data\_b7

\_audit\_creation\_method SHELXL-97

\_chemical\_name\_systematic

;

?

;

\_chemical\_name\_common ?

\_chemical\_melting\_point ?

\_chemical\_formula\_moiety ?

\_chemical\_formula\_sum

'Ca1.48 Fe6.01 Mg0.44 Mn4.06 O232 P8'

\_chemical\_formula\_weight 1388.37

loop\_

\_atom\_type\_symbol

\_atom\_type\_description

\_atom\_type\_scat\_dispersion\_real

\_atom\_type\_scat\_dispersion\_imag

\_atom\_type\_scat\_source

'O' 'O2-' 0.0080 0.0060

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'P' 'P' 0.1023 0.0942

'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'

'Mn' 'Mn' 0.3368 0.7283

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Fe' 'Fe' 0.3463 0.8444

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Mg' 'Mg' 0.0486 0.0363

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting ?

\_symmetry\_space\_group\_name\_H-M ?

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 8.8072(10)

\_cell\_length\_b 11.5131(10)

\_cell\_length\_c 6.1372(10)

\_cell\_angle\_alpha 90.00

\_cell\_angle\_beta 99.24

\_cell\_angle\_gamma 90.00

\_cell\_volume 614.22(13)

\_cell\_formula\_units\_Z 1

\_cell\_measurement\_temperature 293(2)

\_cell\_measurement\_reflns\_used ?

\_cell\_measurement\_theta\_min ?

\_cell\_measurement\_theta\_max ?

\_exptl\_crystal\_description ?

\_exptl\_crystal\_colour ?

\_exptl\_crystal\_size\_max ?

\_exptl\_crystal\_size\_mid ?

\_exptl\_crystal\_size\_min ?

\_exptl\_crystal\_density\_meas ?

\_exptl\_crystal\_density\_diffrn 3.753

\_exptl\_crystal\_density\_method 'not measured'

\_exptl\_crystal\_F\_000 718

\_exptl\_absorpt\_coefficient\_mu 6.426

\_exptl\_absorpt\_correction\_type ?

\_exptl\_absorpt\_correction\_T\_min ?

\_exptl\_absorpt\_correction\_T\_max ?

\_exptl\_absorpt\_process\_details ?

\_exptl\_special\_details

;

?

;

\_diffrn\_ambient\_temperature 293(2)

\_diffrn\_radiation\_wavelength 0.71073

\_diffrn\_radiation\_type MoK\a

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

\_diffrn\_radiation\_monochromator graphite

\_diffrn\_measurement\_device\_type ?

\_diffrn\_measurement\_method ?

\_diffrn\_detector\_area\_resol\_mean ?

\_diffrn\_reflns\_number 1965

\_diffrn\_reflns\_av\_R\_equivalents 0.0233

\_diffrn\_reflns\_av\_sigmaI/netI 0.0533

\_diffrn\_reflns\_limit\_h\_min -12

\_diffrn\_reflns\_limit\_h\_max 12

\_diffrn\_reflns\_limit\_k\_min 0

\_diffrn\_reflns\_limit\_k\_max 16

\_diffrn\_reflns\_limit\_l\_min 0

\_diffrn\_reflns\_limit\_l\_max 8

\_diffrn\_reflns\_theta\_min 2.94

\_diffrn\_reflns\_theta\_max 30.06

\_reflns\_number\_total 1809

\_reflns\_number\_gt 1331

\_reflns\_threshold\_expression >2sigma(I)

\_computing\_data\_collection ?

\_computing\_cell\_refinement ?

\_computing\_data\_reduction ?

\_computing\_structure\_solution 'SHELXS-97 (Sheldrick, 2008)'

\_computing\_structure\_refinement 'SHELXL-97 (Sheldrick, 2008)'

\_computing\_molecular\_graphics ?

\_computing\_publication\_material ?

\_refine\_special\_details

;

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

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.

