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 ?

M2 M1MN M2 128.56(2) 1\_556 3\_756 ?

M2 M1MN M2 151.68(3) 4\_566 3\_756 ?

06 M2 04 159.73(15) . . ?

06 M2 07 97.78(14) . 3\_656 ?

04 M2 07 100.25(14) . 3\_656 ?

06 M2 O8 87.94(13) . 3\_656 ?

04 M2 O8 92.62(13) . 3\_656 ?

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

06 M2 03 91.92(14) . . ?

04 M2 03 80.24(13) . . ?

07 M2 03 85.90(14) 3\_656 . ?

O8 M2 03 158.52(13) 3\_656 . ?

06 M2 P2 20.46(10) . 1\_554 ?

04 M2 P2 149.54(11) . 1\_554 ?

07 M2 P2 109.10(10) 3\_656 1\_554 ?

O8 M2 P2 67.81(8) 3\_656 1\_554 ?

03 M2 P2 109.23(10) . 1\_554 ?

06 M2 P2 163.86(11) . . ?

04 M2 P2 18.28(10) . . ?

07 M2 P2 95.88(11) 3\_656 . ?

O8 M2 P2 78.43(9) 3\_656 . ?

03 M2 P2 97.60(9) . . ?

P2 M2 P2 144.10(5) 1\_554 . ?

06 M2 P1 117.06(10) . 3\_656 ?

04 M2 P1 81.62(10) . 3\_656 ?

07 M2 P1 19.48(10) 3\_656 3\_656 ?

O8 M2 P1 110.84(9) 3\_656 3\_656 ?

03 M2 P1 88.30(10) . 3\_656 ?

P2 M2 P1 126.38(4) 1\_554 3\_656 ?

P2 M2 P1 76.40(3) . 3\_656 ?

06 M2 P1 84.95(10) . 1\_655 ?

04 M2 P1 94.85(10) . 1\_655 ?

07 M2 P1 63.47(10) 3\_656 1\_655 ?

O8 M2 P1 172.52(9) 3\_656 1\_655 ?

03 M2 P1 24.79(9) . 1\_655 ?

P2 M2 P1 105.22(3) 1\_554 1\_655 ?

P2 M2 P1 108.95(3) . 1\_655 ?

P1 M2 P1 70.66(3) 3\_656 1\_655 ?

06 M2 P2 87.61(10) . 3\_656 ?

04 M2 P2 100.19(10) . 3\_656 ?

07 M2 P2 94.16(11) 3\_656 3\_656 ?

O8 M2 P2 21.47(8) 3\_656 3\_656 ?

03 M2 P2 179.54(10) . 3\_656 ?

P2 M2 P2 70.31(3) 1\_554 3\_656 ?

P2 M2 P2 82.85(3) . 3\_656 ?

P1 M2 P2 91.92(4) 3\_656 3\_656 ?

P1 M2 P2 155.08(4) 1\_655 3\_656 ?

06 M2 M3 78.76(10) . . ?

04 M2 M3 89.78(10) . . ?

07 M2 M3 150.86(11) 3\_656 . ?

O8 M2 M3 36.18(8) 3\_656 . ?

03 M2 M3 122.93(10) . . ?

P2 M2 M3 60.50(3) 1\_554 . ?

P2 M2 M3 85.11(3) . . ?

P1 M2 M3 145.79(4) 3\_656 . ?

P1 M2 M3 143.38(4) 1\_655 . ?

P2 M2 M3 56.96(3) 3\_656 . ?

06 M2 O2 82.52(11) . 3\_656 ?

04 M2 O2 112.39(12) . 3\_656 ?

07 M2 O2 69.95(12) 3\_656 3\_656 ?

O8 M2 O2 47.01(10) 3\_656 3\_656 ?

03 M2 O2 154.10(10) . 3\_656 ?

P2 M2 O2 71.86(6) 1\_554 3\_656 ?

P2 M2 O2 94.18(6) . 3\_656 ?

P1 M2 O2 72.15(6) 3\_656 3\_656 ?

P1 M2 O2 129.33(6) 1\_655 3\_656 ?

P2 M2 O2 25.81(5) 3\_656 3\_656 ?

M3 M2 O2 80.93(6) . 3\_656 ?

06 M2 O1 63.19(11) . 1\_655 ?

04 M2 O1 120.29(12) . 1\_655 ?

07 M2 O1 57.50(12) 3\_656 1\_655 ?

O8 M2 O1 146.69(10) 3\_656 1\_655 ?

03 M2 O1 47.09(10) . 1\_655 ?

P2 M2 O1 83.50(6) 1\_554 1\_655 ?

P2 M2 O1 132.30(6) . 1\_655 ?

P1 M2 O1 72.43(6) 3\_656 1\_655 ?

P1 M2 O1 25.99(6) 1\_655 1\_655 ?

P2 M2 O1 132.62(6) 3\_656 1\_655 ?

M3 M2 O1 138.10(6) . 1\_655 ?

O2 M2 O1 109.13(8) 3\_656 1\_655 ?

06 M2 M1MN 140.78(11) . . ?

04 M2 M1MN 41.69(10) . . ?

07 M2 M1MN 70.09(10) 3\_656 . ?

O8 M2 M1MN 131.20(9) 3\_656 . ?

03 M2 M1MN 51.22(9) . . ?

P2 M2 M1MN 160.21(4) 1\_554 . ?

P2 M2 M1MN 53.06(3) . . ?

P1 M2 M1MN 57.51(3) 3\_656 . ?

P1 M2 M1MN 56.03(3) 1\_655 . ?

P2 M2 M1MN 129.23(3) 3\_656 . ?

M3 M2 M1MN 129.49(3) . . ?

O2 M2 M1MN 123.69(6) 3\_656 . ?

O1 M2 M1MN 79.67(6) 1\_655 . ?

06 M2 M1CA 140.78(11) . . ?

04 M2 M1CA 41.69(10) . . ?

07 M2 M1CA 70.09(10) 3\_656 . ?

O8 M2 M1CA 131.20(9) 3\_656 . ?

03 M2 M1CA 51.22(9) . . ?

P2 M2 M1CA 160.21(4) 1\_554 . ?

P2 M2 M1CA 53.06(3) . . ?

P1 M2 M1CA 57.51(3) 3\_656 . ?

P1 M2 M1CA 56.03(3) 1\_655 . ?

P2 M2 M1CA 129.23(3) 3\_656 . ?

M3 M2 M1CA 129.49(3) . . ?

O2 M2 M1CA 123.69(6) 3\_656 . ?

O1 M2 M1CA 79.67(6) 1\_655 . ?

M1MN M2 M1CA 0.00(3) . . ?

06 M2 O2 94.45(11) . 4\_565 ?

04 M2 O2 67.29(11) . 4\_565 ?

07 M2 O2 167.53(11) 3\_656 4\_565 ?

O8 M2 O2 67.33(10) 3\_656 4\_565 ?

03 M2 O2 91.28(10) . 4\_565 ?

P2 M2 O2 83.30(6) 1\_554 4\_565 ?

P2 M2 O2 72.42(6) . 4\_565 ?

P1 M2 O2 148.48(6) 3\_656 4\_565 ?

P1 M2 O2 115.49(6) 1\_655 4\_565 ?

P2 M2 O2 88.75(6) 3\_656 4\_565 ?

M3 M2 O2 35.30(5) . 4\_565 ?

O2 M2 O2 114.30(3) 3\_656 4\_565 ?

O1 M2 O2 127.50(8) 1\_655 4\_565 ?

M1MN M2 O2 98.74(6) . 4\_565 ?

M1CA M2 O2 98.74(6) . 4\_565 ?

06 M2 O8 148.88(12) . . ?

04 M2 O8 43.66(11) . . ?

07 M2 O8 83.85(12) 3\_656 . ?

O8 M2 O8 63.91(11) 3\_656 . ?

03 M2 O8 119.15(10) . . ?

P2 M2 O8 130.76(6) 1\_554 . ?

P2 M2 O8 25.65(5) . . ?

P1 M2 O8 66.10(6) 3\_656 . ?

P1 M2 O8 122.37(6) 1\_655 . ?

P2 M2 O8 61.31(5) 3\_656 . ?

M3 M2 O8 84.88(5) . . ?

O2 M2 O8 68.77(7) 3\_656 . ?

O1 M2 O8 136.98(8) 1\_655 . ?

M1MN M2 O8 69.01(5) . . ?

M1CA M2 O8 69.01(5) . . ?

O2 M2 O8 86.94(7) 4\_565 . ?

06 M2 04 67.07(11) . 4\_565 ?

04 M2 04 92.78(9) . 4\_565 ?

07 M2 04 143.93(12) 3\_656 4\_565 ?

O8 M2 04 97.24(10) 3\_656 4\_565 ?

03 M2 04 63.23(11) . 4\_565 ?

P2 M2 04 68.16(5) 1\_554 4\_565 ?

P2 M2 04 105.80(6) . 4\_565 ?

P1 M2 04 151.52(6) 3\_656 4\_565 ?

P1 M2 04 82.13(6) 1\_655 4\_565 ?

P2 M2 04 116.56(6) 3\_656 4\_565 ?

M3 M2 04 61.35(6) . 4\_565 ?

O2 M2 04 134.68(8) 3\_656 4\_565 ?

