Electronic Supplementary Information for Dalton Transactions

Multimetallic complexes of group 10 and 11 metals based on polydentate dithiocarbamate ligands.

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Supporting Information — X-Ray Crystallography

The X-ray crystal structure of 2

The C(12)-, C(55)- and C(62)-based phenyl rings in the structure of **2** were found to be disordered. Two partial occupancy orientations were identified in each case, with occupancies of *ca.* 83:17, 65:35 and 70:30% for the C(12)-, C(55)- and C(62)-based phenyl rings respectively. Their geometries were optimised and the non-hydrogen atoms of the major occupancy orientations were refined anisotropically, whilst those of the minor occupancy orientations were refined isotropically. The included dichloromethane solvent molecule was found to be severely disordered. Five partial occupancy orientations were identified of *ca.* 35:32:14:10:9% occupancy, all of which were refined isotropically.

The X-ray crystal structure of 3

The C(19)- and C(26)-based phenyl rings in the structure of **3** were found to be disordered. Two partial occupancy orientations were identified in each case, with occupancies of *ca.* 84:16 and 65:35% for the C(19)- and C(26)-based phenyl rings respectively. Their geometries were optimised and the non-hydrogen atoms of the major occupancy orientations were refined anisotropically, whilst those of the minor occupancy orientations were refined isotropically. The P(20)-based hexafluorophosphate anion was found to be disordered. Two partial occupancy orientations were identified of *ca.* 89 and 11% occupancy, their geometries were optimised, and the atoms of the major occupancy orientation were refined anisotropically, whilst those of the minor occupancy orientation were refined isotropically. The included dichloromethane and ethanol solvent molecules were found to be disordered, and in each case three partial occupancy orientations were identified, with occupancies of *ca.*45:42:13% for the dichloromethane, and *ca.* 54:32:14% for the ethanol. The non-hydrogen atoms of the 54% occupancy ethanol molecule were refined anisotropically, whilst all the others were refined isotropically. The O–H protons of the three

ethanol orientations could not be located, and so the atom list for the asymmetric unit is low by one hydrogen atom.

The X-ray crystal structure of 6

The included dichloromethane solvent molecule in the structure of **6** was found to be disordered. Two partial occupancy orientations were identified of *ca.* 88 and 12% occupancy, and the atoms of the major occupancy orientation were refined anisotropically, whilst those of the minor occupancy orientation were refined isotropically. On the basis of the thermal parameters, the included ethanol molecule was determined to be *ca.* 25% occupancy in the asymmetric unit. The O–H proton of this 25% occupancy ethanol molecule could not be located, and so the atom list for the asymmetric unit is low by $H_{0.25}$.

The X-ray crystal structure of 7

The $AuPMe_3$ unit in the structure of **7** was found to be disordered. In the major occupancy orientation (*ca*. 96%) the unit is bound to S(1), as shown in Fig. S4. In the minor occupancy orientation (*ca.* 4%) it is bound to S(3), as shown in Fig. S5. The atoms of the major occupancy orientation were refined anisotropically, whilst those of the minor occupancy orientation were refined isotropically.

Tables

Table 1. Selected bond lengths (Å) and angles (°) for **2**.

Ni(1)–S(1)	2.2143(7)	Ni(1)–S(3)	2.2162(7)
Ni(1)–P(25)	2.2119(7)	Ni(1)–P(48)	2.2070(7)
Ni(2)–S(9)	2.2230(7)	Ni(2)–S(10)	2.2100(7)
Ni(2)–P(61)	2.2213(7)	Ni(2)–P(84)	2.2007(7)
S(1)–C(2)	1.727(3)	C(2)–N(4)	1.316(3)
C(2)–S(3)	1.711(2)	N(7)–C(8)	1.314(3)
C(8)–S(9)	1.713(2)	C(8)–S(10)	1.718(2)
S(1)–Ni(1)–S(3)	78.41(2)	S(9)–Ni(2)–S(10)	78.27(2)
S(1)–C(2)–S(3)	109.07(13)	S(9)–C(8)–S(10)	109.31(13)

Table 2. Selected bond lengths (Å) and angles (°) for **3**.

Pd(1)–S(1)	2.3516(6)	Pd(1)–S(3)	2.3348(6)
Pd(1)–P(25)	2.3018(6)	Pd(1)–P(48)	2.2923(6)
Pd(2)–S(9)	2.3445(7)	Pd(2)–S(10)	2.3347(6)
Pd(2)–P(61)	2.3110(6)	Pd(2)–P(84)	2.2906(7)
S(1)–C(2)	1.728(2)	C(2)–N(4)	1.313(3)
C(2)–S(3)	1.719(2)	N(7)–C(8)	1.323(3)
C(8)–S(9)	1.723(2)	C(8)–S(10)	1.709(2)
S(1)–Pd(1)–S(3)	75.07(2)	S(9)–Pd(2)–S(10)	74.98(2)
S(1)–C(2)–S(3)	111.88(14)	S(9)–C(8)–S(10)	112.15(13)

Table 3. Selected bond lengths (Å) and angles (°) for **6**.

Au(1)–S(1)	2.3290(10)	Au(1)–P(13)	2.2483(10)
Au(1)···S(3)	3.0756(10)	S(1)–C(2)	1.747(4)
C(2)–N(4)	1.343(5)	C(2)–S(3)	1.695(4)
P(13)–Au(1)–	177.86(3)	Au(1)–S(1)–C(2)	97.67(14)

Table 4. Selected bond lengths (Å) and angles (°) for **7**.

Au(1)–S(1)	2.3233(5)	Au(1)–P(13)	2.2440(6)
Au(1)···S(3)	3.1196(5)	S(1)–C(2)	1.7436(19)
C(2)–N(4)	1.349(2)	C(2)–S(3)	1.6922(19)
P(13)–Au(1)–S(1)	175.07(2)	Au(1)–S(1)–C(2)	99.07(6)

Fig. S1 The molecular structure of the dication in **2** (30% probability ellipsoids).

Fig. S2 The molecular structure of the dication in **3** (30% probability ellipsoids).

Fig. S3 The molecular structure of the centrosymmetric complex **6** (50% probability ellipsoids).

Fig. S4 The molecular structure of the centrosymmetric complex **7** (50% probability ellipsoids).

Fig. S5 The asymmetric unit in the structure of **7** showing the disorder in the binding of the $AuPMe_3$ unit. The major (*ca.* 96%) occupancy orientation is shown with dashed bonds, the minor (*ca.* 4%) with open bonds.

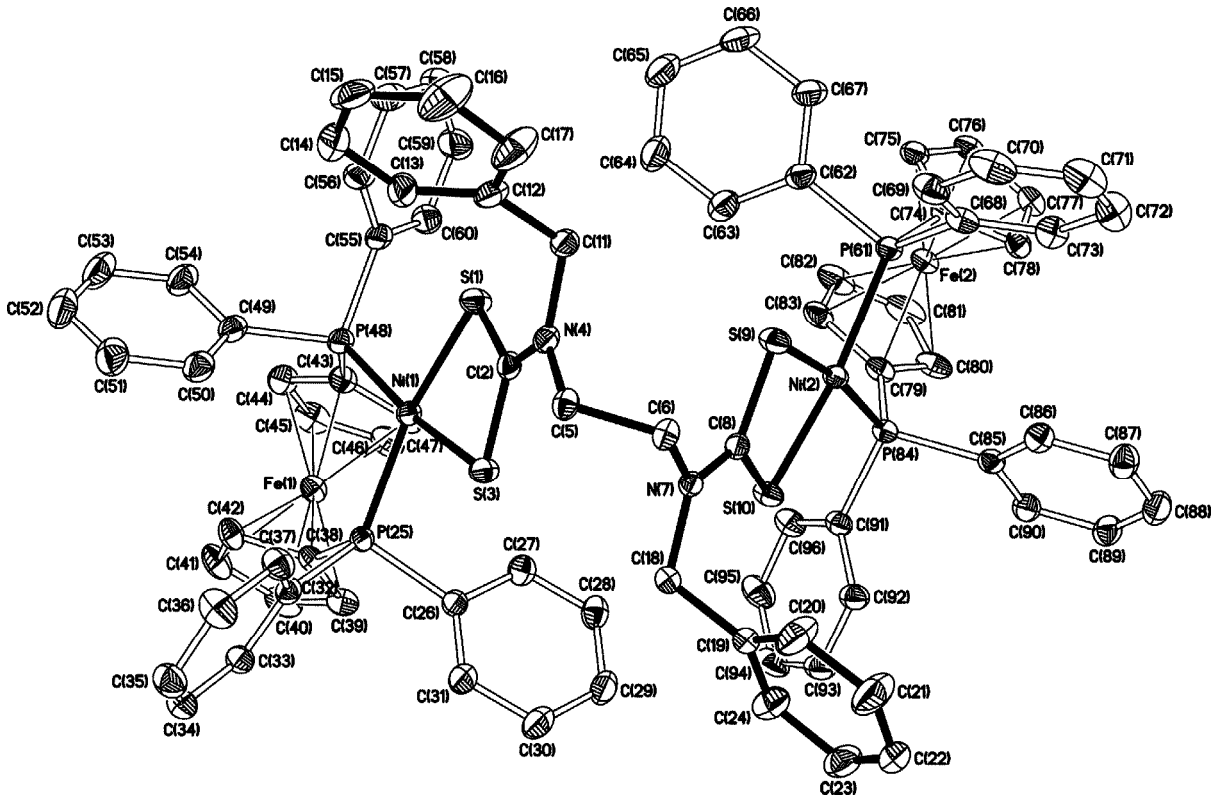
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Fig. S1

