

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.971(5)	C(18)-C(19)	1.442(6)	C(3)-Fe(1)-C(5)	69.4(2)
Pd(1)-N(1)	2.031(4)	C(19)-C(20)	1.427(8)	C(4)-Fe(1)-C(5)	41.0(2)
Pd(1)-Cl(2)	2.3312(11)	C(20)-C(21)	1.448(7)	C(10)-Fe(1)-C(5)	127.6(2)
Pd(1)-Cl(1)	2.4725(12)	C(22)-C(23)	1.362(8)	C(9)-Fe(1)-C(5)	110.1(2)
Pd(2)-C(17)	1.959(4)	C(22)-C(26)	1.413(10)	C(8)-Fe(1)-C(5)	122.8(2)
Pd(2)-N(2)	2.042(3)	C(23)-C(24)	1.375(9)	C(1)-Fe(1)-C(5)	39.5(2)
Pd(2)-Cl(1)	2.3207(11)	C(24)-C(25)	1.385(9)	C(7)-Fe(1)-C(5)	156.2(2)
Pd(2)-Cl(2)	2.4702(11)	C(25)-C(26)	1.364(9)	C(2)-Fe(1)-C(6)	105.9(2)
Fe(1)-C(2)	1.993(4)	C(28)-C(29)	1.521(6)	C(3)-Fe(1)-C(6)	116.9(2)
Fe(1)-C(3)	2.013(5)	C(29)-C(30)	1.513(6)	C(4)-Fe(1)-C(6)	152.7(2)
Fe(1)-C(4)	2.019(6)	C(30)-C(31)	1.474(9)	C(10)-Fe(1)-C(6)	40.7(2)
Fe(1)-C(10)	2.021(5)	C(31)-C(32)	1.420(8)	C(9)-Fe(1)-C(6)	68.3(2)
Fe(1)-C(9)	2.033(5)			C(8)-Fe(1)-C(6)	67.2(2)
Fe(1)-C(8)	2.044(5)	C(1)-Pd(1)-N(1)	81.0(2)	C(1)-Fe(1)-C(6)	126.1(2)
Fe(1)-C(1)	2.045(4)	C(1)-Pd(1)-Cl(2)	94.56(13)	C(7)-Fe(1)-C(6)	39.7(2)
Fe(1)-C(7)	2.047(5)	N(1)-Pd(1)-Cl(2)	171.76(11)	C(5)-Fe(1)-C(6)	163.6(2)
Fe(1)-C(5)	2.069(5)	C(1)-Pd(1)-Cl(1)	173.02(13)	C(26)-Fe(2)-C(25)	39.5(3)
Fe(1)-C(6)	2.070(5)	N(1)-Pd(1)-Cl(1)	97.60(12)	C(26)-Fe(2)-C(21)	118.0(2)
Fe(2)-C(26)	2.017(6)	Cl(2)-Pd(1)-Cl(1)	87.63(4)	C(25)-Fe(2)-C(21)	105.7(2)
Fe(2)-C(25)	2.023(6)	C(17)-Pd(2)-N(2)	81.3(2)	C(26)-Fe(2)-C(20)	153.5(3)
Fe(2)-C(21)	2.029(5)	C(17)-Pd(2)-Cl(1)	92.51(14)	C(25)-Fe(2)-C(20)	119.6(2)
Fe(2)-C(20)	2.034(5)	N(2)-Pd(2)-Cl(1)	173.63(9)	C(21)-Fe(2)-C(20)	41.8(2)
Fe(2)-C(24)	2.037(5)	C(17)-Pd(2)-Cl(2)	177.81(12)	C(26)-Fe(2)-C(24)	66.3(2)
Fe(2)-C(18)	2.038(5)	N(2)-Pd(2)-Cl(2)	98.35(9)	C(25)-Fe(2)-C(24)	39.9(3)
Fe(2)-C(17)	2.039(4)	Cl(1)-Pd(2)-Cl(2)	87.92(4)	C(21)-Fe(2)-C(24)	125.2(2)
Fe(2)-C(22)	2.040(5)	C(2)-Fe(1)-C(3)	41.8(2)	C(20)-Fe(2)-C(24)	108.6(2)
Fe(2)-C(19)	2.049(5)	C(2)-Fe(1)-C(4)	68.5(2)	C(26)-Fe(2)-C(18)	125.7(2)
Fe(2)-C(23)	2.055(5)	C(3)-Fe(1)-C(4)	41.0(2)	C(25)-Fe(2)-C(18)	161.0(2)
O(1)-C(13)	1.423(6)	C(2)-Fe(1)-C(10)	118.9(2)	C(21)-Fe(2)-C(18)	68.9(2)
O(1)-C(16)	1.427(5)	C(3)-Fe(1)-C(10)	152.6(2)	C(20)-Fe(2)-C(18)	69.2(2)
O(2)-C(32)	1.398(7)	C(4)-Fe(1)-C(10)	165.5(2)	C(24)-Fe(2)-C(18)	157.6(2)
O(2)-C(29)	1.429(5)	C(2)-Fe(1)-C(9)	153.8(2)	C(26)-Fe(2)-C(17)	106.5(2)
N(1)-C(11)	1.308(7)	C(3)-Fe(1)-C(9)	164.1(2)	C(25)-Fe(2)-C(17)	122.7(2)
N(1)-C(12)	1.469(7)	C(4)-Fe(1)-C(9)	128.3(2)	C(21)-Fe(2)-C(17)	39.7(2)
N(2)-C(27)	1.311(6)	C(10)-Fe(1)-C(9)	40.1(2)	C(20)-Fe(2)-C(17)	68.9(2)
N(2)-C(28)	1.457(5)	C(2)-Fe(1)-C(8)	163.4(2)	C(24)-Fe(2)-C(17)	159.9(2)
C(1)-C(5)	1.389(6)	C(3)-Fe(1)-C(8)	126.3(2)	C(18)-Fe(2)-C(17)	41.8(2)
C(1)-C(2)	1.412(6)	C(4)-Fe(1)-C(8)	110.3(2)	C(26)-Fe(2)-C(22)	40.8(3)
C(2)-C(3)	1.429(7)	C(10)-Fe(1)-C(8)	66.4(2)	C(25)-Fe(2)-C(22)	67.9(3)
C(2)-C(11)	1.439(7)	C(9)-Fe(1)-C(8)	39.7(2)	C(21)-Fe(2)-C(22)	153.5(2)
C(3)-C(4)	1.410(8)	C(2)-Fe(1)-C(1)	40.9(2)	C(20)-Fe(2)-C(22)	163.9(3)
C(4)-C(5)	1.433(8)	C(3)-Fe(1)-C(1)	69.7(2)	C(24)-Fe(2)-C(22)	67.2(2)
C(6)-C(7)	1.399(7)	C(4)-Fe(1)-C(1)	68.0(2)	C(18)-Fe(2)-C(22)	108.4(2)
C(6)-C(10)	1.423(8)	C(10)-Fe(1)-C(1)	108.6(2)	C(17)-Fe(2)-C(22)	120.6(2)
C(7)-C(8)	1.404(7)	C(9)-Fe(1)-C(1)	120.6(2)	C(26)-Fe(2)-C(19)	164.1(2)
C(8)-C(9)	1.383(7)	C(8)-Fe(1)-C(1)	155.2(2)	C(25)-Fe(2)-C(19)	155.6(2)
C(9)-C(10)	1.390(7)	C(2)-Fe(1)-C(7)	125.1(2)	C(21)-Fe(2)-C(19)	69.5(2)
C(12)-C(13)	1.446(9)	C(3)-Fe(1)-C(7)	106.1(2)	C(20)-Fe(2)-C(19)	40.9(2)
C(13)-C(14)	1.494(7)	C(4)-Fe(1)-C(7)	120.4(2)	C(24)-Fe(2)-C(19)	122.4(2)
C(14)-C(15)	1.387(9)	C(10)-Fe(1)-C(7)	67.0(2)	C(18)-Fe(2)-C(19)	41.3(2)
C(15)-C(16)	1.514(7)	C(9)-Fe(1)-C(7)	67.6(2)	C(17)-Fe(2)-C(19)	69.7(2)
C(17)-C(21)	1.382(6)	C(8)-Fe(1)-C(7)	40.1(2)	C(22)-Fe(2)-C(19)	126.9(3)
C(17)-C(18)	1.455(7)	C(1)-Fe(1)-C(7)	162.8(2)	C(26)-Fe(2)-C(23)	65.3(2)
C(18)-C(27)	1.410(6)	C(2)-Fe(1)-C(5)	67.9(2)	C(25)-Fe(2)-C(23)	65.9(3)

C(21)-Fe(2)-C(23)	163.4(2)	C(1)-C(5)-C(4)	107.3(4)	C(27)-C(18)-Fe(2)	122.3(3)
C(20)-Fe(2)-C(23)	128.4(2)	C(1)-C(5)-Fe(1)	69.3(3)	C(19)-C(18)-Fe(2)	69.8(3)
C(24)-Fe(2)-C(23)	39.3(2)	C(4)-C(5)-Fe(1)	67.6(3)	C(17)-C(18)-Fe(2)	69.1(3)
C(18)-Fe(2)-C(23)	123.7(2)	C(7)-C(6)-C(10)	105.4(4)	C(20)-C(19)-C(18)	107.4(4)
C(17)-Fe(2)-C(23)	156.8(2)	C(7)-C(6)-Fe(1)	69.3(3)	C(20)-C(19)-Fe(2)	69.0(3)
C(22)-Fe(2)-C(23)	38.9(2)	C(10)-C(6)-Fe(1)	67.8(3)	C(18)-C(19)-Fe(2)	68.9(3)
C(19)-Fe(2)-C(23)	111.9(2)	C(6)-C(7)-C(8)	108.7(5)	C(19)-C(20)-C(21)	107.8(4)
Pd(2)-Cl(1)-Pd(1)	88.51(4)	C(6)-C(7)-Fe(1)	71.0(3)	C(19)-C(20)-Fe(2)	70.1(3)
Pd(1)-Cl(2)-Pd(2)	88.32(4)	C(8)-C(7)-Fe(1)	69.8(3)	C(21)-C(20)-Fe(2)	68.9(3)
C(13)-O(1)-C(16)	106.9(3)	C(9)-C(8)-C(7)	109.1(4)	C(17)-C(21)-C(20)	109.0(5)
C(32)-O(2)-C(29)	107.8(4)	C(9)-C(8)-Fe(1)	69.7(3)	C(17)-C(21)-Fe(2)	70.5(3)
C(11)-N(1)-C(12)	121.0(4)	C(7)-C(8)-Fe(1)	70.0(3)	C(20)-C(21)-Fe(2)	69.3(3)
C(11)-N(1)-Pd(1)	115.2(3)	C(8)-C(9)-C(10)	106.8(5)	C(23)-C(22)-C(26)	104.7(6)
C(12)-N(1)-Pd(1)	123.3(4)	C(8)-C(9)-Fe(1)	70.6(3)	C(23)-C(22)-Fe(2)	71.2(3)
C(27)-N(2)-C(28)	120.1(4)	C(10)-C(9)-Fe(1)	69.5(3)	C(26)-C(22)-Fe(2)	68.8(3)
C(27)-N(2)-Pd(2)	115.2(3)	C(9)-C(10)-C(6)	110.0(5)	C(22)-C(23)-C(24)	111.1(6)
C(28)-N(2)-Pd(2)	124.3(3)	C(9)-C(10)-Fe(1)	70.4(3)	C(22)-C(23)-Fe(2)	70.0(3)
C(5)-C(1)-C(2)	108.2(4)	C(6)-C(10)-Fe(1)	71.5(3)	C(24)-C(23)-Fe(2)	69.7(3)
C(5)-C(1)-Pd(1)	138.2(4)	N(1)-C(11)-C(2)	115.5(4)	C(23)-C(24)-C(25)	106.9(5)
C(2)-C(1)-Pd(1)	113.3(3)	C(13)-C(12)-N(1)	114.3(4)	C(23)-C(24)-Fe(2)	71.1(3)
C(5)-C(1)-Fe(1)	71.2(3)	O(1)-C(13)-C(12)	111.2(5)	C(25)-C(24)-Fe(2)	69.5(3)
C(2)-C(1)-Fe(1)	67.6(3)	O(1)-C(13)-C(14)	104.1(4)	C(26)-C(25)-C(24)	107.6(6)
Pd(1)-C(1)-Fe(1)	120.5(2)	C(12)-C(13)-C(14)	113.3(6)	C(26)-C(25)-Fe(2)	70.1(4)
C(1)-C(2)-C(3)	109.5(4)	C(15)-C(14)-C(13)	109.6(5)	C(24)-C(25)-Fe(2)	70.6(4)
C(1)-C(2)-C(11)	114.9(4)	C(14)-C(15)-C(16)	105.3(4)	C(25)-C(26)-C(22)	109.6(6)
C(3)-C(2)-C(11)	134.6(5)	O(1)-C(16)-C(15)	104.9(4)	C(25)-C(26)-Fe(2)	70.5(4)
C(1)-C(2)-Fe(1)	71.5(2)	C(21)-C(17)-C(18)	108.4(4)	C(22)-C(26)-Fe(2)	70.5(3)
C(3)-C(2)-Fe(1)	69.9(3)	C(21)-C(17)-Pd(2)	139.1(4)	N(2)-C(27)-C(18)	115.7(4)
C(11)-C(2)-Fe(1)	115.9(3)	C(18)-C(17)-Pd(2)	112.4(3)	N(2)-C(28)-C(29)	112.4(4)
C(4)-C(3)-C(2)	105.3(5)	C(21)-C(17)-Fe(2)	69.8(3)	O(2)-C(29)-C(30)	106.6(4)
C(4)-C(3)-Fe(1)	69.7(3)	C(18)-C(17)-Fe(2)	69.0(2)	O(2)-C(29)-C(28)	108.6(3)
C(2)-C(3)-Fe(1)	68.4(3)	Pd(2)-C(17)-Fe(2)	123.1(2)	C(30)-C(29)-C(28)	114.0(4)
C(3)-C(4)-C(5)	109.6(4)	C(27)-C(18)-C(19)	137.1(5)	C(31)-C(30)-C(29)	105.5(4)
C(3)-C(4)-Fe(1)	69.3(3)	C(27)-C(18)-C(17)	115.3(4)	C(32)-C(31)-C(30)	105.0(5)
C(5)-C(4)-Fe(1)	71.4(3)	C(19)-C(18)-C(17)	107.4(4)	O(2)-C(32)-C(31)	110.9(6)

