O4 Ca O3 93.76(2) 1_655 . ?
O2 Ca O3 56.37(2) . . ?
O5 Ca O3 78.51(2) 2_645 . ?
O1 Ca O3 81.72(3) 2_645 2_745 ?
O1 Ca O3 78.86(2) 4_666 2_745 ?
O4 Ca O3 55.55(2) 1_655 2_745 ?
O2 Ca O3 159.57(2) . 2_745 ?
O5 Ca O3 74.19(2) 2_645 2_745 ?
O3 Ca O3 142.522(11) . 2_745 ?
O1 Ca O5 146.97(3) 2_645 1_655 ?
O1 Ca O5 76.40(2) 4_666 1_655 ?
O4 Ca O5 74.83(2) 1_655 1_655 ?
O2 Ca O5 77.08(2) . 1_655 ?
O5 Ca O5 137.773(17) 2_645 1_655 ?
O3 Ca O5 72.61(2) . 1_655 ?
O3 Ca O5 112.81(2) 2_745 1_655 ?
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O1 Si O3 115.28(4) . . ?
O2 Si O3 106.73(4) 4_565 . ?
O1 Si O4 108.66(4) . . ?
O2 Si O4 106.19(4) 4_565 . ?
O3 Si O4 105.43(4) . . ?
O4 B O3 107.39(8) 2_655 . ?

O4 B O2 109.02(8) 2_655 . ?
 O3 B O2 107.96(8) . . ?
 O4 B O5 111.89(8) 2_655 . ?
 O3 B O5 109.42(8) . . ?
 O2 B O5 111.02(8) . . ?
 Si O1 Ca 129.86(4) . 2_655 ?
 Si O1 Ca 126.67(4) . 4_465 ?
 Ca O1 Ca 102.18(3) 2_655 4_465 ?
 B O2 Si 122.87(6) . 4_566 ?
 B O2 Ca 100.92(5) . . ?
 Si O2 Ca 122.97(4) 4_566 . ?
 B O3 Si 122.54(6) . . ?
 B O3 Ca 94.06(5) . . ?
 Si O3 Ca 118.86(4) . . ?
 B O3 Ca 92.93(5) . 2_755 ?
 Si O3 Ca 119.04(4) . 2_755 ?
 Ca O3 Ca 103.93(2) . 2_755 ?
 B O4 Si 127.57(6) 2_645 . ?
 B O4 Ca 103.69(5) 2_645 1_455 ?
 Si O4 Ca 121.08(4) . 1_455 ?
 B O5 Ca 120.30(6) . 2_655 ?
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