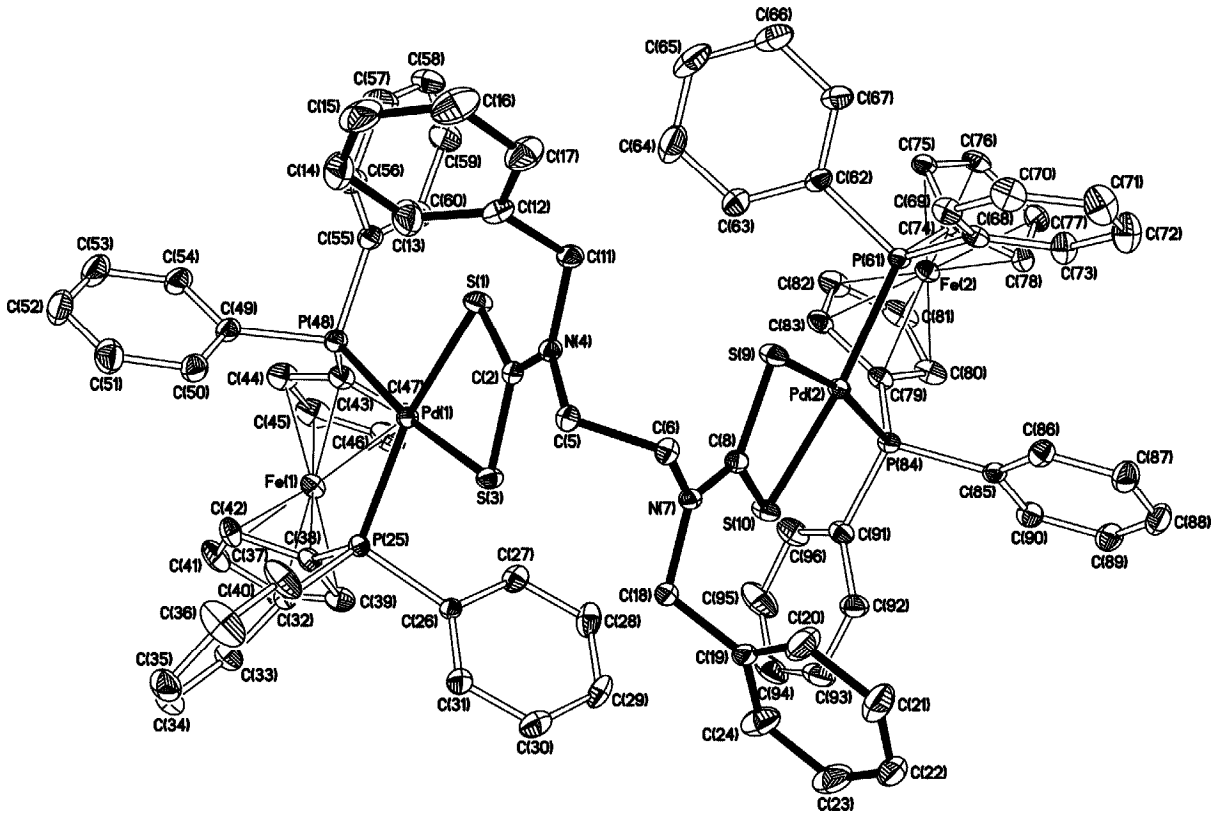
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Fig. S2

