data\_MAGNESIO-HORNBLENDE\_1325

\_publ\_contact\_author

;

 Roberta Oberti

;

\_publ\_contact\_author\_email

;

 oberti@crystal.unipv.it

;

loop\_

\_publ\_author\_name

\_publ\_author\_address

'Oberti R.'

'CNR-IGG, U.O.S. Pavia, Pavia, Italy'

'Boiocchi M.'

'Centro Grandi Strumenti, University of Pavia, Pavia, Italy'

'Hawthorne F.C.'

'Dep. Geological Sciences, University of Manitoba, Winnipeg, Canada'

'Ciriotti M.E.'

'A.M.I., via San Pietro 55, I-10073 Devesi-Cirie, Italy'

\_publ\_section\_title

;

 Magnesio-hornblende from Lüderitz (Namibia):

 mineral description and crystal-chemistry

;

\_audit\_creation\_method 'manually entered'

\_chemical\_name\_systematic ?

\_chemical\_name\_mineral

;

MAGNESIO-HORNBLENDE

;

\_chemical\_compound\_source

;

 Luderitz NAM

;

\_chemical\_name\_common ?

\_chemical\_melting\_point ?

\_chemical\_formula\_moiety ?

\_chemical\_formula\_sum

 'Al1.04 Ca1.75 F0.04 Fe1.34 H1.96 Mg3.51 Na0.56 O23.96 Si7.20'

\_chemical\_formula\_weight 859.50

loop\_

 \_atom\_type\_symbol

 \_atom\_type\_description

 \_atom\_type\_scat\_dispersion\_real

 \_atom\_type\_scat\_dispersion\_imag

 \_atom\_type\_scat\_source

 'O' 'O' 0.0106 0.0060

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'O2-' 'O2-' 0.0106 0.0060

 'Hovesteydt, 1982'

 'F-' 'F-' 0.0140 0.0100

 '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'

 'Al' 'Al' 0.0645 0.0514

 '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'

 'Al3+' 'Al3+' 0.0645 0.0514

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'Si4+' 'Si4+' 0.0817 0.0704

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'Mg2+' 'Mg2+' 0.0490 0.0360

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'Fe2+' 'Fe2+' 0.3460 0.8450

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'Fe3+' 'Fe3+' 0.3460 0.8450

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'Na+' 'Na+' 0.0360 0.0250

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'Ca2+' 'Ca2+' 0.2260 0.3060

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

 'H' 'H' 0.0000 0.0000

 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_space\_group\_crystal\_system monoclinic

\_space\_group\_IT\_number 12

\_space\_group\_name\_H-M\_alt 'C 2/m'

\_space\_group\_name\_Hall '-C 2y'

loop\_

 \_space\_group\_symop\_operation\_xyz

 'x, y, z'

 'x, -y, z'

 'x+1/2, y+1/2, z'

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

 '-x, -y, -z'

 '-x, y, -z'

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

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

\_cell\_length\_a 9.8308(7)

\_cell\_length\_b 18.0659(11)

\_cell\_length\_c 5.2968(4)

\_cell\_angle\_alpha 90

\_cell\_angle\_beta 104.771(6)

\_cell\_angle\_gamma 90

\_cell\_volume 909.64(11)

\_cell\_formula\_units\_Z 2

\_cell\_measurement\_temperature 298(2)

\_cell\_measurement\_reflns\_used 60

\_cell\_measurement\_theta\_min 2

\_cell\_measurement\_theta\_max 30

\_exptl\_crystal\_description 'platy prism'

\_exptl\_crystal\_colour 'green'

\_exptl\_crystal\_density\_meas ?

\_exptl\_crystal\_density\_method ?

\_exptl\_crystal\_density\_diffrn 3.138

\_exptl\_crystal\_F\_000 852.8

\_exptl\_crystal\_size\_max 0.60

\_exptl\_crystal\_size\_mid 0.45

\_exptl\_crystal\_size\_min 0.10

\_exptl\_absorpt\_coefficient\_mu 2.379

\_exptl\_absorpt\_correction\_type psi-scan

\_exptl\_absorpt\_correction\_T\_min 0.68

\_exptl\_absorpt\_correction\_T\_max 0.92

\_exptl\_absorpt\_process\_details

;

 North A.C.T., Phillips D.C. & Mathews F.S. (1968) Acta. Cryst. A24, 351

;

\_exptl\_absorpt\_special\_details ?

