Ag-Catalyzed Selective Fluorination of 6-Substituted 2-Amionpyrazines

Yawei Tian†, Mingzhu Zhao†, Xiaoming Zhao\*, and Gang Zhou

Shanghai Key Lab of Chemical Assessment and Sustainability, Department of Chemistry, Tongji University, 1239 Siping Road, Shanghai 200092, China

*xmzhao08@mail.tongji.edu.cn*

1H NMR Spectrum of Compound **3a** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3a** (565 MHz, CDCl3)



1H NMR Spectrum of Compound **3a'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3a'** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3b** (600 MHz, CDCl3)





19F NMR Spectrum of Compound **3b** (565MHz, CDCl3)

****

1H NMR Spectrum of Compound **3b'** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3b'** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3c** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3c** (565 MHz, CDCl3)



1H NMR Spectrum of Compound **3c'** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3c'** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3d** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3d** (565 MHz, CDCl3)

1H NMR Spectrum of Compound **3d'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3d'** (565 MHz, CDCl3)

1H NMR Spectrum of Compound **3e** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3e** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3e'** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3e'** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3f** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3f** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3f'** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3f'** (565 MHz, CDCl3)

1H NMR Spectrum of Compound **3g** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3g** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3g'** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3g'** (565 MHz, CDCl3)

 ****

1H NMR Spectrum of Compound **3h** (600 MHz, CDCl3)

19F NMR Spectrum of Compound **3h** (565 MHz, CDCl3)



1H NMR Spectrum of Compound **3h'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3h'** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3i** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3i** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3i'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3i'** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3j** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3j** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3j'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3j'** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3k** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3k** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3k'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3k'** (565 MHz, CDCl3)



1H NMR Spectrum of Compound **3l** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3l** (565 MHz, CDCl3)

****

1H NMR Spectrum of Compound **3l'** (600 MHz, CDCl3)



19F NMR Spectrum of Compound **3l'** (565 MHz, CDCl3)



H NMR Spectrum of Compound **3n** (400 MHz, CDCl3)



13C NMR Spectrum of Compound **3n** (151 MHz, CDCl3)



19F NMR Spectrum of Compound **3n** (565 MHz, CDCl3)



1H NMR Spectrum of Compound **4a** (600 MHz, CDCl3)



13C NMR Spectrum of Compound **4a** (151 MHz, CDCl3)



19F NMR Spectrum of Compound **4a** (565 MHz, CDCl3)



**X-ray diffraction parameters and data for 3h'' (ellipsoid contour percent probability of 50%)**

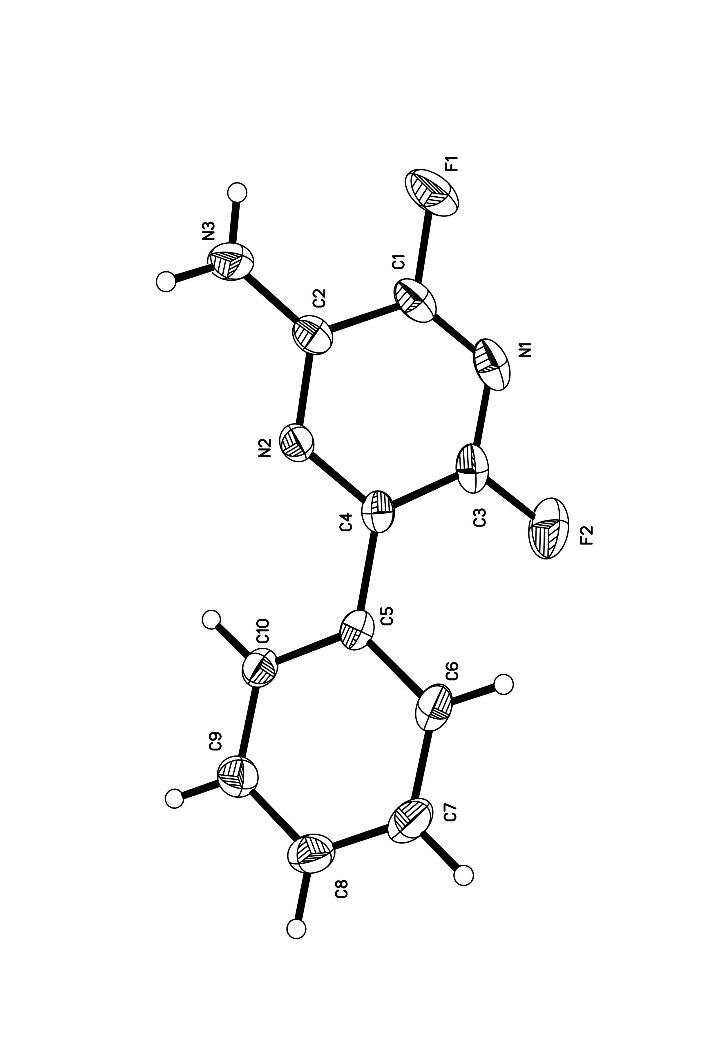


Table 1. Crystal data and structure refinement for mo\_160330B.

Identification code mo\_160330B

Empirical formula C10 H7 F2 N3

Formula weight 207.19

Temperature 293(2) K

Wavelength 0.71073 Å

Crystal system Monoclinic

Space group P2**1**/n

Unit cell dimensions a = 7.2192(4) Å = 90°.

b = 11.5514(6) Å = 96.804(2)°.

c = 10.8370(5) Å  = 90°.

Volume 897.35(8) Å3

Z 4

Density (calculated) 1.534 Mg/m3

Absorption coefficient 0.125 mm-1

F(000) 424

Crystal size 0.350 x 0.320 x 0.250 mm3

Theta range for data collection 3.223 to 27.503°.