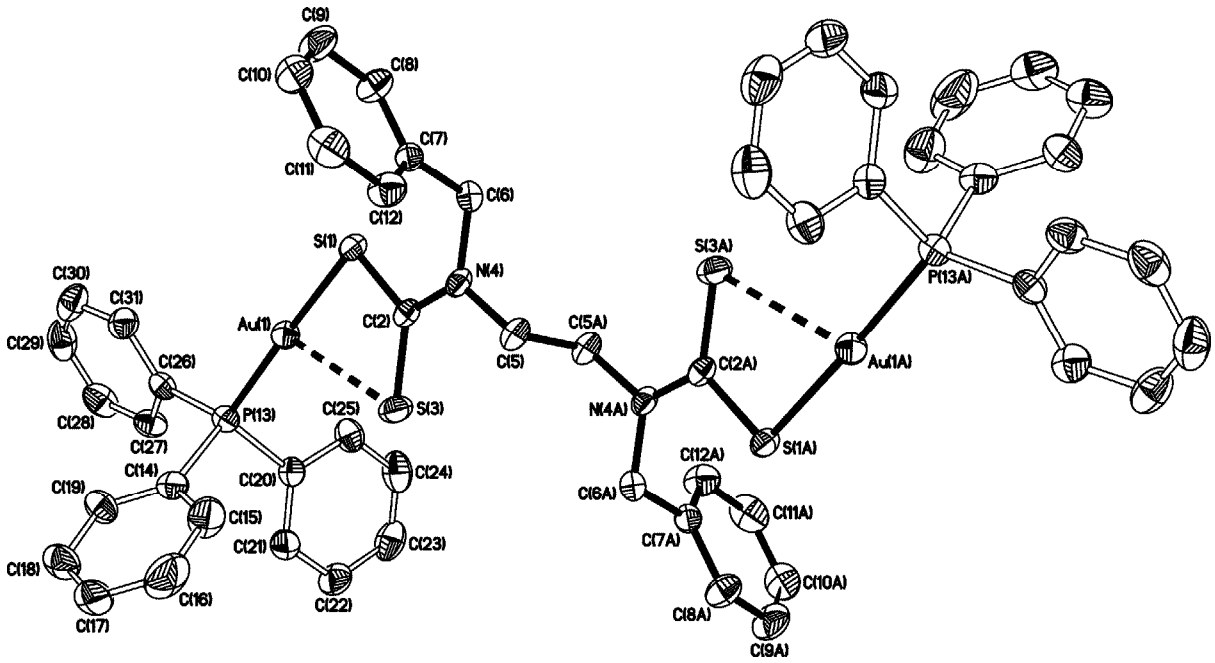

Fig. S3

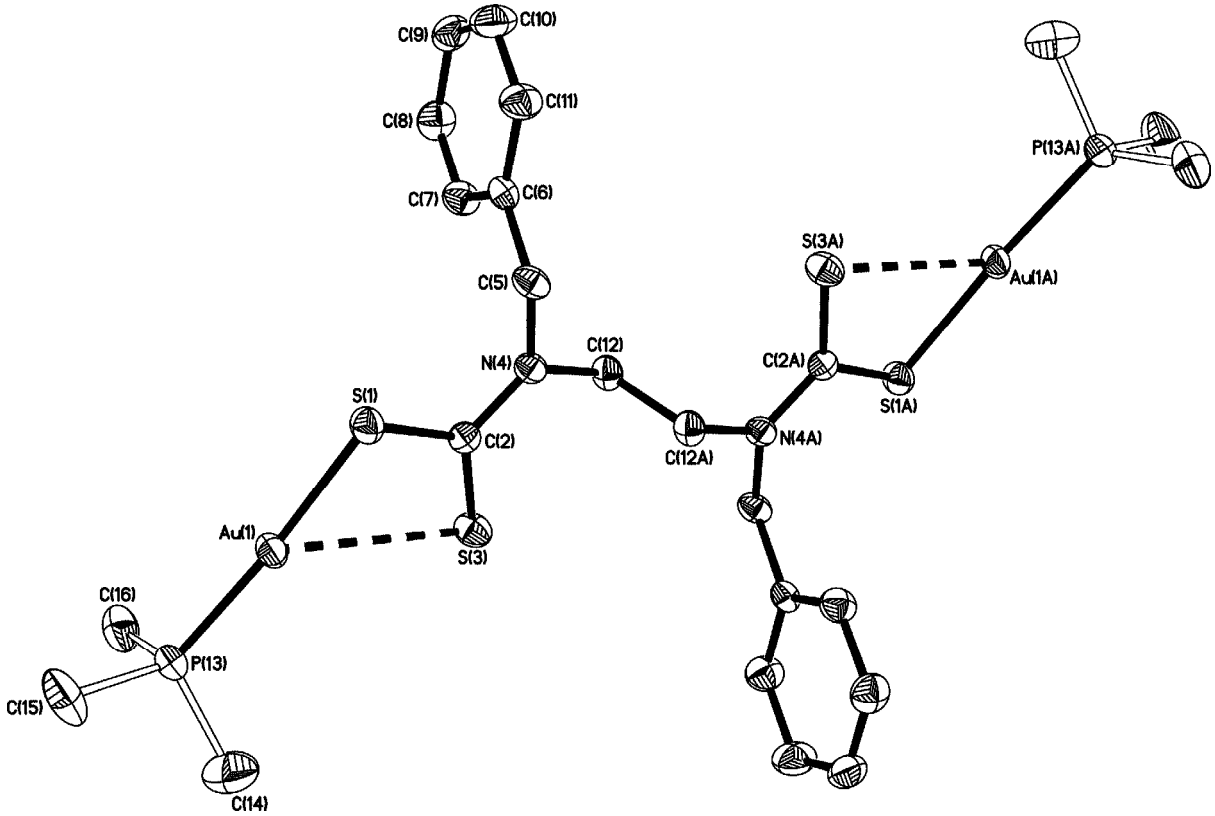

Fig. S4

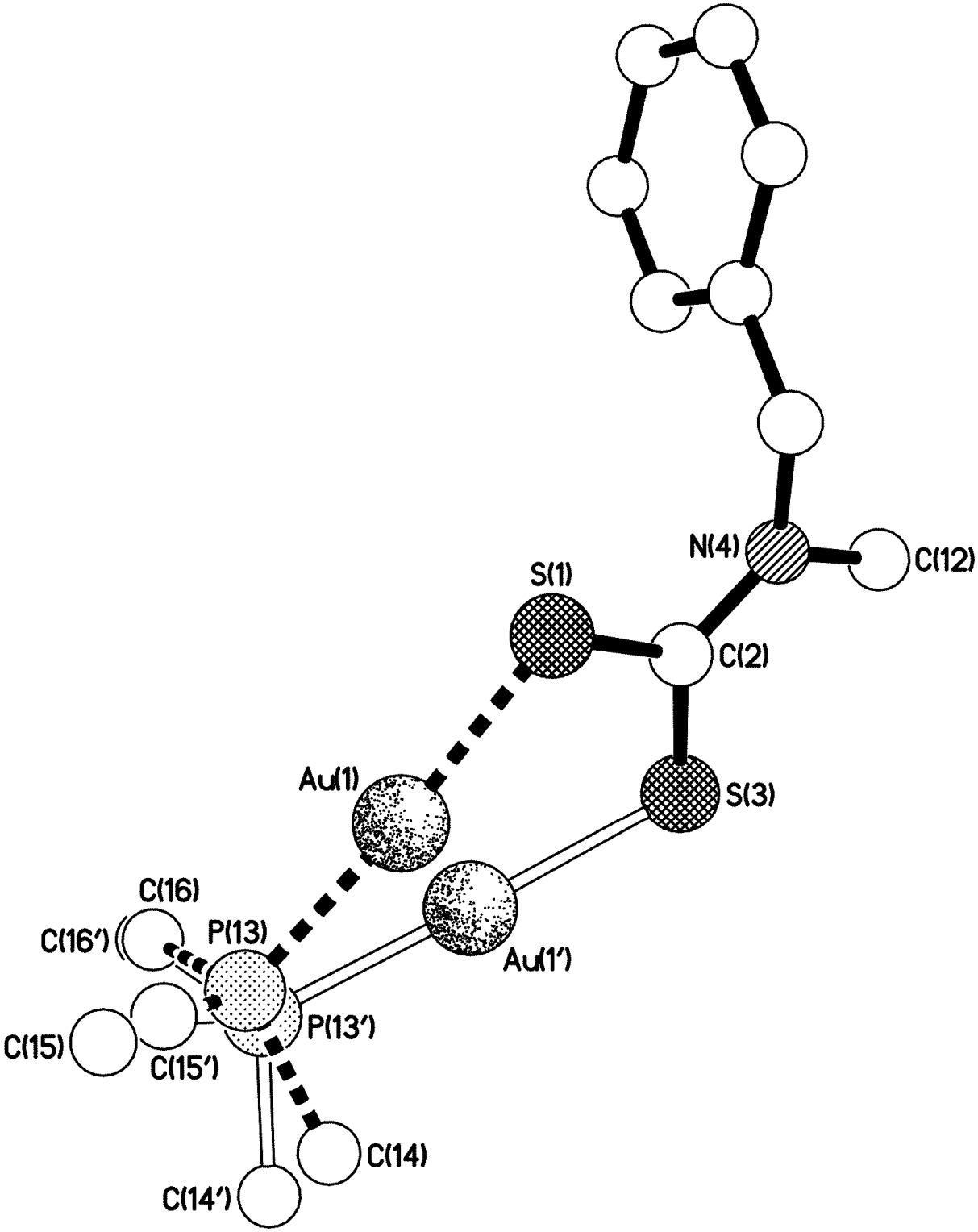

Fig. S5

Table 5. Complete bond lengths [Å] and angles [°] for **2**.

Ni(1)-P(48)	2.2070(7)
Ni(1)-P(25)	2.2119(7)
Ni(1)-S(1)	2.2143(7)
Ni(1)-S(3)	2.2162(7)
Ni(2)-P(84)	2.2007(7)
Ni(2)-S(10)	2.2100(7)
Ni(2)-P(61)	2.2213(7)
Ni(2)-S(9)	2.2230(7)
Fe(1)-C(43)	2.014(3)
Fe(1)-C(38)	2.016(2)
Fe(1)-C(44)	2.027(3)
Fe(1)-C(42)	2.030(3)
Fe(1)-C(47)	2.037(3)
Fe(1)-C(39)	2.052(3)
Fe(1)-C(45)	2.062(3)
Fe(1)-C(41)	2.064(3)
Fe(1)-C(40)	2.065(3)
Fe(1)-C(46)	2.070(3)
Fe(2)-C(79)	2.012(2)
Fe(2)-C(78)	2.018(2)
Fe(2)-C(74)	2.022(2)
Fe(2)-C(83)	2.035(3)
Fe(2)-C(80)	2.038(3)
Fe(2)-C(75)	2.046(3)
Fe(2)-C(77)	2.058(2)
Fe(2)-C(81)	2.063(3)
Fe(2)-C(82)	2.069(3)
Fe(2)-C(76)	2.071(2)
S(1)-C(2)	1.727(3)
C(2)-N(4)	1.316(3)
C(2)-S(3)	1.711(2)
N(4)-C(5)	1.468(3)
N(4)-C(11)	1.479(3)
C(5)-C(6)	1.527(3)
C(6)-N(7)	1.475(3)
N(7)-C(8)	1.314(3)
N(7)-C(18)	1.481(3)
C(8)-S(9)	1.713(2)
C(8)-S(10)	1.718(2)
C(11)-C(12)	1.510(3)
C(11)-C(12')	1.594(11)
C(12)-C(13)	1.3900
C(12)-C(17)	1.3900
C(13)-C(14)	1.3900
C(14)-C(15)	1.3900
C(15)-C(16)	1.3900
C(16)-C(17)	1.3900
C(12')-C(13')	1.3900
C(12')-C(17')	1.3900
C(13')-C(14')	1.3900
C(14')-C(15')	1.3900
C(15')-C(16')	1.3900
C(16')-C(17')	1.3900
C(18)-C(19)	1.506(3)
C(19)-C(24)	1.377(4)
C(19)-C(20)	1.379(4)
C(20)-C(21)	1.387(5)
C(21)-C(22)	1.369(6)

C(22)-C(23)	1.353(5)
C(23)-C(24)	1.390(5)
P(25)-C(38)	1.803(2)
P(25)-C(26)	1.820(2)
P(25)-C(32)	1.829(3)
C(26)-C(31)	1.379(4)
C(26)-C(27)	1.391(4)
C(27)-C(28)	1.386(4)
C(28)-C(29)	1.369(5)
C(29)-C(30)	1.385(5)
C(30)-C(31)	1.389(5)
C(32)-C(37)	1.392(4)
C(32)-C(33)	1.401(3)
C(33)-C(34)	1.379(4)
C(34)-C(35)	1.384(4)
C(35)-C(36)	1.383(5)
C(36)-C(37)	1.387(4)
C(38)-C(42)	1.433(4)
C(38)-C(39)	1.435(4)
C(39)-C(40)	1.428(4)
C(40)-C(41)	1.407(5)
C(41)-C(42)	1.429(4)
C(43)-C(47)	1.438(4)
C(43)-C(44)	1.441(4)
C(43)-P(48)	1.800(3)
C(44)-C(45)	1.417(5)
C(45)-C(46)	1.415(5)
C(46)-C(47)	1.426(4)
P(48)-C(55')	1.802(7)
P(48)-C(49)	1.816(3)
P(48)-C(55)	1.864(3)
C(49)-C(50)	1.389(5)
C(49)-C(54)	1.405(4)
C(50)-C(51)	1.384(5)
C(51)-C(52)	1.386(6)
C(52)-C(53)	1.380(7)
C(53)-C(54)	1.382(5)
C(55)-C(56)	1.3900
C(55)-C(60)	1.3900
C(56)-C(57)	1.3900
C(57)-C(58)	1.3900
C(58)-C(59)	1.3900
C(59)-C(60)	1.3900
C(55')-C(56')	1.3900
C(55')-C(60')	1.3900
C(56')-C(57')	1.3900
C(57')-C(58')	1.3900
C(58')-C(59')	1.3900
C(59')-C(60')	1.3900
P(61)-C(74)	1.814(2)
P(61)-C(62)	1.822(2)
P(61)-C(68)	1.839(3)
P(61)-C(62')	1.846(7)
C(62)-C(63)	1.3900
C(62)-C(67)	1.3900
C(63)-C(64)	1.3900
C(64)-C(65)	1.3900
C(65)-C(66)	1.3900
C(66)-C(67)	1.3900
C(62')-C(63')	1.3900

C(62')-C(67')	1.3900
C(63')-C(64')	1.3900
C(64')-C(65')	1.3900
C(65')-C(66')	1.3900
C(66')-C(67')	1.3900
C(68)-C(69)	1.396(4)
C(68)-C(73)	1.397(4)
C(69)-C(70)	1.401(5)
C(70)-C(71)	1.366(6)
C(71)-C(72)	1.377(5)
C(72)-C(73)	1.388(4)
C(74)-C(78)	1.439(4)
C(74)-C(75)	1.443(4)
C(75)-C(76)	1.420(4)
C(76)-C(77)	1.411(4)
C(77)-C(78)	1.427(4)
C(79)-C(83)	1.443(4)
C(79)-C(80)	1.447(4)
C(79)-P(84)	1.797(3)
C(80)-C(81)	1.423(5)
C(81)-C(82)	1.416(6)
C(82)-C(83)	1.424(4)
P(84)-C(85)	1.816(3)
P(84)-C(91)	1.830(2)
C(85)-C(86)	1.394(4)
C(85)-C(90)	1.398(4)
C(86)-C(87)	1.388(4)
C(87)-C(88)	1.388(5)
C(88)-C(89)	1.381(5)
C(89)-C(90)	1.388(4)
C(91)-C(92)	1.391(4)
C(91)-C(96)	1.392(4)
C(92)-C(93)	1.393(4)
C(93)-C(94)	1.382(5)
C(94)-C(95)	1.386(5)
C(95)-C(96)	1.392(4)