\_diffrn\_ambient\_temperature 298(2)

\_diffrn\_radiation\_wavelength 0.7107

\_diffrn\_radiation\_type MoK\a

\_diffrn\_radiation\_source 'fine-focus sealed tube'

\_diffrn\_radiation\_monochromator graphite

\_diffrn\_measurement\_device\_type 'PHILIPS PW1100'

\_diffrn\_measurement\_method 'omega-2theta scans'

\_diffrn\_standards\_number 3

\_diffrn\_standards\_interval\_count 400

\_diffrn\_standards\_decay\_% 0

\_diffrn\_reflns\_number 2691

\_diffrn\_reflns\_av\_R\_equivalents 0.0260

\_diffrn\_reflns\_limit\_h\_min -13

\_diffrn\_reflns\_limit\_h\_max 13

\_diffrn\_reflns\_limit\_k\_min -25

\_diffrn\_reflns\_limit\_k\_max 25

\_diffrn\_reflns\_limit\_l\_min 0

\_diffrn\_reflns\_limit\_l\_max 7

\_diffrn\_reflns\_theta\_min 2.255

\_diffrn\_reflns\_theta\_max 30.023

\_diffrn\_measured\_fraction\_theta\_max 1.000

\_reflns\_number\_total 1380

\_reflns\_number\_gt 1244

\_reflns\_threshold\_expression 'I > 3\s(I)'

\_reflns\_special\_details ?

\_computing\_data\_collection 'local program'

\_computing\_cell\_refinement 'LAT routine of PW1100 diffractometer'

\_computing\_data\_reduction 'local program'

\_computing\_structure\_refinement 'local program (Cannillo et al., 1983)'

\_refine\_special\_details

;

 Refinement on F against reflections with I > 3sigma(I).

 The threshold expression (\_gt) of I > 3sigma(I) corresponds to the cutoff used

 to discriminate between observed and unobserved reflections for refinement.

 The use of unitary weigth produces unusual values for the calculated

 weighted wR-factor (similar to R).

;

\_refine\_ls\_structure\_factor\_coef F

\_refine\_ls\_matrix\_type full

\_refine\_ls\_weighting\_scheme unit

\_refine\_ls\_hydrogen\_treatment mixed

\_refine\_ls\_extinction\_method none

\_refine\_ls\_number\_reflns 1244

\_refine\_ls\_number\_parameters 118

\_refine\_ls\_number\_restraints 0

\_refine\_ls\_R\_factor\_all 0.0315

\_refine\_ls\_R\_factor\_gt 0.0272

\_refine\_ls\_wR\_factor\_ref 0.0337

\_refine\_ls\_wR\_factor\_gt 0.0312

\_refine\_ls\_restrained\_S\_all 1.806

loop\_

 \_atom\_site\_label

 \_atom\_site\_type\_symbol

 \_atom\_site\_fract\_x

 \_atom\_site\_fract\_y

 \_atom\_site\_fract\_z

 \_atom\_site\_U\_iso\_or\_equiv

 \_atom\_site\_adp\_type

 \_atom\_site\_occupancy

 \_atom\_site\_site\_symmetry\_order

 \_atom\_site\_calc\_flag

 \_atom\_site\_refinement\_flags\_posn

 \_atom\_site\_refinement\_flags\_adp

 \_atom\_site\_refinement\_flags\_occupancy

 \_atom\_site\_disorder\_assembly

 \_atom\_site\_disorder\_group

O1A O 0.1090(2) 0.08794(11) 0.2154(4) 0.0097(5) Uani 0.4(2) 1 d . . P . .

O1B O2- 0.1090(2) 0.08794(11) 0.2154(4) 0.0097(5) Uani 0.6(2) 1 d . . P . .

O2A O 0.1194(2) 0.17303(10) 0.7295(4) 0.0089(5) Uani 0.3(2) 1 d . . P . .

