data\_b5

\_audit\_creation\_method SHELXL-97

\_chemical\_name\_systematic

;

 ?

;

\_chemical\_name\_common ?

\_chemical\_melting\_point ?

\_chemical\_formula\_moiety ?

\_chemical\_formula\_sum

 'Ca2.32 Fe6.62 Mg0.59 Mn2.44 O232 P8'

\_chemical\_formula\_weight 1370.85

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 8.799

\_cell\_length\_b 11.570

\_cell\_length\_c 6.137

\_cell\_angle\_alpha 90.00

\_cell\_angle\_beta 99.32

\_cell\_angle\_gamma 90.00

\_cell\_volume 616.5

\_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 3.692

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

\_exptl\_crystal\_F\_000 712

\_exptl\_absorpt\_coefficient\_mu 6.134

\_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 1969

\_diffrn\_reflns\_av\_R\_equivalents 0.0113

\_diffrn\_reflns\_av\_sigmaI/netI 0.0217

\_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 2.93

\_diffrn\_reflns\_theta\_max 30.05

\_reflns\_number\_total 1813

\_reflns\_number\_gt 1592

\_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 1813

\_refine\_ls\_number\_parameters 121

\_refine\_ls\_number\_restraints 0

\_refine\_ls\_R\_factor\_all 0.0353

\_refine\_ls\_R\_factor\_gt 0.0302

\_refine\_ls\_wR\_factor\_ref 0.1067

\_refine\_ls\_wR\_factor\_gt 0.1022

\_refine\_ls\_goodness\_of\_fit\_ref 0.856

\_refine\_ls\_restrained\_S\_all 0.856

\_refine\_ls\_shift/su\_max 9.428

\_refine\_ls\_shift/su\_mean 0.078

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 0.94688(7) 0.12103(5) 0.83518(10) 0.01875(19) Uani 0.526(13) 1 d P . .

M1MN Mn 0.94688(7) 0.12103(5) 0.83518(10) 0.01875(19) Uani 0.474(13) 1 d P . .

M2 Fe 0.71462(6) 0.07891(5) 0.32686(8) 0.02071(19) Uani 0.960(3) 1 d P . .

M3 Mn 0.36258(5) 0.19165(4) 0.12925(7) 0.01262(17) Uani 1.000(3) 1 d . . .

P1 P 0.09476(8) 0.13445(7) 0.39630(12) 0.00999(19) Uani 1 1 d . . .

P2 P 0.60221(8) 0.08856(6) 0.80641(12) 0.00881(19) Uani 1 1 d . . .

O1 O2- 0.0798(3) 0.0690(2) 0.1773(4) 0.0158(5) Uani 1 1 d . . .

O2 O2- 0.4732(3) 0.17525(19) 0.8292(4) 0.0128(4) Uani 1 1 d . . .

03 O2- 0.9420(3) 0.1925(2) 0.4231(5) 0.0229(5) Uani 1 1 d . . .

04 O2- 0.6894(3) 0.1267(2) 0.6230(4) 0.0136(4) Uani 1 1 d . . .

05 O2- 0.2171(3) 0.2289(2) 0.3832(4) 0.0187(5) Uani 1 1 d . . .

06 O2- 0.7256(2) 0.08990(19) 0.0148(4) 0.0123(4) Uani 1 1 d . . .

07 O2- 0.1420(3) 0.0592(2) 0.5991(4) 0.0178(5) Uani 1 1 d . . .

O8 O2- 0.5350(3) -0.03489(19) 0.7647(4) 0.0125(4) 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 0.0193(3) 0.0126(3) 0.0215(3) -0.0042(2) -0.0052(2) 0.00203(19)

M1MN 0.0193(3) 0.0126(3) 0.0215(3) -0.0042(2) -0.0052(2) 0.00203(19)

M2 0.0212(3) 0.0340(3) 0.0071(3) 0.00027(18) 0.00263(18) 0.0083(2)

M3 0.0143(3) 0.0129(3) 0.0103(3) 0.00021(15) 0.00113(17) 0.00202(15)