P(48)-Ni(1)-P(25)	100.76(3)
P(48)-Ni(1)-S(1)	92.94(3)
P(25)-Ni(1)-S(1)	166.29(3)
P(48)-Ni(1)-S(3)	170.59(3)
P(25)-Ni(1)-S(3)	87.94(2)
S(1)-Ni(1)-S(3)	78.41(2)
P(84)-Ni(2)-S(10)	92.06(2)
P(84)-Ni(2)-P(61)	101.05(3)
S(10)-Ni(2)-P(61)	166.89(3)
P(84)-Ni(2)-S(9)	170.11(3)
S(10)-Ni(2)-S(9)	78.27(2)
P(61)-Ni(2)-S(9)	88.63(2)
C(43)-Fe(1)-C(38)	108.55(10)
C(43)-Fe(1)-C(44)	41.76(11)
C(38)-Fe(1)-C(44)	136.11(12)
C(43)-Fe(1)-C(42)	109.44(12)
C(38)-Fe(1)-C(42)	41.48(10)
C(44)-Fe(1)-C(42)	108.28(13)
C(43)-Fe(1)-C(47)	41.57(12)
C(38)-Fe(1)-C(47)	111.81(11)
C(44)-Fe(1)-C(47)	69.40(12)
C(42)-Fe(1)-C(47)	140.28(11)
C(43)-Fe(1)-C(39)	137.43(10)

C(38)-Fe(1)-C(39)	41.29(10)
C(44)-Fe(1)-C(39)	177.34(12)
C(42)-Fe(1)-C(39)	69.32(11)
C(47)-Fe(1)-C(39)	111.61(12)
C(43)-Fe(1)-C(45)	69.10(12)
C(38)-Fe(1)-C(45)	176.64(13)
C(44)-Fe(1)-C(45)	40.56(14)
C(42)-Fe(1)-C(45)	136.45(13)
C(47)-Fe(1)-C(45)	68.21(12)
C(39)-Fe(1)-C(45)	142.03(13)
C(43)-Fe(1)-C(41)	139.19(13)
C(38)-Fe(1)-C(41)	68.97(10)
C(44)-Fe(1)-C(41)	110.68(13)
C(42)-Fe(1)-C(41)	40.84(11)
C(47)-Fe(1)-C(41)	178.87(12)
C(39)-Fe(1)-C(41)	68.37(13)
C(45)-Fe(1)-C(41)	111.07(13)
C(43)-Fe(1)-C(40)	177.07(11)
C(38)-Fe(1)-C(40)	68.56(10)
C(44)-Fe(1)-C(40)	140.08(12)
C(42)-Fe(1)-C(40)	68.15(12)
C(47)-Fe(1)-C(40)	139.44(14)
C(39)-Fe(1)-C(40)	40.57(12)
C(45)-Fe(1)-C(40)	113.76(12)
C(41)-Fe(1)-C(40)	39.86(15)
C(43)-Fe(1)-C(46)	69.21(12)
C(38)-Fe(1)-C(46)	141.96(12)
C(44)-Fe(1)-C(46)	68.42(14)
C(42)-Fe(1)-C(46)	176.40(13)
C(47)-Fe(1)-C(46)	40.63(12)
C(39)-Fe(1)-C(46)	114.01(13)
C(45)-Fe(1)-C(46)	40.04(15)
C(41)-Fe(1)-C(46)	138.27(12)
C(40)-Fe(1)-C(46)	113.30(13)
C(79)-Fe(2)-C(78)	110.10(11)
C(79)-Fe(2)-C(74)	108.45(10)
C(78)-Fe(2)-C(74)	41.73(10)
C(79)-Fe(2)-C(83)	41.78(12)
C(78)-Fe(2)-C(83)	139.61(11)
C(74)-Fe(2)-C(83)	109.94(12)
C(79)-Fe(2)-C(80)	41.85(11)
C(78)-Fe(2)-C(80)	109.99(12)
C(74)-Fe(2)-C(80)	137.36(11)
C(83)-Fe(2)-C(80)	69.81(13)
C(79)-Fe(2)-C(75)	137.14(11)
C(78)-Fe(2)-C(75)	69.51(10)
C(74)-Fe(2)-C(75)	41.56(10)
C(83)-Fe(2)-C(75)	109.81(12)
C(80)-Fe(2)-C(75)	178.80(11)
C(79)-Fe(2)-C(77)	140.41(12)
C(78)-Fe(2)-C(77)	40.97(10)
C(74)-Fe(2)-C(77)	69.14(10)
C(83)-Fe(2)-C(77)	177.70(12)
C(80)-Fe(2)-C(77)	112.35(12)
C(75)-Fe(2)-C(77)	68.05(11)
C(79)-Fe(2)-C(81)	69.11(11)
C(78)-Fe(2)-C(81)	138.46(14)
C(74)-Fe(2)-C(81)	177.55(11)
C(83)-Fe(2)-C(81)	68.45(14)
C(80)-Fe(2)-C(81)	40.60(13)

C(75)-Fe(2)-C(81)	140.45(13)
C(77)-Fe(2)-C(81)	112.54(13)
C(79)-Fe(2)-C(82)	69.09(11)
C(78)-Fe(2)-C(82)	178.42(14)
C(74)-Fe(2)-C(82)	139.69(14)
C(83)-Fe(2)-C(82)	40.59(13)
C(80)-Fe(2)-C(82)	68.48(15)
C(75)-Fe(2)-C(82)	112.03(14)
C(77)-Fe(2)-C(82)	138.93(12)
C(81)-Fe(2)-C(82)	40.08(17)
C(79)-Fe(2)-C(76)	177.32(11)
C(78)-Fe(2)-C(76)	68.64(10)
C(74)-Fe(2)-C(76)	68.99(10)
C(83)-Fe(2)-C(76)	137.80(12)
C(80)-Fe(2)-C(76)	140.65(12)
C(75)-Fe(2)-C(76)	40.35(11)
C(77)-Fe(2)-C(76)	39.97(12)
C(81)-Fe(2)-C(76)	113.45(11)
C(82)-Fe(2)-C(76)	112.23(12)
C(2)-S(1)-Ni(1)	85.27(8)
N(4)-C(2)-S(3)	124.75(19)
N(4)-C(2)-S(1)	126.12(19)
S(3)-C(2)-S(1)	109.07(13)
C(2)-S(3)-Ni(1)	85.59(8)
C(2)-N(4)-C(5)	121.0(2)
C(2)-N(4)-C(11)	121.3(2)
C(5)-N(4)-C(11)	117.55(19)
N(4)-C(5)-C(6)	113.53(19)
N(7)-C(6)-C(5)	113.30(18)
C(8)-N(7)-C(6)	120.71(19)
C(8)-N(7)-C(18)	120.05(18)
C(6)-N(7)-C(18)	119.04(18)
N(7)-C(8)-S(9)	125.57(17)
N(7)-C(8)-S(10)	125.12(17)
S(9)-C(8)-S(10)	109.31(13)
C(8)-S(9)-Ni(2)	85.99(8)
C(8)-S(10)-Ni(2)	86.29(8)
N(4)-C(11)-C(12)	113.3(2)
N(4)-C(11)-C(12')	108.7(4)
C(13)-C(12)-C(17)	120.0
C(13)-C(12)-C(11)	121.6(2)
C(17)-C(12)-C(11)	118.4(2)
C(14)-C(13)-C(12)	120.0
C(13)-C(14)-C(15)	120.0
C(16)-C(15)-C(14)	120.0
C(15)-C(16)-C(17)	120.0
C(16)-C(17)-C(12)	120.0
C(13')-C(12')-C(17')	120.0
C(13')-C(12')-C(11)	114.4(12)
C(17')-C(12')-C(11)	125.6(12)
C(14')-C(13')-C(12')	120.0
C(13')-C(14')-C(15')	120.0
C(16')-C(15')-C(14')	120.0
C(15')-C(16')-C(17')	120.0
C(16')-C(17')-C(12')	120.0
N(7)-C(18)-C(19)	112.10(18)
C(24)-C(19)-C(20)	117.7(3)
C(24)-C(19)-C(18)	120.3(2)
C(20)-C(19)-C(18)	122.0(2)
C(19)-C(20)-C(21)	121.0(3)

C(22)-C(21)-C(20)	120.0(3)
C(23)-C(22)-C(21)	119.9(3)
C(22)-C(23)-C(24)	120.2(3)
C(19)-C(24)-C(23)	121.2(3)
C(38)-P(25)-C(26)	104.58(11)
C(38)-P(25)-C(32)	100.47(11)
C(26)-P(25)-C(32)	106.64(11)
C(38)-P(25)-Ni(1)	122.47(8)
C(26)-P(25)-Ni(1)	104.32(8)
C(32)-P(25)-Ni(1)	116.99(8)
C(31)-C(26)-C(27)	119.1(2)
C(31)-C(26)-P(25)	122.7(2)
C(27)-C(26)-P(25)	117.9(2)
C(28)-C(27)-C(26)	120.5(3)
C(29)-C(28)-C(27)	120.2(3)
C(28)-C(29)-C(30)	119.8(3)
C(29)-C(30)-C(31)	120.2(3)
C(26)-C(31)-C(30)	120.2(3)
C(37)-C(32)-C(33)	118.9(2)
C(37)-C(32)-P(25)	121.75(19)
C(33)-C(32)-P(25)	119.37(18)
C(34)-C(33)-C(32)	120.4(2)
C(33)-C(34)-C(35)	120.4(3)
C(36)-C(35)-C(34)	119.7(3)
C(35)-C(36)-C(37)	120.4(3)
C(36)-C(37)-C(32)	120.2(3)
C(42)-C(38)-C(39)	108.1(2)
C(42)-C(38)-P(25)	124.83(19)
C(39)-C(38)-P(25)	127.1(2)
C(42)-C(38)-Fe(1)	69.77(15)
C(39)-C(38)-Fe(1)	70.69(15)
P(25)-C(38)-Fe(1)	126.05(13)
C(40)-C(39)-C(38)	106.9(3)
C(40)-C(39)-Fe(1)	70.21(18)
C(38)-C(39)-Fe(1)	68.02(15)
C(41)-C(40)-C(39)	109.3(2)
C(41)-C(40)-Fe(1)	70.02(18)
C(39)-C(40)-Fe(1)	69.22(16)
C(40)-C(41)-C(42)	108.0(3)
C(40)-C(41)-Fe(1)	70.13(17)
C(42)-C(41)-Fe(1)	68.31(15)
C(41)-C(42)-C(38)	107.7(3)
C(41)-C(42)-Fe(1)	70.84(16)
C(38)-C(42)-Fe(1)	68.75(14)
C(47)-C(43)-C(44)	107.0(2)
C(47)-C(43)-P(48)	123.5(2)
C(44)-C(43)-P(48)	129.5(2)
C(47)-C(43)-Fe(1)	70.07(15)
C(44)-C(43)-Fe(1)	69.61(16)
P(48)-C(43)-Fe(1)	122.97(14)
C(45)-C(44)-C(43)	108.0(3)
C(45)-C(44)-Fe(1)	71.02(18)
C(43)-C(44)-Fe(1)	68.63(16)
C(46)-C(45)-C(44)	108.9(3)
C(46)-C(45)-Fe(1)	70.32(17)
C(44)-C(45)-Fe(1)	68.42(16)
C(45)-C(46)-C(47)	108.0(3)
C(45)-C(46)-Fe(1)	69.64(18)
C(47)-C(46)-Fe(1)	68.43(16)
C(46)-C(47)-C(43)	108.2(3)