O2B O2- 0.1194(2) 0.17303(10) 0.7295(4) 0.0089(5) Uani 0.7(2) 1 d . . P . .

O3A F- 0.1108(3) 0.0000 0.7149(5) 0.0102(8) Uani 0.02(6) 2 d S T P . .

O3B O- 0.1108(3) 0.0000 0.7149(5) 0.0102(8) Uani 0.98(6) 2 d S T P . .

O4A O 0.3680(2) 0.24863(11) 0.7904(4) 0.0119(5) Uani 0.5(2) 1 d . . P . .

O4B O2- 0.3680(2) 0.24863(11) 0.7904(4) 0.0119(5) Uani 0.5(2) 1 d . . P . .

O5A O 0.3482(2) 0.13658(11) 0.1022(4) 0.0120(5) Uani 0.5(2) 1 d . . P . .

O5B O2- 0.3482(2) 0.13658(1) 0.1022(4) 0.0120(5) Uani 0.5(2) 1 d . . P . .

O6A O 0.3435(2) 0.11837(11) 0.5944(4) 0.0118(5) Uani 0.2(2) 1 d . . P . .

O6B O2- 0.3435(2) 0.11837(11) 0.5944(4) 0.0118(5) Uani 0.8(2) 1 d . . P . .

O7A O 0.3361(3) 0.0000 0.2858(6) 0.0134(8) Uani 0.01(11) 2 d S T P . .

O7B O2- 0.3361(3) 0.0000 0.2858(6) 0.0134(8) Uani 0.99(11) 2 d S T P . .

T1A Al 0.28034(7) 0.08481(4) 0.29774(14) 0.0057(2) Uani 0.02(13) 1 d . . P . .

T1B Si 0.28034(7) 0.08481(4) 0.29774(14) 0.0057(2) Uani 0.10(13) 1 d . . P . .

T1C Al3+ 0.28034(7) 0.08481(4) 0.29774(14) 0.0057(2) Uani 0.18(13) 1 d . . P . .

T1D Si4+ 0.28034(7) 0.08481(4) 0.29774(14) 0.0057(2) Uani 0.70(13) 1 d . . P . .

T2A Si 0.29007(7) 0.17183(4) 0.80727(13) 0.0065(2) Uani 0.37(12) 1 d . . P . .

T2B Si4+ 0.29007(7) 0.17183(4) 0.80727(13) 0.0065(2) Uani 0.63(12) 1 d . . P . .

M1A Mg2+ 0.0000 0.08892(5) 0.5000 0.0078(2) Uani 0.730(5) 2 d S T P . .

M1B Fe2+ 0.0000 0.08892(5) 0.5000 0.0078(2) Uani 0.270(5) 2 d S T P . .

M2A Mg2+ 0.0000 0.17739(5) 0.0000 0.0065(3) Uani 0.683(5) 2 d S T P . .

M2B Al3+ 0.0000 0.17739(5) 0.0000 0.0065(3) Uani 0.121(5) 2 d S T P . .

M2C Fe2+ 0.0000 0.17739(5) 0.0000 0.0065(3) Uani 0.098(5) 2 d S T P . .

M2D Fe3+ 0.0000 0.17739(5) 0.0000 0.0065(3) Uani 0.098(5) 2 d S T P . .

M3A Mg2+ 0.0000 0.0000 0.0000 0.0072(4) Uani 0.686(4) 4 d S T P . .

M3B Fe2+ 0.0000 0.0000 0.0000 0.0072(4) Uani 0.220(4) 4 d S T P . .

M3C Fe3+ 0.0000 0.0000 0.0000 0.0072(4) Uani 0.094(4) 4 d S T P . .

M4A Na+ 0.0000 0.27851(5) 0.5000 0.0097(2) Uani 0.123(11) 2 d S T P . .

M4B Ca2+ 0.0000 0.27851(5) 0.5000 0.0097(2) Uani 0.877(11) 2 d S T P . .

A Na+ 0.0000 0.5000 0.0000 0.025 Uiso 0.081(7) 4 d S . P . .

AM Na+ 0.028(6) 0.5000 0.081(14) 0.025 Uiso 0.038(5) 2 d S . P . .