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.0784(2)	0.05288(15)	0.0646(2)	0.00028(15)	0.00657(14)	0.0033(2)
Pd(2)	0.0751(2)	0.05488(14)	0.05796(14)	-0.00229(14)	0.00777(13)	0.00215(15)
Fe(1)	0.0780(3)	0.0681(3)	0.0784(3)	0.0041(3)	0.0250(3)	0.0037(3)
Fe(2)	0.0812(3)	0.0680(3)	0.0646(3)	-0.0019(3)	0.0106(3)	0.0029(3)
Cl(1)	0.0803(6)	0.0597(6)	0.1097(8)	-0.0112(6)	0.0205(6)	-0.0067(5)
Cl(2)	0.0770(6)	0.0597(5)	0.0855(7)	-0.0078(5)	0.0070(5)	0.0022(5)
O(1)	0.0582(14)	0.072(2)	0.120(2)	-0.005(2)	0.003(2)	0.0003(14)
O(2)	0.081(2)	0.114(2)	0.068(2)	-0.023(2)	0.0103(14)	-0.012(2)
N(1)	0.096(2)	0.075(2)	0.072(2)	0.004(2)	-0.009(2)	0.009(2)
N(2)	0.078(2)	0.058(2)	0.059(2)	-0.001(2)	0.0111(14)	0.001(2)
C(1)	0.109(3)	0.054(2)	0.073(2)	0.007(2)	0.023(2)	-0.002(2)
C(2)	0.119(3)	0.073(3)	0.062(2)	0.007(2)	0.023(2)	0.016(3)
C(3)	0.175(4)	0.103(4)	0.102(3)	0.025(3)	0.083(2)	0.051(3)
C(4)	0.099(3)	0.104(4)	0.148(4)	0.014(4)	0.060(3)	0.012(3)
C(5)	0.096(2)	0.070(3)	0.144(4)	-0.002(3)	0.057(2)	-0.008(3)
C(6)	0.072(2)	0.096(3)	0.101(3)	0.027(3)	-0.018(2)	-0.012(3)
C(7)	0.110(3)	0.068(3)	0.096(3)	-0.004(3)	0.008(3)	0.009(3)
C(8)	0.075(2)	0.114(4)	0.095(3)	0.004(3)	0.011(2)	0.018(3)
C(9)	0.120(3)	0.098(4)	0.089(3)	-0.014(3)	0.027(3)	0.006(3)
C(10)	0.094(3)	0.117(4)	0.093(3)	0.036(3)	0.029(2)	0.016(3)
C(11)	0.165(5)	0.074(3)	0.045(2)	0.010(2)	-0.017(3)	0.016(3)
C(12)	0.134(4)	0.079(3)	0.146(5)	-0.022(4)	-0.056(4)	0.034(3)
C(13)	0.081(3)	0.064(3)	0.149(5)	-0.027(3)	0.005(3)	0.011(2)
C(14)	0.107(4)	0.105(4)	0.412(10)	-0.089(6)	0.086(5)	0.011(4)
C(15)	0.089(3)	0.088(3)	0.101(3)	-0.002(3)	0.013(3)	-0.004(3)
C(16)	0.092(3)	0.059(2)	0.092(3)	-0.010(2)	0.005(3)	0.005(2)
C(17)	0.078(2)	0.076(3)	0.058(2)	-0.001(2)	0.002(2)	-0.004(2)
C(18)	0.095(3)	0.070(2)	0.067(2)	0.004(2)	0.017(2)	0.013(2)
C(19)	0.091(3)	0.085(3)	0.094(3)	0.006(3)	0.021(2)	0.024(3)
C(20)	0.078(2)	0.104(4)	0.084(3)	-0.006(3)	0.004(2)	0.016(3)
C(21)	0.077(2)	0.088(3)	0.083(3)	-0.010(3)	0.000(2)	0.003(3)
C(22)	0.121(4)	0.122(4)	0.067(3)	-0.001(3)	-0.005(3)	-0.036(4)
C(23)	0.152(4)	0.094(4)	0.063(2)	-0.005(3)	0.012(3)	0.010(4)
C(24)	0.111(3)	0.144(5)	0.074(3)	0.005(3)	0.028(2)	-0.014(4)
C(25)	0.165(5)	0.087(4)	0.111(4)	0.015(4)	0.001(4)	-0.030(4)
C(26)	0.141(4)	0.122(4)	0.077(3)	0.019(3)	0.003(3)	0.050(4)
C(27)	0.106(3)	0.064(2)	0.057(2)	0.004(2)	0.023(2)	-0.001(2)
C(28)	0.090(2)	0.063(2)	0.073(2)	-0.012(2)	0.025(2)	-0.006(2)
C(29)	0.090(3)	0.072(3)	0.068(2)	0.004(2)	0.016(2)	0.008(2)
C(30)	0.072(3)	0.109(4)	0.097(3)	-0.001(3)	0.010(2)	-0.002(3)
C(31)	0.101(4)	0.180(7)	0.132(4)	-0.050(5)	0.017(4)	-0.049(4)
C(32)	0.126(4)	0.139(5)	0.128(4)	-0.068(4)	0.002(4)	-0.010(4)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	-0.1142(5)	0.3086(5)	0.5629(4)	0.080
H(4A)	-0.2666(5)	0.1918(5)	0.4344(5)	0.080
H(5A)	-0.1387(4)	0.0686(5)	0.3224(4)	0.080
H(6A)	0.0813(4)	0.4755(5)	0.3699(4)	0.080
H(7A)	-0.1510(5)	0.5029(4)	0.3821(4)	0.080
H(8A)	-0.2754(4)	0.3838(6)	0.2408(4)	0.080
H(9A)	-0.1236(5)	0.2776(5)	0.1414(4)	0.080
H(10A)	0.0954(5)	0.3323(5)	0.2218(4)	0.080
H(11A)	0.1727(5)	0.3328(5)	0.5660(3)	0.080
H(12A)	0.4279(5)	0.2196(5)	0.4780(5)	0.080
H(12B)	0.3840(5)	0.3235(5)	0.5379(5)	0.080
H(13A)	0.3528(4)	0.3154(4)	0.3205(5)	0.080
H(14A)	0.5391(5)	0.3810(6)	0.3113(8)	0.080
H(14B)	0.5790(5)	0.3289(6)	0.4238(8)	0.080
H(15A)	0.5730(4)	0.5429(5)	0.3645(4)	0.080
H(15B)	0.6041(4)	0.4913(5)	0.4786(4)	0.080
H(16A)	0.4147(4)	0.5307(4)	0.5195(4)	0.080
H(16B)	0.3999(4)	0.6090(4)	0.4195(4)	0.080
H(19A)	0.6744(4)	-0.3633(5)	0.1829(4)	0.080
H(20A)	0.7923(4)	-0.1767(5)	0.2058(4)	0.080
H(21A)	0.6359(4)	-0.0240(5)	0.2449(4)	0.080
H(22A)	0.3649(5)	-0.2533(6)	-0.0479(4)	0.080
H(23A)	0.5811(5)	-0.3044(6)	-0.0833(4)	0.080
H(24A)	0.7227(5)	-0.1383(6)	-0.0534(4)	0.080
H(25A)	0.5933(6)	0.0242(6)	-0.0037(5)	0.080
H(26A)	0.3727(6)	-0.0441(6)	-0.0021(4)	0.080
H(27A)	0.3895(4)	-0.4082(4)	0.1798(3)	0.080
H(28A)	0.1252(4)	-0.3017(4)	0.2621(3)	0.080
H(28B)	0.1833(4)	-0.4065(4)	0.2141(3)	0.080
H(29A)	0.0976(4)	-0.2242(4)	0.0844(3)	0.080
H(30A)	-0.0957(4)	-0.2827(5)	0.0828(4)	0.080
H(30B)	-0.0485(4)	-0.3902(5)	0.1468(4)	0.080
H(31A)	-0.0937(5)	-0.3719(7)	-0.0675(5)	0.080
H(31B)	-0.1035(5)	-0.4813(7)	-0.0008(5)	0.080
H(32A)	0.0933(5)	-0.5133(6)	0.0017(5)	0.080
H(32B)	0.0761(5)	-0.4450(6)	-0.1045(5)	0.080

Tables for *syn*-(+)-(R_p,R,R,R_p)-4bTable 1. Atomic coordinates [$\times 10^5$ for Pd, Fe; $\times 10^4$ for other atoms] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.67002(3)	0.33201(3)	0.75091(3)	0.05848(9)
Pd(2)	0.81801(3)	0.11211(3)	0.63821(3)	0.06222(10)
Fe(1)	0.43505(7)	0.39610(6)	0.90844(6)	0.0692(2)
Fe(2)	1.07637(7)	-0.06652(6)	0.64599(6)	0.0742(2)
Br(1)	0.90118(5)	0.27430(4)	0.73841(4)	0.0730(2)
Br(2)	0.60594(5)	0.14083(4)	0.71274(5)	0.0792(2)
O(1)	0.8386(3)	0.5826(4)	0.9780(3)	0.0918(13)
O(2)	0.6750(3)	-0.2346(3)	0.6070(3)	0.0925(14)
N(1)	0.7006(4)	0.4964(3)	0.7821(3)	0.0680(12)
N(2)	0.7653(4)	-0.0121(3)	0.5340(3)	0.0784(14)
C(1)	0.4997(4)	0.3769(4)	0.7674(3)	0.0618(13)
C(2)	0.4836(4)	0.4906(4)	0.7897(4)	0.070(2)
C(3)	0.3555(4)	0.5113(4)	0.8049(4)	0.083(2)
C(4)	0.2890(5)	0.4149(5)	0.7912(4)	0.093(2)
C(5)	0.3718(4)	0.3283(5)	0.7644(4)	0.080(2)
C(6)	0.4422(7)	0.2729(6)	1.0134(6)	0.131(3)
C(7)	0.5610(5)	0.3157(7)	1.0141(5)	0.110(2)
C(8)	0.5526(7)	0.4260(7)	1.0394(5)	0.121(3)
C(9)	0.4418(7)	0.4554(6)	1.0580(4)	0.121(3)
C(10)	0.3698(6)	0.3530(8)	1.0404(5)	0.131(3)
C(11)	0.6059(5)	0.5546(4)	0.8031(4)	0.073(2)
C(12)	0.8274(4)	0.5500(3)	0.7942(4)	0.0665(15)
C(13)	0.8986(4)	0.5280(5)	0.8991(4)	0.075(2)
C(14)	1.0344(5)	0.5747(7)	0.9152(4)	0.100(2)
C(15)	1.0411(5)	0.6470(8)	0.9986(6)	0.186(3)
C(16)	0.9241(6)	0.6621(6)	1.0288(6)	0.148(3)
C(17)	0.9871(4)	0.0742(4)	0.5980(4)	0.073(2)
C(18)	0.9778(5)	-0.0091(5)	0.5181(4)	0.084(2)
C(19)	1.1109(6)	-0.0261(5)	0.5030(5)	0.127(2)
C(20)	1.1850(6)	0.0357(5)	0.5696(6)	0.134(2)
C(21)	1.1094(4)	0.0986(5)	0.6253(5)	0.093(2)
C(22)	0.9941(6)	-0.2112(5)	0.6757(5)	0.108(2)
C(23)	1.1219(6)	-0.2302(5)	0.6702(5)	0.097(2)
C(24)	1.1889(6)	-0.1643(6)	0.7476(4)	0.104(2)
C(25)	1.1125(6)	-0.1048(7)	0.8030(5)	0.113(3)
C(26)	0.9874(6)	-0.1357(5)	0.7571(4)	0.107(2)
C(27)	0.8575(6)	-0.0509(5)	0.4863(4)	0.092(2)
C(28)	0.6382(6)	-0.0573(5)	0.5194(5)	0.126(2)
C(29)	0.6104(5)	-0.1321(4)	0.6064(6)	0.113(2)
C(30)	0.4684(6)	-0.1598(6)	0.5938(10)	0.214(5)
C(31)	0.4589(5)	-0.2771(5)	0.5872(5)	0.094(2)
C(32)	0.5885(5)	-0.3160(4)	0.5627(5)	0.079(2)

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.924(4)	C(18)-C(27)	1.382(8)	C(3)-Fe(1)-C(1)	69.6(2)
Pd(1)-N(1)	2.042(4)	C(18)-C(19)	1.465(9)	C(10)-Fe(1)-C(9)	42.2(3)
Pd(1)-Br(2)	2.4372(7)	C(19)-C(20)	1.315(9)	C(8)-Fe(1)-C(9)	36.9(3)
Pd(1)-Br(1)	2.5741(8)	C(20)-C(21)	1.374(9)	C(6)-Fe(1)-C(9)	68.3(3)
Pd(2)-C(17)	1.985(5)	C(22)-C(23)	1.386(9)	C(7)-Fe(1)-C(9)	66.3(3)
Pd(2)-N(2)	2.040(4)	C(22)-C(26)	1.397(9)	C(2)-Fe(1)-C(9)	122.2(3)
Pd(2)-Br(1)	2.4439(7)	C(23)-C(24)	1.394(8)	C(4)-Fe(1)-C(9)	126.1(3)
Pd(2)-Br(2)	2.5838(9)	C(24)-C(25)	1.355(9)	C(3)-Fe(1)-C(9)	109.8(3)
Fe(1)-C(10)	1.989(7)	C(25)-C(26)	1.428(9)	C(1)-Fe(1)-C(9)	154.7(2)
Fe(1)-C(8)	1.992(6)	C(28)-C(29)	1.500(10)	C(10)-Fe(1)-C(5)	123.9(3)
Fe(1)-C(6)	2.005(7)	C(29)-C(30)	1.530(8)	C(8)-Fe(1)-C(5)	158.1(3)
Fe(1)-C(7)	2.024(6)	C(30)-C(31)	1.422(10)	C(6)-Fe(1)-C(5)	107.0(3)
Fe(1)-C(2)	2.028(5)	C(31)-C(32)	1.525(8)	C(7)-Fe(1)-C(5)	121.5(3)
Fe(1)-C(4)	2.026(5)			C(2)-Fe(1)-C(5)	68.2(2)
Fe(1)-C(3)	2.030(5)	C(1)-Pd(1)-N(1)	80.3(2)	C(4)-Fe(1)-C(5)	41.2(2)
Fe(1)-C(1)	2.039(5)	C(1)-Pd(1)-Br(2)	92.78(13)	C(3)-Fe(1)-C(5)	67.9(2)
Fe(1)-C(9)	2.047(6)	N(1)-Pd(1)-Br(2)	173.00(11)	C(1)-Fe(1)-C(5)	42.2(2)
Fe(1)-C(5)	2.056(5)	C(1)-Pd(1)-Br(1)	177.19(13)	C(9)-Fe(1)-C(5)	162.6(3)
Fe(2)-C(18)	1.956(5)	N(1)-Pd(1)-Br(1)	98.50(11)	C(18)-Fe(2)-C(19)	43.6(3)
Fe(2)-C(19)	1.986(7)	Br(2)-Pd(1)-Br(1)	88.47(2)	C(18)-Fe(2)-C(26)	120.0(2)
Fe(2)-C(26)	1.999(6)	C(17)-Pd(2)-N(2)	80.6(2)	C(19)-Fe(2)-C(26)	158.3(3)
Fe(2)-C(17)	2.002(5)	C(17)-Pd(2)-Br(1)	92.7(2)	C(18)-Fe(2)-C(17)	42.4(2)
Fe(2)-C(22)	2.012(6)	N(2)-Pd(2)-Br(1)	169.78(13)	C(19)-Fe(2)-C(17)	69.1(2)
Fe(2)-C(24)	2.028(6)	C(17)-Pd(2)-Br(2)	171.6(2)	C(26)-Fe(2)-C(17)	109.1(2)
Fe(2)-C(20)	2.030(7)	N(2)-Pd(2)-Br(2)	99.64(13)	C(18)-Fe(2)-C(22)	105.7(2)
Fe(2)-C(21)	2.047(6)	Br(1)-Pd(2)-Br(2)	88.11(2)	C(19)-Fe(2)-C(22)	121.9(3)
Fe(2)-C(23)	2.048(6)	C(10)-Fe(1)-C(8)	64.8(3)	C(26)-Fe(2)-C(22)	40.8(3)
Fe(2)-C(25)	2.060(7)	C(10)-Fe(1)-C(6)	38.3(3)	C(17)-Fe(2)-C(22)	126.6(2)
O(1)-C(16)	1.419(8)	C(8)-Fe(1)-C(6)	66.4(3)	C(18)-Fe(2)-C(24)	162.2(2)
O(1)-C(13)	1.430(6)	C(10)-Fe(1)-C(7)	64.7(3)	C(19)-Fe(2)-C(24)	125.2(3)
O(2)-C(32)	1.412(6)	C(8)-Fe(1)-C(7)	40.1(3)	C(26)-Fe(2)-C(24)	65.7(2)
O(2)-C(29)	1.413(6)	C(6)-Fe(1)-C(7)	39.5(3)	C(17)-Fe(2)-C(24)	155.0(2)
N(1)-C(11)	1.284(6)	C(10)-Fe(1)-C(2)	160.7(3)	C(22)-Fe(2)-C(24)	66.7(3)
N(1)-C(12)	1.482(6)	C(8)-Fe(1)-C(2)	110.1(3)	C(18)-Fe(2)-C(20)	69.5(2)
N(2)-C(27)	1.309(7)	C(6)-Fe(1)-C(2)	159.3(3)	C(19)-Fe(2)-C(20)	38.2(3)
N(2)-C(28)	1.443(7)	C(7)-Fe(1)-C(2)	124.4(2)	C(26)-Fe(2)-C(20)	162.5(3)
C(1)-C(2)	1.417(7)	C(10)-Fe(1)-C(4)	110.4(2)	C(17)-Fe(2)-C(20)	67.0(2)
C(1)-C(5)	1.474(6)	C(8)-Fe(1)-C(4)	160.1(3)	C(22)-Fe(2)-C(20)	155.3(3)
C(2)-C(3)	1.420(7)	C(6)-Fe(1)-C(4)	122.8(3)	C(24)-Fe(2)-C(20)	110.1(3)
C(2)-C(11)	1.499(7)	C(7)-Fe(1)-C(4)	157.7(3)	C(18)-Fe(2)-C(21)	68.1(2)
C(3)-C(4)	1.360(8)	C(2)-Fe(1)-C(4)	67.7(2)	C(19)-Fe(2)-C(21)	65.4(3)
C(4)-C(5)	1.436(8)	C(10)-Fe(1)-C(3)	125.4(3)	C(26)-Fe(2)-C(21)	127.2(2)
C(6)-C(10)	1.310(11)	C(8)-Fe(1)-C(3)	126.2(3)	C(17)-Fe(2)-C(21)	38.3(2)
C(6)-C(7)	1.361(10)	C(6)-Fe(1)-C(3)	157.8(3)	C(22)-Fe(2)-C(21)	162.9(2)
C(7)-C(8)	1.376(11)	C(7)-Fe(1)-C(3)	161.7(3)	C(24)-Fe(2)-C(21)	123.6(2)
C(8)-C(9)	1.280(11)	C(2)-Fe(1)-C(3)	41.0(2)	C(20)-Fe(2)-C(21)	39.4(2)
C(9)-C(10)	1.455(11)	C(4)-Fe(1)-C(3)	39.2(2)	C(18)-Fe(2)-C(23)	124.0(2)
C(12)-C(13)	1.482(7)	C(10)-Fe(1)-C(1)	158.3(3)	C(19)-Fe(2)-C(23)	108.0(3)
C(13)-C(14)	1.534(7)	C(8)-Fe(1)-C(1)	121.9(3)	C(26)-Fe(2)-C(23)	67.2(3)
C(14)-C(15)	1.378(11)	C(6)-Fe(1)-C(1)	122.0(3)	C(17)-Fe(2)-C(23)	163.3(2)
C(15)-C(16)	1.362(9)	C(7)-Fe(1)-C(1)	105.9(2)	C(22)-Fe(2)-C(23)	39.9(2)
C(17)-C(21)	1.330(7)	C(2)-Fe(1)-C(1)	40.8(2)	C(24)-Fe(2)-C(23)	40.0(2)
C(17)-C(18)	1.433(8)	C(4)-Fe(1)-C(1)	70.3(2)	C(20)-Fe(2)-C(23)	121.5(3)

