Supplementary materials for X-ray crystallographic data of *anti*-[Pd(μ-NH2)(Ph)(PEt3)]2 (**1**) (Tables 1-1 to 5-1) and [Pd(dppe)(NH2)]2(OTf)2 (**2**) (Tables 1-2 to 5-2): crystal data, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters.

Parent-amido (NH2) palladium(II) complexes: synthesis, reactions, and catalytic hydroamination

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Table 1-1. Crystal data and structure refinement for *anti*-[Pd(μ-NH2)(Ph)(PEt3)]2 (**1**).

Chemical formula C24H44N2P2Pd2

Formula weight 635.41

Temperature 293(2) K

Wavelength 0.71069 Å

Crystal system Monoclinic

Space group P21/n

Unit cell dimensions a = 13.228(2) Å α = 90.000(10) deg.

b = 18.132(2) Å β = 101.410(10) deg.

c = 24.745(2) Å γ = 90.000(10) deg.

Volume 5817.8(12) Å3

Z 4

Density (calculated) 1.451 Mg/m3

Absorption coefficient 1.360 mm-1

F(000) 2688

Crystal size 0.80 x 0.50 x 0.25 mm

Theta range for data collection 2.02 to 22.56 deg.

Index ranges 0≤h≤14, 0≤k≤19,

-26≤l≤26

Reflections collected 7990

Independent reflections 7614 [R(int) = 0.0373]

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 7613 / 0 / 540

Goodness-of-fit on F2 1.122

Final R indices [I>2σ(I)]*a*  R1 = 0.0547, wR2 = 0.1417

R indices (all data)*a*  R1 = 0.0715, wR2 = 0.1504

Largest diff. peak and hole 0.743 and -0.717 e Å-3

*a*R1 = Σ⎪⎪Fo⎪ - ⎪Fc⎪⎪/Σ⎪Fo⎪; wR2 = [Σw(Fo2 - Fc2)2/ΣwFo4]1/2

Table 2-1. Atomic coordinates (×104) and equivalent isotropic displacement parameters (Å2×103) for **1**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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

x y z U(eq)

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

Pd(1) 5994(1) 8523(1) -2395(1) 58(1)

Pd(2) 7028(1) 8115(1) -1262(1) 61(1)

P(1) 5088(2) 9536(2) -2686(1) 73(1)

P(2) 6833(2) 7116(2) -764(1) 76(1)

N(1) 7143(6) 8991(5) -1781(3) 72(2)

N(2) 6803(6) 7595(4) -2047(3) 67(2)

C(1) 4979(7) 7930(5) -2929(3) 59(2)

C(2) 5199(7) 7649(6) -3411(4) 69(3)

C(3) 4488(9) 7240(6) -3781(4) 80(3)

C(4) 3539(9) 7082(6) -3680(4) 82(3)

C(5) 3306(8) 7335(6) -3198(4) 82(3)

C(6) 4010(8) 7743(6) -2837(4) 77(3)

C(7) 5733(8) 10419(6) -2548(5) 86(3)

C(8) 6697(11) 10516(7) -2766(5) 106(4)

C(9) 3988(9) 9656(8) -2358(6) 114(4)

C(10) 4252(13) 9569(9) -1741(7) 139(6)

C(11) 4435(11) 9594(7) -3408(5) 112(5)

C(12) 5108(16) 9538(10) -3825(6) 158(7)

C(13) 7227(8) 8761(5) -595(3) 63(2)

C(14) 6417(9) 9055(5) -401(4) 79(3)

C(15) 6547(11) 9508(6) 68(5) 92(4)

C(16) 7509(14) 9653(8) 353(5) 105(4)

C(17) 8326(12) 9385(7) 173(5) 106(4)

C(18) 8196(9) 8930(6) -282(4) 87(3)

C(19) 6769(13) 7269(8) -39(5) 130(5)

C(20) 6667(15) 6552(9) 315(6) 152(6)

C(21) 7931(16) 6425(9) -695(7) 160(7)

C(22) 8919(14) 6783(12) -321(8) 179(8)

C(23) 5847(17) 6480(10) -1090(7) 204(9)

C(24) 4732(13) 6999(13) -1185(9) 206(10)

Pd(3) 4183(1) 6794(1) 2324(1) 54(1)

Pd(4) 3034(1) 7111(1) 1204(1) 54(1)

P(3) 5192(2) 5830(2) 2617(1) 69(1)

P(4) 3142(2) 8063(2) 644(1) 69(1)

N(3) 3011(5) 6261(4) 1764(3) 62(2)

N(4) 3300(6) 7682(4) 1968(3) 60(2)

C(31) 5214(7) 7448(5) 2795(4) 61(2)

C(32) 5069(8) 7713(6) 3304(4) 78(3)

C(33) 5794(11) 8171(7) 3628(5) 99(4)

C(34) 6656(10) 8377(7) 3452(6) 103(4)

C(35) 6804(9) 8152(7) 2958(5) 105(4)

C(36) 6079(8) 7697(6) 2635(4) 82(3)

C(37) 5836(9) 5805(7) 3337(4) 92(4)

C(38) 5100(12) 5764(8) 3745(5) 119(5)

C(39) 4560(9) 4942(6) 2523(5) 98(4)

C(40) 5198(14) 4251(8) 2688(7) 154(7)

C(41) 6254(9) 5750(8) 2272(5) 112(4)

C(42) 5964(15) 5741(11) 1656(7) 171(8)

C(43) 2847(8) 6411(6) 572(4) 67(3)

C(44) 3664(10) 6133(7) 366(5) 102(4)

C(45) 3535(14) 5616(8) -70(6) 122(5)

C(46) 2581(18) 5378(8) -292(6) 122(6)

C(47) 1755(13) 5638(8) -106(5) 114(5)

C(48) 1898(9) 6156(6) 321(4) 87(3)

C(491) 4454(15) 8242(11) 534(9) 108(8)

C(492) 4190(28) 8652(21) 895(15) 83(16)

C(50) 5268(10) 8236(8) 1039(6) 117(5)

C(511) 2853(14) 8980(10) 916(7) 83(7)

C(512) 1958(28) 8667(21) 513(16) 109(15)

C(52) 1779(12) 9036(9) 1078(8) 145(6)

C(531) 2332(18) 8060(11) -54(8) 81(7)

C(541) 1225(24) 8065(16) -30(13) 137(11)

C(532) 3060(25) 7776(17) -140(13) 113(11)

C(542) 3115(29) 8389(21) -517(16) 150(15)

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

Table 3-1. Bond lengths [Å] and angles [°] for **1**.