O1 M2 04 86.87(8) 1\_655 4\_565 ?

M1MN M2 04 100.40(6) . 4\_565 ?

M1CA M2 04 100.40(6) . 4\_565 ?

O2 M2 04 41.30(7) 4\_565 4\_565 ?

O8 M2 04 126.42(7) . 4\_565 ?

06 M2 O2 41.87(11) . 1\_554 ?

04 M2 O2 124.46(12) . 1\_554 ?

07 M2 O2 133.37(11) 3\_656 1\_554 ?

O8 M2 O2 55.98(10) 3\_656 1\_554 ?

03 M2 O2 111.94(11) . 1\_554 ?

P2 M2 O2 25.10(5) 1\_554 1\_554 ?

P2 M2 O2 122.03(6) . 1\_554 ?

P1 M2 O2 148.26(6) 3\_656 1\_554 ?

P1 M2 O2 118.76(6) 1\_655 1\_554 ?

P2 M2 O2 67.69(6) 3\_656 1\_554 ?

M3 M2 O2 36.93(5) . 1\_554 ?

O2 M2 O2 80.37(8) 3\_656 1\_554 ?

O1 M2 O2 102.98(8) 1\_655 1\_554 ?

M1MN M2 O2 154.02(6) . 1\_554 ?

M1CA M2 O2 154.02(6) . 1\_554 ?

O2 M2 O2 58.80(6) 4\_565 1\_554 ?

O8 M2 O2 118.18(7) . 1\_554 ?

04 M2 O2 54.48(8) 4\_565 1\_554 ?

06 M2 O1 138.57(12) . 3\_656 ?

04 M2 O1 58.21(11) . 3\_656 ?

07 M2 O1 42.09(11) 3\_656 3\_656 ?

O8 M2 O1 115.54(10) 3\_656 3\_656 ?

03 M2 O1 77.90(11) . 3\_656 ?

P2 M2 O1 150.86(6) 1\_554 3\_656 ?

P2 M2 O1 56.81(6) . 3\_656 ?

P1 M2 O1 24.55(5) 3\_656 3\_656 ?

P1 M2 O1 69.04(6) 1\_655 3\_656 ?

P2 M2 O1 102.45(6) 3\_656 3\_656 ?

M3 M2 O1 140.06(6) . 3\_656 ?

O2 M2 O1 89.57(8) 3\_656 3\_656 ?

O1 M2 O1 81.66(9) 1\_655 3\_656 ?

M1MN M2 O1 35.19(5) . 3\_656 ?

M1CA M2 O1 35.19(5) . 3\_656 ?

O2 M2 O1 125.44(8) 4\_565 3\_656 ?

O8 M2 O1 55.73(8) . 3\_656 ?

04 M2 O1 135.41(8) 4\_565 3\_656 ?

O2 M2 O1 169.83(8) 1\_554 3\_656 ?

06 M2 O8 36.69(11) . 1\_554 ?

04 M2 O8 148.66(11) . 1\_554 ?

07 M2 O8 94.96(11) 3\_656 1\_554 ?

O8 M2 O8 56.06(11) 3\_656 1\_554 ?

03 M2 O8 128.37(10) . 1\_554 ?

P2 M2 O8 23.51(5) 1\_554 1\_554 ?

P2 M2 O8 133.35(6) . 1\_554 ?

P1 M2 O8 108.52(6) 3\_656 1\_554 ?

P1 M2 O8 116.47(5) 1\_655 1\_554 ?

P2 M2 O8 51.17(5) 3\_656 1\_554 ?

M3 M2 O8 64.90(5) . 1\_554 ?

O2 M2 O8 48.46(7) 3\_656 1\_554 ?

O1 M2 O8 90.98(7) 1\_655 1\_554 ?

M1MN M2 O8 164.96(5) . 1\_554 ?

M1CA M2 O8 164.96(5) . 1\_554 ?

O2 M2 O8 96.30(7) 4\_565 1\_554 ?

O8 M2 O8 112.22(8) . 1\_554 ?

04 M2 O8 90.74(7) 4\_565 1\_554 ?

O2 M2 O8 39.75(7) 1\_554 1\_554 ?

O1 M2 O8 132.15(7) 3\_656 1\_554 ?

06 M2 07 104.02(12) . 1\_655 ?

04 M2 07 81.55(12) . 1\_655 ?

07 M2 07 48.28(14) 3\_656 1\_655 ?

O8 M2 07 160.34(10) 3\_656 1\_655 ?

03 M2 07 38.77(11) . 1\_655 ?

P2 M2 07 124.35(6) 1\_554 1\_655 ?

P2 M2 07 91.50(6) . 1\_655 ?

P1 M2 07 49.86(6) 3\_656 1\_655 ?

P1 M2 07 23.29(5) 1\_655 1\_655 ?

P2 M2 07 141.39(6) 3\_656 1\_655 ?

M3 M2 07 160.78(6) . 1\_655 ?

O2 M2 07 118.23(8) 3\_656 1\_655 ?

O1 M2 07 40.85(8) 1\_655 1\_655 ?

M1MN M2 07 39.87(6) . 1\_655 ?

M1CA M2 07 39.87(6) . 1\_655 ?

O2 M2 07 125.89(8) 4\_565 1\_655 ?

O8 M2 07 100.13(7) . 1\_655 ?

04 M2 07 101.77(8) 4\_565 1\_655 ?

O2 M2 07 141.63(8) 1\_554 1\_655 ?

O1 M2 07 45.77(8) 3\_656 1\_655 ?

O8 M2 07 128.03(8) 1\_554 1\_655 ?

06 M2 M1CA 28.53(10) . 1\_554 ?

04 M2 M1CA 146.40(11) . 1\_554 ?

07 M2 M1CA 83.09(10) 3\_656 1\_554 ?

O8 M2 M1CA 116.35(8) 3\_656 1\_554 ?

03 M2 M1CA 66.57(9) . 1\_554 ?

P2 M2 M1CA 48.94(3) 1\_554 1\_554 ?

P2 M2 M1CA 164.17(4) . 1\_554 ?

P1 M2 M1CA 101.76(3) 3\_656 1\_554 ?

P1 M2 M1CA 56.46(3) 1\_655 1\_554 ?

P2 M2 M1CA 112.98(3) 3\_656 1\_554 ?

M3 M2 M1CA 103.50(2) . 1\_554 ?

O2 M2 M1CA 100.24(6) 3\_656 1\_554 ?

O1 M2 M1CA 35.62(6) 1\_655 1\_554 ?

M1MN M2 M1CA 112.44(3) . 1\_554 ?

M1CA M2 M1CA 112.44(3) . 1\_554 ?

O2 M2 M1CA 106.93(6) 4\_565 1\_554 ?

O8 M2 M1CA 165.28(6) . 1\_554 ?

04 M2 M1CA 68.23(5) 4\_565 1\_554 ?

O2 M2 M1CA 67.42(5) 1\_554 1\_554 ?

O1 M2 M1CA 116.39(6) 3\_656 1\_554 ?

O8 M2 M1CA 62.36(5) 1\_554 1\_554 ?

07 M2 M1CA 75.97(6) 1\_655 1\_554 ?

06 M2 M1MN 28.53(10) . 1\_554 ?

04 M2 M1MN 146.40(11) . 1\_554 ?

07 M2 M1MN 83.09(10) 3\_656 1\_554 ?

O8 M2 M1MN 116.35(8) 3\_656 1\_554 ?

03 M2 M1MN 66.57(9) . 1\_554 ?

P2 M2 M1MN 48.94(3) 1\_554 1\_554 ?

P2 M2 M1MN 164.17(4) . 1\_554 ?

P1 M2 M1MN 101.76(3) 3\_656 1\_554 ?

P1 M2 M1MN 56.46(3) 1\_655 1\_554 ?

P2 M2 M1MN 112.98(3) 3\_656 1\_554 ?

M3 M2 M1MN 103.50(2) . 1\_554 ?

O2 M2 M1MN 100.24(6) 3\_656 1\_554 ?

O1 M2 M1MN 35.62(6) 1\_655 1\_554 ?

M1MN M2 M1MN 112.44(3) . 1\_554 ?

M1CA M2 M1MN 112.44(3) . 1\_554 ?

O2 M2 M1MN 106.93(6) 4\_565 1\_554 ?

O8 M2 M1MN 165.28(6) . 1\_554 ?

04 M2 M1MN 68.23(5) 4\_565 1\_554 ?

O2 M2 M1MN 67.42(5) 1\_554 1\_554 ?

O1 M2 M1MN 116.39(6) 3\_656 1\_554 ?

O8 M2 M1MN 62.36(5) 1\_554 1\_554 ?

07 M2 M1MN 75.97(6) 1\_655 1\_554 ?

M1CA M2 M1MN 0.00(2) 1\_554 1\_554 ?

06 M2 P2 87.79(10) . 4\_565 ?

04 M2 P2 71.97(10) . 4\_565 ?

07 M2 P2 155.28(11) 3\_656 4\_565 ?

O8 M2 P2 88.75(8) 3\_656 4\_565 ?

03 M2 P2 69.79(9) . 4\_565 ?

P2 M2 P2 84.04(3) 1\_554 4\_565 ?

P2 M2 P2 83.35(3) . 4\_565 ?