;

\_refine\_ls\_structure\_factor\_coef Fsqd

\_refine\_ls\_matrix\_type full

\_refine\_ls\_weighting\_scheme calc

\_refine\_ls\_weighting\_details

'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'

\_atom\_sites\_solution\_primary direct

\_atom\_sites\_solution\_secondary difmap

\_atom\_sites\_solution\_hydrogens geom

\_refine\_ls\_hydrogen\_treatment mixed

\_refine\_ls\_extinction\_method none

\_refine\_ls\_extinction\_coef ?

\_refine\_ls\_number\_reflns 1809

\_refine\_ls\_number\_parameters 121

\_refine\_ls\_number\_restraints 0

\_refine\_ls\_R\_factor\_all 0.0582

\_refine\_ls\_R\_factor\_gt 0.0383

\_refine\_ls\_wR\_factor\_ref 0.1137

\_refine\_ls\_wR\_factor\_gt 0.1013

\_refine\_ls\_goodness\_of\_fit\_ref 0.733

\_refine\_ls\_restrained\_S\_all 0.733

\_refine\_ls\_shift/su\_max 7.059

\_refine\_ls\_shift/su\_mean 0.058

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\_symmetry\_multiplicity

\_atom\_site\_calc\_flag

\_atom\_site\_refinement\_flags

\_atom\_site\_disorder\_assembly

\_atom\_site\_disorder\_group

M1CA Ca 0.94553(10) 0.11949(7) 0.83855(14) 0.0177(2) Uani 0.296(18) 1 d P . .

M1MN Mn 0.94553(10) 0.11949(7) 0.83855(14) 0.0177(2) Uani 0.704(18) 1 d P . .

M2 Fe 0.71681(9) 0.07890(7) 0.32800(11) 0.0206(3) Uani 0.978(4) 1 d P . .

M3 Mn 0.36221(8) 0.19132(6) 0.12839(11) 0.0122(2) Uani 1.000(4) 1 d . . .

P1 P 0.09324(13) 0.13515(10) 0.39559(17) 0.0092(3) Uani 1 1 d . . .

P2 P 0.60317(12) 0.08852(10) 0.80651(17) 0.0085(3) Uani 1 1 d . . .

O1 O2- 0.0785(4) 0.0684(3) 0.1771(6) 0.0156(7) Uani 1 1 d . . .

O2 O2- 0.4761(4) 0.1766(3) 0.8296(5) 0.0125(6) Uani 1 1 d . . .

03 O2- 0.9415(4) 0.1965(3) 0.4193(6) 0.0211(8) Uani 1 1 d . . .

04 O2- 0.6926(4) 0.1269(3) 0.6237(5) 0.0132(6) Uani 1 1 d . . .

05 O2- 0.2170(4) 0.2278(3) 0.3815(6) 0.0182(7) Uani 1 1 d . . .

06 O2- 0.7262(4) 0.0887(3) 0.0154(5) 0.0122(6) Uani 1 1 d . . .

07 O2- 0.1384(4) 0.0600(3) 0.5998(6) 0.0201(8) Uani 1 1 d . . .

O8 O2- 0.5339(4) -0.0346(3) 0.7629(5) 0.0107(6) Uani 1 1 d . . .

loop\_

\_atom\_site\_aniso\_label

\_atom\_site\_aniso\_U\_11

\_atom\_site\_aniso\_U\_22

\_atom\_site\_aniso\_U\_33

\_atom\_site\_aniso\_U\_23

\_atom\_site\_aniso\_U\_13

\_atom\_site\_aniso\_U\_12

M1CA 0.0194(4) 0.0133(4) 0.0185(4) -0.0040(3) -0.0032(3) 0.0018(3)

M1MN 0.0194(4) 0.0133(4) 0.0185(4) -0.0040(3) -0.0032(3) 0.0018(3)

M2 0.0219(4) 0.0353(5) 0.0049(3) 0.0003(3) 0.0027(3) 0.0087(3)

M3 0.0154(4) 0.0134(3) 0.0076(3) 0.0000(2) 0.0017(2) 0.0020(2)

P1 0.0097(5) 0.0119(5) 0.0064(4) -0.0003(4) 0.0025(4) -0.0005(4)