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

Pd(1)-C(1) 2.000(9)

Pd(1)-N(2) 2.085(7)

Pd(1)-N(1) 2.104(7)

Pd(1)-P(1) 2.233(3)

Pd(2)-C(13) 1.998(9)

Pd(2)-N(1) 2.067(7)

Pd(2)-N(2) 2.127(7)

Pd(2)-P(2) 2.235(3)

P(1)-C(7) 1.814(11)

P(1)-C(9) 1.813(13)

P(1)-C(11) 1.827(12)

P(2)-C(23) 1.81(2)

P(2)-C(19) 1.832(12)

P(2)-C(21) 1.90(2)

C(1)-C(2) 1.382(12)

C(1)-C(6) 1.387(13)

C(2)-C(3) 1.389(13)

C(3)-C(4) 1.357(14)

C(4)-C(5) 1.368(14)

C(5)-C(6) 1.373(13)

C(7)-C(8) 1.49(2)

C(9)-C(10) 1.51(2)

C(11)-C(12) 1.49(2)

C(13)-C(14) 1.365(14)

C(13)-C(18) 1.395(13)

C(14)-C(15) 1.41(2)

C(15)-C(16) 1.35(2)

C(16)-C(17) 1.34(2)

C(17)-C(18) 1.38(2)

C(19)-C(20) 1.59(2)

C(21)-C(22) 1.58(2)

C(23)-C(24) 1.73(3)

Pd(3)-C(31) 1.998(9)

Pd(3)-N(4) 2.080(7)

Pd(3)-N(3) 2.100(7)

Pd(3)-P(3) 2.231(3)

Pd(4)-C(43) 1.992(10)

Pd(4)-N(3) 2.076(7)

Pd(4)-N(4) 2.122(7)

Pd(4)-P(4) 2.236(3)

P(3)-C(41) 1.789(12)

P(3)-C(39) 1.808(11)

P(3)-C(37) 1.817(10)

P(4)-C(492) 1.76(4)

P(4)-C(491) 1.84(2)

P(4)-C(531) 1.85(2)

P(4)-C(511) 1.86(2)

P(4)-C(512) 1.89(4)

P(4)-C(532) 1.99(3)

C(31)-C(36) 1.359(13)

C(31)-C(32) 1.397(12)

C(32)-C(33) 1.39(2)

C(33)-C(34) 1.35(2)

C(34)-C(35) 1.34(2)

C(35)-C(36) 1.390(14)

C(37)-C(38) 1.54(2)

C(39)-C(40) 1.52(2)

C(41)-C(42) 1.50(2)

C(43)-C(48) 1.367(13)

C(43)-C(44) 1.38(2)

C(44)-C(45) 1.42(2)

C(45)-C(46) 1.34(2)

C(46)-C(47) 1.35(2)

C(47)-C(48) 1.40(2)

C(491)-C(492) 1.26(4)

C(491)-C(50) 1.48(2)

C(492)-C(50) 1.59(4)

C(492)-C(511) 1.88(4)

C(511)-C(512) 1.50(4)

C(511)-C(52) 1.55(2)

C(512)-C(52) 1.61(4)

C(512)-C(541) 1.85(5)

C(512)-C(531) 1.92(4)

C(531)-C(532) 1.15(3)

C(531)-C(541) 1.48(3)

C(531)-C(542) 1.79(4)

C(532)-C(542) 1.46(4)

C(1)-Pd(1)-N(2) 93.5(3)

C(1)-Pd(1)-N(1) 171.3(3)

N(2)-Pd(1)-N(1) 77.8(3)

C(1)-Pd(1)-P(1) 89.0(3)

N(2)-Pd(1)-P(1) 174.3(2)

N(1)-Pd(1)-P(1) 99.5(2)

C(1)-Pd(1)-Pd(2) 128.0(3)

N(2)-Pd(1)-Pd(2) 45.9(2)

N(1)-Pd(1)-Pd(2) 44.3(2)

P(1)-Pd(1)-Pd(2) 128.94(8)

C(13)-Pd(2)-N(1) 92.8(3)

C(13)-Pd(2)-N(2) 170.4(3)

N(1)-Pd(2)-N(2) 77.7(3)

C(13)-Pd(2)-P(2) 91.7(3)

N(1)-Pd(2)-P(2) 175.1(2)

N(2)-Pd(2)-P(2) 97.7(2)

C(13)-Pd(2)-Pd(1) 126.6(3)

N(1)-Pd(2)-Pd(1) 45.3(2)

N(2)-Pd(2)-Pd(1) 44.8(2)

P(2)-Pd(2)-Pd(1) 130.02(8)

C(7)-P(1)-C(9) 101.5(6)

C(7)-P(1)-C(11) 104.2(6)

C(9)-P(1)-C(11) 99.4(7)

C(7)-P(1)-Pd(1) 117.6(4)

C(9)-P(1)-Pd(1) 112.5(5)

C(11)-P(1)-Pd(1) 118.8(4)

C(23)-P(2)-C(19) 111.4(8)

C(23)-P(2)-C(21) 95.2(10)

C(19)-P(2)-C(21) 101.2(7)

C(23)-P(2)-Pd(2) 115.0(6)

C(19)-P(2)-Pd(2) 116.7(5)

C(21)-P(2)-Pd(2) 114.5(5)

Pd(2)-N(1)-Pd(1) 90.4(3)

Pd(1)-N(2)-Pd(2) 89.3(3)

C(2)-C(1)-C(6) 114.2(9)

C(2)-C(1)-Pd(1) 122.7(7)

C(6)-C(1)-Pd(1) 123.0(7)

C(1)-C(2)-C(3) 122.3(9)

C(4)-C(3)-C(2) 121.5(9)

C(3)-C(4)-C(5) 117.7(10)

C(4)-C(5)-C(6) 120.4(10)

C(5)-C(6)-C(1) 123.7(9)

C(8)-C(7)-P(1) 116.2(8)

C(10)-C(9)-P(1) 113.3(9)

C(12)-C(11)-P(1) 116.1(10)

C(14)-C(13)-C(18) 114.8(10)

C(14)-C(13)-Pd(2) 122.3(8)

C(18)-C(13)-Pd(2) 122.9(9)

C(13)-C(14)-C(15) 122.8(11)

C(16)-C(15)-C(14) 119.6(13)

C(17)-C(16)-C(15) 119.6(12)

C(16)-C(17)-C(18) 120.7(13)

C(17)-C(18)-C(13) 122.5(12)

C(20)-C(19)-P(2) 116.2(10)

C(22)-C(21)-P(2) 108.0(12)

C(24)-C(23)-P(2) 103.5(12)

C(31)-Pd(3)-N(4) 92.8(3)

C(31)-Pd(3)-N(3) 171.0(3)

N(4)-Pd(3)-N(3) 78.3(3)

C(31)-Pd(3)-P(3) 88.8(3)

N(4)-Pd(3)-P(3) 173.6(2)

N(3)-Pd(3)-P(3) 99.8(2)

C(31)-Pd(3)-Pd(4) 126.8(3)

N(4)-Pd(3)-Pd(4) 46.2(2)

N(3)-Pd(3)-Pd(4) 44.9(2)

P(3)-Pd(3)-Pd(4) 128.61(8)

C(43)-Pd(4)-N(3) 92.0(3)

C(43)-Pd(4)-N(4) 169.6(3)

N(3)-Pd(4)-N(4) 77.9(3)

C(43)-Pd(4)-P(4) 91.0(3)

N(3)-Pd(4)-P(4) 176.1(2)

N(4)-Pd(4)-P(4) 98.9(2)