C(46)-C(47)-Fe(1)	70.94(16)
C(43)-C(47)-Fe(1)	68.36(15)
C(43)-P(48)-C(55')	110.8(4)
C(43)-P(48)-C(49)	107.06(12)
C(55')-P(48)-C(49)	97.2(4)
C(43)-P(48)-C(55)	101.0(2)
C(49)-P(48)-C(55)	105.0(2)
C(43)-P(48)-Ni(1)	116.54(9)
C(55')-P(48)-Ni(1)	112.3(4)
C(49)-P(48)-Ni(1)	111.10(10)
C(55)-P(48)-Ni(1)	115.01(15)
C(50)-C(49)-C(54)	119.2(3)
C(50)-C(49)-P(48)	119.9(2)
C(54)-C(49)-P(48)	120.9(3)
C(51)-C(50)-C(49)	120.6(3)
C(50)-C(51)-C(52)	119.8(4)
C(53)-C(52)-C(51)	120.2(3)
C(52)-C(53)-C(54)	120.4(3)
C(53)-C(54)-C(49)	119.8(4)
C(56)-C(55)-C(60)	120.0
C(56)-C(55)-P(48)	117.2(2)
C(60)-C(55)-P(48)	122.8(2)
C(57)-C(56)-C(55)	120.0
C(56)-C(57)-C(58)	120.0
C(59)-C(58)-C(57)	120.0
C(60)-C(59)-C(58)	120.0
C(59)-C(60)-C(55)	120.0
C(56')-C(55')-C(60')	120.0
C(56')-C(55')-P(48)	123.0(5)
C(60')-C(55')-P(48)	116.7(5)
C(55')-C(56')-C(57')	120.0
C(58')-C(57')-C(56')	120.0
C(57')-C(58')-C(59')	120.0
C(58')-C(59')-C(60')	120.0
C(59')-C(60')-C(55')	120.0
C(74)-P(61)-C(62)	101.09(19)
C(74)-P(61)-C(68)	103.93(11)
C(62)-P(61)-C(68)	108.5(2)
C(74)-P(61)-C(62')	106.3(4)
C(68)-P(61)-C(62')	98.8(4)
C(74)-P(61)-Ni(2)	123.62(8)
C(62)-P(61)-Ni(2)	106.59(14)
C(68)-P(61)-Ni(2)	111.97(8)
C(62')-P(61)-Ni(2)	109.3(4)
C(63)-C(62)-C(67)	120.0
C(63)-C(62)-P(61)	119.1(2)
C(67)-C(62)-P(61)	120.9(2)
C(62)-C(63)-C(64)	120.0
C(63)-C(64)-C(65)	120.0
C(64)-C(65)-C(66)	120.0
C(67)-C(66)-C(65)	120.0
C(66)-C(67)-C(62)	120.0
C(63')-C(62')-C(67')	120.0
C(63')-C(62')-P(61)	118.3(6)
C(67')-C(62')-P(61)	121.7(6)
C(64')-C(63')-C(62')	120.0
C(63')-C(64')-C(65')	120.0
C(64')-C(65')-C(66')	120.0
C(67')-C(66')-C(65')	120.0
C(66')-C(67')-C(62')	120.0

C(69)-C(68)-C(73)	118.1(3)
C(69)-C(68)-P(61)	121.4(2)
C(73)-C(68)-P(61)	120.48(19)
C(68)-C(69)-C(70)	120.0(3)
C(71)-C(70)-C(69)	120.8(3)
C(70)-C(71)-C(72)	120.0(3)
C(71)-C(72)-C(73)	120.0(3)
C(72)-C(73)-C(68)	121.1(3)
C(78)-C(74)-C(75)	107.0(2)
C(78)-C(74)-P(61)	128.36(19)
C(75)-C(74)-P(61)	124.58(19)
C(78)-C(74)-Fe(2)	68.99(13)
C(75)-C(74)-Fe(2)	70.10(14)
P(61)-C(74)-Fe(2)	123.39(12)
C(76)-C(75)-C(74)	108.1(2)
C(76)-C(75)-Fe(2)	70.78(15)
C(74)-C(75)-Fe(2)	68.34(14)
C(77)-C(76)-C(75)	108.4(2)
C(77)-C(76)-Fe(2)	69.52(14)
C(75)-C(76)-Fe(2)	68.88(14)
C(76)-C(77)-C(78)	108.7(2)
C(76)-C(77)-Fe(2)	70.51(15)
C(78)-C(77)-Fe(2)	68.03(14)
C(77)-C(78)-C(74)	107.8(2)
C(77)-C(78)-Fe(2)	71.00(14)
C(74)-C(78)-Fe(2)	69.28(14)
C(83)-C(79)-C(80)	107.5(2)
C(83)-C(79)-P(84)	123.5(2)
C(80)-C(79)-P(84)	128.9(2)
C(83)-C(79)-Fe(2)	69.97(15)
C(80)-C(79)-Fe(2)	70.07(15)
P(84)-C(79)-Fe(2)	123.71(13)
C(81)-C(80)-C(79)	107.3(3)
C(81)-C(80)-Fe(2)	70.62(18)
C(79)-C(80)-Fe(2)	68.08(15)
C(82)-C(81)-C(80)	109.0(3)
C(82)-C(81)-Fe(2)	70.19(18)
C(80)-C(81)-Fe(2)	68.77(15)
C(81)-C(82)-C(83)	108.5(3)
C(81)-C(82)-Fe(2)	69.73(18)
C(83)-C(82)-Fe(2)	68.41(15)
C(82)-C(83)-C(79)	107.7(3)
C(82)-C(83)-Fe(2)	71.00(17)
C(79)-C(83)-Fe(2)	68.25(15)
C(79)-P(84)-C(85)	106.67(12)
C(79)-P(84)-C(91)	102.91(11)
C(85)-P(84)-C(91)	101.81(11)
C(79)-P(84)-Ni(2)	116.30(9)
C(85)-P(84)-Ni(2)	111.27(8)
C(91)-P(84)-Ni(2)	116.41(8)
C(86)-C(85)-C(90)	119.5(2)
C(86)-C(85)-P(84)	120.08(19)
C(90)-C(85)-P(84)	120.4(2)
C(87)-C(86)-C(85)	120.1(3)
C(86)-C(87)-C(88)	120.0(3)
C(89)-C(88)-C(87)	120.4(3)
C(88)-C(89)-C(90)	120.1(3)
C(89)-C(90)-C(85)	120.1(3)
C(92)-C(91)-C(96)	119.4(2)
C(92)-C(91)-P(84)	119.4(2)

C(96)-C(91)-P(84)	121.3(2)
C(91)-C(92)-C(93)	120.6(3)
C(94)-C(93)-C(92)	119.7(3)
C(93)-C(94)-C(95)	120.0(3)
C(94)-C(95)-C(96)	120.4(3)
C(95)-C(96)-C(91)	119.9(3)

Table 6. Complete bond lengths [Å] and angles [°] for **3**.

Pd(1)-P(48)	2.2923(6)
Pd(1)-P(25)	2.3018(6)
Pd(1)-S(3)	2.3348(6)
Pd(1)-S(1)	2.3516(6)
Pd(2)-P(84)	2.2906(7)
Pd(2)-P(61)	2.3110(6)
Pd(2)-S(10)	2.3347(6)
Pd(2)-S(9)	2.3445(7)
Fe(1)-C(43)	2.015(3)
Fe(1)-C(42)	2.020(3)
Fe(1)-C(38)	2.024(2)
Fe(1)-C(47)	2.027(3)
Fe(1)-C(44)	2.027(3)
Fe(1)-C(39)	2.048(3)
Fe(1)-C(45)	2.049(3)
Fe(1)-C(46)	2.050(3)
Fe(1)-C(41)	2.058(3)
Fe(1)-C(40)	2.065(3)
Fe(2)-C(79)	2.012(2)
Fe(2)-C(78)	2.020(3)
Fe(2)-C(74)	2.028(3)
Fe(2)-C(83)	2.029(3)
Fe(2)-C(80)	2.038(3)
Fe(2)-C(75)	2.043(3)
Fe(2)-C(81)	2.059(3)
Fe(2)-C(77)	2.060(3)
Fe(2)-C(82)	2.066(3)
Fe(2)-C(76)	2.066(2)
S(1)-C(2)	1.728(2)
C(2)-N(4)	1.313(3)
C(2)-S(3)	1.719(2)
N(4)-C(11)	1.471(3)
N(4)-C(5)	1.474(3)
C(5)-C(6)	1.526(3)
C(6)-N(7)	1.470(3)
N(7)-C(8)	1.323(3)
N(7)-C(18)	1.479(3)
C(8)-S(10)	1.709(2)
C(8)-S(9)	1.723(2)
C(11)-C(12)	1.514(4)
C(12)-C(13)	1.368(4)
C(12)-C(17)	1.383(4)
C(13)-C(14)	1.396(4)
C(14)-C(15)	1.359(6)
C(15)-C(16)	1.364(6)
C(16)-C(17)	1.382(5)
C(18)-C(19)	1.498(3)
C(18)-C(19')	1.550(11)
C(19)-C(20)	1.3900