P1 0.0088(3) 0.0121(3) 0.0091(3) -0.0009(2) 0.0017(2) -0.0007(2)

P2 0.0091(3) 0.0108(3) 0.0067(3) 0.0002(2) 0.0017(2) 0.0010(2)

O1 0.0198(11) 0.0159(10) 0.0118(10) -0.0039(8) 0.0027(8) -0.0009(8)

O2 0.0121(9) 0.0144(10) 0.0124(10) 0.0016(8) 0.0032(8) 0.0040(8)

03 0.0137(11) 0.0352(15) 0.0211(12) -0.0061(10) 0.0067(9) 0.0090(10)

04 0.0145(10) 0.0188(11) 0.0080(9) 0.0015(8) 0.0037(8) -0.0011(8)

05 0.0246(12) 0.0194(11) 0.0125(10) 0.0007(9) 0.0043(9) -0.0135(9)

06 0.0095(9) 0.0207(11) 0.0066(9) 0.0008(7) 0.0009(7) 0.0012(8)

07 0.0245(12) 0.0150(10) 0.0131(10) 0.0039(8) 0.0004(9) -0.0034(9)

O8 0.0128(9) 0.0130(10) 0.0120(9) 0.0004(7) 0.0031(7) -0.0005(8)

\_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 2.212(2) 3\_656 ?

M1CA 03 2.226(3) 4\_566 ?

M1CA O1 2.312(2) 1\_656 ?

M1CA 06 2.415(2) 1\_556 ?

M1CA 04 2.424(2) . ?

M1CA 07 2.523(3) 1\_655 ?

M1CA 03 2.654(3) . ?

M1CA 05 2.920(3) 4\_666 ?

M1CA P2 3.0326(9) . ?

M1CA P1 3.1112(9) 4\_666 ?

M1CA P1 3.1791(10) 1\_655 ?

M1CA P1 3.2743(9) 3\_656 ?

M1MN O1 2.212(2) 3\_656 ?

M1MN 03 2.226(3) 4\_566 ?

M1MN O1 2.312(2) 1\_656 ?

M1MN 06 2.415(2) 1\_556 ?

M1MN 04 2.424(2) . ?

M1MN 07 2.523(3) 1\_655 ?

M1MN M2 3.4757(8) . ?

M1MN M1CA 3.4925(12) 3\_757 ?

M1MN M2 3.9391(8) 1\_556 ?

M1MN M2 4.0213(8) 3\_756 ?

M1MN M2 4.0246(8) 4\_566 ?

M2 06 1.937(2) . ?

M2 04 1.946(2) . ?

M2 07 2.041(3) 3\_656 ?

M2 O8 2.236(2) 3\_656 ?

M2 03 2.386(3) . ?

M2 P2 3.1889(9) 1\_554 ?

M2 P2 3.2549(9) . ?

M2 P1 3.2971(9) 3\_656 ?

M2 P1 3.3647(9) 1\_655 ?

M2 P2 3.3848(9) 3\_656 ?

M2 M3 3.3986(7) . ?

M2 O2 3.433(2) 3\_656 ?

M2 O1 3.484(2) 1\_655 ?

M2 O2 3.552(2) 4\_565 ?

M2 O8 3.582(2) . ?

M2 O2 3.603(2) 1\_554 ?

M2 04 3.623(2) 4\_565 ?

M2 O1 3.698(2) 3\_656 ?

M2 O8 3.790(2) 1\_554 ?

M2 07 3.867(3) 1\_655 ?

M2 M1CA 3.9392(8) 1\_554 ?

M2 M1MN 3.9392(8) 1\_554 ?

M2 P2 3.9693(9) 4\_565 ?

M2 05 3.983(3) 3\_656 ?

M2 06 3.998(2) 4\_566 ?

M2 M1MN 4.0213(8) 3\_756 ?

M2 M1CA 4.0213(8) 3\_756 ?

M2 M1CA 4.0247(8) 4\_565 ?

M2 M1MN 4.0247(8) 4\_565 ?

M2 O2 4.169(2) . ?

M2 M3 4.1810(7) 3\_655 ?

M2 O1 4.194(2) 3\_655 ?