C(43)-Pd(4)-Pd(3) 125.2(3)

N(3)-Pd(4)-Pd(3) 45.6(2)

N(4)-Pd(4)-Pd(3) 45.0(2)

P(4)-Pd(4)-Pd(3) 130.55(8)

C(41)-P(3)-C(39) 104.7(7)

C(41)-P(3)-C(37) 101.9(6)

C(39)-P(3)-C(37) 102.7(5)

C(41)-P(3)-Pd(3) 112.6(4)

C(39)-P(3)-Pd(3) 115.1(4)

C(37)-P(3)-Pd(3) 118.2(4)

C(492)-P(4)-C(491) 41.0(12)

C(492)-P(4)-C(531) 127.1(13)

C(491)-P(4)-C(531) 104.6(10)

C(492)-P(4)-C(511) 62.3(14)

C(491)-P(4)-C(511) 99.5(9)

C(531)-P(4)-C(511) 102.6(9)

C(492)-P(4)-C(512) 106(2)

C(491)-P(4)-C(512) 130.4(13)

C(531)-P(4)-C(512) 62.1(14)

C(511)-P(4)-C(512) 47.2(12)

C(492)-P(4)-C(532) 113(2)

C(491)-P(4)-C(532) 76.8(11)

C(531)-P(4)-C(532) 34.5(9)

C(511)-P(4)-C(532) 127.6(11)

C(512)-P(4)-C(532) 96(2)

C(492)-P(4)-Pd(4) 113.1(12)

C(491)-P(4)-Pd(4) 114.0(6)

C(531)-P(4)-Pd(4) 118.8(6)

C(511)-P(4)-Pd(4) 115.0(5)

C(512)-P(4)-Pd(4) 113.7(11)

C(532)-P(4)-Pd(4) 113.8(9)

Pd(4)-N(3)-Pd(3) 89.5(3)

Pd(3)-N(4)-Pd(4) 88.8(3)

C(36)-C(31)-C(32) 114.9(9)

C(36)-C(31)-Pd(3) 123.0(7)

C(32)-C(31)-Pd(3) 122.1(7)

C(33)-C(32)-C(31) 121.4(11)

C(34)-C(33)-C(32) 120.5(11)

C(35)-C(34)-C(33) 119.6(11)

C(34)-C(35)-C(36) 119.7(12)

C(31)-C(36)-C(35) 123.7(10)

C(38)-C(37)-P(3) 114.2(8)

C(40)-C(39)-P(3) 118.7(10)

C(42)-C(41)-P(3) 114.8(10)

C(48)-C(43)-C(44) 115.1(10)

C(48)-C(43)-Pd(4) 122.2(9)

C(44)-C(43)-Pd(4) 122.6(8)

C(43)-C(44)-C(45) 122.7(13)

C(46)-C(45)-C(44) 119(2)

C(45)-C(46)-C(47) 120(2)

C(46)-C(47)-C(48) 119.6(14)

C(43)-C(48)-C(47) 123.1(13)

C(492)-C(491)-C(50) 70(2)

C(492)-C(491)-P(4) 66(2)

C(50)-C(491)-P(4) 115.0(13)

C(491)-C(492)-C(50) 61(2)

C(491)-C(492)-P(4) 73(2)

C(50)-C(492)-P(4) 114(2)

C(491)-C(492)-C(511) 127(3)

C(50)-C(492)-C(511) 162(3)

P(4)-C(492)-C(511) 61.4(13)

C(491)-C(50)-C(492) 48.5(14)

C(512)-C(511)-C(52) 64(2)

C(512)-C(511)-P(4) 67(2)

C(52)-C(511)-P(4) 114.6(12)

C(512)-C(511)-C(492) 119(2)

C(52)-C(511)-C(492) 161(2)

P(4)-C(511)-C(492) 56.3(13)

C(511)-C(512)-C(52) 60(2)

C(511)-C(512)-C(541) 160(3)

C(52)-C(512)-C(541) 137(3)

C(511)-C(512)-P(4) 66(2)

C(52)-C(512)-P(4) 111(2)

C(541)-C(512)-P(4) 95(2)

C(511)-C(512)-C(531) 115(2)

C(52)-C(512)-C(531) 167(3)

C(541)-C(512)-C(531) 46.0(14)

P(4)-C(512)-C(531) 57.9(13)

C(511)-C(52)-C(512) 57(2)

C(532)-C(531)-C(541) 152(3)

C(532)-C(531)-C(542) 55(2)

C(541)-C(531)-C(542) 137(2)

C(532)-C(531)-P(4) 80(2)

C(541)-C(531)-P(4) 111(2)

C(542)-C(531)-P(4) 107(2)

C(532)-C(531)-C(512) 137(3)

C(541)-C(531)-C(512) 64(2)

C(542)-C(531)-C(512) 123(2)

P(4)-C(531)-C(512) 60.0(13)

C(531)-C(541)-C(512) 70(2)

C(531)-C(532)-C(542) 86(3)

C(531)-C(532)-P(4) 66(2)

C(542)-C(532)-P(4) 115(2)

C(532)-C(542)-C(531) 40(2)

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Symmetry transformations used to generate equivalent atoms:

Table 4-1. Anisotropic displacement parameters (Å2×103) for **1**. The anisotropic displacement factor exponent takes the form: -2π2[h2a\*2U11 + ⋅⋅⋅⋅ + 2hka\*b\*U12].

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

U11 U22 U33 U23 U13 U12

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

Pd(1) 55(1) 74(1) 43(1) -2(1) 4(1) 0(1)

Pd(2) 60(1) 76(1) 44(1) 1(1) 5(1) -3(1)

P(1) 67(2) 78(2) 67(2) -4(1) -2(1) 4(1)

P(2) 95(2) 74(2) 59(2) 1(1) 17(1) -3(2)

N(1) 68(5) 92(6) 50(4) 9(4) -3(4) -17(4)

N(2) 61(5) 81(6) 59(5) -5(4) 8(4) 8(4)

C(1) 62(6) 72(6) 44(5) 4(4) 9(4) 4(5)

C(2) 60(6) 89(7) 56(6) -4(5) 8(5) 7(5)

C(3) 92(8) 97(8) 47(6) -24(6) 4(5) 5(7)

C(4) 75(7) 92(8) 66(7) -12(6) -13(6) -9(6)

C(5) 62(6) 99(8) 86(8) -20(7) 15(6) -4(6)

C(6) 80(7) 94(8) 60(6) -17(6) 20(5) -5(6)

C(7) 84(8) 89(8) 81(8) -9(6) 12(6) 7(6)

C(8) 129(11) 91(9) 105(10) -8(7) 36(8) -9(8)

C(9) 74(8) 120(11) 149(13) -1(10) 22(8) 11(7)

C(10) 138(13) 149(14) 153(15) -27(12) 82(12) 1(11)

C(11) 127(11) 85(9) 104(10) 7(8) -27(9) 28(8)

C(12) 226(20) 156(15) 72(9) 29(10) -15(11) 37(14)

C(13) 88(7) 62(6) 35(5) 3(4) 2(5) -11(5)