Index ranges -9<=h<=9, -15<=k<=15, -14<=l<=13

Reflections collected 21988

Independent reflections 2038 [R(int) = 0.0222]

Completeness to theta = 25.242° 99.1 %

Absorption correction Semi-empirical from equivalents

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 2038 / 116 / 144

Goodness-of-fit on F2 1.108

Final R indices [I>2sigma(I)] R1 = 0.0510, wR2 = 0.1537

R indices (all data) R1 = 0.0591, wR2 = 0.1609

Largest diff. peak and hole 0.322 and -0.435 e.Å-3

Table 2. Atomic coordinates ( x 104) and equivalent isotropic displacement parameters (Å2x 103)

for mo\_160330B. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

F(1) 3391(2) 6884(1) 8207(1) 76(1)

N(1) 2910(2) 8200(1) 6672(2) 56(1)

C(1) 3335(3) 7152(2) 7001(2) 50(1)

N(2) 3810(2) 6549(1) 4996(1) 36(1)

F(2) 2375(2) 9497(1) 5163(2) 89(1)

C(2) 3765(2) 6272(2) 6182(1) 40(1)

N(3) 4125(2) 5181(2) 6580(1) 56(1)

C(3) 2921(3) 8431(1) 5476(2) 50(1)

C(4) 3399(2) 7641(1) 4615(1) 38(1)

C(5) 3486(2) 7910(1) 3289(1) 38(1)

C(7) 4174(3) 9200(2) 1651(2) 58(1)

C(6) 4070(3) 8989(1) 2897(2) 50(1)

C(9) 3127(3) 7285(2) 1144(2) 49(1)

C(10) 3023(2) 7062(1) 2388(2) 41(1)

C(8) 3689(3) 8356(2) 776(2) 55(1)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Table 3. Bond lengths [Å] and angles [°] for mo\_160330B.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

F(1)-C(1) 1.339(2)

N(1)-C(1) 1.288(3)

N(1)-C(3) 1.324(2)

C(1)-C(2) 1.409(2)

N(2)-C(2) 1.329(2)

N(2)-C(4) 1.350(2)

F(2)-C(3) 1.325(2)

C(2)-N(3) 1.347(2)

N(3)-H(3A) 0.851(16)

N(3)-H(3B) 0.871(16)

C(3)-C(4) 1.378(2)

C(4)-C(5) 1.479(2)

C(5)-C(10) 1.395(2)

C(5)-C(6) 1.398(2)

C(7)-C(8) 1.375(3)

C(7)-C(6) 1.383(2)

C(7)-H(7) 0.9300

C(6)-H(6) 0.9300

C(9)-C(8) 1.376(3)

C(9)-C(10) 1.383(2)

C(9)-H(9) 0.9300

C(10)-H(10) 0.9300

C(8)-H(8) 0.9300

C(1)-N(1)-C(3) 115.58(14)

N(1)-C(1)-F(1) 117.81(15)

N(1)-C(1)-C(2) 124.52(16)

F(1)-C(1)-C(2) 117.67(18)

C(2)-N(2)-C(4) 119.41(13)

N(2)-C(2)-N(3) 120.62(14)

N(2)-C(2)-C(1) 117.91(16)

N(3)-C(2)-C(1) 121.46(15)

C(2)-N(3)-H(3A) 123.1(18)

C(2)-N(3)-H(3B) 120.8(14)

H(3A)-N(3)-H(3B) 116(2)

N(1)-C(3)-F(2) 113.73(15)

N(1)-C(3)-C(4) 124.08(17)

F(2)-C(3)-C(4) 122.17(18)

N(2)-C(4)-C(3) 118.41(15)

N(2)-C(4)-C(5) 117.36(13)

C(3)-C(4)-C(5) 124.23(15)

C(10)-C(5)-C(6) 117.97(15)

C(10)-C(5)-C(4) 119.92(13)

C(6)-C(5)-C(4) 122.10(14)

C(8)-C(7)-C(6) 120.60(16)

C(8)-C(7)-H(7) 119.7

C(6)-C(7)-H(7) 119.7

C(7)-C(6)-C(5) 120.47(16)

C(7)-C(6)-H(6) 119.8

C(5)-C(6)-H(6) 119.8

C(8)-C(9)-C(10) 120.15(17)

C(8)-C(9)-H(9) 119.9

C(10)-C(9)-H(9) 119.9

C(9)-C(10)-C(5) 120.99(15)

C(9)-C(10)-H(10) 119.5

C(5)-C(10)-H(10) 119.5

C(7)-C(8)-C(9) 119.81(17)

C(7)-C(8)-H(8) 120.1

C(9)-C(8)-H(8) 120.1

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for mo\_160330B. The anisotropic

displacement factor exponent takes the form: -22[ h2 a\*2U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

U11 U22 U33 U23 U13 U12

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

F(1) 96(1) 99(1) 36(1) -13(1) 20(1) -6(1)

N(1) 57(1) 58(1) 55(1) -25(1) 15(1) -4(1)

C(1) 51(1) 64(1) 36(1) -14(1) 12(1) -7(1)

N(2) 39(1) 36(1) 34(1) -4(1) 6(1) -1(1)

F(2) 118(1) 47(1) 104(1) -13(1) 24(1) 17(1)

C(2) 38(1) 49(1) 35(1) -3(1) 8(1) -2(1)

N(3) 76(1) 58(1) 38(1) 10(1) 19(1) 11(1)

C(3) 54(1) 38(1) 60(1) -14(1) 11(1) 0(1)

C(4) 37(1) 33(1) 44(1) -6(1) 4(1) -3(1)

C(5) 37(1) 31(1) 44(1) 1(1) 4(1) 2(1)

C(7) 65(1) 40(1) 72(1) 16(1) 21(1) 4(1)

C(6) 55(1) 32(1) 63(1) 0(1) 10(1) -2(1)

C(9) 54(1) 50(1) 43(1) 0(1) 2(1) 3(1)

C(10) 45(1) 34(1) 44(1) 2(1) 3(1) -2(1)

C(8) 60(1) 55(1) 50(1) 15(1) 14(1) 12(1)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Table 5. Hydrogen coordinates ( x 104) and isotropic displacement parameters (Å2x 10 3)

for mo\_160330B.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

H(3A) 4030(40) 4960(20) 7318(17) 78(7)

H(3B) 4550(30) 4668(16) 6097(18) 56(6)

H(7) 4575 9919 1402 69

H(6) 4391 9569 3478 60

H(9) 2817 6710 555 59

H(10) 2639 6336 2627 49

H(8) 3741 8510 -61 66

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Table 6. Torsion angles [°] for mo\_160330B.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(3)-N(1)-C(1)-F(1) 178.27(15)

C(3)-N(1)-C(1)-C(2) -1.0(3)

C(4)-N(2)-C(2)-N(3) 178.37(14)