M2 06 4.209(2) 1\_556 ?

M2 05 4.321(2) 2\_645 ?

M2 04 4.325(2) 1\_554 ?

M2 03 4.329(3) 4\_565 ?

M2 04 4.330(2) 3\_656 ?

M2 03 4.455(3) 3\_756 ?

M3 05 2.034(2) 4\_565 ?

M3 O8 2.082(2) 3\_656 ?

M3 O2 2.107(2) 4\_565 ?

M3 05 2.214(3) . ?

M3 O2 2.226(2) 1\_554 ?

M3 M2 4.1810(7) 3\_655 ?

M3 M2 4.5464(7) 2\_655 ?

M3 M2 4.6848(7) 4\_565 ?

M3 M2 4.7049(7) 3\_656 ?

M3 M2 5.5385(7) 4\_566 ?

P1 07 1.520(2) . ?

P1 O1 1.529(2) . ?

P1 03 1.535(2) 1\_455 ?

P1 05 1.545(2) . ?

P1 M1CA 3.1111(9) 4\_465 ?

P1 M1CA 3.1791(10) 1\_455 ?

P1 M1CA 3.2744(9) 3\_656 ?

P1 M2 3.2971(9) 3\_656 ?

P1 M2 3.3647(9) 1\_455 ?

P1 M1CA 3.4820(9) 1\_454 ?

P1 M2 5.5329(9) 4\_465 ?

P1 M2 5.5691(9) 3\_655 ?

P2 04 1.527(2) . ?

P2 O2 1.538(2) . ?

P2 06 1.538(2) 1\_556 ?

P2 O8 1.551(2) . ?

P2 M2 3.1889(9) 1\_556 ?

P2 M2 3.3848(9) 3\_656 ?

P2 M2 3.9693(9) 4\_566 ?

O1 M1MN 2.212(2) 3\_656 ?

O1 M1CA 2.212(2) 3\_656 ?

O1 M1CA 2.312(2) 1\_454 ?

O1 M1MN 2.312(2) 1\_454 ?

O1 M2 3.484(2) 1\_455 ?

O1 M2 3.698(2) 3\_656 ?

O1 M2 4.194(2) 3\_655 ?

O2 M3 2.107(2) 4\_566 ?

O2 M3 2.226(2) 1\_556 ?

O2 M2 3.433(2) 3\_656 ?

O2 M2 3.552(2) 4\_566 ?

O2 M2 3.603(2) 1\_556 ?

03 P1 1.535(2) 1\_655 ?

03 M1MN 2.226(3) 4\_565 ?

03 M1CA 2.226(3) 4\_565 ?

03 M2 4.329(3) 4\_566 ?

03 M2 4.455(3) 3\_756 ?

03 M2 4.692(3) 4\_565 ?

04 M2 3.623(2) 4\_566 ?

04 M2 4.325(2) 1\_556 ?

04 M2 4.330(2) 3\_656 ?

05 M3 2.034(2) 4\_566 ?

05 M1CA 2.920(3) 4\_465 ?

05 M2 3.984(3) 3\_656 ?

05 M2 4.321(2) 2\_655 ?

05 M2 4.710(2) 1\_455 ?

06 P2 1.538(2) 1\_554 ?

06 M1CA 2.415(2) 1\_554 ?

06 M1MN 2.415(2) 1\_554 ?

06 M2 3.998(2) 4\_565 ?

06 M2 4.209(2) 1\_554 ?

06 M2 4.537(2) 3\_655 ?

07 M2 2.041(3) 3\_656 ?

07 M1CA 2.523(3) 1\_455 ?

07 M1MN 2.523(3) 1\_455 ?

07 M2 3.867(3) 1\_455 ?

O8 M3 2.082(2) 3\_656 ?

O8 M2 2.236(2) 3\_656 ?

O8 M2 3.790(2) 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 03 165.01(9) 3\_656 4\_566 ?

O1 M1CA O1 78.94(9) 3\_656 1\_656 ?

03 M1CA O1 93.37(9) 4\_566 1\_656 ?

O1 M1CA 06 77.21(8) 3\_656 1\_556 ?