C(21)-Fe(2)-C(23)	156.7(2)	C(3)-C(4)-Fe(1)	70.6(3)	C(17)-C(18)-C(19)	102.6(5)
C(18)-Fe(2)-C(25)	156.1(3)	C(5)-C(4)-Fe(1)	70.5(3)	C(27)-C(18)-Fe(2)	119.3(4)
C(19)-Fe(2)-C(25)	158.8(3)	C(4)-C(5)-C(1)	107.1(5)	C(17)-C(18)-Fe(2)	70.5(3)
C(26)-Fe(2)-C(25)	41.2(2)	C(4)-C(5)-Fe(1)	68.3(3)	C(19)-C(18)-Fe(2)	69.3(3)
C(17)-Fe(2)-C(25)	120.8(3)	C(1)-C(5)-Fe(1)	68.3(3)	C(20)-C(19)-C(18)	109.7(6)
C(22)-Fe(2)-C(25)	69.3(3)	C(10)-C(6)-C(7)	107.1(7)	C(20)-C(19)-Fe(2)	72.7(4)
C(24)-Fe(2)-C(25)	38.7(3)	C(10)-C(6)-Fe(1)	70.2(4)	C(18)-C(19)-Fe(2)	67.1(3)
C(20)-Fe(2)-C(25)	124.7(3)	C(7)-C(6)-Fe(1)	71.0(4)	C(19)-C(20)-C(21)	108.3(6)
C(21)-Fe(2)-C(25)	109.5(3)	C(6)-C(7)-C(8)	106.2(6)	C(19)-C(20)-Fe(2)	69.1(4)
C(23)-Fe(2)-C(25)	68.0(3)	C(6)-C(7)-Fe(1)	69.5(4)	C(21)-C(20)-Fe(2)	71.0(4)
Pd(2)-Br(1)-Pd(1)	88.30(2)	C(8)-C(7)-Fe(1)	68.7(4)	C(17)-C(21)-C(20)	110.8(6)
Pd(1)-Br(2)-Pd(2)	88.22(2)	C(9)-C(8)-C(7)	113.8(7)	C(17)-C(21)-Fe(2)	69.0(3)
C(16)-O(1)-C(13)	108.8(4)	C(9)-C(8)-Fe(1)	73.9(4)	C(20)-C(21)-Fe(2)	69.7(4)
C(32)-O(2)-C(29)	108.6(4)	C(7)-C(8)-Fe(1)	71.2(4)	C(23)-C(22)-C(26)	107.1(5)
C(11)-N(1)-C(12)	117.6(4)	C(8)-C(9)-C(10)	102.2(7)	C(23)-C(22)-Fe(2)	71.4(4)
C(11)-N(1)-Pd(1)	117.7(3)	C(8)-C(9)-Fe(1)	69.2(4)	C(26)-C(22)-Fe(2)	69.1(4)
C(12)-N(1)-Pd(1)	124.3(3)	C(10)-C(9)-Fe(1)	66.7(3)	C(22)-C(23)-C(24)	106.1(6)
C(27)-N(2)-C(28)	123.1(5)	C(6)-C(10)-C(9)	110.7(6)	C(22)-C(23)-Fe(2)	68.7(3)
C(27)-N(2)-Pd(2)	114.6(3)	C(6)-C(10)-Fe(1)	71.5(4)	C(24)-C(23)-Fe(2)	69.2(4)
C(28)-N(2)-Pd(2)	122.2(4)	C(9)-C(10)-Fe(1)	71.0(4)	C(25)-C(24)-C(23)	113.3(6)
C(2)-C(1)-C(5)	104.8(4)	N(1)-C(11)-C(2)	112.5(4)	C(25)-C(24)-Fe(2)	71.9(4)
C(2)-C(1)-Pd(1)	115.8(3)	N(1)-C(12)-C(13)	111.3(4)	C(23)-C(24)-Fe(2)	70.8(3)
C(5)-C(1)-Pd(1)	139.4(4)	O(1)-C(13)-C(12)	110.1(4)	C(24)-C(25)-C(26)	103.4(6)
C(2)-C(1)-Fe(1)	69.2(3)	O(1)-C(13)-C(14)	103.5(4)	C(24)-C(25)-Fe(2)	69.4(4)
C(5)-C(1)-Fe(1)	69.5(3)	C(12)-C(13)-C(14)	114.4(4)	C(26)-C(25)-Fe(2)	67.1(3)
Pd(1)-C(1)-Fe(1)	124.2(2)	C(15)-C(14)-C(13)	106.7(5)	C(22)-C(26)-C(25)	110.1(6)
C(3)-C(2)-C(1)	110.0(4)	C(16)-C(15)-C(14)	110.7(6)	C(22)-C(26)-Fe(2)	70.1(4)
C(3)-C(2)-C(11)	136.2(5)	C(15)-C(16)-O(1)	109.2(6)	C(25)-C(26)-Fe(2)	71.7(4)
C(1)-C(2)-C(11)	113.4(4)	C(21)-C(17)-C(18)	108.5(5)	N(2)-C(27)-C(18)	116.6(5)
C(3)-C(2)-Fe(1)	69.6(3)	C(21)-C(17)-Pd(2)	139.7(5)	N(2)-C(28)-C(29)	113.8(5)
C(1)-C(2)-Fe(1)	70.0(3)	C(18)-C(17)-Pd(2)	111.8(3)	O(2)-C(29)-C(28)	112.8(6)
C(11)-C(2)-Fe(1)	120.4(3)	C(21)-C(17)-Fe(2)	72.7(3)	O(2)-C(29)-C(30)	106.2(5)
C(4)-C(3)-C(2)	108.7(5)	C(18)-C(17)-Fe(2)	67.1(3)	C(28)-C(29)-C(30)	110.0(6)
C(4)-C(3)-Fe(1)	70.3(3)	Pd(2)-C(17)-Fe(2)	121.4(3)	C(31)-C(30)-C(29)	106.6(5)
C(2)-C(3)-Fe(1)	69.5(3)	C(27)-C(18)-C(17)	116.2(5)	C(30)-C(31)-C(32)	105.1(5)
C(3)-C(4)-C(5)	109.3(5)	C(27)-C(18)-C(19)	141.0(5)	O(2)-C(32)-C(31)	104.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.0646(2)	0.05488(15)	0.0552(2)	-0.0032(2)	0.00502(14)	0.0006(2)
Pd(2)	0.0686(2)	0.0547(2)	0.0617(2)	-0.0004(2)	0.0022(2)	0.0027(2)
Fe(1)	0.0725(4)	0.0691(4)	0.0667(4)	-0.0039(3)	0.0118(3)	0.0011(3)
Fe(2)	0.0722(4)	0.0707(4)	0.0833(5)	0.0004(4)	0.0237(3)	0.0033(3)
Br(1)	0.0680(3)	0.0628(2)	0.0852(3)	-0.0088(3)	-0.0015(2)	0.0037(2)
Br(2)	0.0762(3)	0.0630(2)	0.0989(3)	-0.0118(3)	0.0139(3)	-0.0060(2)
O(1)	0.062(2)	0.138(3)	0.073(2)	-0.029(2)	0.001(2)	-0.002(2)
O(2)	0.063(2)	0.067(2)	0.146(3)	-0.013(2)	0.009(2)	0.008(2)
N(1)	0.073(2)	0.077(2)	0.055(2)	0.003(2)	0.011(2)	0.007(2)
N(2)	0.093(3)	0.048(2)	0.091(3)	-0.002(2)	0.002(2)	0.004(2)
C(1)	0.058(2)	0.062(2)	0.061(2)	-0.014(2)	-0.007(2)	0.015(2)
C(2)	0.061(2)	0.079(3)	0.068(3)	-0.012(3)	0.001(2)	-0.003(2)
C(3)	0.070(3)	0.083(3)	0.094(4)	-0.007(3)	0.012(3)	0.031(2)
C(4)	0.086(3)	0.101(4)	0.094(4)	-0.012(4)	0.017(3)	0.008(3)
C(5)	0.063(2)	0.081(3)	0.091(3)	-0.015(3)	-0.004(2)	0.003(3)
C(6)	0.202(7)	0.080(4)	0.109(5)	0.020(4)	0.014(5)	-0.015(5)
C(7)	0.089(3)	0.144(5)	0.099(4)	0.027(4)	0.014(3)	0.043(4)
C(8)	0.167(6)	0.103(4)	0.089(4)	-0.008(4)	0.004(4)	-0.022(5)
C(9)	0.205(6)	0.099(4)	0.061(3)	-0.024(3)	0.033(4)	0.015(5)
C(10)	0.100(4)	0.212(8)	0.077(4)	0.012(5)	0.006(3)	-0.047(5)
C(11)	0.097(3)	0.061(2)	0.060(3)	0.012(2)	0.009(2)	0.000(3)
C(12)	0.074(3)	0.043(2)	0.082(3)	0.001(2)	0.006(2)	-0.003(2)
C(13)	0.077(3)	0.080(3)	0.068(3)	-0.004(3)	0.005(2)	0.003(3)
C(14)	0.087(3)	0.139(5)	0.074(3)	-0.009(4)	0.007(3)	0.010(4)
C(15)	0.115(4)	0.308(8)	0.148(5)	-0.117(6)	0.063(4)	-0.138(4)
C(16)	0.102(4)	0.160(5)	0.185(5)	-0.116(4)	0.029(4)	-0.020(4)
C(17)	0.061(2)	0.072(3)	0.082(3)	0.013(3)	-0.007(2)	0.001(2)
C(18)	0.107(4)	0.080(3)	0.071(3)	-0.013(3)	0.030(3)	-0.007(3)
C(19)	0.191(5)	0.088(4)	0.122(4)	-0.015(4)	0.090(3)	0.033(4)
C(20)	0.127(4)	0.105(4)	0.194(5)	0.033(4)	0.109(3)	-0.001(4)
C(21)	0.072(3)	0.087(4)	0.127(4)	-0.008(4)	0.038(3)	-0.002(3)
C(22)	0.090(4)	0.092(4)	0.136(5)	0.038(4)	-0.010(4)	-0.012(3)
C(23)	0.124(4)	0.069(3)	0.100(4)	0.014(3)	0.023(3)	0.032(3)
C(24)	0.097(4)	0.127(4)	0.085(4)	-0.010(4)	0.000(3)	0.035(4)
C(25)	0.115(4)	0.135(5)	0.084(4)	-0.012(4)	-0.008(4)	0.015(5)
C(26)	0.138(4)	0.099(4)	0.094(3)	0.032(3)	0.056(3)	0.041(3)
C(27)	0.130(4)	0.070(3)	0.070(3)	-0.021(3)	-0.005(3)	0.028(3)
C(28)	0.126(4)	0.057(3)	0.169(6)	-0.015(4)	-0.080(4)	0.022(3)
C(29)	0.099(4)	0.060(3)	0.172(6)	-0.047(3)	-0.006(4)	0.011(3)
C(30)	0.080(4)	0.102(5)	0.469(15)	-0.069(8)	0.073(6)	-0.004(4)
C(31)	0.088(4)	0.093(4)	0.096(4)	-0.012(3)	-0.003(3)	0.013(3)
C(32)	0.085(3)	0.057(2)	0.095(4)	-0.015(3)	0.008(3)	-0.003(3)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	0.3211(4)	0.5811(4)	0.8230(4)	0.080
H(4A)	0.2009(5)	0.4062(5)	0.7994(4)	0.080
H(5A)	0.3487(4)	0.2523(5)	0.7509(4)	0.080
H(6A)	0.4172(7)	0.1979(6)	0.9968(6)	0.080
H(7A)	0.6354(5)	0.2757(7)	1.0006(5)	0.080
H(8A)	0.6221(7)	0.4773(7)	1.0419(5)	0.080
H(9A)	0.4145(7)	0.5265(6)	1.0798(4)	0.080
H(10A)	0.2818(6)	0.3438(8)	1.0489(5)	0.080
H(11A)	0.6126(5)	0.6303(4)	0.8259(4)	0.080
H(12A)	0.8745(4)	0.5209(3)	0.7417(4)	0.080
H(12B)	0.8183(4)	0.6285(3)	0.7838(4)	0.080
H(13A)	0.9004(4)	0.4497(5)	0.9123(4)	0.080
H(14A)	1.0955(5)	0.5156(7)	0.9246(4)	0.080
H(14B)	1.0494(5)	0.6175(7)	0.8553(4)	0.080
H(15A)	1.0924(5)	0.6101(8)	1.0553(6)	0.080
H(15B)	1.0825(5)	0.7152(8)	0.9851(6)	0.080
H(16A)	0.8978(6)	0.7361(6)	1.0089(6)	0.080
H(16B)	0.9253(6)	0.6543(6)	1.1031(6)	0.080
H(19A)	1.1397(6)	-0.0771(5)	0.4541(5)	0.080
H(20A)	1.2764(6)	0.0363(5)	0.5799(6)	0.080
H(21A)	1.1387(4)	0.1474(5)	0.6823(5)	0.080
H(22A)	0.9249(6)	-0.2450(5)	0.6312(5)	0.080
H(23A)	1.1577(6)	-0.2772(5)	0.6216(5)	0.080
H(24A)	1.2800(6)	-0.1586(6)	0.7589(4)	0.080
H(25A)	1.1352(6)	-0.0547(7)	0.8603(5)	0.080
H(26A)	0.9090(6)	-0.1087(5)	0.7772(4)	0.080
H(27A)	0.8399(6)	-0.1040(5)	0.4308(4)	0.080
H(28A)	0.5772(6)	0.0019(5)	0.5103(5)	0.080
H(28B)	0.6279(6)	-0.1011(5)	0.4566(5)	0.080
H(29A)	0.6355(5)	-0.0954(4)	0.6720(6)	0.080
H(30A)	0.4287(6)	-0.1333(6)	0.6518(10)	0.080
H(30B)	0.4285(6)	-0.1252(6)	0.5308(10)	0.080
H(31A)	0.4392(5)	-0.3085(5)	0.6517(5)	0.080
H(31B)	0.3936(5)	-0.2982(5)	0.5318(5)	0.080
H(32A)	0.5899(5)	-0.3228(4)	0.4886(5)	0.080
H(32B)	0.6095(5)	-0.3864(4)	0.5951(5)	0.080