P1 M2 P2 147.88(3) 3\_656 4\_565 ?

P1 M2 P2 93.28(3) 1\_655 4\_565 ?

P2 M2 P2 110.18(2) 3\_656 4\_565 ?

M3 M2 P2 53.84(2) . 4\_565 ?

O2 M2 P2 134.77(6) 3\_656 4\_565 ?

O1 M2 P2 105.31(6) 1\_655 4\_565 ?

M1MN M2 P2 90.39(3) . 4\_565 ?

M1CA M2 P2 90.39(3) . 4\_565 ?

O2 M2 P2 22.73(5) 4\_565 4\_565 ?

O8 M2 P2 103.68(5) . 4\_565 ?

04 M2 P2 22.84(5) 4\_565 4\_565 ?

O2 M2 P2 63.84(6) 1\_554 4\_565 ?

O1 M2 P2 124.09(6) 3\_656 4\_565 ?

O8 M2 P2 103.52(5) 1\_554 4\_565 ?

07 M2 P2 107.00(6) 1\_655 4\_565 ?

M1CA M2 P2 91.00(3) 1\_554 4\_565 ?

M1MN M2 P2 91.00(3) 1\_554 4\_565 ?

06 M2 05 118.15(11) . 3\_656 ?

04 M2 05 82.12(11) . 3\_656 ?

07 M2 05 33.33(12) 3\_656 3\_656 ?

O8 M2 05 88.68(10) 3\_656 3\_656 ?

03 M2 05 110.11(11) . 3\_656 ?

P2 M2 05 118.80(6) 1\_554 3\_656 ?

P2 M2 05 70.61(6) . 3\_656 ?

P1 M2 05 22.16(6) 3\_656 3\_656 ?

P1 M2 05 92.62(6) 1\_655 3\_656 ?

P2 M2 05 70.14(6) 3\_656 3\_656 ?

M3 M2 05 123.99(6) . 3\_656 ?

O2 M2 05 52.90(7) 3\_656 3\_656 ?

O1 M2 05 90.81(8) 1\_655 3\_656 ?

M1MN M2 05 72.03(5) . 3\_656 ?

M1CA M2 05 72.03(5) . 3\_656 ?

O2 M2 05 139.17(8) 4\_565 3\_656 ?

O8 M2 05 52.37(7) . 3\_656 ?

04 M2 05 172.38(8) 4\_565 3\_656 ?

O2 M2 05 133.14(8) 1\_554 3\_656 ?

O1 M2 05 36.98(7) 3\_656 3\_656 ?

O8 M2 05 96.56(7) 1\_554 3\_656 ?

07 M2 05 71.97(7) 1\_655 3\_656 ?

M1CA M2 05 113.38(6) 1\_554 3\_656 ?

M1MN M2 05 113.38(6) 1\_554 3\_656 ?

P2 M2 05 153.81(6) 4\_565 3\_656 ?

06 M2 06 103.13(10) . 4\_566 ?

04 M2 06 57.20(11) . 4\_566 ?

07 M2 06 134.61(11) 3\_656 4\_566 ?

O8 M2 06 105.26(10) 3\_656 4\_566 ?

03 M2 06 53.91(10) . 4\_566 ?

P2 M2 06 104.11(5) 1\_554 4\_566 ?

P2 M2 06 72.69(5) . 4\_566 ?

P1 M2 06 125.71(5) 3\_656 4\_566 ?

P1 M2 06 78.69(5) 1\_655 4\_566 ?

P2 M2 06 126.20(6) 3\_656 4\_566 ?

M3 M2 06 73.51(5) . 4\_566 ?

O2 M2 06 151.97(8) 3\_656 4\_566 ?

O1 M2 06 97.66(7) 1\_655 4\_566 ?

M1MN M2 06 68.22(5) . 4\_566 ?

M1CA M2 06 68.22(5) . 4\_566 ?

O2 M2 06 38.60(7) 4\_565 4\_566 ?

O8 M2 06 97.25(7) . 4\_566 ?

04 M2 06 36.61(7) 4\_565 4\_566 ?

O2 M2 06 85.86(7) 1\_554 4\_566 ?

O1 M2 06 102.63(7) 3\_656 4\_566 ?

O8 M2 06 125.22(7) 1\_554 4\_566 ?

07 M2 06 87.42(7) 1\_655 4\_566 ?

M1CA M2 06 96.75(5) 1\_554 4\_566 ?

M1MN M2 06 96.75(5) 1\_554 4\_566 ?

P2 M2 06 22.34(5) 4\_565 4\_566 ?

05 M2 06 136.95(7) 3\_656 4\_566 ?

06 M2 M1CA 82.19(10) . 4\_565 ?

04 M2 M1CA 82.46(10) . 4\_565 ?

07 M2 M1CA 112.27(11) 3\_656 4\_565 ?

O8 M2 M1CA 132.18(9) 3\_656 4\_565 ?

03 M2 M1CA 27.16(9) . 4\_565 ?

P2 M2 M1CA 93.54(3) 1\_554 4\_565 ?

P2 M2 M1CA 100.52(3) . 4\_565 ?

P1 M2 M1CA 115.31(3) 3\_656 4\_565 ?

P1 M2 M1CA 48.97(3) 1\_655 4\_565 ?

P2 M2 M1CA 152.66(3) 3\_656 4\_565 ?

M3 M2 M1CA 96.05(3) . 4\_565 ?

O2 M2 M1CA 164.71(6) 3\_656 4\_565 ?

O1 M2 M1CA 63.44(6) 1\_655 4\_565 ?

M1MN M2 M1CA 69.63(2) . 4\_565 ?

M1CA M2 M1CA 69.63(2) . 4\_565 ?

O2 M2 M1CA 66.99(5) 4\_565 4\_565 ?

O8 M2 M1CA 126.11(5) . 4\_565 ?

04 M2 M1CA 36.26(6) 4\_565 4\_565 ?

O2 M2 M1CA 88.22(6) 1\_554 4\_565 ?

O1 M2 M1CA 101.95(6) 3\_656 4\_565 ?

O8 M2 M1CA 116.70(5) 1\_554 4\_565 ?

07 M2 M1CA 65.93(5) 1\_655 4\_565 ?

M1CA M2 M1CA 65.72(2) 1\_554 4\_565 ?

M1MN M2 M1CA 65.72(2) 1\_554 4\_565 ?

P2 M2 M1CA 44.42(2) 4\_565 4\_565 ?

05 M2 M1CA 136.75(6) 3\_656 4\_565 ?

06 M2 M1CA 34.74(5) 4\_566 4\_565 ?

06 M2 M1MN 82.19(10) . 4\_565 ?

04 M2 M1MN 82.46(10) . 4\_565 ?

07 M2 M1MN 112.27(11) 3\_656 4\_565 ?

O8 M2 M1MN 132.18(9) 3\_656 4\_565 ?

03 M2 M1MN 27.16(9) . 4\_565 ?

P2 M2 M1MN 93.54(3) 1\_554 4\_565 ?

P2 M2 M1MN 100.52(3) . 4\_565 ?

P1 M2 M1MN 115.31(3) 3\_656 4\_565 ?

P1 M2 M1MN 48.97(3) 1\_655 4\_565 ?

P2 M2 M1MN 152.66(3) 3\_656 4\_565 ?

M3 M2 M1MN 96.05(3) . 4\_565 ?

O2 M2 M1MN 164.71(6) 3\_656 4\_565 ?

O1 M2 M1MN 63.44(6) 1\_655 4\_565 ?

M1MN M2 M1MN 69.63(2) . 4\_565 ?

M1CA M2 M1MN 69.63(2) . 4\_565 ?

O2 M2 M1MN 66.99(5) 4\_565 4\_565 ?

O8 M2 M1MN 126.11(5) . 4\_565 ?

04 M2 M1MN 36.26(6) 4\_565 4\_565 ?

O2 M2 M1MN 88.22(6) 1\_554 4\_565 ?

O1 M2 M1MN 101.95(6) 3\_656 4\_565 ?

O8 M2 M1MN 116.70(5) 1\_554 4\_565 ?

07 M2 M1MN 65.93(5) 1\_655 4\_565 ?

M1CA M2 M1MN 65.72(2) 1\_554 4\_565 ?

M1MN M2 M1MN 65.72(2) 1\_554 4\_565 ?

P2 M2 M1MN 44.42(2) 4\_565 4\_565 ?

05 M2 M1MN 136.75(6) 3\_656 4\_565 ?

06 M2 M1MN 34.74(5) 4\_566 4\_565 ?

M1CA M2 M1MN 0.000(11) 4\_565 4\_565 ?

06 M2 M1MN 68.23(10) . 3\_756 ?

04 M2 M1MN 126.70(10) . 3\_756 ?

07 M2 M1MN 31.72(10) 3\_656 3\_756 ?

O8 M2 M1MN 123.14(9) 3\_656 3\_756 ?

03 M2 M1MN 76.26(9) . 3\_756 ?

P2 M2 M1MN 83.71(3) 1\_554 3\_756 ?

P2 M2 M1MN 126.71(3) . 3\_756 ?

P1 M2 M1MN 50.86(3) 3\_656 3\_756 ?

P1 M2 M1MN 51.67(3) 1\_655 3\_756 ?

P2 M2 M1MN 103.57(3) 3\_656 3\_756 ?