03 M1CA 06 89.15(9) 4\_566 1\_556 ?

O1 M1CA 06 82.72(8) 1\_656 1\_556 ?

O1 M1CA 04 85.61(8) 3\_656 . ?

03 M1CA 04 92.91(9) 4\_566 . ?

O1 M1CA 04 141.85(8) 1\_656 . ?

06 M1CA 04 59.79(7) 1\_556 . ?

O1 M1CA 07 77.09(8) 3\_656 1\_655 ?

03 M1CA 07 117.11(9) 4\_566 1\_655 ?

O1 M1CA 07 99.01(8) 1\_656 1\_655 ?

06 M1CA 07 153.38(8) 1\_556 1\_655 ?

04 M1CA 07 111.28(8) . 1\_655 ?

O1 M1CA 03 106.94(9) 3\_656 . ?

03 M1CA 03 86.05(7) 4\_566 . ?

O1 M1CA 03 150.96(9) 1\_656 . ?

06 M1CA 03 126.26(8) 1\_556 . ?

04 M1CA 03 67.05(8) . . ?

07 M1CA 03 56.55(7) 1\_655 . ?

O1 M1CA 05 132.44(8) 3\_656 4\_666 ?

03 M1CA 05 56.41(8) 4\_566 4\_666 ?

O1 M1CA 05 77.24(8) 1\_656 4\_666 ?

06 M1CA 05 138.26(8) 1\_556 4\_666 ?

04 M1CA 05 135.47(8) . 4\_666 ?

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

03 M1CA 05 78.36(8) . 4\_666 ?

O1 M1CA P2 77.01(7) 3\_656 . ?

03 M1CA P2 94.34(7) 4\_566 . ?

O1 M1CA P2 112.01(6) 1\_656 . ?

06 M1CA P2 30.16(5) 1\_556 . ?

04 M1CA P2 29.93(5) . . ?

07 M1CA P2 134.32(6) 1\_655 . ?

03 M1CA P2 96.97(6) . . ?

05 M1CA P2 150.43(5) 4\_666 . ?

O1 M1CA P1 161.51(7) 3\_656 4\_666 ?

03 M1CA P1 27.58(7) 4\_566 4\_666 ?

O1 M1CA P1 89.25(6) 1\_656 4\_666 ?

06 M1CA P1 115.66(6) 1\_556 4\_666 ?

04 M1CA P1 112.11(6) . 4\_666 ?

07 M1CA P1 90.96(6) 1\_655 4\_666 ?

03 M1CA P1 76.91(7) . 4\_666 ?

05 M1CA P1 29.47(5) 4\_666 4\_666 ?

P2 M1CA P1 120.96(3) . 4\_666 ?

O1 M1CA P1 94.30(6) 3\_656 1\_655 ?

03 M1CA P1 100.65(7) 4\_566 1\_655 ?

O1 M1CA P1 124.47(6) 1\_656 1\_655 ?

06 M1CA P1 149.88(6) 1\_556 1\_655 ?

04 M1CA P1 91.07(6) . 1\_655 ?

07 M1CA P1 28.03(5) 1\_655 1\_655 ?

03 M1CA P1 28.76(5) . 1\_655 ?

05 M1CA P1 67.55(5) 4\_666 1\_655 ?

P2 M1CA P1 119.96(3) . 1\_655 ?

P1 M1CA P1 80.63(2) 4\_666 1\_655 ?

O1 M1CA P1 23.58(6) 3\_656 3\_656 ?

03 M1CA P1 167.14(7) 4\_566 3\_656 ?

O1 M1CA P1 99.43(6) 1\_656 3\_656 ?

06 M1CA P1 91.23(6) 1\_556 3\_656 ?

04 M1CA P1 76.24(6) . 3\_656 ?

07 M1CA P1 62.20(6) 1\_655 3\_656 ?

03 M1CA P1 83.37(6) . 3\_656 ?

05 M1CA P1 127.78(5) 4\_666 3\_656 ?

P2 M1CA P1 79.76(2) . 3\_656 ?

P1 M1CA P1 152.68(2) 4\_666 3\_656 ?