C(4)-N(2)-C(2)-C(1) -1.8(2)

N(1)-C(1)-C(2)-N(2) 2.8(3)

F(1)-C(1)-C(2)-N(2) -176.42(14)

N(1)-C(1)-C(2)-N(3) -177.32(17)

F(1)-C(1)-C(2)-N(3) 3.4(3)

C(1)-N(1)-C(3)-F(2) 176.37(17)

C(1)-N(1)-C(3)-C(4) -1.9(3)

C(2)-N(2)-C(4)-C(3) -0.8(2)

C(2)-N(2)-C(4)-C(5) 179.42(13)

N(1)-C(3)-C(4)-N(2) 2.8(3)

F(2)-C(3)-C(4)-N(2) -175.29(16)

N(1)-C(3)-C(4)-C(5) -177.40(16)

F(2)-C(3)-C(4)-C(5) 4.5(3)

N(2)-C(4)-C(5)-C(10) 33.0(2)

C(3)-C(4)-C(5)-C(10) -146.81(16)

N(2)-C(4)-C(5)-C(6) -145.36(15)

C(3)-C(4)-C(5)-C(6) 34.8(2)

C(8)-C(7)-C(6)-C(5) 0.6(3)

C(10)-C(5)-C(6)-C(7) 0.2(2)

C(4)-C(5)-C(6)-C(7) 178.56(15)

C(8)-C(9)-C(10)-C(5) -0.2(3)

C(6)-C(5)-C(10)-C(9) -0.4(2)

C(4)-C(5)-C(10)-C(9) -178.81(14)

C(6)-C(7)-C(8)-C(9) -1.2(3)

C(10)-C(9)-C(8)-C(7) 1.0(3)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo\_160330B [Å and °].

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

D-H...A d(D-H) d(H...A) d(D...A) <(DHA)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

N(3)-H(3B)...N(2)#1 0.871(16) 2.261(16) 3.120(2) 169.2(19)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

**X-ray diffraction parameters and data for Ag(dppm)1n (ellipsoid contour percent probability of 50%)**

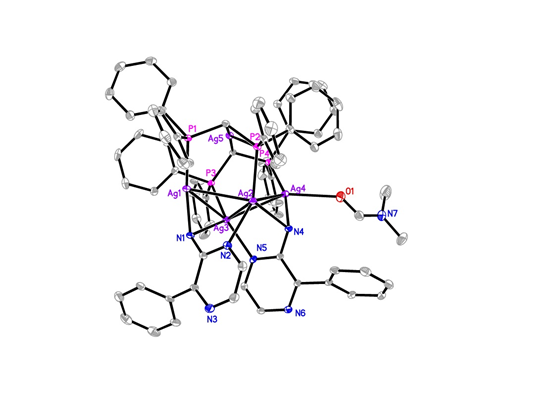


Table 1. Crystal data and structure refinement for mo\_170221b.

Identification code mo\_170221b

Empirical formula C73 H65 Ag5 Cl N7 O5 P4

Formula weight 1819.00

Temperature 150(2) K

Wavelength 0.71073 Å

Crystal system Monoclinic

Space group P21/n

Unit cell dimensions a = 17.9280(10) Å = 90°.

b = 19.9811(9) Å = 103.802(2)°.

c = 19.9625(11) Å  = 90°.

Volume 6944.5(6) Å3

Z 4

Density (calculated) 1.740 Mg/m3

Absorption coefficient 1.572 mm-1

F(000) 3616

Crystal size 0.430 x 0.280 x 0.060 mm3

Theta range for data collection 2.928 to 27.528°.

Index ranges -23<=h<=23, -25<=k<=25, -25<=l<=23

Reflections collected 109627

Independent reflections 15939 [R(int) = 0.0331]

Completeness to theta = 25.242° 99.8 %

Absorption correction Semi-empirical from equivalents

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 15939 / 44 / 897

Goodness-of-fit on F2 1.092

Final R indices [I>2sigma(I)] R1 = 0.0289, wR2 = 0.0566

R indices (all data) R1 = 0.0404, wR2 = 0.0621

Largest diff. peak and hole 0.961 and -1.037 e.Å-3

Table 2. Atomic coordinates ( x 104) and equivalent isotropic displacement parameters (Å2x 103)

for mo\_170221b. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

x y z U(eq)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Ag(1) 3825(1) 8210(1) 7158(1) 20(1)

Cl(1) 7931(1) 6721(1) 7810(1) 70(1)

Ag(2) 4729(1) 6997(1) 6943(1) 21(1)

Ag(3) 3291(1) 6795(1) 7523(1) 17(1)

Ag(4) 3533(1) 5802(1) 6490(1) 20(1)

Ag(5) 2868(1) 7432(1) 5627(1) 18(1)

P(1) 3874(1) 8683(1) 6094(1) 16(1)

P(2) 4594(1) 7390(1) 5786(1) 17(1)

P(3) 2072(1) 7059(1) 6788(1) 15(1)

P(4) 2261(1) 5983(1) 5834(1) 16(1)

O(1) 3953(2) 4647(1) 6121(1) 53(1)

O(2A) 7110(3) 6676(3) 7463(3) 89(2)

O(3A) 8198(3) 6144(2) 7418(3) 65(2)

O(4A) 8281(3) 7268(2) 7590(3) 76(2)

O(5A) 8054(6) 6562(4) 8485(3) 118(3)

O(2B) 7385(7) 6314(6) 8002(9) 115(5)

O(3B) 8571(6) 6682(6) 8466(4) 72(4)

O(4B) 7637(6) 7417(4) 7904(6) 90(4)

O(5B) 8233(9) 6713(8) 7251(5) 118(3)

N(1) 4023(1) 7742(1) 8135(1) 17(1)

N(2) 5203(1) 7306(1) 8069(1) 20(1)

N(3) 5694(2) 7270(1) 9502(1) 28(1)

N(4) 4620(1) 5847(1) 7260(1) 18(1)

N(5) 4127(1) 6104(1) 8203(1) 17(1)

N(6) 5128(1) 5215(1) 9041(1) 20(1)

C(1) 4741(2) 9201(1) 6208(1) 19(1)

C(2) 5401(2) 8972(2) 6673(2) 25(1)

C(3) 6090(2) 9316(2) 6752(2) 33(1)

C(4) 6126(2) 9899(2) 6390(2) 34(1)