Tables for *syn*-(+)-(R_p,R,R,R_p)-5aTable 1. Atomic coordinates [$\times 10^5$ for Pd, Fe; $\times 10^4$ for other atoms] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	1.053552(7)	0.610988(8)	0.03430(3)	0.06293(6)
Pd(2)	0.959096(8)	0.640065(8)	0.20695(2)	0.06448(6)
Fe(1)	1.15122(2)	0.64238(2)	-0.23335(5)	0.07523(13)
Fe(2)	0.93378(2)	0.68962(2)	0.49652(5)	0.07846(14)
Cl(1)	1.04178(3)	0.62348(3)	0.26476(8)	0.0692(2)
Cl(2)	1.01140(3)	0.67710(3)	-0.00225(8)	0.0824(2)
O(1)	1.21438(8)	0.59010(11)	0.1522(3)	0.0879(8)
O(2)	0.88224(12)	0.75976(11)	0.1235(3)	0.1174(10)
N(1)	1.08655(8)	0.54833(9)	0.0456(3)	0.0648(7)
N(2)	0.87693(9)	0.64225(9)	0.1741(3)	0.0719(7)
C(1)	1.06485(13)	0.60159(14)	-0.1433(4)	0.0793(10)
C(2)	1.08508(11)	0.55627(13)	-0.1685(3)	0.0723(9)
C(3)	1.09397(13)	0.55431(15)	-0.3054(4)	0.0925(11)
C(4)	1.0784(2)	0.5958(2)	-0.3588(4)	0.1044(12)
C(5)	1.06072(13)	0.6254(2)	-0.2642(4)	0.0925(11)
C(6)	1.2104(2)	0.7368(2)	-0.2237(5)	0.110(2)
C(7)	1.2131(2)	0.7082(2)	-0.1113(4)	0.110(2)
C(8)	1.23280(15)	0.6648(2)	-0.1376(5)	0.1054(14)
C(9)	1.2422(2)	0.6693(2)	-0.2698(6)	0.127(2)
C(10)	1.2285(2)	0.7126(2)	-0.3232(4)	0.1097(14)
C(11)	1.09873(11)	0.53061(12)	-0.0584(3)	0.0694(9)
C(12)	1.12645(13)	0.48752(12)	-0.0738(4)	0.0886(11)
C(13)	1.09999(11)	0.53087(11)	0.1725(3)	0.0680(9)
C(14)	1.16244(12)	0.58309(12)	0.2254(3)	0.0720(9)
C(15)	1.1739(2)	0.5663(2)	0.3634(4)	0.108(2)
C(16)	1.2330(2)	0.5630(2)	0.3505(6)	0.154(2)
C(17)	1.2428(2)	0.5602(2)	0.2194(5)	0.1217(15)
C(18)	0.92395(12)	0.61929(12)	0.3754(4)	0.0765(10)
C(19)	0.86504(13)	0.62102(14)	0.3887(4)	0.0889(12)
C(20)	0.8473(2)	0.6125(2)	0.5194(4)	0.1028(13)
C(21)	0.8940(2)	0.6043(2)	0.5865(4)	0.1091(14)
C(22)	0.93805(15)	0.60635(15)	0.4987(4)	0.0867(11)
C(23)	1.0002(2)	0.7727(2)	0.4159(4)	0.110(2)
C(24)	0.9435(2)	0.7751(2)	0.4356(4)	0.112(2)
C(25)	0.9295(2)	0.7649(2)	0.5744(4)	0.127(2)
C(26)	0.9808(2)	0.7596(2)	0.6281(5)	0.125(2)
C(27)	1.0224(2)	0.7621(2)	0.5332(5)	0.125(2)
C(28)	0.84099(12)	0.63215(14)	0.2744(4)	0.0814(11)
C(29)	0.77969(14)	0.6317(2)	0.2753(5)	0.1082(15)
C(30)	0.86122(13)	0.6599(2)	0.0533(4)	0.0886(11)
C(31)	0.8948(2)	0.7285(2)	0.0291(5)	0.1038(13)
C(32)	0.8760(2)	0.7470(2)	-0.0905(5)	0.163(2)
C(33)	0.8658(3)	0.7958(3)	-0.0580(6)	0.196(2)
C(34)	0.8670(2)	0.7988(2)	0.0689(6)	0.155(2)

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.916(4)	C(18)-C(19)	1.466(5)	C(3)-Fe(1)-C(8)	121.9(2)
Pd(1)-N(1)	2.058(2)	C(19)-C(20)	1.423(6)	C(4)-Fe(1)-C(8)	157.9(2)
Pd(1)-Cl(2)	2.3394(9)	C(19)-C(28)	1.421(6)	C(10)-Fe(1)-C(8)	68.6(2)
Pd(1)-Cl(1)	2.4750(9)	C(20)-C(21)	1.438(6)	C(6)-Fe(1)-C(5)	108.7(2)
Pd(2)-C(18)	1.921(4)	C(21)-C(22)	1.399(6)	C(9)-Fe(1)-C(5)	159.0(2)
Pd(2)-N(2)	2.062(2)	C(23)-C(27)	1.421(7)	C(7)-Fe(1)-C(5)	124.1(2)
Pd(2)-Cl(1)	2.3292(8)	C(23)-C(24)	1.430(7)	C(2)-Fe(1)-C(5)	67.99(14)
Pd(2)-Cl(2)	2.4747(9)	C(24)-C(25)	1.489(7)	C(3)-Fe(1)-C(5)	68.15(15)
Fe(1)-C(6)	2.020(3)	C(25)-C(26)	1.437(8)	C(4)-Fe(1)-C(5)	40.4(2)
Fe(1)-C(9)	2.013(4)	C(26)-C(27)	1.403(7)	C(10)-Fe(1)-C(5)	123.1(2)
Fe(1)-C(7)	2.020(4)	C(28)-C(29)	1.492(5)	C(8)-Fe(1)-C(5)	159.0(2)
Fe(1)-C(2)	2.024(2)	C(30)-C(31)	1.472(5)	C(6)-Fe(1)-C(1)	120.3(2)
Fe(1)-C(3)	2.036(3)	C(31)-C(32)	1.485(7)	C(9)-Fe(1)-C(1)	160.4(2)
Fe(1)-C(4)	2.042(4)	C(32)-C(33)	1.375(9)	C(7)-Fe(1)-C(1)	105.7(2)
Fe(1)-C(10)	2.039(3)	C(33)-C(34)	1.335(9)	C(2)-Fe(1)-C(1)	41.42(14)
Fe(1)-C(8)	2.046(4)			C(3)-Fe(1)-C(1)	70.34(14)
Fe(1)-C(5)	2.059(3)	C(1)-Pd(1)-N(1)	80.44(14)	C(4)-Fe(1)-C(1)	68.35(15)
Fe(1)-C(1)	2.057(3)	C(1)-Pd(1)-Cl(2)	93.56(12)	C(10)-Fe(1)-C(1)	156.0(2)
Fe(2)-C(19)	2.023(3)	N(1)-Pd(1)-Cl(2)	173.23(7)	C(8)-Fe(1)-C(1)	121.9(2)
Fe(2)-C(20)	2.021(3)	C(1)-Pd(1)-Cl(1)	178.47(10)	C(5)-Fe(1)-C(1)	40.4(2)
Fe(2)-C(27)	2.033(4)	N(1)-Pd(1)-Cl(1)	98.50(8)	C(19)-Fe(2)-C(20)	41.2(2)
Fe(2)-C(23)	2.043(4)	Cl(2)-Pd(1)-Cl(1)	87.55(3)	C(19)-Fe(2)-C(27)	155.2(2)
Fe(2)-C(21)	2.037(4)	C(18)-Pd(2)-N(2)	81.31(13)	C(20)-Fe(2)-C(27)	161.8(2)
Fe(2)-C(26)	2.046(4)	C(18)-Pd(2)-Cl(1)	91.46(11)	C(19)-Fe(2)-C(23)	120.5(2)
Fe(2)-C(18)	2.053(3)	N(2)-Pd(2)-Cl(1)	170.71(7)	C(20)-Fe(2)-C(23)	156.2(2)
Fe(2)-C(25)	2.062(6)	C(18)-Pd(2)-Cl(2)	174.52(8)	C(27)-Fe(2)-C(23)	40.8(2)
Fe(2)-C(24)	2.079(4)	N(2)-Pd(2)-Cl(2)	99.96(8)	C(19)-Fe(2)-C(21)	68.9(2)
Fe(2)-C(22)	2.087(4)	Cl(1)-Pd(2)-Cl(2)	87.79(3)	C(20)-Fe(2)-C(21)	41.5(2)
O(1)-C(17)	1.420(6)	C(6)-Fe(1)-C(9)	66.1(2)	C(27)-Fe(2)-C(21)	123.9(2)
O(1)-C(14)	1.418(4)	C(6)-Fe(1)-C(7)	40.3(2)	C(23)-Fe(2)-C(21)	160.6(2)
O(2)-C(34)	1.315(6)	C(9)-Fe(1)-C(7)	66.2(2)	C(19)-Fe(2)-C(26)	163.0(2)
O(2)-C(31)	1.377(6)	C(6)-Fe(1)-C(2)	155.8(2)	C(20)-Fe(2)-C(26)	125.9(2)
N(1)-C(11)	1.264(4)	C(9)-Fe(1)-C(2)	125.4(2)	C(27)-Fe(2)-C(26)	40.2(2)
N(1)-C(13)	1.486(4)	C(7)-Fe(1)-C(2)	120.24(15)	C(23)-Fe(2)-C(26)	67.4(2)
N(2)-C(28)	1.313(5)	C(6)-Fe(1)-C(3)	161.0(2)	C(21)-Fe(2)-C(26)	108.8(2)
N(2)-C(30)	1.453(5)	C(9)-Fe(1)-C(3)	109.7(2)	C(19)-Fe(2)-C(18)	42.16(14)
C(1)-C(5)	1.421(6)	C(7)-Fe(1)-C(3)	157.1(2)	C(20)-Fe(2)-C(18)	70.38(15)
C(1)-C(2)	1.444(5)	C(2)-Fe(1)-C(3)	42.12(15)	C(27)-Fe(2)-C(18)	118.3(2)
C(2)-C(11)	1.432(5)	C(6)-Fe(1)-C(4)	126.4(2)	C(23)-Fe(2)-C(18)	106.0(2)
C(2)-C(3)	1.459(5)	C(9)-Fe(1)-C(4)	124.8(2)	C(21)-Fe(2)-C(18)	68.7(2)
C(3)-C(4)	1.368(6)	C(7)-Fe(1)-C(4)	161.7(2)	C(26)-Fe(2)-C(18)	154.1(2)
C(4)-C(5)	1.416(6)	C(2)-Fe(1)-C(4)	67.59(14)	C(19)-Fe(2)-C(25)	124.7(2)
C(6)-C(10)	1.379(7)	C(3)-Fe(1)-C(4)	39.2(2)	C(20)-Fe(2)-C(25)	106.7(2)
C(6)-C(7)	1.391(7)	C(6)-Fe(1)-C(10)	39.7(2)	C(27)-Fe(2)-C(25)	69.8(2)
C(7)-C(8)	1.390(7)	C(9)-Fe(1)-C(10)	39.7(2)	C(23)-Fe(2)-C(25)	69.4(2)
C(8)-C(9)	1.403(8)	C(7)-Fe(1)-C(10)	67.4(2)	C(21)-Fe(2)-C(25)	121.1(2)
C(9)-C(10)	1.378(7)	C(2)-Fe(1)-C(10)	162.1(2)	C(26)-Fe(2)-C(25)	40.9(2)
C(11)-C(12)	1.517(5)	C(3)-Fe(1)-C(10)	125.0(2)	C(18)-Fe(2)-C(25)	162.7(2)
C(13)-C(14)	1.522(3)	C(4)-Fe(1)-C(10)	110.6(2)	C(19)-Fe(2)-C(24)	106.8(2)
C(14)-C(15)	1.569(5)	C(6)-Fe(1)-C(8)	68.0(2)	C(20)-Fe(2)-C(24)	120.8(2)
C(15)-C(16)	1.491(7)	C(9)-Fe(1)-C(8)	40.4(2)	C(27)-Fe(2)-C(24)	69.4(2)
C(16)-C(17)	1.404(9)	C(7)-Fe(1)-C(8)	40.0(2)	C(23)-Fe(2)-C(24)	40.6(2)
C(18)-C(22)	1.416(6)	C(2)-Fe(1)-C(8)	106.09(14)	C(21)-Fe(2)-C(24)	157.7(2)