C(14) 100(8) 62(7) 76(7) -7(6) 18(6) -12(6)

C(15) 133(11) 65(7) 84(8) 5(7) 32(8) 9(7)

C(16) 160(14) 106(11) 42(6) -3(6) -2(8) -10(10)

C(17) 132(12) 102(11) 70(8) -5(7) -13(8) -33(9)

C(18) 81(8) 97(9) 73(7) 7(7) -7(6) -13(6)

C(19) 228(17) 105(10) 70(8) 14(7) 60(9) -15(11)

C(20) 235(19) 124(12) 111(11) 39(10) 71(12) 6(12)

C(21) 243(19) 117(12) 139(13) 25(10) 82(14) 60(13)

C(22) 126(13) 236(22) 162(17) 54(16) -1(12) 22(14)

C(23) 299(22) 153(15) 131(12) 23(11) -28(13) -128(15)

C(24) 94(11) 296(26) 214(22) 89(20) -4(13) -46(14)

Pd(3) 51(1) 68(1) 41(1) 3(1) 5(1) -1(1)

Pd(4) 56(1) 61(1) 42(1) 4(1) 3(1) -2(1)

P(3) 58(2) 81(2) 61(2) 10(1) -1(1) 8(1)

P(4) 79(2) 71(2) 55(2) 12(1) 10(1) -4(1)

N(3) 56(4) 70(5) 56(4) 15(4) 4(3) -8(4)

N(4) 69(5) 58(5) 55(4) 1(4) 16(4) 7(4)

C(31) 50(5) 80(7) 51(5) -7(5) 0(4) 0(5)

C(32) 85(7) 88(8) 60(6) -9(6) 14(5) 0(6)

C(33) 121(11) 106(10) 61(7) -30(7) -1(7) 12(8)

C(34) 77(8) 106(10) 113(11) -47(8) -16(8) -3(7)

C(35) 79(8) 129(11) 106(10) -42(9) 16(7) -17(7)

C(36) 70(7) 110(9) 67(7) -28(6) 14(5) -21(6)

C(37) 91(8) 95(9) 73(7) 22(6) -27(6) 4(7)

C(38) 137(12) 131(12) 83(9) 37(8) 10(8) 0(9)

C(39) 109(9) 81(8) 90(8) -6(7) -10(7) 0(7)

C(40) 181(16) 86(10) 162(15) 2(10) -44(12) 30(10)

C(41) 94(9) 143(12) 104(10) 22(9) 30(8) 35(8)

C(42) 189(17) 226(20) 121(13) 32(13) 88(13) 79(15)

C(43) 79(7) 74(7) 42(5) 7(5) -5(5) 0(6)

C(44) 110(10) 109(10) 84(8) -23(8) 10(7) 8(8)

C(45) 154(15) 119(12) 90(10) -18(9) 18(10) 37(11)

C(46) 197(19) 75(10) 79(10) -1(7) -12(12) 19(11)

C(47) 142(13) 95(11) 76(9) 8(8) -47(9) -20(9)

C(48) 101(9) 85(8) 64(7) -1(6) -11(6) -16(7)

C(50) 90(9) 146(12) 113(11) 2(9) 14(8) -28(9)

C(52) 126(12) 118(12) 202(18) 23(12) 59(12) 37(10)

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

Table 5-1. Hydrogen coordinates (×104) and isotropic displacement parameters (Å2×103) for **1**.

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

x y z U(eq)

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

H(1A) 7763(6) 9024(5) -1878(3) 87

H(1B) 6961(6) 9426(5) -1654(3) 87

H(2A) 7391(6) 7513(4) -2168(3) 81

H(2B) 6416(6) 7184(4) -2071(3) 81

H(2) 5846(7) 7736(6) -3492(4) 83

H(3) 4665(9) 7071(6) -4104(4) 96

H(4) 3064(9) 6812(6) -3930(4) 98

H(5) 2666(8) 7229(6) -3115(4) 99

H(6) 3827(8) 7904(6) -2513(4) 93

H(7A) 5252(8) 10803(6) -2704(5) 103

H(7B) 5896(8) 10492(6) -2152(5) 103

H(8A) 6975 10998 -2671 128

H(8B) 6546 10463 -3160 128

H(8C) 7191 10149 -2607 128

H(9A) 3700(9) 10143(8) -2446(6) 137

H(9B) 3463(9) 9298(8) -2509(6) 137

H(10A) 3642 9639 -1591 167

H(10B) 4760 9929 -1588 167

H(10C) 4521 9083 -1651 167

H(11A) 3925(11) 9204(7) -3479(5) 135

H(11B) 4068(11) 10060(7) -3462(5) 135

H(12A) 4692 9575 -4188 189

H(12B) 5461 9073 -3785 189

H(12C) 5604 9931 -3768 189

H(14) 5751(9) 8950(5) -588(4) 95

H(15) 5976(11) 9708(6) 182(5) 111

H(16) 7602(14) 9936(8) 673(5) 126

H(17) 8988(12) 9508(7) 357(5) 127

H(18) 8777(9) 8728(6) -384(4) 104

H(3A) 3201(5) 5821(4) 1647(3) 74

H(3B) 2412(5) 6224(4) 1882(3) 74

H(4A) 3660(6) 8103(4) 1966(3) 72

H(4B) 2726(6) 7758(4) 2104(3) 72

H(32) 4476(8) 7582(6) 3430(4) 93

H(33) 5683(11) 8335(7) 3967(5) 119

H(34) 7144(10) 8673(7) 3673(6) 124

H(35) 7389(9) 8299(7) 2831(5) 126

H(36) 6192(8) 7556(6) 2291(4) 99

H(37A) 6291(9) 5381(7) 3394(4) 111

H(37B) 6260(9) 6243(7) 3417(4) 111

H(38A) 5494 5752 4115 143

H(38B) 4689 5325 3676 143

H(38C) 4658 6189 3699 143

H(39A) 4006(9) 4947(6) 2728(5) 117

H(39B) 4242(9) 4896(6) 2136(5) 117

H(40A) 4763 3825 2615 184

H(40B) 5498 4272 3074 184

H(40C) 5735 4221 2479 184

H(41A) 6721(9) 6159(8) 2383(5) 135

H(41B) 6626(9) 5299(8) 2393(5) 135

H(42A) 6575 5695 1504 205

H(42B) 5615 6192 1529 205

H(42C) 5515 5331 1539 205

H(44) 4327(10) 6291(7) 521(5) 123

H(45) 4102(14) 5443(8) -202(6) 146

H(46) 2488(18) 5032(8) -576(6) 147

H(47) 1095(13) 5473(8) -260(5) 137

H(48) 1320(9) 6336(6) 439(4) 105

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

Table 1-2. Crystal data and structure refinement for [Pd(dppe)(μ-NH2)]2(OTf)2 (**2**).

Chemical formula C54H52F6N2O6P4Pd2S2

Formula weight 1339.78

Temperature 293(2) K

Wavelength 0.71069 Å

Crystal system Monoclinic

Space group P21/n

Unit cell dimensions a = 11.4478(7) Å α = 90.000(8) deg.

b = 43.540(3) Å β = 104.127(6) deg.

c = 11.7208(8) Å γ = 90.000(6) deg.