C(5) 5473(2) 10132(2) 5939(2) 33(1)

C(6) 4784(2) 9786(2) 5839(2) 26(1)

C(7) 3129(2) 9259(1) 5658(1) 20(1)

N(7) 4179(2) 3532(1) 6208(2) 36(1)

C(8) 2745(2) 9184(2) 4973(2) 27(1)

C(9) 2213(2) 9664(2) 4653(2) 34(1)

C(10) 2070(2) 10220(2) 5009(2) 34(1)

C(11) 2460(2) 10301(2) 5692(2) 35(1)

C(12) 2979(2) 9821(2) 6015(2) 29(1)

C(13) 3865(2) 8008(1) 5505(1) 19(1)

C(14) 5511(2) 7704(1) 5659(1) 20(1)

C(15) 6194(2) 7502(2) 6109(2) 28(1)

C(16) 6897(2) 7764(2) 6055(2) 36(1)

C(17) 6919(2) 8234(2) 5554(2) 39(1)

C(18) 6250(2) 8435(2) 5105(2) 37(1)

C(19) 5545(2) 8169(2) 5149(2) 27(1)

C(20) 4332(2) 6732(2) 5136(2) 22(1)

C(21) 4467(2) 6067(2) 5320(2) 30(1)

C(22) 4241(2) 5564(2) 4834(2) 40(1)

C(23) 3891(2) 5726(2) 4164(2) 44(1)

C(24) 3752(2) 6383(2) 3975(2) 49(1)

C(25) 3964(2) 6889(2) 4458(2) 37(1)

C(26) 1858(2) 7952(1) 6791(1) 18(1)

C(27) 1533(2) 8315(2) 6195(2) 24(1)

C(28) 1378(2) 8993(2) 6247(2) 36(1)

C(29) 1527(2) 9305(2) 6884(2) 37(1)

C(30) 1831(2) 8945(2) 7474(2) 35(1)

C(31) 2001(2) 8272(2) 7430(2) 26(1)

C(32) 1288(2) 6731(1) 7139(1) 19(1)

C(33) 527(2) 6835(2) 6814(2) 44(1)

C(34) -56(2) 6608(2) 7104(2) 51(1)

C(35) 112(2) 6274(2) 7721(2) 35(1)

C(36) 861(2) 6171(2) 8049(2) 43(1)

C(37) 1450(2) 6397(2) 7760(2) 34(1)

C(38) 1970(2) 6834(1) 5903(1) 16(1)

C(39) 1547(2) 5450(1) 6098(1) 20(1)

C(40) 1759(2) 5078(2) 6689(2) 38(1)

C(41) 1216(3) 4726(2) 6939(2) 54(1)

C(42) 461(2) 4750(2) 6608(2) 43(1)

C(43) 234(2) 5120(2) 6015(2) 50(1)

C(44) 778(2) 5468(2) 5757(2) 42(1)

C(45) 2092(2) 5776(1) 4920(1) 19(1)

C(46) 2321(2) 5139(2) 4761(2) 28(1)

C(47) 2140(2) 4918(2) 4079(2) 33(1)

C(48) 1750(2) 5331(2) 3562(2) 34(1)

C(49) 1551(2) 5969(2) 3712(2) 36(1)

C(50) 1718(2) 6195(2) 4396(2) 29(1)

C(51) 5907(2) 7078(2) 8388(2) 26(1)

C(52) 6142(2) 7050(2) 9092(2) 33(1)

C(53) 5016(2) 7526(1) 9202(1) 20(1)

C(54) 4518(2) 7752(2) 9654(1) 22(1)

C(55) 4195(2) 8389(2) 9588(2) 30(1)

C(56) 3718(2) 8590(2) 10007(2) 39(1)

C(57) 3554(2) 8150(2) 10488(2) 45(1)

C(58) 3879(2) 7523(2) 10562(2) 44(1)

C(59) 4366(2) 7324(2) 10155(2) 32(1)

C(60) 4741(2) 7541(1) 8461(1) 17(1)

C(61) 4635(1) 5753(1) 7938(1) 16(1)

C(62) 4144(2) 6029(1) 8877(1) 18(1)

C(63) 4629(2) 5589(1) 9291(1) 21(1)

C(64) 5149(2) 5298(1) 8389(1) 17(1)

C(65) 5710(2) 4876(2) 8133(1) 22(1)

C(66) 5716(2) 4187(2) 8237(2) 30(1)

C(67) 6255(2) 3790(2) 8028(2) 39(1)

C(68) 6801(2) 4081(2) 7736(2) 42(1)

C(69) 6803(2) 4765(2) 7636(2) 38(1)

C(70) 6252(2) 5161(2) 7825(2) 26(1)

C(71) 4311(2) 4160(2) 6403(2) 39(1)

C(72) 4606(3) 2975(2) 6587(2) 54(1)

C(73) 3571(3) 3370(3) 5617(3) 85(2)

Table 3. Bond lengths [Å] and angles [°] for mo\_170221b.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Ag(1)-N(1) 2.116(2)

Ag(1)-P(1) 2.3452(7)

Ag(1)-Ag(2) 3.0026(3)

Ag(1)-Ag(3) 3.1261(3)

Cl(1)-O(5A) 1.349(5)

Cl(1)-O(5B) 1.351(7)

Cl(1)-O(4A) 1.383(4)

Cl(1)-O(2B) 1.396(7)

Cl(1)-O(2A) 1.473(5)

Cl(1)-O(4B) 1.515(7)

Cl(1)-O(3B) 1.523(7)

Cl(1)-O(3A) 1.533(4)

Ag(2)-N(2) 2.289(2)

Ag(2)-P(2) 2.3957(7)

Ag(2)-N(4) 2.403(2)

Ag(2)-Ag(3) 3.0945(3)

Ag(2)-Ag(4) 3.1935(3)

Ag(3)-N(5) 2.242(2)

Ag(3)-P(3) 2.3826(7)

Ag(3)-N(1) 2.455(2)

Ag(3)-Ag(4) 2.9679(3)

Ag(4)-N(4) 2.177(2)

Ag(4)-P(4) 2.3700(7)

Ag(4)-O(1) 2.589(3)

Ag(5)-C(38) 2.178(3)

Ag(5)-C(13) 2.189(3)