C(26)-Fe(2)-C(24)	68.6(2)	C(3)-C(4)-Fe(1)	70.2(2)	C(28)-C(19)-C(18)	115.5(3)
C(18)-Fe(2)-C(24)	123.7(2)	C(5)-C(4)-Fe(1)	70.5(2)	C(20)-C(19)-Fe(2)	69.3(2)
C(25)-Fe(2)-C(24)	42.2(2)	C(4)-C(5)-C(1)	108.5(4)	C(28)-C(19)-Fe(2)	124.5(2)
C(19)-Fe(2)-C(22)	67.95(15)	C(4)-C(5)-Fe(1)	69.1(2)	C(18)-C(19)-Fe(2)	70.0(2)
C(20)-Fe(2)-C(22)	68.3(2)	C(1)-C(5)-Fe(1)	69.7(2)	C(19)-C(20)-C(21)	106.7(4)
C(27)-Fe(2)-C(22)	107.2(2)	C(10)-C(6)-C(7)	108.7(4)	C(19)-C(20)-Fe(2)	69.5(2)
C(23)-Fe(2)-C(22)	124.7(2)	C(10)-C(6)-Fe(1)	70.9(2)	C(21)-C(20)-Fe(2)	69.8(2)
C(21)-Fe(2)-C(22)	39.6(2)	C(7)-C(6)-Fe(1)	69.8(2)	C(22)-C(21)-C(20)	108.7(4)
C(26)-Fe(2)-C(22)	121.7(2)	C(6)-C(7)-C(8)	109.6(4)	C(22)-C(21)-Fe(2)	72.1(2)
C(18)-Fe(2)-C(22)	40.00(15)	C(6)-C(7)-Fe(1)	69.9(2)	C(20)-C(21)-Fe(2)	68.6(2)
C(25)-Fe(2)-C(22)	156.0(2)	C(8)-C(7)-Fe(1)	71.0(2)	C(21)-C(22)-C(18)	110.1(4)
C(24)-Fe(2)-C(22)	160.8(2)	C(7)-C(8)-C(9)	104.1(4)	C(21)-C(22)-Fe(2)	68.3(3)
Pd(2)-Cl(1)-Pd(1)	86.01(3)	C(7)-C(8)-Fe(1)	69.0(2)	C(18)-C(22)-Fe(2)	68.7(2)
Pd(1)-Cl(2)-Pd(2)	85.80(3)	C(9)-C(8)-Fe(1)	68.5(2)	C(27)-C(23)-C(24)	110.3(4)
C(17)-O(1)-C(14)	107.7(3)	C(10)-C(9)-C(8)	111.7(5)	C(27)-C(23)-Fe(2)	69.2(2)
C(34)-O(2)-C(31)	108.1(4)	C(10)-C(9)-Fe(1)	71.1(2)	C(24)-C(23)-Fe(2)	71.1(2)
C(11)-N(1)-C(13)	123.7(3)	C(8)-C(9)-Fe(1)	71.1(3)	C(23)-C(24)-C(25)	106.3(4)
C(11)-N(1)-Pd(1)	116.8(2)	C(6)-C(10)-C(9)	105.9(4)	C(23)-C(24)-Fe(2)	68.4(3)
C(13)-N(1)-Pd(1)	119.3(2)	C(6)-C(10)-Fe(1)	69.4(2)	C(25)-C(24)-Fe(2)	68.3(3)
C(28)-N(2)-C(30)	120.4(3)	C(9)-C(10)-Fe(1)	69.1(2)	C(26)-C(25)-C(24)	105.2(4)
C(28)-N(2)-Pd(2)	115.4(2)	N(1)-C(11)-C(2)	113.7(3)	C(26)-C(25)-Fe(2)	68.9(3)
C(30)-N(2)-Pd(2)	123.9(2)	N(1)-C(11)-C(12)	126.3(3)	C(24)-C(25)-Fe(2)	69.5(3)
C(5)-C(1)-C(2)	105.7(3)	C(2)-C(11)-C(12)	120.0(3)	C(27)-C(26)-C(25)	111.2(4)
C(5)-C(1)-Pd(1)	141.0(3)	N(1)-C(13)-C(14)	111.1(2)	C(27)-C(26)-Fe(2)	69.4(3)
C(2)-C(1)-Pd(1)	113.3(3)	O(1)-C(14)-C(13)	111.3(3)	C(25)-C(26)-Fe(2)	70.1(3)
C(5)-C(1)-Fe(1)	69.9(2)	O(1)-C(14)-C(15)	105.5(3)	C(23)-C(27)-C(26)	106.8(5)
C(2)-C(1)-Fe(1)	68.0(2)	C(13)-C(14)-C(15)	110.7(2)	C(23)-C(27)-Fe(2)	70.0(2)
Pd(1)-C(1)-Fe(1)	124.3(2)	C(16)-C(15)-C(14)	103.5(4)	C(26)-C(27)-Fe(2)	70.4(2)
C(11)-C(2)-C(1)	115.5(3)	C(17)-C(16)-C(15)	106.5(4)	N(2)-C(28)-C(19)	114.3(3)
C(11)-C(2)-C(3)	135.3(3)	C(16)-C(17)-O(1)	109.0(4)	N(2)-C(28)-C(29)	125.5(4)
C(1)-C(2)-C(3)	108.6(3)	C(22)-C(18)-C(19)	105.7(3)	C(19)-C(28)-C(29)	120.2(4)
C(11)-C(2)-Fe(1)	119.1(2)	C(22)-C(18)-Pd(2)	140.8(3)	N(2)-C(30)-C(31)	114.1(3)
C(1)-C(2)-Fe(1)	70.5(2)	C(19)-C(18)-Pd(2)	113.3(3)	O(2)-C(31)-C(30)	110.8(3)
C(3)-C(2)-Fe(1)	69.4(2)	C(22)-C(18)-Fe(2)	71.3(2)	O(2)-C(31)-C(32)	104.5(4)
C(4)-C(3)-C(2)	106.2(3)	C(19)-C(18)-Fe(2)	67.9(2)	C(30)-C(31)-C(32)	114.3(3)
C(4)-C(3)-Fe(1)	70.6(2)	Pd(2)-C(18)-Fe(2)	120.03(13)	C(33)-C(32)-C(31)	105.8(5)
C(2)-C(3)-Fe(1)	68.5(2)	C(20)-C(19)-C(28)	135.8(4)	C(34)-C(33)-C(32)	106.7(6)
C(3)-C(4)-C(5)	111.0(4)	C(20)-C(19)-C(18)	108.7(4)	O(2)-C(34)-C(33)	113.7(6)

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA}^2 \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.05130(6)	0.06107(7)	0.07908(12)	-0.00432(8)	-0.00023(8)	0.03008(5)
Pd(2)	0.05647(7)	0.05987(7)	0.08149(13)	-0.00764(9)	-0.00336(8)	0.03236(5)
Fe(1)	0.0750(2)	0.0868(2)	0.0743(2)	0.0106(2)	0.0062(2)	0.04824(12)
Fe(2)	0.0788(2)	0.0907(2)	0.0703(2)	0.0057(2)	0.0116(2)	0.04572(14)
Cl(1)	0.0589(2)	0.0693(2)	0.0845(4)	-0.0060(3)	-0.0032(3)	0.0360(2)
Cl(2)	0.0931(3)	0.0937(3)	0.0867(5)	0.0058(3)	0.0081(3)	0.0664(2)
O(1)	0.0594(8)	0.1068(12)	0.0927(14)	0.0190(11)	0.0074(9)	0.0380(7)
O(2)	0.1575(13)	0.1261(11)	0.113(2)	-0.0011(13)	-0.0097(14)	0.1039(8)
N(1)	0.0479(7)	0.0545(8)	0.0896(15)	-0.0049(10)	0.0032(9)	0.0238(6)
N(2)	0.0626(8)	0.0656(9)	0.094(2)	-0.0142(10)	-0.0080(10)	0.0369(6)
C(1)	0.0675(11)	0.0791(13)	0.095(2)	-0.0120(14)	-0.0054(14)	0.0396(9)
C(2)	0.0574(10)	0.0689(11)	0.092(2)	-0.0157(12)	-0.0010(12)	0.0324(8)
C(3)	0.0959(13)	0.1050(14)	0.096(2)	-0.0257(15)	-0.009(2)	0.0648(10)
C(4)	0.120(2)	0.157(2)	0.072(2)	-0.023(2)	-0.016(2)	0.0955(13)
C(5)	0.0918(12)	0.125(2)	0.087(2)	-0.009(2)	-0.0175(13)	0.0741(10)
C(6)	0.109(2)	0.088(2)	0.137(3)	0.020(2)	0.011(2)	0.0515(14)
C(7)	0.081(2)	0.109(2)	0.092(2)	0.020(2)	-0.004(2)	0.012(2)
C(8)	0.0665(14)	0.100(2)	0.134(3)	0.045(2)	0.001(2)	0.0299(12)
C(9)	0.0852(14)	0.114(2)	0.195(5)	0.028(3)	0.017(3)	0.0606(12)
C(10)	0.111(2)	0.135(2)	0.098(2)	0.045(2)	0.036(2)	0.0732(14)
C(11)	0.0501(10)	0.0590(11)	0.094(2)	-0.0072(12)	-0.0035(12)	0.0237(8)
C(12)	0.0970(14)	0.0717(12)	0.108(3)	-0.0069(14)	0.015(2)	0.0501(9)
C(13)	0.0598(10)	0.0554(10)	0.088(2)	0.0027(11)	0.0090(12)	0.0278(8)
C(14)	0.0696(10)	0.0675(10)	0.084(2)	0.0078(12)	0.0043(13)	0.0378(8)
C(15)	0.115(2)	0.111(2)	0.084(2)	0.012(2)	-0.008(2)	0.047(2)
C(16)	0.134(2)	0.139(3)	0.181(4)	0.045(2)	-0.045(3)	0.062(2)
C(17)	0.1173(15)	0.174(2)	0.116(3)	-0.012(2)	-0.010(2)	0.1048(12)
C(18)	0.0635(11)	0.0670(12)	0.100(2)	-0.0002(14)	0.0011(14)	0.0337(8)
C(19)	0.0601(12)	0.0767(14)	0.125(3)	0.014(2)	0.016(2)	0.0308(10)
C(20)	0.095(2)	0.111(2)	0.107(2)	0.042(2)	0.040(2)	0.0553(13)
C(21)	0.094(2)	0.150(2)	0.098(2)	0.048(2)	0.0424(15)	0.0729(13)
C(22)	0.0927(15)	0.0826(14)	0.089(2)	0.0166(14)	0.002(2)	0.0467(11)
C(23)	0.106(2)	0.092(2)	0.103(3)	-0.012(2)	0.002(2)	0.028(2)
C(24)	0.147(3)	0.080(2)	0.107(3)	-0.012(2)	-0.026(2)	0.055(2)
C(25)	0.145(2)	0.175(2)	0.099(3)	-0.022(2)	0.006(2)	0.109(2)
C(26)	0.131(2)	0.167(3)	0.092(3)	-0.036(2)	-0.004(2)	0.085(2)
C(27)	0.092(2)	0.125(3)	0.134(3)	-0.035(3)	-0.007(3)	0.037(2)
C(28)	0.0575(11)	0.0768(13)	0.112(2)	0.000(2)	-0.0055(14)	0.0354(9)
C(29)	0.0755(13)	0.136(2)	0.128(3)	0.007(2)	0.004(2)	0.0640(12)
C(30)	0.0740(11)	0.109(2)	0.096(2)	-0.023(2)	-0.0242(14)	0.0557(9)
C(31)	0.1049(14)	0.137(2)	0.100(3)	0.014(2)	0.004(2)	0.0830(11)
C(32)	0.180(2)	0.274(3)	0.116(3)	0.060(3)	0.023(2)	0.174(2)
C(33)	0.232(3)	0.265(3)	0.165(4)	0.105(3)	0.037(3)	0.179(2)
C(34)	0.201(3)	0.149(2)	0.174(5)	0.011(3)	-0.025(3)	0.132(2)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	1.10731(13)	0.52809(15)	-0.3477(4)	0.080
H(4A)	1.0808(2)	0.6044(2)	-0.4484(4)	0.080
H(5A)	1.04863(13)	0.6567(2)	-0.2786(4)	0.080
H(6A)	1.1983(2)	0.7686(2)	-0.2302(5)	0.080
H(7A)	1.2032(2)	0.7169(2)	-0.0281(4)	0.080
H(8A)	1.23931(15)	0.6387(2)	-0.0783(5)	0.080
H(9A)	1.2558(2)	0.6445(2)	-0.3169(6)	0.080
H(10A)	1.2321(2)	0.7246(2)	-0.4112(4)	0.080
H(12A)	1.13322(13)	0.47511(12)	0.0088(4)	0.080
H(12B)	1.09780(13)	0.45057(12)	-0.1213(4)	0.080
H(12C)	1.16605(13)	0.50975(12)	-0.1181(4)	0.080
H(13A)	1.10244(11)	0.49297(11)	0.1648(3)	0.080
H(13B)	1.06586(11)	0.52237(11)	0.2295(3)	0.080
H(14A)	1.16197(12)	0.62217(12)	0.2262(3)	0.080
H(15A)	1.1393(2)	0.5262(2)	0.3898(4)	0.080
H(15B)	1.1792(2)	0.5982(2)	0.4236(4)	0.080
H(16A)	1.2293(2)	0.5267(2)	0.3939(6)	0.080
H(16B)	1.2681(2)	0.6002(2)	0.3863(6)	0.080
H(17A)	1.2872(2)	0.5811(2)	0.2011(5)	0.080
H(17B)	1.2238(2)	0.5169(2)	0.1929(5)	0.080
H(20A)	0.8109(2)	0.6120(2)	0.5556(4)	0.080
H(21A)	0.8944(2)	0.5985(2)	0.6768(4)	0.080
H(22A)	0.97479(15)	0.60345(15)	0.5197(4)	0.080
H(23A)	1.0189(2)	0.7766(2)	0.3336(4)	0.080
H(24A)	0.9185(2)	0.7799(2)	0.3709(4)	0.080
H(25A)	0.8942(2)	0.7642(2)	0.6163(4)	0.080
H(26A)	0.9834(2)	0.7516(2)	0.7167(5)	0.080
H(27A)	1.0598(2)	0.7589(2)	0.5446(5)	0.080
H(29A)	0.77092(14)	0.6402(2)	0.1908(5)	0.080
H(29B)	0.74674(14)	0.5908(2)	0.3020(5)	0.080
H(29C)	0.78163(14)	0.6633(2)	0.3325(5)	0.080
H(30A)	0.81653(13)	0.6444(2)	0.0510(4)	0.080
H(30B)	0.87097(13)	0.6390(2)	-0.0130(4)	0.080
H(31A)	0.9395(2)	0.7436(2)	0.0257(5)	0.080
H(32A)	0.8367(2)	0.7123(2)	-0.1200(5)	0.080
H(32B)	0.9074(2)	0.7583(2)	-0.1556(5)	0.080
H(33A)	0.8272(3)	0.7906(3)	-0.0931(6)	0.080
H(33B)	0.9004(3)	0.8341(3)	-0.0910(6)	0.080
H(34A)	0.8962(2)	0.8409(2)	0.0975(6)	0.080
H(34B)	0.8254(2)	0.7882(2)	0.0969(6)	0.080