A2 Na+ 0.0000 0.478(2) 0.0000 0.025 Uiso 0.076(5) 2 d S . P . .

M42 Fe2+ 0.0000 0.2549(10) 0.5000 0.013 Uiso 0.045(2) 2 d S . P . .

H H 0.196(6) 0.0000 0.758(10) 0.013 Uiso 0.98 2 d S . P . .

loop\_

 \_atom\_site\_aniso\_label

 \_atom\_site\_aniso\_U\_11

 \_atom\_site\_aniso\_U\_22

 \_atom\_site\_aniso\_U\_33

 \_atom\_site\_aniso\_U\_12

 \_atom\_site\_aniso\_U\_13

 \_atom\_site\_aniso\_U\_23

O1A 0.0087(8) 0.0131(8) 0.0075(8) -0.0021(7) 0.0025(6) -0.0010(7)

O1B 0.0087(8) 0.0131(8) 0.0075(8) -0.0021(7) 0.0025(6) -0.0010(7)

O2A 0.0072(8) 0.0094(8) 0.0098(8) 0.0010(6) 0.0018(6) 0.0014(7)

O2B 0.0072(8) 0.0094(8) 0.0098(8) 0.0010(6) 0.0018(6) 0.0014(7)

O3A 0.0112(14) 0.0098(13) 0.0101(13) 0.0000 0.0033(10) 0.0000

O3B 0.0112(14) 0.0098(13) 0.0101(13) 0.0000 0.0033(10) 0.0000

O4A 0.0153(9) 0.0086(8) 0.0124(9) -0.0024(7) 0.0045(7) 0.0000(7)

O4B 0.0153(9) 0.0086(8) 0.0124(9) -0.0024(7) 0.0045(7) 0.0000(7)

O5A 0.0083(8) 0.0165(8) 0.0110(8) 0.0012(7) 0.0019(7) 0.0058(7)

O5B 0.0083(8) 0.0165(8) 0.0110(8) 0.0012(7) 0.0019(7) 0.0058(7)

O6A 0.0076(8) 0.0154(8) 0.0122(9) 0.0000(7) 0.0023(7) -0.0034(7)

O6B 0.0076(8) 0.0154(8) 0.0122(9) 0.0000(7) 0.0023(7) -0.0034(7)

O7A 0.0118(12) 0.0089(12) 0.0192(14) 0.0000 0.0037(11) 0.0000

O7B 0.0118(12) 0.0089(12) 0.0192(14) 0.0000 0.0037(11) 0.0000

T1A 0.0054(3) 0.0060(3) 0.0059(3) -0.0003(3) 0.0015(2) 0.0005(2)

T1B 0.0054(3) 0.0060(3) 0.0059(3) -0.0003(3) 0.0015(2) 0.0005(2)

T1C 0.0054(3) 0.0060(3) 0.0059(3) -0.0003(3) 0.0015(2) 0.0005(2)

T1D 0.0054(3) 0.0060(3) 0.0059(3) -0.0003(3) 0.0015(2) 0.0005(2)

T2A 0.0062(3) 0.0068(3) 0.0068(3) -0.0007(3) 0.0021(2) 0.0007(2)

T2B 0.0062(3) 0.0068(3) 0.0068(3) -0.0007(3) 0.0021(2) 0.0007(2)

M1A 0.0096(4) 0.0078(3) 0.0068(4) 0.0000 0.0034(3) 0.0000

M1B 0.0096(4) 0.0078(3) 0.0068(4) 0.0000 0.0034(3) 0.0000

M2A 0.0074(5) 0.0055(5) 0.0073(5) 0.0000 0.0027(3) 0.0000

M2B 0.0074(5) 0.0055(5) 0.0073(5) 0.0000 0.0027(3) 0.0000

M2C 0.0074(5) 0.0055(5) 0.0073(5) 0.0000 0.0027(3) 0.0000

M2D 0.0074(5) 0.0055(5) 0.0073(5) 0.0000 0.0027(3) 0.0000

M3A 0.0086(6) 0.0066(7) 0.0067(6) 0.0000 0.0022(4) 0.0000

M3B 0.0086(6) 0.0066(7) 0.0067(6) 0.0000 0.0022(4) 0.0000

M3C 0.0086(6) 0.0066(7) 0.0067(6) 0.0000 0.0022(4) 0.0000

M4A 0.0104(4) 0.0096(3) 0.0114(4) 0.0000 0.0071(3) 0.0000

M4B 0.0104(4) 0.0096(3) 0.0114(4) 0.0000 0.0071(3) 0.0000

\_geom\_special\_details

;

 Geometry data (distances and angles) are reported only for T, M and A

 sites flagged by the A suffix.