Ag(5)-P(2) 3.0351(7)

P(1)-C(13) 1.787(3)

P(1)-C(7) 1.819(3)

P(1)-C(1) 1.837(3)

P(2)-C(13) 1.789(3)

P(2)-C(20) 1.827(3)

P(2)-C(14) 1.833(3)

P(3)-C(38) 1.791(3)

P(3)-C(26) 1.825(3)

P(3)-C(32) 1.835(3)

P(4)-C(38) 1.794(3)

P(4)-C(45) 1.826(3)

P(4)-C(39) 1.836(3)

O(1)-C(71) 1.227(4)

N(1)-C(60) 1.358(3)

N(1)-H(1A) 0.79(3)

N(2)-C(51) 1.350(4)

N(2)-C(60) 1.352(4)

N(3)-C(53) 1.323(4)

N(3)-C(52) 1.351(4)

N(4)-C(61) 1.360(3)

N(4)-H(4A) 0.82(3)

N(5)-C(62) 1.347(3)

N(5)-C(61) 1.353(3)

N(6)-C(64) 1.323(3)

N(6)-C(63) 1.350(4)

C(1)-C(6) 1.393(4)

C(1)-C(2) 1.396(4)

C(2)-C(3) 1.388(4)

C(2)-H(2) 0.9500

C(3)-C(4) 1.381(5)

C(3)-H(3) 0.9500

C(4)-C(5) 1.377(5)

C(4)-H(4) 0.9500

C(5)-C(6) 1.388(4)

C(5)-H(5) 0.9500

C(6)-H(6) 0.9500

C(7)-C(8) 1.385(4)

C(7)-C(12) 1.390(4)

N(7)-C(71) 1.318(4)

N(7)-C(73) 1.439(5)

N(7)-C(72) 1.456(5)

C(8)-C(9) 1.395(4)

C(8)-H(8) 0.9500

C(9)-C(10) 1.377(5)

C(9)-H(9) 0.9500

C(10)-C(11) 1.384(5)

C(10)-H(10) 0.9500

C(11)-C(12) 1.384(4)

C(11)-H(11) 0.9500

C(12)-H(12) 0.9500

C(13)-H(13) 1.0000

C(14)-C(19) 1.391(4)

C(14)-C(15) 1.393(4)

C(15)-C(16) 1.393(4)

C(15)-H(15) 0.9500

C(16)-C(17) 1.380(5)

C(16)-H(16) 0.9500

C(17)-C(18) 1.375(5)

C(17)-H(17) 0.9500

C(18)-C(19) 1.393(4)

C(18)-H(18) 0.9500

C(19)-H(19) 0.9500

C(20)-C(21) 1.384(4)

C(20)-C(25) 1.394(4)

C(21)-C(22) 1.389(5)

C(21)-H(21) 0.9500

C(22)-C(23) 1.374(5)

C(22)-H(22) 0.9500

C(23)-C(24) 1.371(6)

C(23)-H(23) 0.9500

C(24)-C(25) 1.386(5)

C(24)-H(24) 0.9500

C(25)-H(25) 0.9500

C(26)-C(31) 1.393(4)

C(26)-C(27) 1.397(4)

C(27)-C(28) 1.393(4)

C(27)-H(27) 0.9500

C(28)-C(29) 1.382(5)

C(28)-H(28) 0.9500

C(29)-C(30) 1.378(5)

C(29)-H(29) 0.9500

C(30)-C(31) 1.386(4)

C(30)-H(30) 0.9500

C(31)-H(31) 0.9500

C(32)-C(37) 1.376(4)

C(32)-C(33) 1.379(4)

C(33)-C(34) 1.386(5)

C(33)-H(33) 0.9500

C(34)-C(35) 1.371(5)

C(34)-H(34) 0.9500

C(35)-C(36) 1.361(5)

C(35)-H(35) 0.9500

C(36)-C(37) 1.395(5)

C(36)-H(36) 0.9500

C(37)-H(37) 0.9500

C(38)-H(38) 1.0000

C(39)-C(40) 1.370(4)

C(39)-C(44) 1.385(4)

C(40)-C(41) 1.385(5)

C(40)-H(40) 0.9500

C(41)-C(42) 1.359(6)

C(41)-H(41) 0.9500

C(42)-C(43) 1.372(6)

C(42)-H(42) 0.9500

C(43)-C(44) 1.394(5)

C(43)-H(43) 0.9500

C(44)-H(44) 0.9500

C(45)-C(50) 1.382(4)

C(45)-C(46) 1.397(4)

C(46)-C(47) 1.394(4)

C(46)-H(46) 0.9500

C(47)-C(48) 1.376(5)

C(47)-H(47) 0.9500

C(48)-C(49) 1.377(5)

C(48)-H(48) 0.9500

C(49)-C(50) 1.399(4)

C(49)-H(49) 0.9500

C(50)-H(50) 0.9500

C(51)-C(52) 1.368(4)

C(51)-H(51) 0.9500

C(52)-H(52) 0.9500

C(53)-C(60) 1.443(4)

C(53)-C(54) 1.481(4)

C(54)-C(59) 1.391(4)

C(54)-C(55) 1.392(4)

C(55)-C(56) 1.391(5)

C(55)-H(55) 0.9500

C(56)-C(57) 1.383(5)

C(56)-H(56) 0.9500

C(57)-C(58) 1.374(6)

C(57)-H(57) 0.9500

C(58)-C(59) 1.385(5)

C(58)-H(58) 0.9500

C(59)-H(59) 0.9500

C(61)-C(64) 1.445(4)

C(62)-C(63) 1.366(4)

C(62)-H(62) 0.9500

C(63)-H(63) 0.9500

C(64)-C(65) 1.492(4)

C(65)-C(70) 1.389(4)

C(65)-C(66) 1.392(4)

C(66)-C(67) 1.390(5)

C(66)-H(66) 0.9500

C(67)-C(68) 1.383(6)

C(67)-H(67) 0.9500

C(68)-C(69) 1.380(6)

C(68)-H(68) 0.9500

C(69)-C(70) 1.387(4)

C(69)-H(69) 0.9500

C(70)-H(70) 0.9500

C(71)-H(71) 0.9500

C(72)-H(72A) 0.9800

C(72)-H(72B) 0.9800

C(72)-H(72C) 0.9800

C(73)-H(73A) 0.9800

C(73)-H(73B) 0.9800

C(73)-H(73C) 0.9800

N(1)-Ag(1)-P(1) 168.24(7)