C(19)-C(24)	1.3900
C(20)-C(21)	1.3900
C(21)-C(22)	1.3900
C(22)-C(23)	1.3900
C(23)-C(24)	1.3900
C(19')-C(20')	1.3900
C(19')-C(24')	1.3900
C(20')-C(21')	1.3900
C(21')-C(22')	1.3900
C(22')-C(23')	1.3900
C(23')-C(24')	1.3900
P(25)-C(38)	1.790(3)
P(25)-C(26)	1.804(3)
P(25)-C(32)	1.827(2)
P(25)-C(26')	1.846(7)
C(26)-C(27)	1.3900
C(26)-C(31)	1.3900
C(27)-C(28)	1.3900
C(28)-C(29)	1.3900
C(29)-C(30)	1.3900
C(30)-C(31)	1.3900
C(26')-C(27')	1.3900
C(26')-C(31')	1.3900
C(27')-C(28')	1.3900
C(28')-C(29')	1.3900
C(29')-C(30')	1.3900
C(30')-C(31')	1.3900
C(32)-C(37)	1.373(4)
C(32)-C(33)	1.394(3)
C(33)-C(34)	1.386(4)
C(34)-C(35)	1.373(4)
C(35)-C(36)	1.369(5)
C(36)-C(37)	1.393(4)
C(38)-C(39)	1.432(4)
C(38)-C(42)	1.438(4)
C(39)-C(40)	1.433(4)
C(40)-C(41)	1.415(5)
C(41)-C(42)	1.425(4)
C(43)-C(47)	1.429(4)
C(43)-C(44)	1.448(4)
C(43)-P(48)	1.792(3)
C(44)-C(45)	1.409(5)
C(45)-C(46)	1.410(5)
C(46)-C(47)	1.422(4)
P(48)-C(49)	1.816(3)
P(48)-C(55)	1.825(3)
C(49)-C(50)	1.384(4)
C(49)-C(54)	1.395(4)
C(50)-C(51)	1.379(4)
C(51)-C(52)	1.378(5)
C(52)-C(53)	1.361(5)
C(53)-C(54)	1.383(4)
C(55)-C(60)	1.372(4)
C(55)-C(56)	1.400(4)
C(56)-C(57)	1.375(4)
C(57)-C(58)	1.386(6)
C(58)-C(59)	1.347(6)
C(59)-C(60)	1.406(4)
P(61)-C(74)	1.806(2)
P(61)-C(62)	1.810(3)

P(61)-C(68)	1.830(3)
C(62)-C(67)	1.389(4)
C(62)-C(63)	1.395(4)
C(63)-C(64)	1.397(4)
C(64)-C(65)	1.398(6)
C(65)-C(66)	1.373(5)
C(66)-C(67)	1.374(4)
C(68)-C(73)	1.390(4)
C(68)-C(69)	1.391(4)
C(69)-C(70)	1.385(4)
C(70)-C(71)	1.379(4)
C(71)-C(72)	1.382(4)
C(72)-C(73)	1.387(4)
C(74)-C(75)	1.437(3)
C(74)-C(78)	1.438(3)
C(75)-C(76)	1.423(4)
C(76)-C(77)	1.424(4)
C(77)-C(78)	1.426(4)
C(79)-C(83)	1.434(4)
C(79)-C(80)	1.442(4)
C(79)-P(84)	1.796(3)
C(80)-C(81)	1.437(4)
C(81)-C(82)	1.409(5)
C(82)-C(83)	1.421(4)
P(84)-C(91)	1.812(3)
P(84)-C(85)	1.815(3)
C(85)-C(86)	1.384(4)
C(85)-C(90)	1.398(4)
C(86)-C(87)	1.389(4)
C(87)-C(88)	1.393(4)
C(88)-C(89)	1.374(5)
C(89)-C(90)	1.369(4)
C(91)-C(96)	1.385(4)
C(91)-C(92)	1.405(4)
C(92)-C(93)	1.392(4)
C(93)-C(94)	1.378(5)
C(94)-C(95)	1.375(5)
C(95)-C(96)	1.386(4)

P(48)-Pd(1)-P(25)	99.27(2)
P(48)-Pd(1)-S(3)	170.12(2)
P(25)-Pd(1)-S(3)	90.25(2)
P(48)-Pd(1)-S(1)	95.41(2)
P(25)-Pd(1)-S(1)	165.31(2)
S(3)-Pd(1)-S(1)	75.07(2)
P(84)-Pd(2)-P(61)	99.49(2)
P(84)-Pd(2)-S(10)	94.27(2)
P(61)-Pd(2)-S(10)	166.19(2)
P(84)-Pd(2)-S(9)	169.19(2)
P(61)-Pd(2)-S(9)	91.23(2)
S(10)-Pd(2)-S(9)	74.98(2)
C(43)-Fe(1)-C(42)	109.36(12)
C(43)-Fe(1)-C(38)	109.47(10)
C(42)-Fe(1)-C(38)	41.67(10)
C(43)-Fe(1)-C(47)	41.39(11)
C(42)-Fe(1)-C(47)	139.64(11)
C(38)-Fe(1)-C(47)	111.69(11)
C(43)-Fe(1)-C(44)	41.98(11)
C(42)-Fe(1)-C(44)	108.52(13)

C(38)-Fe(1)-C(44)	137.41(12)
C(47)-Fe(1)-C(44)	69.58(12)
C(43)-Fe(1)-C(39)	138.78(11)
C(42)-Fe(1)-C(39)	69.31(12)
C(38)-Fe(1)-C(39)	41.16(10)
C(47)-Fe(1)-C(39)	112.34(12)
C(44)-Fe(1)-C(39)	177.77(13)
C(43)-Fe(1)-C(45)	69.14(12)
C(42)-Fe(1)-C(45)	136.80(13)
C(38)-Fe(1)-C(45)	177.80(13)
C(47)-Fe(1)-C(45)	68.52(13)
C(44)-Fe(1)-C(45)	40.43(13)
C(39)-Fe(1)-C(45)	140.97(13)
C(43)-Fe(1)-C(46)	69.15(12)
C(42)-Fe(1)-C(46)	176.86(13)
C(38)-Fe(1)-C(46)	141.25(13)
C(47)-Fe(1)-C(46)	40.82(12)
C(44)-Fe(1)-C(46)	68.48(15)
C(39)-Fe(1)-C(46)	113.68(14)
C(45)-Fe(1)-C(46)	40.23(14)
C(43)-Fe(1)-C(41)	138.20(13)
C(42)-Fe(1)-C(41)	40.88(11)
C(38)-Fe(1)-C(41)	69.23(11)
C(47)-Fe(1)-C(41)	179.03(13)
C(44)-Fe(1)-C(41)	109.56(13)
C(39)-Fe(1)-C(41)	68.54(13)
C(45)-Fe(1)-C(41)	110.55(13)
C(46)-Fe(1)-C(41)	138.59(13)
C(43)-Fe(1)-C(40)	177.83(12)
C(42)-Fe(1)-C(40)	68.47(12)
C(38)-Fe(1)-C(40)	68.90(11)
C(47)-Fe(1)-C(40)	140.30(13)
C(44)-Fe(1)-C(40)	138.35(13)
C(39)-Fe(1)-C(40)	40.77(12)
C(45)-Fe(1)-C(40)	112.44(13)
C(46)-Fe(1)-C(40)	113.02(13)
C(41)-Fe(1)-C(40)	40.14(13)
C(79)-Fe(2)-C(78)	110.11(10)
C(79)-Fe(2)-C(74)	109.84(10)
C(78)-Fe(2)-C(74)	41.62(10)
C(79)-Fe(2)-C(83)	41.55(11)
C(78)-Fe(2)-C(83)	138.60(11)
C(74)-Fe(2)-C(83)	109.85(11)
C(79)-Fe(2)-C(80)	41.70(10)
C(78)-Fe(2)-C(80)	111.09(12)
C(74)-Fe(2)-C(80)	139.39(11)
C(83)-Fe(2)-C(80)	69.49(12)
C(79)-Fe(2)-C(75)	139.02(10)
C(78)-Fe(2)-C(75)	69.23(11)
C(74)-Fe(2)-C(75)	41.34(10)
C(83)-Fe(2)-C(75)	110.81(11)
C(80)-Fe(2)-C(75)	179.17(11)
C(79)-Fe(2)-C(81)	69.24(11)
C(78)-Fe(2)-C(81)	140.41(13)
C(74)-Fe(2)-C(81)	177.86(13)
C(83)-Fe(2)-C(81)	68.14(13)
C(80)-Fe(2)-C(81)	41.06(12)
C(75)-Fe(2)-C(81)	138.23(12)
C(79)-Fe(2)-C(77)	138.87(11)
C(78)-Fe(2)-C(77)	40.91(10)