 All esds are estimated using the full covariance matrix.

;

loop\_

 \_geom\_bond\_atom\_site\_label\_1

 \_geom\_bond\_atom\_site\_label\_2

 \_geom\_bond\_distance

 \_geom\_bond\_site\_symmetry\_2

 \_geom\_bond\_publ\_flag

T1A O1A 1.630(2) . ?

T1A O7A 1.6337(12) . ?

T1A O6A 1.651(2) . ?

T1A O5A 1.657(2) . ?

T2A O4A 1.598(2) . ?

T2A O2A 1.623(2) . ?

T2A O5A 1.648(2) 1\_556 ?

T2A O6A 1.668(2) . ?

M1A O1A 2.060(2) 6\_556 ?

M1A O1A 2.060(2) . ?

M1A O3A 2.105(2) 5\_556 ?

M1A O3A 2.105(2) . ?

M1A O2A 2.106(2) 6\_556 ?

M1A O2A 2.106(2) . ?

M2A O4A 1.992(2) 7\_556 ?

M2A O4A 1.992(2) 4\_454 ?

M2A O2A 2.072(2) 6\_556 ?

M2A O2A 2.072(2) 1\_554 ?

M2A O1A 2.107(2) . ?

M2A O1A 2.107(2) 6 ?

M3A O3A 2.075(3) 5\_556 ?

M3A O3A 2.075(3) 1\_554 ?

M3A O1A 2.086(2) 5 ?

M3A O1A 2.086(2) 2 ?

M3A O1A 2.086(2) 6 ?

M3A O1A 2.086(2) . ?

M4A O4A 2.304(2) 4\_455 ?

M4A O4A 2.304(2) 7\_556 ?

M4A O2A 2.400(2) . ?

M4A O2A 2.400(2) 6\_556 ?

M4A O6A 2.545(2) 7\_556 ?

M4A O6A 2.545(2) 4\_455 ?

M4A O5A 2.723(2) 7\_556 ?

M4A O5A 2.723(2) 4\_455 ?

A O7A 2.477(3) 3\_455 ?

A O7A 2.477(3) 7 ?

A O5A 3.003(2) 8 ?

A O5A 3.003(2) 4\_455 ?

A O5A 3.003(2) 3\_455 ?

A O5A 3.003(2) 7 ?

A O6A 3.142(2) 8\_556 ?

A O6A 3.142(2) 4\_454 ?

A O6A 3.142(2) 3\_454 ?

A O6A 3.142(2) 7\_556 ?

AM O7A 2.40(5) 3\_455 ?

AM O7A 2.63(6) 7 ?

AM O6A 2.83(5) 8\_556 ?

AM O6A 2.83(5) 7\_556 ?

AM O5A 3.02(3) 8 ?

AM O5A 3.02(3) 7 ?

AM O5A 3.05(3) 4\_455 ?

AM O5A 3.05(3) 3\_455 ?

AM O7A 3.28(7) 7\_556 ?

A2 O7A 2.507(6) 3\_455 ?

A2 O7A 2.507(6) 7 ?

A2 O5A 2.69(3) 4\_455 ?

A2 O5A 2.69(3) 7 ?

A2 O6A 2.89(2) 4\_454 ?

A2 O6A 2.89(2) 7\_556 ?

M42 O2A 2.077(13) . ?

M42 O2A 2.077(13) 6\_556 ?

M42 O4A 2.253(2) 4\_455 ?

M42 O4A 2.253(2) 7\_556 ?

M42 O6A 2.872(14) 7\_556 ?

M42 O6A 2.872(14) 4\_455 ?