N(1)-Ag(1)-Ag(2) 78.31(7)

P(1)-Ag(1)-Ag(2) 93.327(19)

N(1)-Ag(1)-Ag(3) 51.56(6)

P(1)-Ag(1)-Ag(3) 130.937(19)

Ag(2)-Ag(1)-Ag(3) 60.613(7)

O(5A)-Cl(1)-O(4A) 121.7(5)

O(5B)-Cl(1)-O(2B) 131.7(9)

O(5A)-Cl(1)-O(2A) 111.2(5)

O(4A)-Cl(1)-O(2A) 112.2(3)

O(5B)-Cl(1)-O(4B) 109.4(7)

O(2B)-Cl(1)-O(4B) 102.3(6)

O(5B)-Cl(1)-O(3B) 110.0(7)

O(2B)-Cl(1)-O(3B) 99.7(7)

O(4B)-Cl(1)-O(3B) 98.9(6)

O(5A)-Cl(1)-O(3A) 109.6(4)

O(4A)-Cl(1)-O(3A) 102.2(3)

O(2A)-Cl(1)-O(3A) 96.5(3)

N(2)-Ag(2)-P(2) 141.85(6)

N(2)-Ag(2)-N(4) 91.95(8)

P(2)-Ag(2)-N(4) 124.80(6)

N(2)-Ag(2)-Ag(1) 74.24(6)

P(2)-Ag(2)-Ag(1) 86.531(19)

N(4)-Ag(2)-Ag(1) 130.77(6)

N(2)-Ag(2)-Ag(3) 79.33(6)

P(2)-Ag(2)-Ag(3) 120.098(19)

N(4)-Ag(2)-Ag(3) 69.46(6)

Ag(1)-Ag(2)-Ag(3) 61.669(7)

N(2)-Ag(2)-Ag(4) 123.14(6)

P(2)-Ag(2)-Ag(4) 93.712(19)

N(4)-Ag(2)-Ag(4) 42.96(5)

Ag(1)-Ag(2)-Ag(4) 107.154(9)

Ag(3)-Ag(2)-Ag(4) 56.300(7)

N(5)-Ag(3)-P(3) 153.11(6)

N(5)-Ag(3)-N(1) 88.44(8)

P(3)-Ag(3)-N(1) 116.00(6)

N(5)-Ag(3)-Ag(4) 79.71(6)

P(3)-Ag(3)-Ag(4) 89.122(18)

N(1)-Ag(3)-Ag(4) 135.39(6)

N(5)-Ag(3)-Ag(2) 79.08(6)

P(3)-Ag(3)-Ag(2) 117.665(19)

N(1)-Ag(3)-Ag(2) 72.05(6)

Ag(4)-Ag(3)-Ag(2) 63.535(7)

N(5)-Ag(3)-Ag(1) 120.05(6)

P(3)-Ag(3)-Ag(1) 86.720(18)

N(1)-Ag(3)-Ag(1) 42.47(5)

Ag(4)-Ag(3)-Ag(1) 109.812(9)

Ag(2)-Ag(3)-Ag(1) 57.718(7)

N(4)-Ag(4)-P(4) 164.71(7)

N(4)-Ag(4)-O(1) 88.03(10)

P(4)-Ag(4)-O(1) 106.61(7)

N(4)-Ag(4)-Ag(3) 74.67(7)

P(4)-Ag(4)-Ag(3) 90.076(19)

O(1)-Ag(4)-Ag(3) 153.44(6)

N(4)-Ag(4)-Ag(2) 48.78(6)

P(4)-Ag(4)-Ag(2) 122.359(19)

O(1)-Ag(4)-Ag(2) 121.71(7)

Ag(3)-Ag(4)-Ag(2) 60.165(7)

C(38)-Ag(5)-C(13) 171.61(10)

C(38)-Ag(5)-P(2) 138.97(7)

C(13)-Ag(5)-P(2) 35.60(7)

C(13)-P(1)-C(7) 105.79(13)

C(13)-P(1)-C(1) 112.33(13)

C(7)-P(1)-C(1) 101.84(13)

C(13)-P(1)-Ag(1) 107.23(9)

C(7)-P(1)-Ag(1) 120.46(9)

C(1)-P(1)-Ag(1) 109.20(9)

C(13)-P(2)-C(20) 103.24(13)

C(13)-P(2)-C(14) 109.36(13)

C(20)-P(2)-C(14) 103.55(13)

C(13)-P(2)-Ag(2) 115.34(9)

C(20)-P(2)-Ag(2) 113.52(10)

C(14)-P(2)-Ag(2) 110.95(9)

C(13)-P(2)-Ag(5) 45.44(9)

C(20)-P(2)-Ag(5) 82.12(9)

C(14)-P(2)-Ag(5) 154.35(10)

Ag(2)-P(2)-Ag(5) 88.67(2)

C(38)-P(3)-C(26) 106.07(13)

C(38)-P(3)-C(32) 112.29(12)

C(26)-P(3)-C(32) 99.64(12)

C(38)-P(3)-Ag(3) 114.50(9)

C(26)-P(3)-Ag(3) 112.19(9)

C(32)-P(3)-Ag(3) 111.09(9)

C(38)-P(4)-C(45) 108.00(13)

C(38)-P(4)-C(39) 107.01(13)

C(45)-P(4)-C(39) 101.26(12)

C(38)-P(4)-Ag(4) 111.16(9)

C(45)-P(4)-Ag(4) 115.22(9)

C(39)-P(4)-Ag(4) 113.45(9)

C(71)-O(1)-Ag(4) 137.1(2)

C(60)-N(1)-Ag(1) 120.22(18)

C(60)-N(1)-Ag(3) 110.14(17)

Ag(1)-N(1)-Ag(3) 85.97(8)

C(60)-N(1)-H(1A) 112(2)

Ag(1)-N(1)-H(1A) 115(2)

Ag(3)-N(1)-H(1A) 110(2)

C(51)-N(2)-C(60) 118.4(2)

C(51)-N(2)-Ag(2) 117.28(19)

C(60)-N(2)-Ag(2) 121.87(17)