M3 M2 M1MN 142.75(3) . 3\_756 ?

O2 M2 M1MN 78.19(6) 3\_656 3\_756 ?

O1 M2 M1MN 32.79(6) 1\_655 3\_756 ?

M1MN M2 M1MN 87.72(3) . 3\_756 ?

M1CA M2 M1MN 87.72(3) . 3\_756 ?

O2 M2 M1MN 157.89(6) 4\_565 3\_756 ?

O8 M2 M1MN 115.04(6) . 3\_756 ?

04 M2 M1MN 116.82(6) 4\_565 3\_756 ?

O2 M2 M1MN 108.66(6) 1\_554 3\_756 ?

O1 M2 M1MN 70.34(6) 3\_656 3\_756 ?

O8 M2 M1MN 78.19(5) 1\_554 3\_756 ?

07 M2 M1MN 51.03(6) 1\_655 3\_756 ?

M1CA M2 M1MN 51.44(2) 1\_554 3\_756 ?

M1MN M2 M1MN 51.44(2) 1\_554 3\_756 ?

P2 M2 M1MN 137.48(3) 4\_565 3\_756 ?

05 M2 M1MN 62.94(6) 3\_656 3\_756 ?

06 M2 M1MN 129.59(5) 4\_566 3\_756 ?

M1CA M2 M1MN 96.09(2) 4\_565 3\_756 ?

M1MN M2 M1MN 96.09(2) 4\_565 3\_756 ?

06 M2 M1CA 68.23(10) . 3\_756 ?

04 M2 M1CA 126.70(10) . 3\_756 ?

07 M2 M1CA 31.72(10) 3\_656 3\_756 ?

O8 M2 M1CA 123.14(9) 3\_656 3\_756 ?

03 M2 M1CA 76.26(9) . 3\_756 ?

P2 M2 M1CA 83.71(3) 1\_554 3\_756 ?

P2 M2 M1CA 126.71(3) . 3\_756 ?

P1 M2 M1CA 50.86(3) 3\_656 3\_756 ?

P1 M2 M1CA 51.67(3) 1\_655 3\_756 ?

P2 M2 M1CA 103.57(3) 3\_656 3\_756 ?

M3 M2 M1CA 142.75(3) . 3\_756 ?

O2 M2 M1CA 78.19(6) 3\_656 3\_756 ?

O1 M2 M1CA 32.79(6) 1\_655 3\_756 ?

M1MN M2 M1CA 87.72(3) . 3\_756 ?

M1CA M2 M1CA 87.72(3) . 3\_756 ?

O2 M2 M1CA 157.89(6) 4\_565 3\_756 ?

O8 M2 M1CA 115.04(6) . 3\_756 ?

04 M2 M1CA 116.82(6) 4\_565 3\_756 ?

O2 M2 M1CA 108.66(6) 1\_554 3\_756 ?

O1 M2 M1CA 70.34(6) 3\_656 3\_756 ?

O8 M2 M1CA 78.19(5) 1\_554 3\_756 ?

07 M2 M1CA 51.03(6) 1\_655 3\_756 ?

M1CA M2 M1CA 51.44(2) 1\_554 3\_756 ?

M1MN M2 M1CA 51.44(2) 1\_554 3\_756 ?

P2 M2 M1CA 137.48(3) 4\_565 3\_756 ?

05 M2 M1CA 62.94(6) 3\_656 3\_756 ?

06 M2 M1CA 129.59(5) 4\_566 3\_756 ?

M1CA M2 M1CA 96.09(2) 4\_565 3\_756 ?

M1MN M2 M1CA 96.09(2) 4\_565 3\_756 ?

M1MN M2 M1CA 0.00(3) 3\_756 3\_756 ?

06 M2 O2 145.55(11) . . ?

04 M2 O2 24.00(11) . . ?

07 M2 O2 115.09(11) 3\_656 . ?

O8 M2 O2 69.40(9) 3\_656 . ?

03 M2 O2 100.04(10) . . ?

P2 M2 O2 128.02(5) 1\_554 . ?

P2 M2 O2 19.30(5) . . ?

P1 M2 O2 95.63(5) 3\_656 . ?

P1 M2 O2 117.99(5) 1\_655 . ?

P2 M2 O2 80.34(5) 3\_656 . ?

M3 M2 O2 67.58(5) . . ?

O2 M2 O2 98.68(7) 3\_656 . ?

O1 M2 O2 143.86(7) 1\_655 . ?

M1MN M2 O2 65.61(5) . . ?

M1CA M2 O2 65.61(5) . . ?

O2 M2 O2 53.44(6) 4\_565 . ?

O8 M2 O2 37.20(7) . . ?

04 M2 O2 89.69(7) 4\_565 . ?

O2 M2 O2 104.06(8) 1\_554 . ?

O1 M2 O2 75.81(7) 3\_656 . ?

O8 M2 O2 125.05(7) 1\_554 . ?

07 M2 O2 105.48(7) 1\_655 . ?

M1CA M2 O2 157.44(5) 1\_554 . ?

M1MN M2 O2 157.44(5) 1\_554 . ?

P2 M2 O2 66.85(5) 4\_565 . ?

05 M2 O2 87.91(7) 3\_656 . ?

06 M2 O2 61.16(7) 4\_566 . ?

M1CA M2 O2 93.92(5) 4\_565 . ?

M1MN M2 O2 93.92(5) 4\_565 . ?

M1MN M2 O2 145.98(5) 3\_756 . ?

M1CA M2 O2 145.98(5) 3\_756 . ?

06 M2 M3 53.64(10) . 3\_655 ?

04 M2 M3 143.98(10) . 3\_655 ?

07 M2 M3 66.03(10) 3\_656 3\_655 ?

O8 M2 M3 67.20(8) 3\_656 3\_655 ?

03 M2 M3 128.55(9) . 3\_655 ?

P2 M2 M3 50.35(2) 1\_554 3\_655 ?

P2 M2 M3 126.13(3) . 3\_655 ?

P1 M2 M3 78.68(3) 3\_656 3\_655 ?

P1 M2 M3 106.47(3) 1\_655 3\_655 ?

P2 M2 M3 51.12(2) 3\_656 3\_655 ?

M3 M2 M3 89.86(2) . 3\_655 ?

O2 M2 M3 32.38(5) 3\_656 3\_655 ?

O1 M2 M3 81.69(6) 1\_655 3\_655 ?

M1MN M2 M3 135.76(3) . 3\_655 ?

M1CA M2 M3 135.76(3) . 3\_655 ?

O2 M2 M3 124.21(6) 4\_565 3\_655 ?

O8 M2 M3 100.49(6) . 3\_655 ?

04 M2 M3 118.24(5) 4\_565 3\_655 ?

O2 M2 M3 69.59(6) 1\_554 3\_655 ?

O1 M2 M3 102.54(6) 3\_656 3\_655 ?

O8 M2 M3 29.84(5) 1\_554 3\_655 ?

07 M2 M3 107.23(6) 1\_655 3\_655 ?

M1CA M2 M3 67.88(2) 1\_554 3\_655 ?

M1MN M2 M3 67.88(2) 1\_554 3\_655 ?

P2 M2 M3 133.32(3) 4\_565 3\_655 ?

05 M2 M3 68.49(5) 3\_656 3\_655 ?

06 M2 M3 154.45(5) 4\_566 3\_655 ?

M1CA M2 M3 133.34(3) 4\_565 3\_655 ?

M1MN M2 M3 133.34(3) 4\_565 3\_655 ?

M1MN M2 M3 56.932(19) 3\_756 3\_655 ?

M1CA M2 M3 56.932(19) 3\_756 3\_655 ?

O2 M2 M3 130.43(5) . 3\_655 ?

06 M2 O1 36.70(11) . 3\_655 ?

04 M2 O1 158.81(12) . 3\_655 ?

07 M2 O1 61.12(11) 3\_656 3\_655 ?

O8 M2 O1 104.30(10) 3\_656 3\_655 ?

03 M2 O1 87.95(10) . 3\_655 ?

P2 M2 O1 51.38(5) 1\_554 3\_655 ?

P2 M2 O1 156.02(6) . 3\_655 ?

P1 M2 O1 80.49(5) 3\_656 3\_655 ?

P1 M2 O1 68.49(5) 1\_655 3\_655 ?

P2 M2 O1 91.68(5) 3\_656 3\_655 ?

M3 M2 O1 111.41(5) . 3\_655 ?

O2 M2 O1 72.49(7) 3\_656 3\_655 ?

O1 M2 O1 42.52(9) 1\_655 3\_655 ?

M1MN M2 O1 117.78(5) . 3\_655 ?

M1CA M2 O1 117.78(5) . 3\_655 ?

O2 M2 O1 131.00(7) 4\_565 3\_655 ?

O8 M2 O1 134.69(7) . 3\_655 ?

04 M2 O1 97.55(7) 4\_565 3\_655 ?

O2 M2 O1 76.28(7) 1\_554 3\_655 ?

O1 M2 O1 102.24(8) 3\_656 3\_655 ?

O8 M2 O1 49.99(7) 1\_554 3\_655 ?

07 M2 O1 78.26(7) 1\_655 3\_655 ?

M1CA M2 O1 30.92(5) 1\_554 3\_655 ?