P2 0.0093(5) 0.0117(5) 0.0046(4) 0.0004(4) 0.0016(4) 0.0007(4)

O1 0.0222(17) 0.0159(15) 0.0089(14) -0.0041(12) 0.0032(13) -0.0007(13)

O2 0.0108(14) 0.0184(16) 0.0084(14) 0.0014(12) 0.0015(11) 0.0062(12)

03 0.0129(16) 0.033(2) 0.0190(17) -0.0066(15) 0.0074(14) 0.0051(14)

04 0.0153(15) 0.0206(16) 0.0051(13) -0.0001(12) 0.0057(12) -0.0021(13)

05 0.0237(18) 0.0198(17) 0.0121(15) 0.0003(13) 0.0063(14) -0.0119(14)

06 0.0117(14) 0.0205(16) 0.0044(13) -0.0001(12) 0.0018(11) 0.0003(12)

07 0.031(2) 0.0163(17) 0.0114(15) 0.0048(13) -0.0003(14) -0.0060(15)

O8 0.0108(14) 0.0114(14) 0.0104(13) -0.0011(11) 0.0028(11) -0.0018(11)

\_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.

;

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

M1CA O1 2.174(3) 3\_656 ?

M1CA 03 2.177(4) 4\_566 ?

M1CA O1 2.292(4) 1\_656 ?

M1CA 06 2.389(3) 1\_556 ?

M1CA 04 2.401(3) . ?

M1CA 07 2.510(4) 1\_655 ?

M1CA 03 2.716(4) . ?

M1CA 05 2.946(4) 4\_666 ?

M1CA P2 3.0112(14) . ?

M1CA P1 3.1062(14) 4\_666 ?

M1CA P1 3.2018(14) 1\_655 ?

M1CA P1 3.2586(14) 3\_656 ?

M1MN O1 2.174(3) 3\_656 ?

M1MN 03 2.177(4) 4\_566 ?

M1MN O1 2.292(4) 1\_656 ?

M1MN 06 2.389(3) 1\_556 ?

M1MN 04 2.401(3) . ?

M1MN 07 2.510(4) 1\_655 ?

M1MN M1CA 3.4362(16) 3\_757 ?

M1MN M2 3.4737(11) . ?

M1MN M2 3.9043(13) 1\_556 ?

M1MN M2 4.0098(12) 4\_566 ?

M1MN M2 4.0103(12) 3\_756 ?

M2 06 1.937(3) . ?

M2 04 1.941(3) . ?

M2 07 2.049(4) 3\_656 ?

M2 O8 2.247(3) 3\_656 ?

M2 03 2.389(4) . ?

M2 P2 3.1981(13) 1\_554 ?

M2 P2 3.2531(13) . ?

M2 P1 3.2920(14) 3\_656 ?

M2 P1 3.3378(14) 1\_655 ?

M2 P2 3.4046(14) 3\_656 ?

M2 M3 3.4206(11) . ?

M2 O2 3.456(4) 3\_656 ?

M2 O1 3.459(4) 1\_655 ?

M2 O2 3.525(3) 4\_565 ?

M2 O8 3.579(3) . ?

M2 04 3.606(3) 4\_565 ?

M2 O2 3.610(3) 1\_554 ?

M2 O1 3.687(4) 3\_656 ?

M2 O8 3.813(3) 1\_554 ?

M2 07 3.824(4) 1\_655 ?

M2 M1CA 3.9043(13) 1\_554 ?

M2 M1MN 3.9043(13) 1\_554 ?

M2 P2 3.9545(14) 4\_565 ?

M2 05 3.956(4) 3\_656 ?

M2 06 3.993(3) 4\_566 ?

M2 M1CA 4.0098(12) 4\_565 ?

M2 M1MN 4.0098(12) 4\_565 ?

M2 M1MN 4.0103(12) 3\_756 ?

M2 M1CA 4.0103(12) 3\_756 ?

M2 O2 4.163(3) . ?

M2 M3 4.1692(11) 3\_655 ?

M2 O1 4.187(3) 3\_655 ?

M2 06 4.208(3) 1\_556 ?