C(53)-N(3)-C(52) 117.8(3)

C(61)-N(4)-Ag(4) 119.95(18)

C(61)-N(4)-Ag(2) 114.27(18)

Ag(4)-N(4)-Ag(2) 88.26(8)

C(61)-N(4)-H(4A) 109(2)

Ag(4)-N(4)-H(4A) 111(2)

Ag(2)-N(4)-H(4A) 113(2)

C(62)-N(5)-C(61) 118.5(2)

C(62)-N(5)-Ag(3) 121.69(18)

C(61)-N(5)-Ag(3) 119.84(17)

C(64)-N(6)-C(63) 118.1(2)

C(6)-C(1)-C(2) 118.8(3)

C(6)-C(1)-P(1) 124.1(2)

C(2)-C(1)-P(1) 117.1(2)

C(3)-C(2)-C(1) 120.2(3)

C(3)-C(2)-H(2) 119.9

C(1)-C(2)-H(2) 119.9

C(4)-C(3)-C(2) 120.6(3)

C(4)-C(3)-H(3) 119.7

C(2)-C(3)-H(3) 119.7

C(5)-C(4)-C(3) 119.3(3)

C(5)-C(4)-H(4) 120.4

C(3)-C(4)-H(4) 120.4

C(4)-C(5)-C(6) 121.0(3)

C(4)-C(5)-H(5) 119.5

C(6)-C(5)-H(5) 119.5

C(5)-C(6)-C(1) 120.1(3)

C(5)-C(6)-H(6) 120.0

C(1)-C(6)-H(6) 120.0

C(8)-C(7)-C(12) 118.8(3)

C(8)-C(7)-P(1) 122.7(2)

C(12)-C(7)-P(1) 118.4(2)

C(71)-N(7)-C(73) 120.3(3)

C(71)-N(7)-C(72) 122.5(3)

C(73)-N(7)-C(72) 117.1(3)

C(7)-C(8)-C(9) 120.2(3)

C(7)-C(8)-H(8) 119.9

C(9)-C(8)-H(8) 119.9

C(10)-C(9)-C(8) 120.6(3)

C(10)-C(9)-H(9) 119.7

C(8)-C(9)-H(9) 119.7

C(9)-C(10)-C(11) 119.3(3)

C(9)-C(10)-H(10) 120.3

C(11)-C(10)-H(10) 120.3

C(12)-C(11)-C(10) 120.3(3)

C(12)-C(11)-H(11) 119.8

C(10)-C(11)-H(11) 119.8

C(11)-C(12)-C(7) 120.7(3)

C(11)-C(12)-H(12) 119.6

C(7)-C(12)-H(12) 119.6

P(1)-C(13)-P(2) 115.05(15)

P(1)-C(13)-Ag(5) 101.65(12)

P(2)-C(13)-Ag(5) 98.96(13)

P(1)-C(13)-H(13) 113.2

P(2)-C(13)-H(13) 113.2

Ag(5)-C(13)-H(13) 113.2

C(19)-C(14)-C(15) 118.6(3)

C(19)-C(14)-P(2) 121.9(2)

C(15)-C(14)-P(2) 119.4(2)

C(16)-C(15)-C(14) 121.0(3)

C(16)-C(15)-H(15) 119.5

C(14)-C(15)-H(15) 119.5

C(17)-C(16)-C(15) 119.6(3)

C(17)-C(16)-H(16) 120.2

C(15)-C(16)-H(16) 120.2

C(18)-C(17)-C(16) 120.1(3)

C(18)-C(17)-H(17) 120.0

C(16)-C(17)-H(17) 120.0

C(17)-C(18)-C(19) 120.6(3)

C(17)-C(18)-H(18) 119.7

C(19)-C(18)-H(18) 119.7

C(14)-C(19)-C(18) 120.1(3)

C(14)-C(19)-H(19) 120.0

C(18)-C(19)-H(19) 120.0

C(21)-C(20)-C(25) 119.1(3)

C(21)-C(20)-P(2) 120.2(2)

C(25)-C(20)-P(2) 120.7(2)

C(20)-C(21)-C(22) 120.4(3)

C(20)-C(21)-H(21) 119.8

C(22)-C(21)-H(21) 119.8

C(23)-C(22)-C(21) 120.0(3)

C(23)-C(22)-H(22) 120.0

C(21)-C(22)-H(22) 120.0

C(24)-C(23)-C(22) 120.2(3)

C(24)-C(23)-H(23) 119.9

C(22)-C(23)-H(23) 119.9

C(23)-C(24)-C(25) 120.4(4)

C(23)-C(24)-H(24) 119.8

C(25)-C(24)-H(24) 119.8

C(24)-C(25)-C(20) 119.9(3)

C(24)-C(25)-H(25) 120.0

C(20)-C(25)-H(25) 120.0

C(31)-C(26)-C(27) 119.4(3)

C(31)-C(26)-P(3) 117.3(2)

C(27)-C(26)-P(3) 123.3(2)

C(28)-C(27)-C(26) 119.4(3)

C(28)-C(27)-H(27) 120.3

C(26)-C(27)-H(27) 120.3

C(29)-C(28)-C(27) 120.6(3)

C(29)-C(28)-H(28) 119.7

C(27)-C(28)-H(28) 119.7

C(30)-C(29)-C(28) 120.1(3)

C(30)-C(29)-H(29) 119.9

C(28)-C(29)-H(29) 119.9

C(29)-C(30)-C(31) 119.9(3)

C(29)-C(30)-H(30) 120.0

C(31)-C(30)-H(30) 120.0

C(30)-C(31)-C(26) 120.6(3)

C(30)-C(31)-H(31) 119.7

C(26)-C(31)-H(31) 119.7

C(37)-C(32)-C(33) 118.0(3)

C(37)-C(32)-P(3) 120.0(2)

C(33)-C(32)-P(3) 121.9(2)

C(32)-C(33)-C(34) 121.0(3)

C(32)-C(33)-H(33) 119.5

C(34)-C(33)-H(33) 119.5

C(35)-C(34)-C(33) 120.5(3)

C(35)-C(34)-H(34) 119.7

C(33)-C(34)-H(34) 119.7

C(36)-C(35)-C(34) 119.2(3)

C(36)-C(35)-H(35) 120.4

C(34)-C(35)-H(35) 120.4

C(35)-C(36)-C(37) 120.5(3)