Tables for *syn*-($-$)-(S_p,S,S,S_p)-5aTable 1. Atomic coordinates [$\times 10^5$ for Pd, Fe; $\times 10^4$ for other atoms] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.64037(3)	0.68090(3)	0.38962(8)	0.0692(2)
Pd(2)	0.61101(3)	0.55741(3)	0.56208(7)	0.0660(2)
Fe(1)	0.68885(7)	0.75504(7)	0.09918(14)	0.0849(4)
Fe(2)	0.64216(7)	0.49120(6)	0.83028(14)	0.0792(4)
Cl(1)	0.62399(11)	0.58184(10)	0.3321(3)	0.0747(6)
Cl(2)	0.67720(12)	0.66571(10)	0.5988(3)	0.0871(7)
O(1)	0.7611(4)	0.8771(4)	0.4686(10)	0.126(3)
O(2)	0.5904(3)	0.3762(3)	0.4439(7)	0.090(2)
N(1)	0.6419(4)	0.7643(4)	0.4211(8)	0.076(2)
N(2)	0.5489(3)	0.4625(3)	0.5514(8)	0.069(2)
C(1)	0.6185(4)	0.6955(4)	0.2228(10)	0.075(2)
C(2)	0.6213(5)	0.7553(5)	0.2104(12)	0.086(3)
C(3)	0.6123(6)	0.7650(6)	0.0798(14)	0.115(4)
C(4)	0.6029(7)	0.7100(7)	0.0108(14)	0.122(5)
C(5)	0.6058(5)	0.6675(5)	0.0994(12)	0.097(3)
C(6)	0.7734(6)	0.7718(9)	0.1769(17)	0.127(5)
C(7)	0.7601(7)	0.7374(8)	0.0593(18)	0.134(5)
C(8)	0.7577(8)	0.7773(8)	-0.0340(14)	0.136(5)
C(9)	0.7633(8)	0.8344(8)	0.0205(14)	0.135(5)
C(10)	0.7734(6)	0.8309(7)	0.1563(17)	0.130(5)
C(11)	0.6332(5)	0.7910(4)	0.3215(13)	0.087(3)
C(12)	0.6306(7)	0.8505(6)	0.3179(17)	0.131(5)
C(13)	0.6588(6)	0.7969(5)	0.5452(12)	0.096(3)
C(14)	0.7274(7)	0.8332(5)	0.5642(15)	0.113(4)
C(15)	0.7471(11)	0.8722(8)	0.6876(17)	0.181(9)
C(16)	0.7992(11)	0.9314(8)	0.6486(22)	0.210(11)
C(17)	0.8017(9)	0.9326(7)	0.5218(19)	0.158(7)
C(18)	0.6011(5)	0.5367(5)	0.7435(10)	0.081(3)
C(19)	0.5560(5)	0.4709(4)	0.7643(10)	0.078(3)
C(20)	0.5536(6)	0.4607(5)	0.9015(12)	0.094(3)
C(21)	0.5981(7)	0.5183(6)	0.9550(12)	0.112(4)
C(22)	0.6261(6)	0.5646(5)	0.8618(11)	0.097(3)
C(23)	0.7128(6)	0.4855(6)	0.9205(14)	0.114(4)
C(24)	0.6692(6)	0.4282(6)	0.8650(21)	0.136(6)
C(25)	0.6673(7)	0.4363(8)	0.7320(15)	0.114(5)
C(26)	0.7096(7)	0.4975(8)	0.7071(15)	0.114(4)
C(27)	0.7383(6)	0.5280(6)	0.8167(14)	0.110(4)
C(28)	0.5300(4)	0.4319(4)	0.6547(10)	0.070(2)
C(29)	0.4862(4)	0.3607(4)	0.6694(11)	0.091(3)
C(30)	0.5310(4)	0.4306(4)	0.4231(9)	0.069(2)
C(31)	0.5833(5)	0.4208(4)	0.3708(9)	0.077(2)
C(32)	0.5666(7)	0.3937(7)	0.2319(11)	0.114(4)
C(33)	0.5630(7)	0.3308(7)	0.2461(18)	0.138(6)
C(34)	0.5590(7)	0.3166(5)	0.3773(17)	0.122(4)

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.918(10)	C(19)-C(20)	1.46(2)	C(7)-Fe(1)-C(6)	41.0(6)
Pd(1)-N(1)	2.046(8)	C(20)-C(21)	1.40(2)	C(2)-Fe(1)-C(6)	120.5(6)
Pd(1)-Cl(1)	2.326(2)	C(21)-C(22)	1.39(2)	C(8)-Fe(1)-C(6)	67.0(6)
Pd(1)-Cl(2)	2.474(3)	C(23)-C(24)	1.40(2)	C(4)-Fe(1)-C(6)	160.8(7)
Pd(2)-C(18)	1.957(11)	C(23)-C(27)	1.42(2)	C(9)-Fe(1)-C(6)	69.3(7)
Pd(2)-N(2)	2.043(7)	C(24)-C(25)	1.42(2)	C(10)-Fe(1)-C(6)	41.5(6)
Pd(2)-Cl(2)	2.342(2)	C(25)-C(26)	1.35(2)	C(1)-Fe(1)-C(6)	106.8(5)
Pd(2)-Cl(1)	2.472(3)	C(26)-C(27)	1.36(2)	C(3)-Fe(1)-C(5)	68.8(5)
Fe(1)-C(3)	2.012(12)	C(28)-C(29)	1.528(12)	C(7)-Fe(1)-C(5)	106.3(6)
Fe(1)-C(7)	2.035(14)	C(30)-C(31)	1.514(12)	C(2)-Fe(1)-C(5)	68.0(4)
Fe(1)-C(2)	2.025(11)	C(31)-C(32)	1.571(15)	C(8)-Fe(1)-C(5)	121.6(6)
Fe(1)-C(8)	2.042(14)	C(32)-C(33)	1.50(2)	C(4)-Fe(1)-C(5)	40.3(5)
Fe(1)-C(4)	2.043(12)	C(33)-C(34)	1.41(2)	C(9)-Fe(1)-C(5)	156.3(6)
Fe(1)-C(9)	2.055(15)			C(10)-Fe(1)-C(5)	161.2(6)
Fe(1)-C(10)	2.057(13)	C(1)-Pd(1)-N(1)	80.2(4)	C(1)-Fe(1)-C(5)	40.2(4)
Fe(1)-C(1)	2.064(10)	C(1)-Pd(1)-Cl(1)	92.1(3)	C(6)-Fe(1)-C(5)	124.6(6)
Fe(1)-C(6)	2.063(14)	N(1)-Pd(1)-Cl(1)	170.3(2)	C(24)-Fe(2)-C(25)	41.4(7)
Fe(1)-C(5)	2.085(11)	C(1)-Pd(1)-Cl(2)	175.5(3)	C(24)-Fe(2)-C(21)	125.1(7)
Fe(2)-C(24)	1.989(12)	N(1)-Pd(1)-Cl(2)	100.3(2)	C(25)-Fe(2)-C(21)	161.1(7)
Fe(2)-C(25)	2.016(12)	Cl(1)-Pd(1)-Cl(2)	87.78(9)	C(24)-Fe(2)-C(19)	125.4(5)
Fe(2)-C(21)	2.008(13)	C(18)-Pd(2)-N(2)	80.5(4)	C(25)-Fe(2)-C(19)	106.6(4)
Fe(2)-C(19)	2.028(10)	C(18)-Pd(2)-Cl(2)	93.3(3)	C(21)-Fe(2)-C(19)	69.0(5)
Fe(2)-C(23)	2.034(11)	N(2)-Pd(2)-Cl(2)	173.1(2)	C(24)-Fe(2)-C(23)	40.6(5)
Fe(2)-C(26)	2.040(15)	C(18)-Pd(2)-Cl(1)	178.8(3)	C(25)-Fe(2)-C(23)	69.1(5)
Fe(2)-C(20)	2.045(11)	N(2)-Pd(2)-Cl(1)	98.8(2)	C(21)-Fe(2)-C(23)	109.3(6)
Fe(2)-C(18)	2.047(10)	Cl(2)-Pd(2)-Cl(1)	87.47(9)	C(19)-Fe(2)-C(23)	162.8(5)
Fe(2)-C(22)	2.046(10)	C(3)-Fe(1)-C(7)	161.7(7)	C(24)-Fe(2)-C(26)	66.9(7)
Fe(2)-C(27)	2.058(13)	C(3)-Fe(1)-C(2)	41.5(5)	C(25)-Fe(2)-C(26)	38.9(5)
O(1)-C(17)	1.34(2)	C(7)-Fe(1)-C(2)	154.7(6)	C(21)-Fe(2)-C(26)	159.3(6)
O(1)-C(14)	1.40(2)	C(3)-Fe(1)-C(8)	126.1(6)	C(19)-Fe(2)-C(26)	120.1(5)
O(2)-C(31)	1.413(11)	C(7)-Fe(1)-C(8)	40.3(6)	C(23)-Fe(2)-C(26)	67.7(6)
O(2)-C(34)	1.443(14)	C(2)-Fe(1)-C(8)	163.6(5)	C(24)-Fe(2)-C(20)	110.5(5)
N(1)-C(11)	1.304(14)	C(3)-Fe(1)-C(4)	41.6(5)	C(25)-Fe(2)-C(20)	124.3(6)
N(1)-C(13)	1.476(15)	C(7)-Fe(1)-C(4)	123.4(7)	C(21)-Fe(2)-C(20)	40.3(5)
N(2)-C(28)	1.267(12)	C(2)-Fe(1)-C(4)	69.2(5)	C(19)-Fe(2)-C(20)	42.0(5)
N(2)-C(30)	1.509(13)	C(8)-Fe(1)-C(4)	108.6(7)	C(23)-Fe(2)-C(20)	125.7(6)
C(1)-C(5)	1.43(2)	C(3)-Fe(1)-C(9)	106.4(6)	C(26)-Fe(2)-C(20)	158.0(6)
C(1)-C(2)	1.432(13)	C(7)-Fe(1)-C(9)	70.7(7)	C(24)-Fe(2)-C(18)	160.8(7)
C(2)-C(11)	1.40(2)	C(2)-Fe(1)-C(9)	124.6(6)	C(25)-Fe(2)-C(18)	121.8(5)
C(2)-C(3)	1.43(2)	C(8)-Fe(1)-C(9)	41.4(6)	C(21)-Fe(2)-C(18)	67.9(5)
C(3)-C(4)	1.44(2)	C(4)-Fe(1)-C(9)	120.8(6)	C(19)-Fe(2)-C(18)	41.4(4)
C(4)-C(5)	1.42(2)	C(3)-Fe(1)-C(10)	119.7(6)	C(23)-Fe(2)-C(18)	155.2(5)
C(6)-C(10)	1.46(2)	C(7)-Fe(1)-C(10)	70.8(7)	C(26)-Fe(2)-C(18)	105.8(5)
C(6)-C(7)	1.44(2)	C(2)-Fe(1)-C(10)	106.3(6)	C(20)-Fe(2)-C(18)	69.2(4)
C(7)-C(8)	1.40(2)	C(8)-Fe(1)-C(10)	68.8(7)	C(24)-Fe(2)-C(22)	158.8(7)
C(8)-C(9)	1.45(2)	C(4)-Fe(1)-C(10)	156.4(7)	C(25)-Fe(2)-C(22)	157.2(6)
C(9)-C(10)	1.46(2)	C(9)-Fe(1)-C(10)	41.6(6)	C(21)-Fe(2)-C(22)	40.1(4)
C(11)-C(12)	1.489(13)	C(3)-Fe(1)-C(1)	69.6(5)	C(19)-Fe(2)-C(22)	68.8(5)
C(13)-C(14)	1.47(2)	C(7)-Fe(1)-C(1)	118.7(5)	C(23)-Fe(2)-C(22)	121.7(5)
C(14)-C(15)	1.54(2)	C(2)-Fe(1)-C(1)	41.0(4)	C(26)-Fe(2)-C(22)	122.6(6)
C(15)-C(16)	1.43(3)	C(8)-Fe(1)-C(1)	154.7(5)	C(20)-Fe(2)-C(22)	68.2(4)
C(16)-C(17)	1.33(2)	C(4)-Fe(1)-C(1)	68.7(5)	C(18)-Fe(2)-C(22)	40.1(5)
C(18)-C(22)	1.40(2)	C(9)-Fe(1)-C(1)	161.9(5)	C(24)-Fe(2)-C(27)	66.6(5)
C(18)-C(19)	1.439(13)	C(10)-Fe(1)-C(1)	123.9(5)	C(25)-Fe(2)-C(27)	66.1(6)
C(19)-C(28)	1.426(14)	C(3)-Fe(1)-C(6)	156.1(7)	C(21)-Fe(2)-C(27)	125.7(6)

C(19)-Fe(2)-C(27)	154.4(5)	C(1)-C(5)-Fe(1)	69.1(6)	C(18)-C(19)-Fe(2)	70.0(6)
C(23)-Fe(2)-C(27)	40.5(5)	C(10)-C(6)-C(7)	109.8(14)	C(20)-C(19)-Fe(2)	69.6(6)
C(26)-Fe(2)-C(27)	38.8(5)	C(10)-C(6)-Fe(1)	69.0(8)	C(21)-C(20)-C(19)	106.3(9)
C(20)-Fe(2)-C(27)	162.3(6)	C(7)-C(6)-Fe(1)	68.4(9)	C(21)-C(20)-Fe(2)	68.4(7)
C(18)-Fe(2)-C(27)	119.7(5)	C(8)-C(7)-C(6)	105.7(15)	C(19)-C(20)-Fe(2)	68.3(6)
C(22)-Fe(2)-C(27)	107.8(5)	C(8)-C(7)-Fe(1)	70.1(9)	C(20)-C(21)-C(22)	110.7(12)
Pd(1)-Cl(1)-Pd(2)	86.08(9)	C(6)-C(7)-Fe(1)	70.5(8)	C(20)-C(21)-Fe(2)	71.3(7)
Pd(2)-Cl(2)-Pd(1)	85.71(8)	C(7)-C(8)-C(9)	112.0(14)	C(22)-C(21)-Fe(2)	71.4(7)
C(17)-O(1)-C(14)	109.3(12)	C(7)-C(8)-Fe(1)	69.6(8)	C(21)-C(22)-C(18)	108.2(10)
C(31)-O(2)-C(34)	107.8(9)	C(9)-C(8)-Fe(1)	69.8(9)	C(21)-C(22)-Fe(2)	68.5(7)
C(11)-N(1)-C(13)	120.7(8)	C(8)-C(9)-C(10)	105.6(14)	C(18)-C(22)-Fe(2)	70.0(6)
C(11)-N(1)-Pd(1)	116.1(7)	C(8)-C(9)-Fe(1)	68.8(8)	C(24)-C(23)-C(27)	104.4(13)
C(13)-N(1)-Pd(1)	122.8(7)	C(10)-C(9)-Fe(1)	69.3(8)	C(24)-C(23)-Fe(2)	68.0(7)
C(28)-N(2)-C(30)	122.4(7)	C(9)-C(10)-C(6)	106.6(15)	C(27)-C(23)-Fe(2)	70.6(7)
C(28)-N(2)-Pd(2)	117.8(7)	C(9)-C(10)-Fe(1)	69.2(9)	C(23)-C(24)-C(25)	109.5(14)
C(30)-N(2)-Pd(2)	119.6(6)	C(6)-C(10)-Fe(1)	69.5(8)	C(23)-C(24)-Fe(2)	71.5(7)
C(5)-C(1)-C(2)	107.1(9)	N(1)-C(11)-C(2)	113.2(8)	C(25)-C(24)-Fe(2)	70.3(8)
C(5)-C(1)-Pd(1)	139.1(7)	N(1)-C(11)-C(12)	127.3(12)	C(26)-C(25)-C(24)	106.6(13)
C(2)-C(1)-Pd(1)	113.4(8)	C(2)-C(11)-C(12)	119.4(12)	C(26)-C(25)-Fe(2)	71.5(8)
C(5)-C(1)-Fe(1)	70.7(7)	C(14)-C(13)-N(1)	111.9(10)	C(24)-C(25)-Fe(2)	68.3(7)
C(2)-C(1)-Fe(1)	68.1(6)	O(1)-C(14)-C(13)	115.0(12)	C(25)-C(26)-C(27)	109.9(15)
Pd(1)-C(1)-Fe(1)	119.7(4)	O(1)-C(14)-C(15)	104.5(11)	C(25)-C(26)-Fe(2)	69.6(8)
C(11)-C(2)-C(1)	116.6(10)	C(13)-C(14)-C(15)	113.4(14)	C(27)-C(26)-Fe(2)	71.3(9)
C(11)-C(2)-C(3)	134.5(10)	C(16)-C(15)-C(14)	103.2(17)	C(26)-C(27)-C(23)	109.6(12)
C(1)-C(2)-C(3)	108.9(10)	C(17)-C(16)-C(15)	108.5(16)	C(26)-C(27)-Fe(2)	69.9(8)
C(11)-C(2)-Fe(1)	124.6(7)	O(1)-C(17)-C(16)	113.1(16)	C(23)-C(27)-Fe(2)	68.8(7)
C(1)-C(2)-Fe(1)	70.9(6)	C(22)-C(18)-C(19)	108.2(9)	N(2)-C(28)-C(19)	112.9(8)
C(3)-C(2)-Fe(1)	68.8(8)	C(22)-C(18)-Pd(2)	140.4(8)	N(2)-C(28)-C(29)	126.8(10)
C(2)-C(3)-C(4)	107.2(10)	C(19)-C(18)-Pd(2)	111.3(8)	C(19)-C(28)-C(29)	120.3(9)
C(2)-C(3)-Fe(1)	69.7(6)	C(22)-C(18)-Fe(2)	69.9(6)	N(2)-C(30)-C(31)	110.9(7)
C(4)-C(3)-Fe(1)	70.3(7)	C(19)-C(18)-Fe(2)	68.6(6)	O(2)-C(31)-C(30)	111.3(8)
C(5)-C(4)-C(3)	107.9(12)	Pd(2)-C(18)-Fe(2)	123.0(5)	O(2)-C(31)-C(32)	106.6(8)
C(5)-C(4)-Fe(1)	71.5(6)	C(28)-C(19)-C(18)	117.3(9)	C(30)-C(31)-C(32)	110.1(8)
C(3)-C(4)-Fe(1)	68.0(7)	C(28)-C(19)-C(20)	135.8(9)	C(33)-C(32)-C(31)	102.1(11)
C(4)-C(5)-C(1)	108.9(10)	C(18)-C(19)-C(20)	106.5(9)	C(34)-C(33)-C(32)	108.0(11)
C(4)-C(5)-Fe(1)	68.3(7)	C(28)-C(19)-Fe(2)	120.0(6)	C(33)-C(34)-O(2)	106.9(11)