C(74)-Fe(2)-C(77)	69.29(10)
C(83)-Fe(2)-C(77)	179.09(12)
C(80)-Fe(2)-C(77)	111.34(12)
C(75)-Fe(2)-C(77)	68.36(11)
C(81)-Fe(2)-C(77)	112.71(13)
C(79)-Fe(2)-C(82)	69.22(11)
C(78)-Fe(2)-C(82)	179.18(11)
C(74)-Fe(2)-C(82)	138.00(13)
C(83)-Fe(2)-C(82)	40.58(12)
C(80)-Fe(2)-C(82)	68.76(13)
C(75)-Fe(2)-C(82)	110.93(12)
C(81)-Fe(2)-C(82)	39.96(14)
C(77)-Fe(2)-C(82)	139.91(12)
C(79)-Fe(2)-C(76)	178.77(11)
C(78)-Fe(2)-C(76)	68.70(11)
C(74)-Fe(2)-C(76)	69.10(10)
C(83)-Fe(2)-C(76)	139.19(11)
C(80)-Fe(2)-C(76)	138.78(11)
C(75)-Fe(2)-C(76)	40.51(10)
C(81)-Fe(2)-C(76)	111.84(11)
C(77)-Fe(2)-C(76)	40.37(11)
C(82)-Fe(2)-C(76)	111.96(11)
C(2)-S(1)-Pd(1)	85.39(8)
N(4)-C(2)-S(3)	123.48(18)
N(4)-C(2)-S(1)	124.58(18)
S(3)-C(2)-S(1)	111.88(14)
C(2)-S(3)-Pd(1)	86.13(8)
C(2)-N(4)-C(11)	121.8(2)
C(2)-N(4)-C(5)	120.9(2)
C(11)-N(4)-C(5)	116.9(2)
N(4)-C(5)-C(6)	113.40(19)
N(7)-C(6)-C(5)	113.4(2)
C(8)-N(7)-C(6)	121.32(19)
C(8)-N(7)-C(18)	119.6(2)
C(6)-N(7)-C(18)	118.78(19)
N(7)-C(8)-S(10)	124.26(18)
N(7)-C(8)-S(9)	123.58(18)
S(10)-C(8)-S(9)	112.15(13)
C(8)-S(9)-Pd(2)	86.04(8)
C(8)-S(10)-Pd(2)	86.67(8)
N(4)-C(11)-C(12)	112.5(2)
C(13)-C(12)-C(17)	118.6(3)
C(13)-C(12)-C(11)	121.7(3)
C(17)-C(12)-C(11)	119.5(3)
C(12)-C(13)-C(14)	120.5(3)
C(15)-C(14)-C(13)	120.3(4)
C(14)-C(15)-C(16)	119.4(3)
C(15)-C(16)-C(17)	120.8(4)
C(16)-C(17)-C(12)	120.2(3)
N(7)-C(18)-C(19)	112.2(2)
N(7)-C(18)-C(19')	112.9(7)
C(20)-C(19)-C(24)	120.0
C(20)-C(19)-C(18)	120.1(2)
C(24)-C(19)-C(18)	119.9(2)
C(21)-C(20)-C(19)	120.0
C(20)-C(21)-C(22)	120.0
C(23)-C(22)-C(21)	120.0
C(22)-C(23)-C(24)	120.0
C(23)-C(24)-C(19)	120.0
C(20')-C(19')-C(24')	120.0

C(20')-C(19')-C(18)	124.8(11)
C(24')-C(19')-C(18)	115.0(11)
C(21')-C(20')-C(19')	120.0
C(20')-C(21')-C(22')	120.0
C(23')-C(22')-C(21')	120.0
C(22')-C(23')-C(24')	120.0
C(23')-C(24')-C(19')	120.0
C(38)-P(25)-C(26)	107.06(19)
C(38)-P(25)-C(32)	101.90(11)
C(26)-P(25)-C(32)	106.25(18)
C(38)-P(25)-C(26')	102.6(3)
C(32)-P(25)-C(26')	108.1(3)
C(38)-P(25)-Pd(1)	121.79(8)
C(26)-P(25)-Pd(1)	103.55(15)
C(32)-P(25)-Pd(1)	115.26(8)
C(26')-P(25)-Pd(1)	106.0(3)
C(27)-C(26)-C(31)	120.0
C(27)-C(26)-P(25)	117.5(3)
C(31)-C(26)-P(25)	122.2(3)
C(26)-C(27)-C(28)	120.0
C(27)-C(28)-C(29)	120.0
C(30)-C(29)-C(28)	120.0
C(31)-C(30)-C(29)	120.0
C(30)-C(31)-C(26)	120.0
C(27')-C(26')-C(31')	120.0
C(27')-C(26')-P(25)	118.5(6)
C(31')-C(26')-P(25)	121.2(6)
C(26')-C(27')-C(28')	120.0
C(27')-C(28')-C(29')	120.0
C(30')-C(29')-C(28')	120.0
C(31')-C(30')-C(29')	120.0
C(30')-C(31')-C(26')	120.0
C(37)-C(32)-C(33)	118.7(2)
C(37)-C(32)-P(25)	121.3(2)
C(33)-C(32)-P(25)	120.0(2)
C(34)-C(33)-C(32)	120.4(3)
C(35)-C(34)-C(33)	120.4(3)
C(36)-C(35)-C(34)	119.5(3)
C(35)-C(36)-C(37)	120.6(3)
C(32)-C(37)-C(36)	120.4(3)
C(39)-C(38)-C(42)	107.4(2)
C(39)-C(38)-P(25)	127.7(2)
C(42)-C(38)-P(25)	124.8(2)
C(39)-C(38)-Fe(1)	70.30(15)
C(42)-C(38)-Fe(1)	69.01(15)
P(25)-C(38)-Fe(1)	126.62(13)
C(38)-C(39)-C(40)	107.7(3)
C(38)-C(39)-Fe(1)	68.54(15)
C(40)-C(39)-Fe(1)	70.26(17)
C(41)-C(40)-C(39)	108.6(3)
C(41)-C(40)-Fe(1)	69.69(17)
C(39)-C(40)-Fe(1)	68.97(16)
C(40)-C(41)-C(42)	108.1(3)
C(40)-C(41)-Fe(1)	70.17(17)
C(42)-C(41)-Fe(1)	68.11(15)
C(41)-C(42)-C(38)	108.2(3)
C(41)-C(42)-Fe(1)	71.01(16)
C(38)-C(42)-Fe(1)	69.33(14)
C(47)-C(43)-C(44)	107.0(3)
C(47)-C(43)-P(48)	124.1(2)

C(44)-C(43)-P(48)	128.8(2)
C(47)-C(43)-Fe(1)	69.73(15)
C(44)-C(43)-Fe(1)	69.45(16)
P(48)-C(43)-Fe(1)	123.16(13)
C(45)-C(44)-C(43)	107.7(3)
C(45)-C(44)-Fe(1)	70.61(18)
C(43)-C(44)-Fe(1)	68.58(15)
C(44)-C(45)-C(46)	109.0(3)
C(44)-C(45)-Fe(1)	68.96(17)
C(46)-C(45)-Fe(1)	69.94(17)
C(45)-C(46)-C(47)	108.2(3)
C(45)-C(46)-Fe(1)	69.83(19)
C(47)-C(46)-Fe(1)	68.70(16)
C(46)-C(47)-C(43)	108.1(3)
C(46)-C(47)-Fe(1)	70.47(17)
C(43)-C(47)-Fe(1)	68.87(15)
C(43)-P(48)-C(49)	108.51(13)
C(43)-P(48)-C(55)	105.07(13)
C(49)-P(48)-C(55)	102.61(12)
C(43)-P(48)-Pd(1)	115.35(9)
C(49)-P(48)-Pd(1)	111.63(9)
C(55)-P(48)-Pd(1)	112.71(9)
C(50)-C(49)-C(54)	118.9(3)
C(50)-C(49)-P(48)	120.1(2)
C(54)-C(49)-P(48)	120.9(2)
C(51)-C(50)-C(49)	120.4(3)
C(52)-C(51)-C(50)	120.0(3)
C(53)-C(52)-C(51)	120.3(3)
C(52)-C(53)-C(54)	120.4(3)
C(53)-C(54)-C(49)	119.9(3)
C(60)-C(55)-C(56)	119.0(3)
C(60)-C(55)-P(48)	121.8(2)
C(56)-C(55)-P(48)	119.1(2)
C(57)-C(56)-C(55)	120.7(3)
C(56)-C(57)-C(58)	119.8(4)
C(59)-C(58)-C(57)	120.0(3)
C(58)-C(59)-C(60)	121.2(4)
C(55)-C(60)-C(59)	119.4(3)
C(74)-P(61)-C(62)	102.93(11)
C(74)-P(61)-C(68)	104.95(11)
C(62)-P(61)-C(68)	104.43(13)
C(74)-P(61)-Pd(2)	122.92(8)
C(62)-P(61)-Pd(2)	108.72(9)
C(68)-P(61)-Pd(2)	111.19(7)
C(67)-C(62)-C(63)	119.2(3)
C(67)-C(62)-P(61)	121.4(2)
C(63)-C(62)-P(61)	119.4(2)
C(62)-C(63)-C(64)	120.4(3)
C(63)-C(64)-C(65)	118.9(3)
C(66)-C(65)-C(64)	120.4(3)
C(65)-C(66)-C(67)	120.6(3)
C(66)-C(67)-C(62)	120.6(3)
C(73)-C(68)-C(69)	118.2(2)
C(73)-C(68)-P(61)	121.0(2)
C(69)-C(68)-P(61)	120.6(2)
C(70)-C(69)-C(68)	121.2(3)
C(71)-C(70)-C(69)	119.9(3)
C(70)-C(71)-C(72)	119.7(3)
C(71)-C(72)-C(73)	120.4(3)
C(72)-C(73)-C(68)	120.6(3)