C(35)-C(36)-H(36) 119.7

C(37)-C(36)-H(36) 119.7

C(32)-C(37)-C(36) 120.9(3)

C(32)-C(37)-H(37) 119.6

C(36)-C(37)-H(37) 119.6

P(3)-C(38)-P(4) 110.53(14)

P(3)-C(38)-Ag(5) 101.80(12)

P(4)-C(38)-Ag(5) 104.79(12)

P(3)-C(38)-H(38) 113.0

P(4)-C(38)-H(38) 113.0

Ag(5)-C(38)-H(38) 113.0

C(40)-C(39)-C(44) 118.4(3)

C(40)-C(39)-P(4) 119.6(2)

C(44)-C(39)-P(4) 121.6(2)

C(39)-C(40)-C(41) 120.8(3)

C(39)-C(40)-H(40) 119.6

C(41)-C(40)-H(40) 119.6

C(42)-C(41)-C(40) 120.7(3)

C(42)-C(41)-H(41) 119.6

C(40)-C(41)-H(41) 119.6

C(41)-C(42)-C(43) 119.6(3)

C(41)-C(42)-H(42) 120.2

C(43)-C(42)-H(42) 120.2

C(42)-C(43)-C(44) 119.9(4)

C(42)-C(43)-H(43) 120.1

C(44)-C(43)-H(43) 120.1

C(39)-C(44)-C(43) 120.5(3)

C(39)-C(44)-H(44) 119.7

C(43)-C(44)-H(44) 119.7

C(50)-C(45)-C(46) 119.8(3)

C(50)-C(45)-P(4) 123.7(2)

C(46)-C(45)-P(4) 116.4(2)

C(47)-C(46)-C(45) 119.8(3)

C(47)-C(46)-H(46) 120.1

C(45)-C(46)-H(46) 120.1

C(48)-C(47)-C(46) 120.1(3)

C(48)-C(47)-H(47) 120.0

C(46)-C(47)-H(47) 120.0

C(47)-C(48)-C(49) 120.2(3)

C(47)-C(48)-H(48) 119.9

C(49)-C(48)-H(48) 119.9

C(48)-C(49)-C(50) 120.3(3)

C(48)-C(49)-H(49) 119.8

C(50)-C(49)-H(49) 119.8

C(45)-C(50)-C(49) 119.6(3)

C(45)-C(50)-H(50) 120.2

C(49)-C(50)-H(50) 120.2

N(2)-C(51)-C(52) 121.6(3)

N(2)-C(51)-H(51) 119.2

C(52)-C(51)-H(51) 119.2

N(3)-C(52)-C(51) 121.8(3)

N(3)-C(52)-H(52) 119.1

C(51)-C(52)-H(52) 119.1

N(3)-C(53)-C(60) 121.6(3)

N(3)-C(53)-C(54) 117.6(2)

C(60)-C(53)-C(54) 120.6(2)

C(59)-C(54)-C(55) 118.6(3)

C(59)-C(54)-C(53) 120.1(3)

C(55)-C(54)-C(53) 121.3(3)

C(56)-C(55)-C(54) 120.7(3)

C(56)-C(55)-H(55) 119.7

C(54)-C(55)-H(55) 119.7

C(57)-C(56)-C(55) 119.7(3)

C(57)-C(56)-H(56) 120.1

C(55)-C(56)-H(56) 120.1

C(58)-C(57)-C(56) 119.9(3)

C(58)-C(57)-H(57) 120.0

C(56)-C(57)-H(57) 120.0

C(57)-C(58)-C(59) 120.5(3)

C(57)-C(58)-H(58) 119.7

C(59)-C(58)-H(58) 119.7

C(58)-C(59)-C(54) 120.4(3)

C(58)-C(59)-H(59) 119.8

C(54)-C(59)-H(59) 119.8

N(2)-C(60)-N(1) 117.8(2)

N(2)-C(60)-C(53) 118.7(2)

N(1)-C(60)-C(53) 123.3(3)

N(5)-C(61)-N(4) 117.5(2)

N(5)-C(61)-C(64) 118.1(2)

N(4)-C(61)-C(64) 124.4(2)

N(5)-C(62)-C(63) 122.3(3)

N(5)-C(62)-H(62) 118.9

C(63)-C(62)-H(62) 118.9

N(6)-C(63)-C(62) 121.1(2)

N(6)-C(63)-H(63) 119.5

C(62)-C(63)-H(63) 119.5

N(6)-C(64)-C(61) 121.9(2)

N(6)-C(64)-C(65) 116.5(2)

C(61)-C(64)-C(65) 121.6(2)

C(70)-C(65)-C(66) 119.3(3)

C(70)-C(65)-C(64) 121.3(3)

C(66)-C(65)-C(64) 119.3(3)

C(67)-C(66)-C(65) 120.1(3)

C(67)-C(66)-H(66) 119.9

C(65)-C(66)-H(66) 119.9

C(68)-C(67)-C(66) 119.9(3)

C(68)-C(67)-H(67) 120.0

C(66)-C(67)-H(67) 120.0

C(69)-C(68)-C(67) 120.3(3)

C(69)-C(68)-H(68) 119.9

C(67)-C(68)-H(68) 119.9

C(68)-C(69)-C(70) 119.9(3)

C(68)-C(69)-H(69) 120.0

C(70)-C(69)-H(69) 120.0

C(69)-C(70)-C(65) 120.4(3)

C(69)-C(70)-H(70) 119.8

C(65)-C(70)-H(70) 119.8

O(1)-C(71)-N(7) 125.6(4)

O(1)-C(71)-H(71) 117.2

N(7)-C(71)-H(71) 117.2

N(7)-C(72)-H(72A) 109.5

N(7)-C(72)-H(72B) 109.5

H(72A)-C(72)-H(72B) 109.5

N(7)-C(72)-H(72C) 109.5

H(72A)-C(72)-H(72C) 109.5

H(72B)-C(72)-H(72C) 109.5

N(7)-C(73)-H(73A) 109.5

N(7)-C(73)-H(73B) 109.5

H(73A)-C(73)-H(73B) 109.5

N(7)-C(73)-H(73C) 109.5

H(73A)-C(73)-H(73C) 109.5

H(73B)-C(73)-H(73C) 109.5

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_