M1MN M2 O1 30.92(5) 1\_554 3\_655 ?

P2 M2 O1 120.28(5) 4\_565 3\_655 ?

05 M2 O1 85.56(7) 3\_656 3\_655 ?

06 M2 O1 127.58(7) 4\_566 3\_655 ?

M1CA M2 O1 95.03(5) 4\_565 3\_655 ?

M1MN M2 O1 95.03(5) 4\_565 3\_655 ?

M1MN M2 O1 32.38(5) 3\_756 3\_655 ?

M1CA M2 O1 32.38(5) 3\_756 3\_655 ?

O2 M2 O1 171.06(7) . 3\_655 ?

M3 M2 O1 41.04(5) 3\_655 3\_655 ?

06 M2 06 173.96(15) . 1\_556 ?

04 M2 06 16.76(11) . 1\_556 ?

07 M2 06 83.85(11) 3\_656 1\_556 ?

O8 M2 06 96.63(10) 3\_656 1\_556 ?

03 M2 06 82.38(10) . 1\_556 ?

P2 M2 06 162.75(6) 1\_554 1\_556 ?

P2 M2 06 18.80(5) . 1\_556 ?

P1 M2 06 64.97(5) 3\_656 1\_556 ?

P1 M2 06 90.63(5) 1\_655 1\_556 ?

P2 M2 06 98.08(5) 3\_656 1\_556 ?

M3 M2 06 102.64(5) . 1\_556 ?

O2 M2 06 103.48(7) 3\_656 1\_556 ?

O1 M2 06 113.49(7) 1\_655 1\_556 ?

M1MN M2 06 34.59(5) . 1\_556 ?

M1CA M2 06 34.59(5) . 1\_556 ?

O2 M2 06 83.74(7) 4\_565 1\_556 ?

O8 M2 06 36.95(7) . 1\_556 ?

04 M2 06 108.29(7) 4\_565 1\_556 ?

O2 M2 06 139.07(7) 1\_554 1\_556 ?

O1 M2 06 42.10(7) 3\_656 1\_556 ?

O8 M2 06 149.16(7) 1\_554 1\_556 ?

07 M2 06 72.71(7) 1\_655 1\_556 ?

M1CA M2 06 147.00(5) 1\_554 1\_556 ?

M1MN M2 06 147.00(5) 1\_554 1\_556 ?

P2 M2 06 88.37(5) 4\_565 1\_556 ?

05 M2 06 66.07(7) 3\_656 1\_556 ?

06 M2 06 71.90(7) 4\_566 1\_556 ?

M1CA M2 06 91.81(5) 4\_565 1\_556 ?

M1MN M2 06 91.81(5) 4\_565 1\_556 ?

M1MN M2 06 112.01(5) 3\_756 1\_556 ?

M1CA M2 06 112.01(5) 3\_756 1\_556 ?

O2 M2 06 35.09(6) . 1\_556 ?

M3 M2 06 131.91(5) 3\_655 1\_556 ?

O1 M2 06 144.26(7) 3\_655 1\_556 ?

06 M2 03 44.77(11) . 4\_565 ?

04 M2 03 120.28(12) . 4\_565 ?

07 M2 03 105.48(12) 3\_656 4\_565 ?

O8 M2 03 121.16(10) 3\_656 4\_565 ?

03 M2 03 49.80(6) . 4\_565 ?

P2 M2 03 59.65(6) 1\_554 4\_565 ?

P2 M2 03 138.01(6) . 4\_565 ?

P1 M2 03 120.49(6) 3\_656 4\_565 ?

P1 M2 03 54.19(5) 1\_655 4\_565 ?

P2 M2 03 129.76(6) 3\_656 4\_565 ?

M3 M2 03 92.45(5) . 4\_565 ?

O2 M2 03 126.88(8) 3\_656 4\_565 ?

O1 M2 03 48.32(7) 1\_655 4\_565 ?

M1MN M2 03 101.00(6) . 4\_565 ?

M1CA M2 03 101.00(6) . 4\_565 ?

O2 M2 03 81.64(7) 4\_565 4\_565 ?

O8 M2 03 163.56(8) . 4\_565 ?

04 M2 03 40.48(7) 4\_565 4\_565 ?

O2 M2 03 65.22(7) 1\_554 4\_565 ?

O1 M2 03 123.17(8) 3\_656 4\_565 ?

O8 M2 03 80.93(7) 1\_554 4\_565 ?

07 M2 03 77.47(7) 1\_655 4\_565 ?

M1CA M2 03 30.29(6) 1\_554 4\_565 ?

M1MN M2 03 30.29(6) 1\_554 4\_565 ?

P2 M2 03 62.35(6) 4\_565 4\_565 ?

05 M2 03 138.71(8) 3\_656 4\_565 ?

06 M2 03 66.51(7) 4\_566 4\_565 ?

M1CA M2 03 37.96(5) 4\_565 4\_565 ?

M1MN M2 03 37.96(5) 4\_565 4\_565 ?

M1MN M2 03 76.36(6) 3\_756 4\_565 ?

M1CA M2 03 76.36(6) 3\_756 4\_565 ?

O2 M2 03 127.27(7) . 4\_565 ?

M3 M2 03 95.72(6) 3\_655 4\_565 ?

O1 M2 03 61.21(7) 3\_655 4\_565 ?

06 M2 03 129.19(7) 1\_556 4\_565 ?

06 M2 05 74.33(11) . 2\_645 ?

04 M2 05 125.89(11) . 2\_645 ?

07 M2 05 39.03(11) 3\_656 2\_645 ?

O8 M2 05 83.55(10) 3\_656 2\_645 ?

03 M2 05 117.08(10) . 2\_645 ?

P2 M2 05 76.68(5) 1\_554 2\_645 ?

P2 M2 05 112.16(5) . 2\_645 ?

P1 M2 05 50.93(5) 3\_656 2\_645 ?

P1 M2 05 92.29(6) 1\_655 2\_645 ?

P2 M2 05 62.80(6) 3\_656 2\_645 ?

M3 M2 05 114.05(5) . 2\_645 ?

O2 M2 05 37.08(7) 3\_656 2\_645 ?

O1 M2 05 73.31(8) 1\_655 2\_645 ?

M1MN M2 05 107.98(5) . 2\_645 ?

M1CA M2 05 107.98(5) . 2\_645 ?

O2 M2 05 149.32(7) 4\_565 2\_645 ?

O8 M2 05 88.78(7) . 2\_645 ?

04 M2 05 141.32(7) 4\_565 2\_645 ?

O2 M2 05 97.38(7) 1\_554 2\_645 ?

O1 M2 05 75.09(7) 3\_656 2\_645 ?

O8 M2 05 57.64(7) 1\_554 2\_645 ?

07 M2 05 84.76(8) 1\_655 2\_645 ?

M1CA M2 05 76.80(5) 1\_554 2\_645 ?

M1MN M2 05 76.80(5) 1\_554 2\_645 ?

P2 M2 05 160.71(5) 4\_565 2\_645 ?

05 M2 05 43.958(15) 3\_656 2\_645 ?

06 M2 05 170.87(7) 4\_566 2\_645 ?

M1CA M2 05 136.51(6) 4\_565 2\_645 ?

M1MN M2 05 136.51(6) 4\_565 2\_645 ?

M1MN M2 05 41.27(5) 3\_756 2\_645 ?

M1CA M2 05 41.27(5) 3\_756 2\_645 ?

O2 M2 05 125.68(7) . 2\_645 ?

M3 M2 05 27.83(5) 3\_655 2\_645 ?

O1 M2 05 45.92(7) 3\_655 2\_645 ?

06 M2 05 110.03(7) 1\_556 2\_645 ?

03 M2 05 107.05(7) 4\_565 2\_645 ?

06 M2 04 6.57(11) . 1\_554 ?

04 M2 04 154.43(15) . 1\_554 ?

07 M2 04 104.16(11) 3\_656 1\_554 ?

O8 M2 04 83.81(9) 3\_656 1\_554 ?

03 M2 04 93.90(10) . 1\_554 ?

P2 M2 04 16.06(5) 1\_554 1\_554 ?

P2 M2 04 157.54(5) . 1\_554 ?

P1 M2 04 123.33(5) 3\_656 1\_554 ?

P1 M2 04 89.31(5) 1\_655 1\_554 ?

P2 M2 04 85.64(5) 3\_656 1\_554 ?

M3 M2 04 72.45(5) . 1\_554 ?

O2 M2 04 83.46(7) 3\_656 1\_554 ?

O1 M2 04 68.71(7) 1\_655 1\_554 ?

M1MN M2 04 144.29(5) . 1\_554 ?

M1CA M2 04 144.29(5) . 1\_554 ?

O2 M2 04 88.14(7) 4\_565 1\_554 ?

O8 M2 04 146.66(7) . 1\_554 ?

04 M2 04 62.76(7) 4\_565 1\_554 ?

O2 M2 04 35.52(7) 1\_554 1\_554 ?

O1 M2 04 145.13(7) 3\_656 1\_554 ?

O8 M2 04 35.86(6) 1\_554 1\_554 ?

07 M2 04 109.35(7) 1\_655 1\_554 ?

M1CA M2 04 33.40(5) 1\_554 1\_554 ?

M1MN M2 04 33.40(5) 1\_554 1\_554 ?