Volume 5665.4(6) Å3

Z 4

Density (calculated) 1.571 Mg/m3

Absorption coefficient 0.891 mm-1

F(000) 2704

Crystal size 0.66 x 0.32 x 0.18 mm

Theta range for data collection 1.85 to 22.47 deg.

Index ranges 0≤h≤12, 0≤k≤46, -12≤l≤12

Reflections collected 7812

Independent reflections 7390 [R(int) = 0.0223]

Refinement method Full-matrix least-squares on F2

Data / restraints / parameters 7390 / 0 / 685

Goodness-of-fit on F2 1.220

Final R indices [I>2σ(I)]*a*  R1 = 0.0502, wR2 = 0.1260

R indices (all data)*a*  R1 = 0.0593, wR2 = 0.1300

Largest diff. peak and hole 0.493 and -0.487 e Å-3

*a*R1 = Σ⎪⎪Fo⎪ - ⎪Fc⎪⎪/Σ⎪Fo⎪; wR2 = [Σw(Fo2 - Fc2)2/ΣwFo4]1/2

Table 2-2. Atomic coordinates (×104) and equivalent isotropic displacement parameters (Å2×103) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

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

x y z U(eq)

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

Pd(1) 9269(1) 1159(1) -817(1) 33(1)

Pd(2) 9446(1) 1414(1) 1659(1) 35(1)

P(1) 7824(2) 1026(1) -2419(2) 36(1)

P(2) 10452(2) 832(1) -1493(2) 39(1)

P(3) 8224(2) 1609(1) 2704(2) 42(1)

P(4) 10720(2) 1365(1) 3438(2) 47(1)

N(1) 8343(5) 1473(2) -11(5) 43(2)

N(2) 10608(5) 1276(2) 648(5) 41(2)

C(1) 7004(7) 1336(2) -3287(7) 41(2)

C(2) 7320(8) 1637(2) -3006(8) 56(2)

C(3) 6753(10) 1881(2) -3682(8) 66(3)

C(4) 5874(8) 1820(2) -4671(9) 64(3)

C(5) 5567(8) 1528(2) -4974(9) 69(3)

C(6) 6106(7) 1279(2) -4305(8) 57(2)

C(7) 6741(7) 756(2) -2104(7) 41(2)

C(8) 6564(8) 739(2) -976(8) 53(2)

C(9) 5754(9) 545(2) -691(9) 67(3)

C(10) 5113(8) 346(2) -1549(10) 65(3)

C(11) 5275(8) 351(2) -2657(10) 61(3)

C(12) 6086(7) 552(2) -2942(8) 49(2)

C(13) 8565(7) 823(2) -3407(7) 46(2)

C(14) 9504(7) 607(2) -2680(7) 49(2)

C(15) 11201(7) 566(2) -370(7) 42(2)

C(16) 10524(9) 426(2) 300(9) 65(3)

C(17) 11047(10) 219(3) 1183(10) 81(3)

C(18) 12249(10) 161(2) 1425(10) 77(3)

C(19) 12938(10) 315(3) 786(10) 85(3)

C(20) 12434(8) 512(2) -95(9) 68(3)

C(21) 11599(7) 1012(2) -2080(7) 44(2)

C(22) 12248(8) 853(2) -2755(8) 60(2)

C(23) 13176(9) 994(3) -3106(9) 76(3)

C(24) 13487(9) 1299(3) -2790(10) 76(3)

C(25) 12852(10) 1457(2) -2141(9) 74(3)

C(26) 11896(8) 1317(2) -1798(8) 59(2)

C(27) 6614(7) 1571(2) 2089(7) 47(2)

C(28) 5873(9) 1832(2) 1851(9) 68(3)

C(29) 4659(10) 1794(3) 1327(12) 92(4)

C(30) 4206(10) 1504(3) 1094(10) 84(3)

C(31) 4924(10) 1253(3) 1321(11) 90(4)

C(32) 6138(8) 1296(2) 1823(9) 68(3)

C(33) 8598(7) 2008(2) 3012(7) 46(2)

C(34) 9127(9) 2175(2) 2270(9) 66(3)

C(35) 9546(10) 2463(2) 2546(12) 84(3)

C(36) 9429(11) 2602(3) 3551(12) 87(4)

C(37) 8876(12) 2447(3) 4300(12) 97(4)

C(38) 8460(10) 2154(3) 4026(9) 79(3)

C(39) 8553(7) 1408(2) 4117(7) 53(2)

C(40) 9847(8) 1351(4) 4571(8) 100(5)

C(41) 11661(7) 1705(2) 3774(7) 48(2)

C(42) 11966(9) 1864(3) 2895(9) 75(3)

C(43) 12606(10) 2138(3) 3107(11) 86(3)

C(44) 12942(11) 2244(3) 4204(15) 97(4)

C(45) 12653(14) 2092(4) 5085(14) 124(5)

C(46) 12033(11) 1818(3) 4890(10) 92(4)

C(47) 11711(8) 1035(2) 3670(7) 53(2)

C(48) 11342(12) 756(3) 4027(10) 90(4)

C(49) 12094(19) 502(3) 4203(13) 120(5)

C(50) 13228(17) 529(4) 4051(13) 118(6)

C(51) 13607(11) 805(3) 3684(11) 97(4)

C(52) 12846(8) 1053(2) 3475(9) 67(3)

S(1) 10694(2) 2142(1) -583(2) 62(1)

O(1) 10998(7) 2440(2) -121(7) 93(2)

O(2) 11598(7) 1916(2) -256(6) 87(2)

O(3) 9512(7) 2045(2) -535(7) 98(3)

C(53) 10509(11) 2193(3) -2151(10) 76(3)

F(1) 10180(7) 1934(2) -2731(6) 111(2)

F(2) 11496(8) 2276(2) -2427(7) 141(3)

F(3) 9688(8) 2397(2) -2593(7) 140(3)

S(2) 6941(3) 429(1) 3419(3) 87(1)

O(4) 6026(8) 419(2) 2359(7) 114(3)

O(5) 6714(11) 245(3) 4361(9) 158(4)

O(6) 7390(13) 713(2) 3782(9) 184(6)

C(54) 8103(14) 216(4) 3133(24) 150(7)

F(4) 9044(10) 216(3) 3998(16) 254(8)

F(5) 7818(12) -57(3) 2762(15) 254(8)

F(6) 8472(13) 369(5) 2265(15) 271(9)

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

Table 3-2. Bond lengths [Å] and angles [°] for **2**.