C(75)-C(74)-C(78)	106.8(2)
C(75)-C(74)-P(61)	125.21(19)
C(78)-C(74)-P(61)	127.90(18)
C(75)-C(74)-Fe(2)	69.92(15)
C(78)-C(74)-Fe(2)	68.89(14)
P(61)-C(74)-Fe(2)	123.65(12)
C(76)-C(75)-C(74)	108.6(2)
C(76)-C(75)-Fe(2)	70.62(15)
C(74)-C(75)-Fe(2)	68.74(14)
C(75)-C(76)-C(77)	108.2(2)
C(75)-C(76)-Fe(2)	68.87(14)
C(77)-C(76)-Fe(2)	69.59(14)
C(76)-C(77)-C(78)	108.0(2)
C(76)-C(77)-Fe(2)	70.04(15)
C(78)-C(77)-Fe(2)	68.00(14)
C(77)-C(78)-C(74)	108.5(2)
C(77)-C(78)-Fe(2)	71.08(15)
C(74)-C(78)-Fe(2)	69.49(14)
C(83)-C(79)-C(80)	107.4(2)
C(83)-C(79)-P(84)	123.4(2)
C(80)-C(79)-P(84)	129.2(2)
C(83)-C(79)-Fe(2)	69.85(14)
C(80)-C(79)-Fe(2)	70.11(15)
P(84)-C(79)-Fe(2)	123.36(14)
C(81)-C(80)-C(79)	106.9(3)
C(81)-C(80)-Fe(2)	70.24(17)
C(79)-C(80)-Fe(2)	68.19(15)
C(82)-C(81)-C(80)	109.0(3)
C(82)-C(81)-Fe(2)	70.29(18)
C(80)-C(81)-Fe(2)	68.70(16)
C(81)-C(82)-C(83)	108.1(3)
C(81)-C(82)-Fe(2)	69.75(18)
C(83)-C(82)-Fe(2)	68.31(16)
C(82)-C(83)-C(79)	108.5(3)
C(82)-C(83)-Fe(2)	71.11(17)
C(79)-C(83)-Fe(2)	68.60(15)
C(79)-P(84)-C(91)	103.61(12)
C(79)-P(84)-C(85)	107.95(12)
C(91)-P(84)-C(85)	102.67(12)
C(79)-P(84)-Pd(2)	114.72(9)
C(91)-P(84)-Pd(2)	115.52(8)
C(85)-P(84)-Pd(2)	111.34(9)
C(86)-C(85)-C(90)	119.4(2)
C(86)-C(85)-P(84)	119.85(19)
C(90)-C(85)-P(84)	120.7(2)
C(85)-C(86)-C(87)	120.2(3)
C(86)-C(87)-C(88)	119.4(3)
C(89)-C(88)-C(87)	120.3(3)
C(90)-C(89)-C(88)	120.4(3)
C(89)-C(90)-C(85)	120.3(3)
C(96)-C(91)-C(92)	118.6(3)
C(96)-C(91)-P(84)	122.3(2)
C(92)-C(91)-P(84)	119.1(2)
C(93)-C(92)-C(91)	120.5(3)
C(94)-C(93)-C(92)	119.6(3)
C(95)-C(94)-C(93)	120.3(3)
C(94)-C(95)-C(96)	120.5(4)
C(91)-C(96)-C(95)	120.4(3)

Table 7. Bond lengths [Å] and angles [°] for **6**.

Au(1)-P(13)	2.2483(10)
Au(1)-S(1)	2.3290(10)
Au(1)-S(3)	3.0756(10)
S(1)-C(2)	1.747(4)
C(2)-N(4)	1.343(5)
C(2)-S(3)	1.695(4)
N(4)-C(6)	1.465(5)
N(4)-C(5)	1.476(5)
C(5)-C(5)#1	1.545(8)
C(6)-C(7)	1.513(5)
C(7)-C(12)	1.377(6)
C(7)-C(8)	1.383(6)
C(8)-C(9)	1.399(6)
C(9)-C(10)	1.370(7)
C(10)-C(11)	1.351(7)
C(11)-C(12)	1.411(6)
P(13)-C(26)	1.817(4)
P(13)-C(14)	1.819(4)
P(13)-C(20)	1.826(4)
C(14)-C(19)	1.373(6)
C(14)-C(15)	1.390(6)
C(15)-C(16)	1.398(8)
C(16)-C(17)	1.357(8)
C(17)-C(18)	1.370(8)
C(18)-C(19)	1.389(7)
C(20)-C(21)	1.387(6)
C(20)-C(25)	1.388(6)
C(21)-C(22)	1.394(6)
C(22)-C(23)	1.389(7)
C(23)-C(24)	1.356(8)
C(24)-C(25)	1.382(7)
C(26)-C(31)	1.393(6)
C(26)-C(27)	1.398(6)
C(27)-C(28)	1.385(6)
C(28)-C(29)	1.392(7)
C(29)-C(30)	1.353(8)
C(30)-C(31)	1.394(6)

P(13)-Au(1)-S(1)	177.86(3)
P(13)-Au(1)-S(3)	111.96(3)
S(1)-Au(1)-S(3)	65.96(3)
C(2)-S(1)-Au(1)	97.67(14)
N(4)-C(2)-S(3)	121.6(3)
N(4)-C(2)-S(1)	116.6(3)
S(3)-C(2)-S(1)	121.8(2)
C(2)-S(3)-Au(1)	74.60(13)
C(2)-N(4)-C(6)	122.9(3)
C(2)-N(4)-C(5)	120.8(3)
C(6)-N(4)-C(5)	116.1(3)
N(4)-C(5)-C(5)#1	108.9(4)
N(4)-C(6)-C(7)	113.8(3)
C(12)-C(7)-C(8)	119.3(4)
C(12)-C(7)-C(6)	121.5(4)
C(8)-C(7)-C(6)	119.2(4)
C(7)-C(8)-C(9)	120.2(4)
C(10)-C(9)-C(8)	120.5(4)
C(11)-C(10)-C(9)	119.2(4)
C(10)-C(11)-C(12)	121.6(5)

C(7)-C(12)-C(11)	119.1(4)
C(26)-P(13)-C(14)	105.04(19)
C(26)-P(13)-C(20)	105.52(18)
C(14)-P(13)-C(20)	106.03(19)
C(26)-P(13)-Au(1)	117.87(14)
C(14)-P(13)-Au(1)	111.76(14)
C(20)-P(13)-Au(1)	109.81(13)
C(19)-C(14)-C(15)	119.1(4)
C(19)-C(14)-P(13)	122.8(3)
C(15)-C(14)-P(13)	118.1(4)
C(14)-C(15)-C(16)	119.3(5)
C(17)-C(16)-C(15)	121.3(6)
C(16)-C(17)-C(18)	119.2(5)
C(17)-C(18)-C(19)	120.7(5)
C(14)-C(19)-C(18)	120.4(5)
C(21)-C(20)-C(25)	119.8(4)
C(21)-C(20)-P(13)	122.6(3)
C(25)-C(20)-P(13)	117.6(3)
C(20)-C(21)-C(22)	119.6(4)
C(23)-C(22)-C(21)	119.8(5)
C(24)-C(23)-C(22)	120.1(4)
C(23)-C(24)-C(25)	121.1(5)
C(24)-C(25)-C(20)	119.6(5)
C(31)-C(26)-C(27)	119.7(4)
C(31)-C(26)-P(13)	118.7(3)
C(27)-C(26)-P(13)	121.5(3)
C(28)-C(27)-C(26)	119.9(4)
C(27)-C(28)-C(29)	119.9(5)
C(30)-C(29)-C(28)	120.2(4)
C(29)-C(30)-C(31)	121.4(5)
C(26)-C(31)-C(30)	119.0(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table 8. Bond lengths [Å] and angles [°] for **7**.

Au(1)-P(13)	2.2440(6)
Au(1)-S(1)	2.3233(5)
Au(1)-S(3)	3.1196(5)
Au(1')-P(13')	2.248(13)
Au(1')-S(3)	2.353(2)
S(1)-C(2)	1.7436(19)
C(2)-N(4)	1.349(2)
C(2)-S(3)	1.6922(19)
N(4)-C(5)	1.459(2)
N(4)-C(12)	1.463(2)
C(5)-C(6)	1.507(3)
C(6)-C(7)	1.384(3)
C(6)-C(11)	1.395(3)
C(7)-C(8)	1.381(3)
C(8)-C(9)	1.374(3)
C(9)-C(10)	1.377(3)
C(10)-C(11)	1.374(3)
C(12)-C(12)#1	1.526(4)
P(13)-C(16)	1.800(3)

P(13)-C(14)	1.801(3)
P(13)-C(15)	1.803(3)
P(13')-C(15')	1.792(13)
P(13')-C(14')	1.795(13)
P(13')-C(16')	1.811(13)

P(13)-Au(1)-S(1)	175.07(2)
P(13')-Au(1')-S(3)	174.4(4)
C(2)-S(1)-Au(1)	99.07(6)
N(4)-C(2)-S(3)	121.49(14)
N(4)-C(2)-S(1)	117.39(14)
S(3)-C(2)-S(1)	121.12(11)
C(2)-S(3)-Au(1')	103.99(9)
C(2)-S(3)-Au(1)	74.17(6)
C(2)-N(4)-C(5)	124.33(16)
C(2)-N(4)-C(12)	121.46(16)
C(5)-N(4)-C(12)	114.20(15)
N(4)-C(5)-C(6)	113.85(15)
C(7)-C(6)-C(11)	117.92(19)
C(7)-C(6)-C(5)	123.38(17)
C(11)-C(6)-C(5)	118.68(17)
C(8)-C(7)-C(6)	120.71(19)
C(9)-C(8)-C(7)	120.6(2)
C(8)-C(9)-C(10)	119.4(2)
C(11)-C(10)-C(9)	120.2(2)
C(10)-C(11)-C(6)	121.1(2)
N(4)-C(12)-C(12)#1	110.41(18)
C(16)-P(13)-C(14)	104.64(17)
C(16)-P(13)-C(15)	104.49(12)
C(14)-P(13)-C(15)	105.49(15)
C(16)-P(13)-Au(1)	114.46(9)
C(14)-P(13)-Au(1)	113.07(11)
C(15)-P(13)-Au(1)	113.73(10)
C(15')-P(13')-C(14')	105.5(10)
C(15')-P(13')-C(16')	104.3(10)
C(14')-P(13')-C(16')	104.4(10)
C(15')-P(13')-Au(1')	114.6(9)
C(14')-P(13')-Au(1')	114.0(9)
C(16')-P(13')-Au(1')	112.9(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1