M2 03 4.299(4) 4\_565 ?

M2 05 4.310(4) 2\_645 ?

M2 04 4.329(3) 1\_554 ?

M2 04 4.364(3) 3\_656 ?

M2 03 4.474(4) 3\_756 ?

M3 05 2.043(3) 4\_565 ?

M3 O8 2.084(3) 3\_656 ?

M3 O2 2.109(3) 4\_565 ?

M3 05 2.205(4) . ?

M3 O2 2.234(3) 1\_554 ?

M3 M2 4.1692(11) 3\_655 ?

M3 M2 4.5306(12) 2\_655 ?

M3 M2 4.6904(11) 4\_565 ?

M3 M2 4.6946(11) 3\_656 ?

M3 M2 5.5569(11) 4\_566 ?

P1 07 1.522(4) . ?

P1 O1 1.533(3) . ?

P1 03 1.539(4) 1\_455 ?

P1 05 1.538(3) . ?

P1 M1CA 3.1062(14) 4\_465 ?

P1 M1CA 3.2018(14) 1\_455 ?

P1 M1CA 3.2587(14) 3\_656 ?

P1 M2 3.2921(14) 3\_656 ?

P1 M2 3.3378(14) 1\_455 ?

P1 M1CA 3.4617(14) 1\_454 ?

P1 M2 5.5004(14) 4\_465 ?

P1 M2 5.5659(14) 3\_655 ?

P2 O2 1.533(3) . ?

P2 04 1.535(3) . ?

P2 06 1.540(3) 1\_556 ?

P2 O8 1.550(3) . ?

P2 M2 3.1981(14) 1\_556 ?

P2 M2 3.4045(14) 3\_656 ?

P2 M2 3.9545(14) 4\_566 ?

O1 M1MN 2.174(3) 3\_656 ?

O1 M1CA 2.174(3) 3\_656 ?

O1 M1CA 2.292(4) 1\_454 ?

O1 M1MN 2.292(4) 1\_454 ?

O1 M2 3.459(4) 1\_455 ?

O1 M2 3.687(4) 3\_656 ?

O1 M2 4.187(3) 3\_655 ?

O2 M3 2.109(3) 4\_566 ?

O2 M3 2.234(3) 1\_556 ?

O2 M2 3.456(4) 3\_656 ?

O2 M2 3.525(3) 4\_566 ?

O2 M2 3.610(3) 1\_556 ?

03 P1 1.539(4) 1\_655 ?

03 M1MN 2.177(4) 4\_565 ?

03 M1CA 2.177(4) 4\_565 ?

03 M2 4.299(4) 4\_566 ?

03 M2 4.474(4) 3\_756 ?

03 M2 4.633(4) 4\_565 ?

04 M2 3.606(3) 4\_566 ?

04 M2 4.328(3) 1\_556 ?

04 M2 4.364(3) 3\_656 ?

05 M3 2.043(3) 4\_566 ?

05 M1CA 2.946(4) 4\_465 ?

05 M2 3.956(4) 3\_656 ?

05 M2 4.310(4) 2\_655 ?

05 M2 4.690(4) 1\_455 ?

06 P2 1.540(3) 1\_554 ?

06 M1CA 2.389(3) 1\_554 ?

06 M1MN 2.389(3) 1\_554 ?

06 M2 3.993(3) 4\_565 ?

06 M2 4.208(3) 1\_554 ?

06 M2 4.555(3) 3\_655 ?

07 M2 2.049(4) 3\_656 ?

07 M1CA 2.510(4) 1\_455 ?

07 M1MN 2.510(4) 1\_455 ?

07 M2 3.824(4) 1\_455 ?

O8 M3 2.084(3) 3\_656 ?

O8 M2 2.247(3) 3\_656 ?

O8 M2 3.813(3) 1\_556 ?

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

O1 M1CA 03 166.68(14) 3\_656 4\_566 ?

O1 M1CA O1 79.42(13) 3\_656 1\_656 ?

03 M1CA O1 93.91(13) 4\_566 1\_656 ?

O1 M1CA 06 78.03(12) 3\_656 1\_556 ?