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

Pd(1)-N(2) 2.067(6)

Pd(1)-N(1) 2.089(6)

Pd(1)-P(2) 2.240(2)

Pd(1)-P(1) 2.255(2)

Pd(1)-Pd(2) 3.0669(8)

Pd(2)-N(1) 2.069(6)

Pd(2)-N(2) 2.075(6)

Pd(2)-P(3) 2.240(2)

Pd(2)-P(4) 2.244(2)

P(1)-C(7) 1.809(8)

P(1)-C(1) 1.811(8)

P(1)-C(13) 1.821(8)

P(2)-C(21) 1.804(8)

P(2)-C(15) 1.807(8)

P(2)-C(14) 1.827(8)

P(3)-C(33) 1.802(8)

P(3)-C(27) 1.815(8)

P(3)-C(39) 1.830(8)

P(4)-C(47) 1.811(9)

P(4)-C(41) 1.816(9)

P(4)-C(40) 1.847(9)

C(1)-C(2) 1.377(11)

C(1)-C(6) 1.394(11)

C(2)-C(3) 1.388(12)

C(3)-C(4) 1.364(13)

C(4)-C(5) 1.344(13)

C(5)-C(6) 1.391(12)

C(7)-C(8) 1.388(11)

C(7)-C(12) 1.398(11)

C(8)-C(9) 1.356(12)

C(9)-C(10) 1.392(13)

C(10)-C(11) 1.356(13)

C(11)-C(12) 1.376(12)

C(13)-C(14) 1.524(11)

C(15)-C(16) 1.373(12)

C(15)-C(20) 1.388(11)

C(16)-C(17) 1.393(13)

C(17)-C(18) 1.359(14)

C(18)-C(19) 1.387(14)

C(19)-C(20) 1.359(13)

C(21)-C(26) 1.389(12)

C(21)-C(22) 1.395(11)

C(22)-C(23) 1.374(13)

C(23)-C(24) 1.40(2)

C(24)-C(25) 1.360(14)

C(25)-C(26) 1.394(12)

C(27)-C(32) 1.322(12)

C(27)-C(28) 1.405(12)

C(28)-C(29) 1.386(14)

C(29)-C(30) 1.37(2)

C(30)-C(31) 1.36(2)

C(31)-C(32) 1.384(13)

C(33)-C(34) 1.382(12)

C(33)-C(38) 1.391(12)

C(34)-C(35) 1.354(14)

C(35)-C(36) 1.36(2)

C(36)-C(37) 1.38(2)

C(37)-C(38) 1.37(2)

C(39)-C(40) 1.467(12)

C(41)-C(42) 1.356(13)

C(41)-C(46) 1.364(13)

C(42)-C(43) 1.391(14)

C(43)-C(44) 1.33(2)

C(44)-C(45) 1.34(2)

C(45)-C(46) 1.38(2)

C(47)-C(52) 1.376(13)

C(47)-C(48) 1.382(14)

C(48)-C(49) 1.39(2)

C(49)-C(50) 1.36(2)

C(50)-C(51) 1.38(2)

C(51)-C(52) 1.37(2)

S(1)-O(2) 1.413(7)

S(1)-O(1) 1.417(7)

S(1)-O(3) 1.432(8)

S(1)-C(53) 1.812(11)

C(53)-F(2) 1.300(12)

C(53)-F(3) 1.304(12)

C(53)-F(1) 1.322(12)

S(2)-O(6) 1.370(9)

S(2)-O(4) 1.416(8)

S(2)-O(5) 1.436(10)

S(2)-C(54) 1.72(2)

C(54)-F(5) 1.28(2)

C(54)-F(4) 1.29(2)

C(54)-F(6) 1.37(2)

N(2)-Pd(1)-N(1) 79.6(2)

N(2)-Pd(1)-P(2) 93.4(2)

N(1)-Pd(1)-P(2) 173.0(2)

N(2)-Pd(1)-P(1) 179.1(2)

N(1)-Pd(1)-P(1) 101.3(2)

P(2)-Pd(1)-P(1) 85.69(7)

N(2)-Pd(1)-Pd(2) 42.3(2)

N(1)-Pd(1)-Pd(2) 42.2(2)

P(2)-Pd(1)-Pd(2) 131.22(6)

P(1)-Pd(1)-Pd(2) 138.34(6)

N(1)-Pd(2)-N(2) 79.9(2)

N(1)-Pd(2)-P(3) 98.8(2)

N(2)-Pd(2)-P(3) 174.6(2)

N(1)-Pd(2)-P(4) 176.9(2)

N(2)-Pd(2)-P(4) 98.1(2)

P(3)-Pd(2)-P(4) 83.03(8)

N(1)-Pd(2)-Pd(1) 42.7(2)

N(2)-Pd(2)-Pd(1) 42.1(2)

P(3)-Pd(2)-Pd(1) 138.50(6)

P(4)-Pd(2)-Pd(1) 136.27(6)

C(7)-P(1)-C(1) 108.2(3)

C(7)-P(1)-C(13) 105.3(4)

C(1)-P(1)-C(13) 105.2(4)

C(7)-P(1)-Pd(1) 113.4(3)

C(1)-P(1)-Pd(1) 116.7(3)

C(13)-P(1)-Pd(1) 107.1(3)

C(21)-P(2)-C(15) 107.3(4)

C(21)-P(2)-C(14) 107.2(4)

C(15)-P(2)-C(14) 107.3(4)

C(21)-P(2)-Pd(1) 114.7(3)

C(15)-P(2)-Pd(1) 111.8(3)

C(14)-P(2)-Pd(1) 108.3(3)

C(33)-P(3)-C(27) 109.6(4)

C(33)-P(3)-C(39) 107.1(4)

C(27)-P(3)-C(39) 106.3(4)

C(33)-P(3)-Pd(2) 108.9(3)

C(27)-P(3)-Pd(2) 117.2(3)

C(39)-P(3)-Pd(2) 107.2(3)

C(47)-P(4)-C(41) 107.3(4)

C(47)-P(4)-C(40) 107.1(5)

C(41)-P(4)-C(40) 105.5(5)

C(47)-P(4)-Pd(2) 117.2(3)

C(41)-P(4)-Pd(2) 109.9(3)

C(40)-P(4)-Pd(2) 109.2(3)

Pd(2)-N(1)-Pd(1) 95.0(2)

Pd(1)-N(2)-Pd(2) 95.6(2)

C(2)-C(1)-C(6) 118.1(8)

C(2)-C(1)-P(1) 120.5(6)

C(6)-C(1)-P(1) 121.2(6)

C(1)-C(2)-C(3) 122.2(8)

C(4)-C(3)-C(2) 118.7(9)

C(5)-C(4)-C(3) 120.0(9)

C(4)-C(5)-C(6) 122.5(9)

C(5)-C(6)-C(1) 118.4(9)

C(8)-C(7)-C(12) 117.2(7)

C(8)-C(7)-P(1) 119.8(6)

C(12)-C(7)-P(1) 123.0(6)

C(9)-C(8)-C(7) 122.4(9)

C(8)-C(9)-C(10) 118.8(9)

C(11)-C(10)-C(9) 120.7(9)

C(10)-C(11)-C(12) 120.1(9)

C(11)-C(12)-C(7) 120.8(9)

C(14)-C(13)-P(1) 108.6(5)

C(13)-C(14)-P(2) 107.5(6)

C(16)-C(15)-C(20) 118.5(8)

C(16)-C(15)-P(2) 117.8(6)

C(20)-C(15)-P(2) 123.5(7)