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.0682(4)	0.0588(4)	0.0805(5)	0.0024(4)	0.0075(4)	0.0317(3)
Pd(2)	0.0679(4)	0.0588(4)	0.0758(4)	0.0038(3)	0.0036(4)	0.0352(3)
Fe(1)	0.1015(10)	0.0858(9)	0.0688(9)	0.0061(7)	-0.0079(7)	0.0477(8)
Fe(2)	0.0948(9)	0.0722(8)	0.0721(8)	-0.0043(7)	-0.0122(7)	0.0428(7)
Cl(1)	0.0776(13)	0.0644(12)	0.084(2)	0.0032(11)	0.0080(12)	0.0367(11)
Cl(2)	0.103(2)	0.0619(12)	0.085(2)	0.0009(11)	-0.0074(13)	0.0330(12)
O(1)	0.131(7)	0.092(5)	0.119(7)	-0.005(5)	0.021(6)	0.027(5)
O(2)	0.112(5)	0.100(5)	0.092(5)	-0.009(4)	-0.016(4)	0.078(4)
N(1)	0.077(5)	0.077(5)	0.074(6)	0.001(4)	0.010(4)	0.038(4)
N(2)	0.059(4)	0.072(4)	0.080(5)	0.004(4)	-0.001(4)	0.034(3)
C(1)	0.073(5)	0.067(5)	0.085(7)	-0.002(5)	-0.013(5)	0.036(4)
C(2)	0.079(6)	0.080(6)	0.110(9)	-0.001(6)	-0.023(6)	0.048(5)
C(3)	0.128(9)	0.100(8)	0.127(11)	-0.005(8)	-0.047(9)	0.065(7)
C(4)	0.143(11)	0.122(10)	0.118(11)	-0.019(8)	-0.061(9)	0.079(9)
C(5)	0.100(8)	0.090(7)	0.097(9)	-0.003(6)	-0.021(6)	0.046(6)
C(6)	0.096(9)	0.161(15)	0.123(13)	0.024(11)	0.016(8)	0.065(9)
C(7)	0.127(11)	0.176(14)	0.119(12)	0.014(13)	0.024(10)	0.090(10)
C(8)	0.187(15)	0.133(12)	0.087(10)	0.034(9)	0.038(9)	0.080(11)
C(9)	0.176(15)	0.119(11)	0.091(11)	0.027(8)	0.009(9)	0.059(10)
C(10)	0.092(9)	0.107(10)	0.143(15)	-0.001(9)	0.021(8)	0.014(8)
C(11)	0.083(6)	0.069(6)	0.118(9)	-0.005(6)	0.011(6)	0.045(5)
C(12)	0.165(12)	0.104(9)	0.165(14)	0.018(9)	0.006(11)	0.097(9)
C(13)	0.111(8)	0.088(7)	0.098(9)	0.010(6)	0.018(7)	0.057(6)
C(14)	0.161(12)	0.087(7)	0.104(9)	-0.015(8)	0.006(10)	0.073(8)
C(15)	0.303(26)	0.114(12)	0.125(14)	-0.052(10)	-0.069(16)	0.104(15)
C(16)	0.306(28)	0.097(12)	0.168(21)	-0.050(12)	-0.110(19)	0.057(15)
C(17)	0.181(16)	0.099(11)	0.143(17)	-0.041(10)	-0.027(12)	0.031(11)
C(18)	0.098(7)	0.072(6)	0.077(7)	0.008(5)	0.020(5)	0.046(5)
C(19)	0.085(6)	0.071(6)	0.092(8)	0.008(5)	0.011(5)	0.049(5)
C(20)	0.128(9)	0.079(6)	0.079(7)	0.017(6)	0.025(7)	0.055(6)
C(21)	0.168(12)	0.090(8)	0.076(7)	0.015(6)	0.018(8)	0.063(8)
C(22)	0.134(9)	0.079(6)	0.082(9)	-0.008(5)	0.010(6)	0.056(6)
C(23)	0.122(9)	0.116(9)	0.107(10)	-0.006(8)	-0.056(8)	0.060(8)
C(24)	0.112(10)	0.093(8)	0.217(21)	0.000(11)	-0.013(11)	0.062(8)
C(25)	0.119(10)	0.162(14)	0.113(11)	-0.052(10)	-0.051(9)	0.108(11)
C(26)	0.095(8)	0.138(11)	0.136(12)	-0.018(10)	-0.031(8)	0.079(9)
C(27)	0.102(8)	0.107(9)	0.114(10)	-0.006(8)	-0.031(8)	0.048(7)
C(28)	0.058(5)	0.069(5)	0.092(7)	0.004(5)	0.011(5)	0.039(4)
C(29)	0.073(6)	0.069(6)	0.110(9)	0.014(6)	0.009(6)	0.020(5)
C(30)	0.060(5)	0.063(5)	0.086(7)	0.009(4)	-0.007(4)	0.032(4)
C(31)	0.087(6)	0.073(5)	0.076(7)	-0.008(5)	-0.011(5)	0.044(5)
C(32)	0.128(10)	0.140(11)	0.078(8)	-0.025(8)	-0.009(7)	0.071(9)
C(33)	0.146(12)	0.119(10)	0.157(16)	-0.070(11)	-0.025(11)	0.072(9)
C(34)	0.170(13)	0.087(7)	0.119(11)	0.003(8)	0.022(10)	0.070(8)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	0.6115(6)	0.8017(6)	0.0443(14)	0.138
H(4A)	0.5956(7)	0.7030(7)	-0.0809(14)	0.147
H(5A)	0.6026(5)	0.6270(5)	0.0782(12)	0.116
H(6A)	0.7781(6)	0.7562(9)	0.2597(17)	0.152
H(7A)	0.7566(7)	0.6960(8)	0.0461(18)	0.161
H(8A)	0.7492(8)	0.7660(8)	-0.1241(14)	0.163
H(9A)	0.7616(8)	0.8686(8)	-0.0247(14)	0.163
H(10A)	0.7793(6)	0.8623(7)	0.2211(17)	0.156
H(12A)	0.6401(7)	0.8696(6)	0.4008(17)	0.197
H(12B)	0.5890(7)	0.8413(6)	0.2929(17)	0.197
H(12C)	0.6610(7)	0.8792(6)	0.2578(17)	0.197
H(13A)	0.6417(6)	0.8252(5)	0.5502(12)	0.115
H(13B)	0.6397(6)	0.7659(5)	0.6126(12)	0.115
H(14A)	0.7430(7)	0.8032(5)	0.5685(15)	0.135
H(15A)	0.7129(11)	0.8774(8)	0.7206(17)	0.217
H(15B)	0.7598(11)	0.8524(8)	0.7522(17)	0.217
H(16A)	0.7938(11)	0.9658(8)	0.6797(22)	0.252
H(16B)	0.8382(11)	0.9364(8)	0.6834(22)	0.252
H(17A)	0.7925(9)	0.9646(7)	0.4910(19)	0.190
H(17B)	0.8443(9)	0.9446(7)	0.4952(19)	0.190
H(20A)	0.5268(6)	0.4210(5)	0.9468(12)	0.113
H(21A)	0.6080(7)	0.5253(6)	1.0460(12)	0.134
H(22A)	0.6585(6)	0.6088(5)	0.8759(11)	0.116
H(23A)	0.7249(6)	0.4940(6)	1.0103(14)	0.137
H(24A)	0.6441(6)	0.3883(6)	0.9108(21)	0.163
H(25A)	0.6414(7)	0.4036(8)	0.6698(15)	0.137
H(26A)	0.7180(7)	0.5172(8)	0.6228(15)	0.137
H(27A)	0.7701(6)	0.5729(6)	0.8234(14)	0.132
H(29A)	0.4730(4)	0.3417(4)	0.5869(11)	0.137
H(29B)	0.4498(4)	0.3528(4)	0.7183(11)	0.137
H(29C)	0.5083(4)	0.3427(4)	0.7122(11)	0.137
H(30A)	0.5229(4)	0.4564(4)	0.3645(9)	0.083
H(30B)	0.4925(4)	0.3900(4)	0.4310(9)	0.083
H(31A)	0.6231(5)	0.4612(4)	0.3702(9)	0.093
H(32A)	0.5266(7)	0.3888(7)	0.2041(11)	0.137
H(32B)	0.5994(7)	0.4206(7)	0.1722(11)	0.137
H(33A)	0.5260(7)	0.2984(7)	0.2021(18)	0.166
H(33B)	0.6003(7)	0.3325(7)	0.2096(18)	0.166
H(34A)	0.5795(7)	0.2922(5)	0.3952(17)	0.147
H(34B)	0.5152(7)	0.2923(5)	0.4035(17)	0.147

Tables for *syn*-(+)-(R_p,R,R,R_p)-6aTable 1. Atomic coordinates [$\times 10^5$ for Pd, Fe; $\times 10^4$ for other atoms] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.68217(3)	0.86953(2)	0.10099(2)	0.07238(8)
Pd(2)	0.77443(3)	0.82365(2)	0.32916(2)	0.06890(7)
Fe(1)	0.52673(6)	0.76219(5)	-0.12787(5)	0.0828(2)
Fe(2)	0.99568(5)	0.80981(5)	0.54827(4)	0.07203(14)
O(1)	0.7769(4)	1.0737(4)	-0.1341(3)	0.1262(14)
O(2)	0.6399(3)	0.5984(4)	0.5468(3)	0.1125(12)
O(3)	0.7547(3)	0.9993(2)	0.1949(2)	0.0855(9)
O(4)	0.8332(5)	1.0429(3)	0.3436(3)	0.1255(14)
O(5)	0.5654(3)	0.8213(3)	0.2840(3)	0.1064(11)
O(6)	0.4177(4)	0.8474(4)	0.1701(3)	0.132(2)
N(1)	0.8169(3)	0.8878(3)	-0.0087(3)	0.0791(10)
N(2)	0.7755(3)	0.6696(3)	0.3697(3)	0.0777(10)
N(3)	0.7930(4)	0.9714(3)	0.2871(2)	0.0785(10)
N(4)	0.5431(3)	0.8380(3)	0.2072(2)	0.0757(9)
C(1)	0.6320(4)	0.7552(4)	0.0142(3)	0.0809(12)
C(2)	0.7143(5)	0.7416(4)	-0.0718(3)	0.0868(13)
C(3)	0.6726(5)	0.6543(4)	-0.1321(4)	0.097(2)
C(4)	0.5638(6)	0.6126(4)	-0.0846(4)	0.102(2)
C(5)	0.5385(5)	0.6724(4)	0.0029(4)	0.0895(14)
C(6)	0.4797(6)	0.8126(7)	-0.2746(5)	0.132(2)
C(7)	0.3684(5)	0.7684(6)	-0.2356(4)	0.116(2)
C(8)	0.3416(6)	0.8160(7)	-0.1463(5)	0.128(2)
C(9)	0.4297(7)	0.9010(5)	-0.1339(5)	0.155(2)
C(10)	0.5209(7)	0.8945(6)	-0.2087(6)	0.152(3)
C(11)	0.8086(4)	0.8215(4)	-0.0797(3)	0.0822(12)
C(12)	0.9090(5)	0.9745(4)	-0.0109(4)	0.0958(15)
C(13)	0.8422(5)	1.0747(5)	-0.0345(4)	0.103(2)
C(14)	0.9389(6)	1.1645(5)	-0.0315(5)	0.125(2)
C(15)	0.8940(9)	1.2243(8)	-0.1268(6)	0.229(4)
C(16)	0.8207(9)	1.1540(5)	-0.1921(5)	0.144(3)
C(17)	0.9547(4)	0.8144(4)	0.3900(3)	0.0776(10)
C(18)	0.9864(4)	0.7132(3)	0.4252(3)	0.0752(11)
C(19)	1.1163(4)	0.7135(4)	0.4759(3)	0.0908(14)
C(20)	1.1636(4)	0.8182(5)	0.4693(3)	0.0974(15)
C(21)	1.0659(4)	0.8793(4)	0.4176(3)	0.0863(13)
C(22)	0.9167(5)	0.9168(5)	0.6423(4)	0.107(2)
C(23)	1.0276(4)	0.8761(4)	0.6929(3)	0.0865(13)
C(24)	1.0096(5)	0.7680(4)	0.7005(3)	0.0874(14)
C(25)	0.8845(5)	0.7416(5)	0.6554(3)	0.0947(15)
C(26)	0.8275(4)	0.8362(5)	0.6186(3)	0.099(2)
C(27)	0.8807(4)	0.6389(3)	0.4129(3)	0.0817(12)
C(28)	0.6603(4)	0.6052(3)	0.3634(3)	0.0800(12)
C(29)	0.5761(4)	0.6273(4)	0.4515(3)	0.0858(13)
C(30)	0.4425(5)	0.5645(4)	0.4435(4)	0.097(2)
C(31)	0.4742(6)	0.4782(5)	0.5209(5)	0.119(2)
C(32)	0.5645(5)	0.5254(4)	0.5988(4)	0.097(2)