03 M1CA 06 89.82(12) 4\_566 1\_556 ?

O1 M1CA 06 83.25(12) 1\_656 1\_556 ?

O1 M1CA 04 86.33(13) 3\_656 . ?

03 M1CA 04 92.45(13) 4\_566 . ?

O1 M1CA 04 143.20(12) 1\_656 . ?

06 M1CA 04 60.55(11) 1\_556 . ?

O1 M1CA 07 76.88(12) 3\_656 1\_655 ?

03 M1CA 07 115.83(13) 4\_566 1\_655 ?

O1 M1CA 07 99.45(12) 1\_656 1\_655 ?

06 M1CA 07 153.77(12) 1\_556 1\_655 ?

04 M1CA 07 110.14(11) . 1\_655 ?

O1 M1CA 03 107.25(12) 3\_656 . ?

03 M1CA 03 84.25(10) 4\_566 . ?

O1 M1CA 03 150.42(12) 1\_656 . ?

06 M1CA 03 126.17(11) 1\_556 . ?

04 M1CA 03 66.32(10) . . ?

07 M1CA 03 56.17(11) 1\_655 . ?

O1 M1CA 05 132.04(12) 3\_656 4\_666 ?

03 M1CA 05 56.06(11) 4\_566 4\_666 ?

O1 M1CA 05 77.47(11) 1\_656 4\_666 ?

06 M1CA 05 138.75(11) 1\_556 4\_666 ?

04 M1CA 05 134.13(11) . 4\_666 ?

07 M1CA 05 66.37(11) 1\_655 4\_666 ?

03 M1CA 05 77.11(11) . 4\_666 ?

O1 M1CA P2 77.88(10) 3\_656 . ?

03 M1CA P2 94.43(10) 4\_566 . ?

O1 M1CA P2 112.90(9) 1\_656 . ?

06 M1CA P2 30.46(8) 1\_556 . ?

04 M1CA P2 30.38(8) . . ?

07 M1CA P2 133.95(9) 1\_655 . ?

03 M1CA P2 96.67(8) . . ?

05 M1CA P2 150.06(7) 4\_666 . ?

O1 M1CA P1 161.05(10) 3\_656 4\_666 ?

03 M1CA P1 27.30(9) 4\_566 4\_666 ?

O1 M1CA P1 89.30(9) 1\_656 4\_666 ?

06 M1CA P1 115.99(9) 1\_556 4\_666 ?

04 M1CA P1 111.38(9) . 4\_666 ?

07 M1CA P1 90.19(9) 1\_655 4\_666 ?

03 M1CA P1 75.61(9) . 4\_666 ?

05 M1CA P1 29.28(7) 4\_666 4\_666 ?

P2 M1CA P1 120.79(4) . 4\_666 ?

O1 M1CA P1 93.92(10) 3\_656 1\_655 ?

03 M1CA P1 99.34(10) 4\_566 1\_655 ?

O1 M1CA P1 124.48(9) 1\_656 1\_655 ?

06 M1CA P1 149.60(8) 1\_556 1\_655 ?

04 M1CA P1 89.97(8) . 1\_655 ?

07 M1CA P1 27.67(8) 1\_655 1\_655 ?

03 M1CA P1 28.68(8) . 1\_655 ?

05 M1CA P1 66.90(7) 4\_666 1\_655 ?

P2 M1CA P1 119.37(4) . 1\_655 ?

P1 M1CA P1 79.90(4) 4\_666 1\_655 ?

O1 M1CA P1 23.48(9) 3\_656 3\_656 ?

03 M1CA P1 166.26(10) 4\_566 3\_656 ?

O1 M1CA P1 99.83(9) 1\_656 3\_656 ?

06 M1CA P1 91.82(8) 1\_556 3\_656 ?

04 M1CA P1 76.55(8) . 3\_656 ?

07 M1CA P1 61.97(8) 1\_655 3\_656 ?

03 M1CA P1 83.77(9) . 3\_656 ?

05 M1CA P1 127.05(7) 4\_666 3\_656 ?

P2 M1CA P1 80.31(3) . 3\_656 ?