C(15)-C(16)-C(17) 120.7(9)

C(18)-C(17)-C(16) 120.4(10)

C(17)-C(18)-C(19) 118.5(9)

C(20)-C(19)-C(18) 121.6(10)

C(19)-C(20)-C(15) 120.1(10)

C(26)-C(21)-C(22) 118.5(8)

C(26)-C(21)-P(2) 118.9(6)

C(22)-C(21)-P(2) 122.5(7)

C(23)-C(22)-C(21) 120.3(9)

C(22)-C(23)-C(24) 120.6(9)

C(25)-C(24)-C(23) 119.4(9)

C(24)-C(25)-C(26) 120.4(10)

C(21)-C(26)-C(25) 120.8(9)

C(32)-C(27)-C(28) 119.5(9)

C(32)-C(27)-P(3) 119.7(7)

C(28)-C(27)-P(3) 120.7(7)

C(29)-C(28)-C(27) 118.8(10)

C(30)-C(29)-C(28) 119.4(11)

C(31)-C(30)-C(29) 121.6(10)

C(30)-C(31)-C(32) 118.1(11)

C(27)-C(32)-C(31) 122.5(10)

C(34)-C(33)-C(38) 117.1(9)

C(34)-C(33)-P(3) 120.1(7)

C(38)-C(33)-P(3) 122.7(7)

C(35)-C(34)-C(33) 121.5(10)

C(34)-C(35)-C(36) 121.0(11)

C(35)-C(36)-C(37) 119.6(11)

C(38)-C(37)-C(36) 119.5(11)

C(37)-C(38)-C(33) 121.3(11)

C(40)-C(39)-P(3) 112.0(6)

C(39)-C(40)-P(4) 114.2(6)

C(42)-C(41)-C(46) 117.9(9)

C(42)-C(41)-P(4) 120.0(7)

C(46)-C(41)-P(4) 122.0(8)

C(41)-C(42)-C(43) 121.6(10)

C(44)-C(43)-C(42) 119.0(12)

C(43)-C(44)-C(45) 120.5(12)

C(44)-C(45)-C(46) 121.1(12)

C(41)-C(46)-C(45) 119.8(12)

C(52)-C(47)-C(48) 118.0(10)

C(52)-C(47)-P(4) 120.8(7)

C(48)-C(47)-P(4) 121.1(9)

C(47)-C(48)-C(49) 121.4(13)

C(50)-C(49)-C(48) 119.5(14)

C(49)-C(50)-C(51) 119.8(14)

C(52)-C(51)-C(50) 120.4(13)

C(51)-C(52)-C(47) 120.7(11)

O(2)-S(1)-O(1) 116.1(5)

O(2)-S(1)-O(3) 114.7(5)

O(1)-S(1)-O(3) 113.8(5)

O(2)-S(1)-C(53) 104.8(5)

O(1)-S(1)-C(53) 103.5(5)

O(3)-S(1)-C(53) 101.5(5)

F(2)-C(53)-F(3) 107.3(10)

F(2)-C(53)-F(1) 105.3(10)

F(3)-C(53)-F(1) 106.7(10)

F(2)-C(53)-S(1) 113.2(9)

F(3)-C(53)-S(1) 112.4(8)

F(1)-C(53)-S(1) 111.5(8)

O(6)-S(2)-O(4) 116.2(6)

O(6)-S(2)-O(5) 112.9(7)

O(4)-S(2)-O(5) 115.0(7)

O(6)-S(2)-C(54) 107.3(9)

O(4)-S(2)-C(54) 104.8(9)

O(5)-S(2)-C(54) 98.3(10)

F(5)-C(54)-F(4) 111(2)

F(5)-C(54)-F(6) 107(2)

F(4)-C(54)-F(6) 103.7(14)

F(5)-C(54)-S(2) 114.9(12)

F(4)-C(54)-S(2) 113(2)

F(6)-C(54)-S(2) 106(2)

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Symmetry transformations used to generate equivalent atoms:

Table 4-2. Anisotropic displacement parameters (Å2×103) for **2**. The anisotropic displacement factor exponent takes the form: -2π2[h2a\*2U11 + ⋅⋅⋅⋅ + 2hka\*b\*U12].

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

U11 U22 U33 U23 U13 U12

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

Pd(1) 29(1) 37(1) 33(1) -2(1) 6(1) 2(1)

Pd(2) 31(1) 41(1) 33(1) -1(1) 7(1) -3(1)

P(1) 32(1) 39(1) 35(1) 1(1) 5(1) 0(1)

P(2) 37(1) 37(1) 41(1) 0(1) 9(1) 6(1)

P(3) 42(1) 48(1) 39(1) 2(1) 14(1) 1(1)

P(4) 34(1) 68(2) 36(1) 3(1) 6(1) -7(1)

N(1) 35(4) 51(4) 40(4) 0(3) 6(3) 4(3)

N(2) 34(3) 44(4) 42(4) -3(3) 4(3) 2(3)

C(1) 34(4) 48(5) 40(5) 8(4) 11(4) 1(4)

C(2) 66(6) 49(6) 47(5) 0(4) 5(4) 2(5)

C(3) 93(8) 38(5) 63(6) 6(5) 14(6) 11(5)

C(4) 58(6) 56(6) 75(7) 27(5) 12(5) 17(5)

C(5) 43(5) 74(7) 77(7) 26(6) -11(5) -6(5)

C(6) 41(5) 59(6) 62(6) 15(5) -3(4) -3(4)

C(7) 36(4) 40(5) 46(5) 3(4) 9(4) -1(4)

C(8) 58(6) 48(5) 56(6) -8(4) 19(5) -12(4)

C(9) 71(7) 68(7) 71(7) 4(6) 36(6) -13(6)

C(10) 46(5) 57(6) 94(8) 8(6) 25(5) -4(5)

C(11) 44(5) 45(5) 87(8) -1(5) 1(5) -2(4)

C(12) 38(5) 49(5) 55(5) 1(4) 2(4) -3(4)

C(13) 42(5) 59(5) 37(4) -3(4) 11(4) -1(4)

C(14) 46(5) 50(5) 50(5) -9(4) 10(4) 7(4)

C(15) 44(5) 33(4) 47(5) 0(4) 6(4) 4(4)

C(16) 55(6) 63(6) 79(7) 31(5) 19(5) 14(5)

C(17) 87(8) 80(8) 82(8) 34(6) 31(6) 9(6)

C(18) 75(8) 72(7) 78(7) 30(6) 9(6) 27(6)

C(19) 57(6) 100(9) 90(8) 33(7) 6(6) 28(6)

C(20) 52(6) 76(7) 75(7) 23(6) 15(5) 24(5)

C(21) 43(5) 50(5) 41(5) 6(4) 14(4) 9(4)

C(22) 68(6) 55(6) 63(6) -3(5) 27(5) 16(5)

C(23) 67(7) 97(9) 81(7) 25(7) 51(6) 35(6)

C(24) 68(7) 88(8) 84(8) 24(7) 38(6) 3(6)

C(25) 85(8) 59(6) 89(8) -8(6) 44(6) -21(6)