P1 M1CA P1 73.08(2) 1\_655 3\_656 ?

O1 M1MN 03 165.01(9) 3\_656 4\_566 ?

O1 M1MN O1 78.94(9) 3\_656 1\_656 ?

03 M1MN O1 93.37(9) 4\_566 1\_656 ?

O1 M1MN 06 77.21(8) 3\_656 1\_556 ?

03 M1MN 06 89.15(9) 4\_566 1\_556 ?

O1 M1MN 06 82.72(8) 1\_656 1\_556 ?

O1 M1MN 04 85.61(8) 3\_656 . ?

03 M1MN 04 92.91(9) 4\_566 . ?

O1 M1MN 04 141.85(8) 1\_656 . ?

06 M1MN 04 59.79(7) 1\_556 . ?

O1 M1MN 07 77.09(8) 3\_656 1\_655 ?

03 M1MN 07 117.11(9) 4\_566 1\_655 ?

O1 M1MN 07 99.01(8) 1\_656 1\_655 ?

06 M1MN 07 153.38(8) 1\_556 1\_655 ?

04 M1MN 07 111.28(8) . 1\_655 ?

O1 M1MN M2 77.63(6) 3\_656 . ?

03 M1MN M2 108.77(7) 4\_566 . ?

O1 M1MN M2 156.39(6) 1\_656 . ?

06 M1MN M2 89.34(6) 1\_556 . ?

04 M1MN M2 32.77(5) . . ?

07 M1MN M2 78.51(6) 1\_655 . ?

O1 M1MN M1CA 40.51(6) 3\_656 3\_757 ?

03 M1MN M1CA 130.59(8) 4\_566 3\_757 ?

O1 M1MN M1CA 38.43(6) 1\_656 3\_757 ?

06 M1MN M1CA 77.05(6) 1\_556 3\_757 ?

04 M1MN M1CA 118.17(6) . 3\_757 ?

07 M1MN M1CA 87.83(6) 1\_655 3\_757 ?

M2 M1MN M1CA 118.08(3) . 3\_757 ?

O1 M1MN M2 80.69(6) 3\_656 1\_556 ?

03 M1MN M2 84.33(7) 4\_566 1\_556 ?

O1 M1MN M2 61.38(6) 1\_656 1\_556 ?

06 M1MN M2 22.35(5) 1\_556 1\_556 ?

04 M1MN M2 81.91(5) . 1\_556 ?

07 M1MN M2 152.96(6) 1\_655 1\_556 ?

M2 M1MN M2 111.57(2) . 1\_556 ?

M1CA M1MN M2 65.20(2) 3\_757 1\_556 ?

O1 M1MN M2 59.88(6) 3\_656 3\_756 ?

03 M1MN M2 131.43(7) 4\_566 3\_756 ?

O1 M1MN M2 77.81(6) 1\_656 3\_756 ?

06 M1MN M2 135.34(6) 1\_556 3\_756 ?

04 M1MN M2 123.22(6) . 3\_756 ?

07 M1MN M2 25.13(5) 1\_655 3\_756 ?

M2 M1MN M2 92.797(18) . 3\_756 ?

M1CA M1MN M2 62.771(19) 3\_757 3\_756 ?

M2 M1MN M2 127.967(17) 1\_556 3\_756 ?

O1 M1MN M2 143.75(7) 3\_656 4\_566 ?

03 M1MN M2 30.38(7) 4\_566 4\_566 ?

O1 M1MN M2 114.66(6) 1\_656 4\_566 ?

06 M1MN M2 71.89(5) 1\_556 4\_566 ?

04 M1MN M2 62.70(6) . 4\_566 ?

07 M1MN M2 128.95(6) 1\_655 4\_566 ?

M2 M1MN M2 83.453(18) . 4\_566 ?

M1CA M1MN M2 141.89(3) 3\_757 4\_566 ?

M2 M1MN M2 77.938(17) 1\_556 4\_566 ?

M2 M1MN M2 152.63(2) 3\_756 4\_566 ?

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07 M2 O8 115.09(9) 3\_656 3\_656 ?

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