P2 M2 04 82.62(5) 4\_565 1\_554 ?

05 M2 04 122.95(7) 3\_656 1\_554 ?

06 M2 04 99.25(6) 4\_566 1\_554 ?

M1CA M2 04 81.35(5) 4\_565 1\_554 ?

M1MN M2 04 81.35(5) 4\_565 1\_554 ?

M1MN M2 04 74.80(5) 3\_756 1\_554 ?

M1CA M2 04 74.80(5) 3\_756 1\_554 ?

O2 M2 04 138.99(6) . 1\_554 ?

M3 M2 04 56.51(5) 3\_655 1\_554 ?

O1 M2 04 43.15(7) 3\_655 1\_554 ?

06 M2 04 170.97(7) 1\_556 1\_554 ?

03 M2 04 45.10(7) 4\_565 1\_554 ?

05 M2 04 79.00(7) 2\_645 1\_554 ?

06 M2 04 105.44(11) . 3\_656 ?

04 M2 04 82.82(12) . 3\_656 ?

07 M2 04 93.09(12) 3\_656 3\_656 ?

O8 M2 04 26.38(9) 3\_656 3\_656 ?

03 M2 04 162.57(10) . 3\_656 ?

P2 M2 04 87.57(5) 1\_554 3\_656 ?

P2 M2 04 65.16(5) . 3\_656 ?

P1 M2 04 85.16(5) 3\_656 3\_656 ?

P1 M2 04 155.77(5) 1\_655 3\_656 ?

P2 M2 04 17.89(4) 3\_656 3\_656 ?

M3 M2 04 60.85(5) . 3\_656 ?

O2 M2 04 35.17(7) 3\_656 3\_656 ?

O1 M2 04 143.66(7) 1\_655 3\_656 ?

M1MN M2 04 112.18(5) . 3\_656 ?

M1CA M2 04 112.18(5) . 3\_656 ?

O2 M2 04 85.96(7) 4\_565 3\_656 ?

O8 M2 04 43.56(7) . 3\_656 ?

04 M2 04 122.02(5) 4\_565 3\_656 ?

O2 M2 04 81.23(7) 1\_554 3\_656 ?

O1 M2 04 89.69(7) 3\_656 3\_656 ?

O8 M2 04 69.06(6) 1\_554 3\_656 ?

07 M2 04 133.98(7) 1\_655 3\_656 ?

M1CA M2 04 130.63(5) 1\_554 3\_656 ?

M1MN M2 04 130.63(5) 1\_554 3\_656 ?

P2 M2 04 108.69(5) 4\_565 3\_656 ?

05 M2 04 63.15(7) 3\_656 3\_656 ?

06 M2 04 118.68(7) 4\_566 3\_656 ?

M1CA M2 04 152.55(5) 4\_565 3\_656 ?

M1MN M2 04 152.55(5) 4\_565 3\_656 ?

M1MN M2 04 111.27(5) 3\_756 3\_656 ?

M1CA M2 04 111.27(5) 3\_756 3\_656 ?

O2 M2 04 64.66(6) . 3\_656 ?

M3 M2 04 65.79(4) 3\_655 3\_656 ?

O1 M2 04 106.81(7) 3\_655 3\_656 ?

06 M2 04 80.21(6) 1\_556 3\_656 ?

03 M2 04 145.97(7) 4\_565 3\_656 ?

05 M2 04 70.35(7) 2\_645 3\_656 ?

04 M2 04 103.20(5) 1\_554 3\_656 ?

06 M2 03 104.55(11) . 3\_756 ?

04 M2 03 92.66(11) . 3\_756 ?

07 M2 03 8.62(11) 3\_656 3\_756 ?

O8 M2 03 120.30(10) 3\_656 3\_756 ?

03 M2 03 80.49(12) . 3\_756 ?

P2 M2 03 117.15(5) 1\_554 3\_756 ?

P2 M2 03 89.92(5) . 3\_756 ?

P1 M2 03 14.76(5) 3\_656 3\_756 ?

P1 M2 03 59.67(5) 1\_655 3\_756 ?

P2 M2 03 99.63(6) 3\_656 3\_756 ?

M3 M2 03 156.48(6) . 3\_756 ?

O2 M2 03 76.52(7) 3\_656 3\_756 ?

O1 M2 03 58.06(7) 1\_655 3\_756 ?

M1MN M2 03 61.47(5) . 3\_756 ?

M1CA M2 03 61.47(5) . 3\_756 ?

O2 M2 03 159.46(7) 4\_565 3\_756 ?

O8 M2 03 80.86(7) . 3\_756 ?

04 M2 03 141.73(8) 4\_565 3\_756 ?

O2 M2 03 141.74(7) 1\_554 3\_756 ?

O1 M2 03 34.49(7) 3\_656 3\_756 ?

O8 M2 03 103.58(7) 1\_554 3\_756 ?

07 M2 03 41.99(7) 1\_655 3\_756 ?

M1CA M2 03 87.14(5) 1\_554 3\_756 ?

M1MN M2 03 87.14(5) 1\_554 3\_756 ?

P2 M2 03 148.25(5) 4\_565 3\_756 ?

05 M2 03 33.81(7) 3\_656 3\_756 ?

06 M2 03 126.70(7) 4\_566 3\_756 ?

M1CA M2 03 107.45(5) 4\_565 3\_756 ?

M1MN M2 03 107.45(5) 4\_565 3\_756 ?

M1MN M2 03 36.83(5) 3\_756 3\_756 ?

M1CA M2 03 36.83(5) 3\_756 3\_756 ?

O2 M2 03 109.22(6) . 3\_756 ?

M3 M2 03 74.60(5) 3\_655 3\_756 ?

O1 M2 03 67.91(7) 3\_655 3\_756 ?

06 M2 03 76.57(6) 1\_556 3\_756 ?

03 M2 03 106.35(4) 4\_565 3\_756 ?

05 M2 03 47.39(7) 2\_645 3\_756 ?

04 M2 03 111.04(7) 1\_554 3\_756 ?

04 M2 03 96.25(7) 3\_656 3\_756 ?

05 M3 O8 145.32(14) 4\_565 3\_656 ?

05 M3 O2 106.71(14) 4\_565 4\_565 ?

O8 M3 O2 107.09(13) 3\_656 4\_565 ?

05 M3 05 94.08(14) 4\_565 . ?

O8 M3 05 102.35(13) 3\_656 . ?

O2 M3 05 74.06(12) 4\_565 . ?

05 M3 O2 74.68(13) 4\_565 1\_554 ?

O8 M3 O2 87.99(12) 3\_656 1\_554 ?

O2 M3 O2 107.54(13) 4\_565 1\_554 ?

05 M3 O2 168.69(13) . 1\_554 ?

05 M3 M2 149.83(10) 4\_565 . ?

O8 M3 M2 39.55(9) 3\_656 . ?

O2 M3 M2 75.05(9) 4\_565 . ?

05 M3 M2 114.78(10) . . ?

O2 M3 M2 76.15(8) 1\_554 . ?

05 M3 M2 79.91(10) 4\_565 3\_655 ?

O8 M3 M2 65.56(9) 3\_656 3\_655 ?

O2 M3 M2 160.73(9) 4\_565 3\_655 ?

05 M3 M2 124.21(9) . 3\_655 ?

O2 M3 M2 55.96(9) 1\_554 3\_655 ?

M2 M3 M2 90.14(2) . 3\_655 ?

05 M3 M2 60.74(10) 4\_565 2\_655 ?

O8 M3 M2 153.85(9) 3\_656 2\_655 ?

O2 M3 M2 47.01(9) 4\_565 2\_655 ?

05 M3 M2 70.06(9) . 2\_655 ?

O2 M3 M2 102.52(9) 1\_554 2\_655 ?

M2 M3 M2 119.45(2) . 2\_655 ?

M2 M3 M2 139.81(2) 3\_655 2\_655 ?

05 M3 M2 80.11(11) 4\_565 4\_565 ?

O8 M3 M2 109.16(9) 3\_656 4\_565 ?

O2 M3 M2 62.55(9) 4\_565 4\_565 ?

05 M3 M2 131.88(9) . 4\_565 ?

O2 M3 M2 45.97(9) 1\_554 4\_565 ?

M2 M3 M2 74.15(3) . 4\_565 ?

M2 M3 M2 101.925(17) 3\_655 4\_565 ?

M2 M3 M2 65.54(2) 2\_655 4\_565 ?

05 M3 M2 133.04(11) 4\_565 3\_656 ?

O8 M3 M2 46.08(9) 3\_656 3\_656 ?

O2 M3 M2 99.95(9) 4\_565 3\_656 ?

05 M3 M2 57.09(9) . 3\_656 ?

O2 M3 M2 132.10(9) 1\_554 3\_656 ?

M2 M3 M2 74.08(2) . 3\_656 ?

M2 M3 M2 87.43(2) 3\_655 3\_656 ?

M2 M3 M2 124.68(2) 2\_655 3\_656 ?

M2 M3 M2 146.841(17) 4\_565 3\_656 ?

05 M3 M2 124.26(11) 4\_565 4\_566 ?

O8 M3 M2 90.08(9) 3\_656 4\_566 ?

O2 M3 M2 17.96(9) 4\_565 4\_566 ?