C(26) 58(6) 71(7) 57(6) -6(5) 28(5) -4(5)

C(27) 41(5) 59(6) 43(5) 2(4) 17(4) 0(4)

C(28) 65(7) 53(6) 88(7) 16(5) 20(6) 6(5)

C(29) 50(7) 94(9) 129(11) 26(8) 17(7) 16(6)

C(30) 46(6) 123(11) 79(8) 6(7) 9(5) -2(7)

C(31) 55(7) 100(10) 113(10) -9(8) 15(7) -17(7)

C(32) 48(6) 72(7) 86(7) -6(6) 18(5) -2(5)

C(33) 45(5) 44(5) 47(5) 1(4) 6(4) 5(4)

C(34) 81(7) 52(6) 68(7) 2(5) 27(6) 1(5)

C(35) 92(8) 54(7) 107(10) 7(7) 25(7) -8(6)

C(36) 88(9) 51(7) 108(10) -12(7) -3(7) -5(6)

C(37) 128(11) 70(8) 91(9) -33(7) 25(8) -3(8)

C(38) 99(9) 77(8) 66(7) -12(6) 31(6) -5(6)

C(39) 52(5) 59(6) 51(5) 7(4) 21(4) 2(4)

C(40) 41(6) 218(15) 43(6) 38(7) 14(5) 3(7)

C(41) 33(4) 55(5) 52(5) -1(4) 5(4) 0(4)

C(42) 63(6) 95(8) 67(7) -17(6) 17(5) -30(6)

C(43) 83(8) 85(8) 91(9) -23(7) 20(7) -37(7)

C(44) 65(8) 85(9) 136(13) -25(9) 16(8) -14(6)

C(45) 131(13) 135(14) 95(11) -69(10) 8(9) -34(11)

C(46) 111(10) 100(9) 55(7) -22(6) 6(6) -26(8)

C(47) 58(6) 47(5) 46(5) 5(4) -4(4) -9(4)

C(48) 110(10) 69(8) 86(8) -10(6) 15(7) -21(7)

C(49) 185(17) 53(8) 105(11) 1(7) 3(12) -4(11)

C(50) 137(14) 86(11) 96(10) -21(8) -39(10) 38(11)

C(51) 76(8) 98(10) 102(10) -20(8) -9(7) 15(8)

C(52) 53(6) 57(6) 83(7) -1(5) 3(5) 3(5)

S(1) 82(2) 45(1) 62(2) -2(1) 28(1) -4(1)

O(1) 120(6) 58(5) 106(6) -29(4) 35(5) -13(4)

O(2) 121(6) 54(4) 81(5) 5(4) 13(4) 32(4)

O(3) 109(6) 94(6) 104(6) 7(5) 54(5) -27(5)

C(53) 78(8) 78(8) 78(8) 6(7) 31(6) -1(6)

F(1) 132(6) 125(6) 74(4) -20(4) 20(4) -6(5)

F(2) 124(6) 217(10) 101(6) -3(6) 63(5) -52(6)

F(3) 173(8) 145(7) 104(6) 45(5) 39(5) 85(7)

S(2) 108(2) 67(2) 75(2) -17(2) 3(2) 6(2)

O(4) 94(6) 144(8) 83(6) -8(5) -20(5) 0(6)

O(5) 197(12) 179(11) 105(8) 40(8) 49(8) -22(9)

O(6) 308(16) 46(5) 139(9) -21(5) -61(9) 3(7)

C(54) 72(11) 112(14) 258(25) -2(15) 26(14) -21(9)

F(4) 82(7) 245(14) 386(22) 98(14) -38(10) 1(8)

F(5) 191(12) 136(9) 423(22) -133(12) 54(13) 37(9)

F(6) 169(12) 404(25) 283(19) -27(17) 140(14) -50(14)

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Table 5-2. Hydrogen coordinates (×104) and isotropic displacement parameters (Å2×103) for **2**.

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

x y z U(eq)

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

H(1A) 8365(5) 1665(2) -283(5) 51

H(1B) 7577(5) 1416(2) -59(5) 51

H(2A) 11078(5) 1430(2) 506(5) 49

H(2B) 11064(5) 1114(2) 960(5) 49

H(2) 7933(8) 1678(2) -2342(8) 67

H(3) 6969(10) 2083(2) -3464(8) 79

H(4) 5486(8) 1980(2) -5137(9) 77

H(5) 4972(8) 1490(2) -5657(9) 83

H(6) 5874(7) 1079(2) -4531(8) 68

H(8) 7018(8) 865(2) -394(8) 64

H(9) 5629(9) 544(2) 64(9) 80

H(10) 4568(8) 208(2) -1360(10) 77

H(11) 4837(8) 218(2) -3225(10) 73

H(12) 6200(7) 553(2) -3701(8) 59

H(13A) 7977(7) 707(2) -3982(7) 55

H(13B) 8950(7) 969(2) -3823(7) 55

H(14A) 9989(7) 517(2) -3167(7) 58

H(14B) 9113(7) 442(2) -2357(7) 58

H(16) 9706(9) 471(2) 164(9) 78

H(17) 10572(10) 120(3) 1609(10) 97

H(18) 12601(10) 20(2) 2006(10) 92

H(19) 13766(10) 282(3) 965(10) 102

H(20) 12915(8) 612(2) -514(9) 81

H(22) 12051(8) 650(2) -2968(8) 72

H(23) 13602(9) 886(3) -3557(9) 91

H(24) 14121(9) 1393(3) -3023(10) 92

H(25) 13056(10) 1659(2) -1924(9) 88

H(26) 11452(8) 1429(2) -1375(8) 71

H(28) 6191(9) 2028(2) 2041(9) 82

H(29) 4156(10) 1964(3) 1137(12) 110

H(30) 3385(10) 1479(3) 771(10) 100

H(31) 4610(10) 1056(3) 1145(11) 108

H(32) 6639(8) 1125(2) 1980(9) 82

H(34) 9196(9) 2088(2) 1565(9) 79

H(35) 9921(10) 2568(2) 2041(12) 101

H(36) 9720(11) 2800(3) 3732(12) 105

H(37) 8785(12) 2541(3) 4986(12) 116

H(38) 8078(10) 2051(3) 4529(9) 94

H(39A) 8262(7) 1529(2) 4684(7) 63

H(39B) 8127(7) 1213(2) 4023(7) 63

H(40A) 9955(8) 1151(4) 4942(8) 120

H(40B) 10170(8) 1503(4) 5171(8) 120

H(42) 11742(9) 1788(3) 2131(9) 90

H(43) 12795(10) 2246(3) 2491(11) 104

H(44) 13383(11) 2425(3) 4357(15) 116

H(45) 12874(14) 2172(4) 5843(14) 148

H(46) 11869(11) 1710(3) 5518(10) 110

H(48) 10573(12) 739(3) 4151(10) 108

H(49) 11825(19) 315(3) 4424(13) 144

H(50) 13749(17) 362(4) 4193(13) 142

H(51) 14383(11) 823(3) 3578(11) 117

H(52) 13099(8) 1235(2) 3197(9) 80

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