P1 M1CA P1 151.67(3) 4\_666 3\_656 ?

P1 M1CA P1 72.80(4) 1\_655 3\_656 ?

O1 M1MN 03 166.68(14) 3\_656 4\_566 ?

O1 M1MN O1 79.42(13) 3\_656 1\_656 ?

03 M1MN O1 93.91(13) 4\_566 1\_656 ?

O1 M1MN 06 78.03(12) 3\_656 1\_556 ?

03 M1MN 06 89.82(12) 4\_566 1\_556 ?

O1 M1MN 06 83.25(12) 1\_656 1\_556 ?

O1 M1MN 04 86.33(13) 3\_656 . ?

03 M1MN 04 92.45(13) 4\_566 . ?

O1 M1MN 04 143.20(12) 1\_656 . ?

06 M1MN 04 60.55(11) 1\_556 . ?

O1 M1MN 07 76.88(12) 3\_656 1\_655 ?

03 M1MN 07 115.83(13) 4\_566 1\_655 ?

O1 M1MN 07 99.45(12) 1\_656 1\_655 ?

06 M1MN 07 153.77(12) 1\_556 1\_655 ?

04 M1MN 07 110.14(11) . 1\_655 ?

O1 M1MN M1CA 40.97(9) 3\_656 3\_757 ?

03 M1MN M1CA 131.38(11) 4\_566 3\_757 ?

O1 M1MN M1CA 38.45(8) 1\_656 3\_757 ?

06 M1MN M1CA 77.90(8) 1\_556 3\_757 ?

04 M1MN M1CA 119.57(9) . 3\_757 ?

07 M1MN M1CA 88.04(9) 1\_655 3\_757 ?

O1 M1MN M2 77.77(9) 3\_656 . ?

03 M1MN M2 107.93(10) 4\_566 . ?

O1 M1MN M2 157.07(9) 1\_656 . ?

06 M1MN M2 89.77(8) 1\_556 . ?

04 M1MN M2 32.54(7) . . ?

07 M1MN M2 77.61(9) 1\_655 . ?

M1CA M1MN M2 118.70(4) 3\_757 . ?

O1 M1MN M2 81.74(10) 3\_656 1\_556 ?

03 M1MN M2 84.95(10) 4\_566 1\_556 ?

O1 M1MN M2 61.53(9) 1\_656 1\_556 ?

06 M1MN M2 22.78(8) 1\_556 1\_556 ?

04 M1MN M2 83.04(8) . 1\_556 ?

07 M1MN M2 153.85(8) 1\_655 1\_556 ?

M1CA M1MN M2 65.87(3) 3\_757 1\_556 ?

M2 M1MN M2 112.44(3) . 1\_556 ?

O1 M1MN M2 144.68(10) 3\_656 4\_566 ?

03 M1MN M2 30.06(9) 4\_566 4\_566 ?

O1 M1MN M2 114.79(9) 1\_656 4\_566 ?

06 M1MN M2 72.25(8) 1\_556 4\_566 ?

04 M1MN M2 62.68(8) . 4\_566 ?

07 M1MN M2 127.74(8) 1\_655 4\_566 ?

M1CA M1MN M2 142.73(4) 3\_757 4\_566 ?

M2 M1MN M2 83.39(3) . 4\_566 ?

M2 M1MN M2 78.24(2) 1\_556 4\_566 ?

O1 M1MN M2 59.52(10) 3\_656 3\_756 ?

03 M1MN M2 130.71(10) 4\_566 3\_756 ?

O1 M1MN M2 78.06(9) 1\_656 3\_756 ?

06 M1MN M2 135.89(8) 1\_556 3\_756 ?

04 M1MN M2 122.74(8) . 3\_756 ?

07 M1MN M2 25.42(8) 1\_655 3\_756 ?

M1CA M1MN M2 62.69(3) 3\_757 3\_756 ?

M2 M1MN M2 92.28(3) . 3\_756 ?

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07 M2 O8 115.40(13) 3\_656 3\_656 ?

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04 M2 03 80.24(13) . . ?

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