05 M3 M2 71.49(9) . 4\_566 ?

O2 M3 M2 113.56(9) 1\_554 4\_566 ?

M2 M3 M2 62.35(2) . 4\_566 ?

M2 M3 M2 152.47(2) 3\_655 4\_566 ?

M2 M3 M2 63.773(18) 2\_655 4\_566 ?

M2 M3 M2 73.031(17) 4\_565 4\_566 ?

M2 M3 M2 83.999(16) 3\_656 4\_566 ?

07 P1 O1 114.2(2) . . ?

07 P1 03 107.4(2) . 1\_455 ?

O1 P1 03 111.1(2) . 1\_455 ?

07 P1 05 110.3(2) . . ?

O1 P1 05 105.1(2) . . ?

03 P1 05 108.7(2) 1\_455 . ?

07 P1 M1CA 131.21(16) . 4\_465 ?

O1 P1 M1CA 112.48(14) . 4\_465 ?

03 P1 M1CA 40.44(15) 1\_455 4\_465 ?

05 P1 M1CA 69.56(15) . 4\_465 ?

07 P1 M1CA 49.98(16) . 1\_455 ?

O1 P1 M1CA 136.50(14) . 1\_455 ?

03 P1 M1CA 57.87(15) 1\_455 1\_455 ?

05 P1 M1CA 118.38(14) . 1\_455 ?

M1CA P1 M1CA 85.81(4) 4\_465 1\_455 ?

07 P1 M1CA 81.20(14) . 3\_656 ?

O1 P1 M1CA 34.40(13) . 3\_656 ?

03 P1 M1CA 115.06(15) 1\_455 3\_656 ?

05 P1 M1CA 128.63(15) . 3\_656 ?

M1CA P1 M1CA 139.13(4) 4\_465 3\_656 ?

M1CA P1 M1CA 107.20(4) 1\_455 3\_656 ?

07 P1 M2 26.68(15) . 3\_656 ?

O1 P1 M2 92.29(14) . 3\_656 ?

03 P1 M2 132.22(16) 1\_455 3\_656 ?

05 P1 M2 104.00(15) . 3\_656 ?

M1CA P1 M2 155.20(4) 4\_465 3\_656 ?

M1CA P1 M2 76.26(3) 1\_455 3\_656 ?

M1CA P1 M2 64.05(3) 3\_656 3\_656 ?

07 P1 M2 96.60(15) . 1\_455 ?

O1 P1 M2 81.42(14) . 1\_455 ?

03 P1 M2 40.59(15) 1\_455 1\_455 ?

05 P1 M2 145.77(16) . 1\_455 ?

M1CA P1 M2 76.87(3) 4\_465 1\_455 ?

M1CA P1 M2 64.13(3) 1\_455 1\_455 ?

M1CA P1 M2 74.87(3) 3\_656 1\_455 ?

M2 P1 M2 109.34(3) 3\_656 1\_455 ?

07 P1 M1CA 142.24(15) . 1\_454 ?

O1 P1 M1CA 31.17(13) . 1\_454 ?

03 P1 M1CA 85.59(14) 1\_455 1\_454 ?

05 P1 M1CA 97.93(14) . 1\_454 ?

M1CA P1 M1CA 81.48(3) 4\_465 1\_454 ?

M1CA P1 M1CA 134.11(4) 1\_455 1\_454 ?

M1CA P1 M1CA 61.41(3) 3\_656 1\_454 ?

M2 P1 M1CA 123.31(4) 3\_656 1\_454 ?

M2 P1 M1CA 70.06(3) 1\_455 1\_454 ?

07 P1 M2 155.89(16) . 4\_465 ?

O1 P1 M2 77.78(14) . 4\_465 ?

03 P1 M2 48.77(15) 1\_455 4\_465 ?

05 P1 M2 84.83(15) . 4\_465 ?

M1CA P1 M2 35.45(2) 4\_465 4\_465 ?

M1CA P1 M2 106.60(3) 1\_455 4\_465 ?

M1CA P1 M2 104.44(3) 3\_656 4\_465 ?

M2 P1 M2 168.27(4) 3\_656 4\_465 ?

M2 P1 M2 63.37(3) 1\_455 4\_465 ?

M1CA P1 M2 46.61(2) 1\_454 4\_465 ?

07 P1 M2 109.46(15) . 3\_655 ?

O1 P1 M2 22.22(14) . 3\_655 ?

03 P1 M2 130.96(14) 1\_455 3\_655 ?

05 P1 M2 87.45(14) . 3\_655 ?

M1CA P1 M2 119.13(3) 4\_465 3\_655 ?

M1CA P1 M2 150.19(3) 1\_455 3\_655 ?

M1CA P1 M2 43.40(2) 3\_656 3\_655 ?

M2 P1 M2 83.49(3) 3\_656 3\_655 ?

M2 P1 M2 103.58(3) 1\_455 3\_655 ?

M1CA P1 M2 45.77(2) 1\_454 3\_655 ?

M2 P1 M2 89.29(2) 4\_465 3\_655 ?

O2 P2 04 110.18(19) . . ?

O2 P2 06 110.41(18) . 1\_556 ?

04 P2 06 103.46(18) . 1\_556 ?

O2 P2 O8 110.35(18) . . ?

04 P2 O8 111.77(18) . . ?

06 P2 O8 110.49(18) 1\_556 . ?

O2 P2 M1CA 130.82(14) . . ?

04 P2 M1CA 52.25(13) . . ?

06 P2 M1CA 51.83(12) 1\_556 . ?

O8 P2 M1CA 118.82(13) . . ?

O2 P2 M2 92.65(12) . 1\_556 ?

04 P2 M2 128.77(13) . 1\_556 ?

06 P2 M2 26.07(12) 1\_556 1\_556 ?

O8 P2 M2 101.09(13) . 1\_556 ?

M1CA P2 M2 77.86(3) . 1\_556 ?

O2 P2 M2 116.15(13) . . ?

04 P2 M2 23.36(13) . . ?

06 P2 M2 118.30(13) 1\_556 . ?

O8 P2 M2 89.01(12) . . ?

M1CA P2 M2 67.23(3) . . ?

M2 P2 M2 144.10(5) 1\_556 . ?

O2 P2 M2 78.98(13) . 3\_656 ?

04 P2 M2 119.17(13) . 3\_656 ?

06 P2 M2 130.32(13) 1\_556 3\_656 ?

O8 P2 M2 32.06(12) . 3\_656 ?

M1CA P2 M2 149.78(4) . 3\_656 ?

M2 P2 M2 109.68(3) 1\_556 3\_656 ?

M2 P2 M2 97.15(3) . 3\_656 ?

O2 P2 M2 62.69(13) . 4\_566 ?

04 P2 M2 65.74(13) . 4\_566 ?

06 P2 M2 80.23(13) 1\_556 4\_566 ?

O8 P2 M2 169.14(13) . 4\_566 ?

M1CA P2 M2 68.76(3) . 4\_566 ?

M2 P2 M2 87.90(3) 1\_556 4\_566 ?

M2 P2 M2 87.14(3) . 4\_566 ?

M2 P2 M2 138.72(4) 3\_656 4\_566 ?

P1 O1 M1MN 122.1(2) . 3\_656 ?

P1 O1 M1CA 122.1(2) . 3\_656 ?

M1MN O1 M1CA 0.00(7) 3\_656 3\_656 ?

P1 O1 M1CA 128.6(2) . 1\_454 ?

M1MN O1 M1CA 100.58(13) 3\_656 1\_454 ?

M1CA O1 M1CA 100.58(13) 3\_656 1\_454 ?

P1 O1 M1MN 128.6(2) . 1\_454 ?

M1MN O1 M1MN 100.58(13) 3\_656 1\_454 ?

M1CA O1 M1MN 100.58(13) 3\_656 1\_454 ?

M1CA O1 M1MN 0.00(6) 1\_454 1\_454 ?

P1 O1 M2 72.58(13) . 1\_455 ?

M1MN O1 M2 87.68(11) 3\_656 1\_455 ?

M1CA O1 M2 87.68(11) 3\_656 1\_455 ?

M1CA O1 M2 82.85(10) 1\_454 1\_455 ?

M1MN O1 M2 82.85(10) 1\_454 1\_455 ?

P1 O1 M2 63.16(13) . 3\_656 ?

M1MN O1 M2 67.05(9) 3\_656 3\_656 ?

M1CA O1 M2 67.05(9) 3\_656 3\_656 ?

M1CA O1 M2 167.43(13) 1\_454 3\_656 ?

M1MN O1 M2 167.43(13) 1\_454 3\_656 ?

M2 O1 M2 98.34(9) 1\_455 3\_656 ?

P1 O1 M2 149.83(18) . 3\_655 ?

M1MN O1 M2 67.34(9) 3\_656 3\_655 ?

M1CA O1 M2 67.34(9) 3\_656 3\_655 ?

M1CA O1 M2 69.57(8) 1\_454 3\_655 ?

M1MN O1 M2 69.57(8) 1\_454 3\_655 ?

M2 O1 M2 137.48(9) 1\_455 3\_655 ?

M2 O1 M2 102.24(8) 3\_656 3\_655 ?

P2 O2 M3 135.12(19) . 4\_566 ?

P2 O2 M3 123.83(18) . 1\_556 ?