M42 O5A 2.985(12) 7\_556 ?

M42 O5A 2.985(12) 4\_455 ?

O3A H 0.81(6) . ?

loop\_

 \_geom\_angle\_atom\_site\_label\_1

 \_geom\_angle\_atom\_site\_label\_2

 \_geom\_angle\_atom\_site\_label\_3

 \_geom\_angle

 \_geom\_angle\_site\_symmetry\_1

 \_geom\_angle\_site\_symmetry\_3

 \_geom\_angle\_publ\_flag

O1A T1A O7A 110.86(12) . . ?

O1A T1A O6A 110.76(10) . . ?

O7A T1A O6A 109.44(13) . . ?

O1A T1A O5A 111.50(10) . . ?

O7A T1A O5A 108.23(12) . . ?

O6A T1A O5A 105.90(10) . . ?

O4A T2A O2A 116.96(11) . . ?

O4A T2A O5A 109.45(11) . 1\_556 ?

O2A T2A O5A 109.39(10) . 1\_556 ?

O4A T2A O6A 103.11(10) . . ?

O2A T2A O6A 108.64(10) . . ?

O5A T2A O6A 108.91(10) 1\_556 . ?

O1A M1A O1A 179.01(11) 6\_556 . ?

O1A M1A O3A 95.45(9) 6\_556 5\_556 ?

O1A M1A O3A 83.79(9) . 5\_556 ?

O1A M1A O3A 83.79(9) 6\_556 . ?

O1A M1A O3A 95.45(9) . . ?

O3A M1A O3A 80.51(12) 5\_556 . ?

O1A M1A O2A 96.39(7) 6\_556 6\_556 ?

O1A M1A O2A 84.32(7) . 6\_556 ?

O3A M1A O2A 95.92(8) 5\_556 6\_556 ?

O3A M1A O2A 176.42(9) . 6\_556 ?

O1A M1A O2A 84.32(7) 6\_556 . ?

O1A M1A O2A 96.39(7) . . ?

O3A M1A O2A 176.42(9) 5\_556 . ?

O3A M1A O2A 95.92(8) . . ?

O2A M1A O2A 87.65(10) 6\_556 . ?

O4A M2A O4A 95.73(12) 7\_556 4\_454 ?

O4A M2A O2A 92.50(8) 7\_556 6\_556 ?

O4A M2A O2A 90.42(8) 4\_454 6\_556 ?

O4A M2A O2A 90.42(8) 7\_556 1\_554 ?

O4A M2A O2A 92.50(8) 4\_454 1\_554 ?

O2A M2A O2A 175.64(12) 6\_556 1\_554 ?

O4A M2A O1A 92.51(7) 7\_556 . ?

O4A M2A O1A 170.26(9) 4\_454 . ?

O2A M2A O1A 84.01(7) 6\_556 . ?

O2A M2A O1A 92.63(7) 1\_554 . ?

O4A M2A O1A 170.26(9) 7\_556 6 ?

O4A M2A O1A 92.51(7) 4\_454 6 ?

O2A M2A O1A 92.63(7) 6\_556 6 ?

O2A M2A O1A 84.01(7) 1\_554 6 ?

O1A M2A O1A 79.81(11) . 6 ?

O3A M3A O3A 180.0 5\_556 1\_554 ?

O3A M3A O1A 96.11(7) 5\_556 5 ?

O3A M3A O1A 83.89(7) 1\_554 5 ?

O3A M3A O1A 83.89(7) 5\_556 2 ?

O3A M3A O1A 96.11(7) 1\_554 2 ?

O1A M3A O1A 80.77(10) 5 2 ?

O3A M3A O1A 96.11(7) 5\_556 6 ?

O3A M3A O1A 83.89(7) 1\_554 6 ?

O1A M3A O1A 99.23(10) 5 6 ?

O1A M3A O1A 180.0 2 6 ?

O3A M3A O1A 83.89(7) 5\_556 . ?

O3A M3A O1A 96.11(7) 1\_554 . ?

O1A M3A O1A 180.0 5 . ?

O1A M3A O1A 99.23(10) 2 . ?

O1A M3A O1A 80.77(10) 6 . ?

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