M3 O2 M3 101.05(13) 4\_566 1\_556 ?

P2 O2 M2 75.21(13) . 3\_656 ?

M3 O2 M2 106.48(12) 4\_566 3\_656 ?

M3 O2 M2 91.66(11) 1\_556 3\_656 ?

P2 O2 M2 94.57(15) . 4\_566 ?

M3 O2 M2 69.64(9) 4\_566 4\_566 ?

M3 O2 M2 106.92(12) 1\_556 4\_566 ?

M2 O2 M2 161.39(10) 3\_656 4\_566 ?

P2 O2 M2 62.24(11) . 1\_556 ?

M3 O2 M2 151.67(14) 4\_566 1\_556 ?

M3 O2 M2 66.92(8) 1\_556 1\_556 ?

M2 O2 M2 99.63(8) 3\_656 1\_556 ?

M2 O2 M2 88.83(8) 4\_566 1\_556 ?

P2 O2 M2 44.54(10) . . ?

M3 O2 M2 90.73(10) 4\_566 . ?

M3 O2 M2 167.64(13) 1\_556 . ?

M2 O2 M2 81.32(7) 3\_656 . ?

M2 O2 M2 80.55(7) 4\_566 . ?

M2 O2 M2 104.06(8) 1\_556 . ?

P1 03 M1MN 112.3(2) 1\_655 4\_565 ?

P1 03 M1CA 112.3(2) 1\_655 4\_565 ?

M1MN 03 M1CA 0.00(4) 4\_565 4\_565 ?

P1 03 M2 114.6(2) 1\_655 . ?

M1MN 03 M2 122.79(16) 4\_565 . ?

M1CA 03 M2 122.79(16) 4\_565 . ?

P1 03 M1CA 93.45(18) 1\_655 . ?

M1MN 03 M1CA 122.35(15) 4\_565 . ?

M1CA 03 M1CA 122.35(15) 4\_565 . ?

M2 03 M1CA 85.50(12) . . ?

P1 03 M2 145.00(18) 1\_655 4\_566 ?

M1MN 03 M2 64.76(9) 4\_565 4\_566 ?

M1CA 03 M2 64.76(9) 4\_565 4\_566 ?

M2 03 M2 92.08(10) . 4\_566 ?

M1CA 03 M2 65.23(7) . 4\_566 ?

P1 03 M2 33.02(12) 1\_655 3\_756 ?

M1MN 03 M2 137.20(13) 4\_565 3\_756 ?

M1CA 03 M2 137.20(13) 4\_565 3\_756 ?

M2 03 M2 99.51(12) . 3\_756 ?

M1CA 03 M2 62.26(7) . 3\_756 ?

M2 03 M2 124.82(9) 4\_566 3\_756 ?

P1 03 M2 116.75(17) 1\_655 4\_565 ?

M1MN 03 M2 45.51(8) 4\_565 4\_565 ?

M1CA 03 M2 45.51(8) 4\_565 4\_565 ?

M2 03 M2 84.22(10) . 4\_565 ?

M1CA 03 M2 149.68(11) . 4\_565 ?

M2 03 M2 86.71(7) 4\_566 4\_565 ?

M2 03 M2 147.77(8) 3\_756 4\_565 ?

P2 04 M2 138.4(2) . . ?

P2 04 M1CA 97.37(16) . . ?

M2 04 M1CA 105.77(14) . . ?

P2 04 M1MN 97.37(16) . . ?

M2 04 M1MN 105.77(14) . . ?

M1CA 04 M1MN 0.00(4) . . ?

P2 04 M2 91.42(14) . 4\_566 ?

M2 04 M2 125.66(13) . 4\_566 ?

M1CA 04 M2 81.06(9) . 4\_566 ?

M1MN 04 M2 81.06(9) . 4\_566 ?

P2 04 M2 35.17(10) . 1\_556 ?

M2 04 M2 154.43(14) . 1\_556 ?

M1CA 04 M2 63.55(7) . 1\_556 ?

M1MN 04 M2 63.55(7) . 1\_556 ?

M2 04 M2 77.41(6) 4\_566 1\_556 ?

P2 04 M2 42.93(10) . 3\_656 ?

M2 04 M2 97.18(12) . 3\_656 ?

M1CA 04 M2 130.34(11) . 3\_656 ?

M1MN 04 M2 130.34(11) . 3\_656 ?

M2 04 M2 119.32(8) 4\_566 3\_656 ?

M2 04 M2 76.80(5) 1\_556 3\_656 ?

P1 05 M3 129.7(2) . 4\_566 ?

P1 05 M3 113.85(19) . . ?

M3 05 M3 104.16(15) 4\_566 . ?

P1 05 M1CA 81.15(16) . 4\_465 ?

M3 05 M1CA 101.33(14) 4\_566 4\_465 ?

M3 05 M1CA 127.22(15) . 4\_465 ?

P1 05 M2 53.84(12) . 3\_656 ?

M3 05 M2 92.48(12) 4\_566 3\_656 ?

M3 05 M2 95.02(12) . 3\_656 ?

M1CA 05 M2 129.18(10) 4\_465 3\_656 ?

P1 05 M2 142.98(19) . 2\_655 ?

M3 05 M2 72.26(9) 4\_566 2\_655 ?

M3 05 M2 81.20(9) . 2\_655 ?

M1CA 05 M2 63.90(7) 4\_465 2\_655 ?

M2 05 M2 162.63(10) 3\_656 2\_655 ?

P1 05 M2 23.60(11) . 1\_455 ?

M3 05 M2 133.42(13) 4\_566 1\_455 ?

M3 05 M2 121.71(12) . 1\_455 ?

M1CA 05 M2 58.12(6) 4\_465 1\_455 ?

M2 05 M2 76.94(6) 3\_656 1\_455 ?

M2 05 M2 119.50(9) 2\_655 1\_455 ?

P1 05 M2 115.08(17) . . ?

M3 05 M2 75.00(11) 4\_566 . ?

M3 05 M2 40.48(7) . . ?

M1CA 05 M2 161.88(10) 4\_465 . ?

M2 05 M2 68.94(6) 3\_656 . ?

M2 05 M2 98.38(7) 2\_655 . ?

M2 05 M2 136.77(8) 1\_455 . ?

P2 06 M2 133.5(2) 1\_554 . ?

P2 06 M1CA 97.71(15) 1\_554 1\_554 ?

M2 06 M1CA 128.70(16) . 1\_554 ?

P2 06 M1MN 97.71(15) 1\_554 1\_554 ?

M2 06 M1MN 128.70(16) . 1\_554 ?

M1CA 06 M1MN 0.00(6) 1\_554 1\_554 ?

P2 06 M2 77.42(13) 1\_554 4\_565 ?

M2 06 M2 109.82(12) . 4\_565 ?

M1CA 06 M2 73.01(8) 1\_554 4\_565 ?

M1MN 06 M2 73.01(8) 1\_554 4\_565 ?

P2 06 M2 42.90(10) 1\_554 1\_554 ?

M2 06 M2 173.96(15) . 1\_554 ?

M1CA 06 M2 55.64(7) 1\_554 1\_554 ?

M1MN 06 M2 55.64(7) 1\_554 1\_554 ?

M2 06 M2 74.97(6) 4\_565 1\_554 ?

P2 06 M2 34.74(10) 1\_554 3\_655 ?

M2 06 M2 105.29(12) . 3\_655 ?

M1CA 06 M2 123.20(10) 1\_554 3\_655 ?

M1MN 06 M2 123.20(10) 1\_554 3\_655 ?

M2 06 M2 107.22(7) 4\_565 3\_655 ?

M2 06 M2 69.34(5) 1\_554 3\_655 ?

P1 07 M2 133.8(2) . 3\_656 ?

P1 07 M1CA 102.35(19) . 1\_455 ?

M2 07 M1CA 122.86(15) 3\_656 1\_455 ?

P1 07 M1MN 102.35(19) . 1\_455 ?

M2 07 M1MN 122.86(15) 3\_656 1\_455 ?

M1CA 07 M1MN 0.00(3) 1\_455 1\_455 ?

P1 07 M2 60.11(13) . 1\_455 ?

M2 07 M2 131.72(14) 3\_656 1\_455 ?

M1CA 07 M2 62.52(8) 1\_455 1\_455 ?

M1MN 07 M2 62.52(8) 1\_455 1\_455 ?

P2 O8 M3 126.60(19) . 3\_656 ?

P2 O8 M2 126.48(18) . 3\_656 ?

M3 O8 M2 104.27(13) 3\_656 3\_656 ?

P2 O8 M2 65.34(11) . . ?

M3 O8 M2 109.13(11) 3\_656 . ?

M2 O8 M2 116.09(11) 3\_656 . ?

P2 O8 M2 55.40(10) . 1\_556 ?

M3 O8 M2 84.60(10) 3\_656 1\_556 ?

M2 O8 M2 123.94(11) 3\_656 1\_556 ?

M2 O8 M2 112.22(8) . 1\_556 ?

\_diffrn\_measured\_fraction\_theta\_max 0.999

\_diffrn\_reflns\_theta\_full 30.06

\_diffrn\_measured\_fraction\_theta\_full 0.999

\_refine\_diff\_density\_max 1.568

\_refine\_diff\_density\_min -1.094

\_refine\_diff\_density\_rms 0.176