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.906(4)	C(13)-C(14)	1.524(9)	C(4)-Fe(1)-C(3)	40.4(2)
Pd(1)-N(1)	2.053(3)	C(14)-C(15)	1.499(11)	C(10)-Fe(1)-C(5)	155.9(2)
Pd(1)-N(4)	2.079(3)	C(15)-C(16)	1.419(11)	C(8)-Fe(1)-C(5)	107.3(3)
Pd(1)-O(3)	2.173(3)	C(17)-C(18)	1.417(6)	C(2)-Fe(1)-C(5)	68.1(2)
Pd(1)-Pd(2)	3.0893(5)	C(17)-C(21)	1.438(6)	C(6)-Fe(1)-C(5)	161.7(3)
Pd(2)-C(17)	1.957(4)	C(18)-C(19)	1.440(6)	C(4)-Fe(1)-C(5)	40.3(2)
Pd(2)-N(3)	2.000(4)	C(18)-C(27)	1.447(6)	C(3)-Fe(1)-C(5)	68.4(2)
Pd(2)-N(2)	2.061(4)	C(19)-C(20)	1.443(9)	C(10)-Fe(1)-C(9)	40.0(3)
Pd(2)-O(5)	2.176(3)	C(20)-C(21)	1.406(7)	C(8)-Fe(1)-C(9)	41.0(3)
Fe(1)-C(10)	2.004(7)	C(22)-C(23)	1.375(7)	C(2)-Fe(1)-C(9)	125.0(2)
Fe(1)-C(8)	2.014(7)	C(22)-C(26)	1.406(8)	C(6)-Fe(1)-C(9)	66.4(3)
Fe(1)-C(2)	2.021(5)	C(23)-C(24)	1.415(8)	C(4)-Fe(1)-C(9)	157.0(3)
Fe(1)-C(6)	2.030(6)	C(24)-C(25)	1.411(7)	C(3)-Fe(1)-C(9)	161.5(3)
Fe(1)-C(4)	2.043(5)	C(25)-C(26)	1.422(8)	C(5)-Fe(1)-C(9)	122.1(2)
Fe(1)-C(3)	2.045(5)	C(28)-C(29)	1.498(6)	C(10)-Fe(1)-C(7)	67.7(3)
Fe(1)-C(5)	2.046(5)	C(29)-C(30)	1.586(7)	C(8)-Fe(1)-C(7)	38.7(3)
Fe(1)-C(9)	2.050(6)	C(30)-C(31)	1.519(8)	C(2)-Fe(1)-C(7)	158.3(2)
Fe(1)-C(7)	2.064(5)	C(31)-C(32)	1.453(8)	C(6)-Fe(1)-C(7)	39.9(2)
Fe(1)-C(1)	2.065(4)			C(4)-Fe(1)-C(7)	110.1(3)
Fe(2)-C(18)	2.018(4)	C(1)-Pd(1)-N(1)	81.4(2)	C(3)-Fe(1)-C(7)	123.3(2)
Fe(2)-C(19)	2.024(5)	C(1)-Pd(1)-N(4)	93.8(2)	C(5)-Fe(1)-C(7)	125.4(2)
Fe(2)-C(26)	2.025(5)	N(1)-Pd(1)-N(4)	175.01(14)	C(9)-Fe(1)-C(7)	65.5(3)
Fe(2)-C(24)	2.034(4)	C(1)-Pd(1)-O(3)	175.4(2)	C(10)-Fe(1)-C(1)	119.7(2)
Fe(2)-C(22)	2.042(6)	N(1)-Pd(1)-O(3)	94.38(13)	C(8)-Fe(1)-C(1)	123.3(2)
Fe(2)-C(25)	2.046(5)	N(4)-Pd(1)-O(3)	90.36(12)	C(2)-Fe(1)-C(1)	41.5(2)
Fe(2)-C(20)	2.056(4)	C(1)-Pd(1)-Pd(2)	117.66(13)	C(6)-Fe(1)-C(1)	156.8(2)
Fe(2)-C(17)	2.058(4)	N(1)-Pd(1)-Pd(2)	120.22(9)	C(4)-Fe(1)-C(1)	68.9(2)
Fe(2)-C(23)	2.061(5)	N(4)-Pd(1)-Pd(2)	60.82(8)	C(3)-Fe(1)-C(1)	69.9(2)
Fe(2)-C(21)	2.081(4)	O(3)-Pd(1)-Pd(2)	62.96(8)	C(5)-Fe(1)-C(1)	40.9(2)
O(1)-C(16)	1.373(8)	C(17)-Pd(2)-N(3)	93.7(2)	C(9)-Fe(1)-C(1)	107.1(2)
O(1)-C(13)	1.409(6)	C(17)-Pd(2)-N(2)	81.4(2)	C(7)-Fe(1)-C(1)	159.8(2)
O(2)-C(29)	1.404(5)	N(3)-Pd(2)-N(2)	174.07(14)	C(18)-Fe(2)-C(19)	41.7(2)
O(2)-C(32)	1.415(6)	C(17)-Pd(2)-O(5)	170.8(2)	C(18)-Fe(2)-C(26)	117.4(2)
O(3)-N(3)	1.279(4)	N(3)-Pd(2)-O(5)	92.8(2)	C(19)-Fe(2)-C(26)	150.6(2)
O(4)-N(3)	1.232(5)	N(2)-Pd(2)-O(5)	92.5(2)	C(18)-Fe(2)-C(24)	126.3(2)
O(5)-N(4)	1.025(5)	C(17)-Pd(2)-Pd(1)	127.85(11)	C(19)-Fe(2)-C(24)	106.0(2)
O(6)-N(4)	1.343(5)	N(3)-Pd(2)-Pd(1)	65.53(9)	C(26)-Fe(2)-C(24)	67.6(2)
N(1)-C(11)	1.254(6)	N(2)-Pd(2)-Pd(1)	115.08(9)	C(18)-Fe(2)-C(22)	152.6(2)
N(1)-C(12)	1.466(6)	O(5)-Pd(2)-Pd(1)	61.03(10)	C(19)-Fe(2)-C(22)	165.5(2)
N(2)-C(27)	1.243(5)	C(10)-Fe(1)-C(8)	69.4(3)	C(26)-Fe(2)-C(22)	40.4(2)
N(2)-C(28)	1.439(5)	C(10)-Fe(1)-C(2)	107.1(2)	C(24)-Fe(2)-C(22)	67.1(2)
C(1)-C(5)	1.436(7)	C(8)-Fe(1)-C(2)	161.5(2)	C(18)-Fe(2)-C(25)	105.4(2)
C(1)-C(2)	1.447(6)	C(10)-Fe(1)-C(6)	40.8(3)	C(19)-Fe(2)-C(25)	115.4(2)
C(2)-C(11)	1.421(7)	C(8)-Fe(1)-C(6)	67.5(3)	C(26)-Fe(2)-C(25)	40.9(2)
C(2)-C(3)	1.422(7)	C(2)-Fe(1)-C(6)	122.4(2)	C(24)-Fe(2)-C(25)	40.5(2)
C(3)-C(4)	1.411(8)	C(10)-Fe(1)-C(4)	161.9(3)	C(22)-Fe(2)-C(25)	68.4(2)
C(4)-C(5)	1.407(7)	C(8)-Fe(1)-C(4)	121.0(3)	C(18)-Fe(2)-C(20)	68.9(2)
C(6)-C(7)	1.397(9)	C(2)-Fe(1)-C(4)	67.9(2)	C(19)-Fe(2)-C(20)	41.4(2)
C(6)-C(10)	1.406(10)	C(6)-Fe(1)-C(4)	126.0(3)	C(26)-Fe(2)-C(20)	167.0(3)
C(7)-C(8)	1.350(9)	C(10)-Fe(1)-C(3)	124.5(3)	C(24)-Fe(2)-C(20)	119.1(2)
C(8)-C(9)	1.424(10)	C(8)-Fe(1)-C(3)	155.9(3)	C(22)-Fe(2)-C(20)	129.4(2)
C(9)-C(10)	1.387(10)	C(2)-Fe(1)-C(3)	40.9(2)	C(25)-Fe(2)-C(20)	151.2(2)
C(12)-C(13)	1.486(8)	C(6)-Fe(1)-C(3)	108.8(3)	C(18)-Fe(2)-C(17)	40.7(2)

C(19)-Fe(2)-C(17)	69.5(2)	C(2)-C(1)-Fe(1)	67.6(2)	C(18)-C(17)-Fe(2)	68.1(2)
C(26)-Fe(2)-C(17)	108.5(2)	Pd(1)-C(1)-Fe(1)	126.3(2)	C(21)-C(17)-Fe(2)	70.5(2)
C(24)-Fe(2)-C(17)	164.3(2)	C(11)-C(2)-C(3)	136.0(5)	Pd(2)-C(17)-Fe(2)	121.6(2)
C(22)-Fe(2)-C(17)	120.5(2)	C(11)-C(2)-C(1)	113.5(4)	C(17)-C(18)-C(19)	109.1(4)
C(25)-Fe(2)-C(17)	126.7(2)	C(3)-C(2)-C(1)	110.3(4)	C(17)-C(18)-C(27)	115.2(3)
C(20)-Fe(2)-C(17)	68.1(2)	C(11)-C(2)-Fe(1)	120.6(3)	C(19)-C(18)-C(27)	135.2(4)
C(18)-Fe(2)-C(23)	165.2(2)	C(3)-C(2)-Fe(1)	70.5(3)	C(17)-C(18)-Fe(2)	71.2(2)
C(19)-Fe(2)-C(23)	127.6(2)	C(1)-C(2)-Fe(1)	70.9(3)	C(19)-C(18)-Fe(2)	69.4(3)
C(26)-Fe(2)-C(23)	67.1(2)	C(4)-C(3)-C(2)	106.4(5)	C(27)-C(18)-Fe(2)	119.6(3)
C(24)-Fe(2)-C(23)	40.4(2)	C(4)-C(3)-Fe(1)	69.7(3)	C(18)-C(19)-C(20)	106.1(4)
C(22)-Fe(2)-C(23)	39.1(2)	C(2)-C(3)-Fe(1)	68.6(3)	C(18)-C(19)-Fe(2)	68.9(3)
C(25)-Fe(2)-C(23)	68.2(2)	C(5)-C(4)-C(3)	109.3(5)	C(20)-C(19)-Fe(2)	70.5(3)
C(20)-Fe(2)-C(23)	109.9(2)	C(5)-C(4)-Fe(1)	70.0(3)	C(21)-C(20)-C(19)	109.0(4)
C(17)-Fe(2)-C(23)	153.7(2)	C(3)-C(4)-Fe(1)	69.9(3)	C(21)-C(20)-Fe(2)	71.1(2)
C(18)-Fe(2)-C(21)	68.3(2)	C(4)-C(5)-C(1)	109.6(5)	C(19)-C(20)-Fe(2)	68.1(3)
C(19)-Fe(2)-C(21)	68.8(2)	C(4)-C(5)-Fe(1)	69.8(3)	C(20)-C(21)-C(17)	108.3(5)
C(26)-Fe(2)-C(21)	129.7(2)	C(1)-C(5)-Fe(1)	70.3(3)	C(20)-C(21)-Fe(2)	69.2(3)
C(24)-Fe(2)-C(21)	153.2(2)	C(7)-C(6)-C(10)	108.0(6)	C(17)-C(21)-Fe(2)	68.8(2)
C(22)-Fe(2)-C(21)	111.1(2)	C(7)-C(6)-Fe(1)	71.4(4)	C(23)-C(22)-C(26)	108.7(5)
C(25)-Fe(2)-C(21)	166.1(2)	C(10)-C(6)-Fe(1)	68.6(4)	C(23)-C(22)-Fe(2)	71.2(3)
C(20)-Fe(2)-C(21)	39.7(2)	C(8)-C(7)-C(6)	109.7(6)	C(26)-C(22)-Fe(2)	69.1(3)
C(17)-Fe(2)-C(21)	40.7(2)	C(8)-C(7)-Fe(1)	68.7(4)	C(22)-C(23)-C(24)	107.8(4)
C(23)-Fe(2)-C(21)	120.8(2)	C(6)-C(7)-Fe(1)	68.8(3)	C(22)-C(23)-Fe(2)	69.7(3)
C(16)-O(1)-C(13)	109.8(5)	C(7)-C(8)-C(9)	106.6(6)	C(24)-C(23)-Fe(2)	68.8(3)
C(29)-O(2)-C(32)	110.9(4)	C(7)-C(8)-Fe(1)	72.7(4)	C(25)-C(24)-C(23)	109.2(4)
N(3)-O(3)-Pd(1)	111.8(2)	C(9)-C(8)-Fe(1)	70.9(4)	C(25)-C(24)-Fe(2)	70.2(3)
N(4)-O(5)-Pd(2)	114.0(3)	C(10)-C(9)-C(8)	108.9(6)	C(23)-C(24)-Fe(2)	70.8(3)
C(11)-N(1)-C(12)	121.4(4)	C(10)-C(9)-Fe(1)	68.2(4)	C(24)-C(25)-C(26)	105.6(5)
C(11)-N(1)-Pd(1)	114.2(3)	C(8)-C(9)-Fe(1)	68.1(4)	C(24)-C(25)-Fe(2)	69.3(3)
C(12)-N(1)-Pd(1)	124.2(3)	C(9)-C(10)-C(6)	106.2(6)	C(26)-C(25)-Fe(2)	68.8(3)
C(27)-N(2)-C(28)	121.3(4)	C(9)-C(10)-Fe(1)	71.8(4)	C(22)-C(26)-C(25)	108.7(4)
C(27)-N(2)-Pd(2)	114.4(3)	C(6)-C(10)-Fe(1)	70.6(4)	C(22)-C(26)-Fe(2)	70.4(3)
C(28)-N(2)-Pd(2)	123.7(3)	N(1)-C(11)-C(2)	117.3(4)	C(25)-C(26)-Fe(2)	70.4(3)
O(4)-N(3)-O(3)	114.0(3)	N(1)-C(12)-C(13)	112.6(4)	N(2)-C(27)-C(18)	117.0(4)
O(4)-N(3)-Pd(2)	126.3(3)	O(1)-C(13)-C(12)	111.2(5)	N(2)-C(28)-C(29)	110.8(3)
O(3)-N(3)-Pd(2)	119.6(3)	O(1)-C(13)-C(14)	107.2(5)	O(2)-C(29)-C(28)	110.9(4)
O(5)-N(4)-O(6)	120.6(4)	C(12)-C(13)-C(14)	111.8(5)	O(2)-C(29)-C(30)	105.5(4)
O(5)-N(4)-Pd(1)	124.1(3)	C(15)-C(14)-C(13)	102.2(6)	C(28)-C(29)-C(30)	112.8(4)
O(6)-N(4)-Pd(1)	115.1(3)	C(16)-C(15)-C(14)	106.0(7)	C(31)-C(30)-C(29)	100.9(4)
C(5)-C(1)-C(2)	104.4(4)	O(1)-C(16)-C(15)	109.9(6)	C(32)-C(31)-C(30)	104.1(5)
C(5)-C(1)-Pd(1)	142.2(3)	C(18)-C(17)-C(21)	107.5(4)	O(2)-C(32)-C(31)	107.1(4)
C(2)-C(1)-Pd(1)	113.4(3)	C(18)-C(17)-Pd(2)	112.0(3)		
C(5)-C(1)-Fe(1)	68.8(2)	C(21)-C(17)-Pd(2)	140.4(4)		

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.0857(2)	0.07072(14)	0.06049(12)	0.00188(12)	0.00312(11)	-0.00282(14)
Pd(2)	0.08381(14)	0.06234(12)	0.06093(12)	-0.00069(11)	0.00780(10)	-0.00205(13)
Fe(1)	0.0958(4)	0.0783(3)	0.0730(3)	-0.0002(3)	-0.0047(3)	-0.0098(3)
Fe(2)	0.0692(2)	0.0828(3)	0.0649(2)	0.0054(3)	0.0098(2)	0.0022(3)
O(1)	0.150(3)	0.116(3)	0.110(2)	0.015(2)	-0.013(2)	-0.049(2)
O(2)	0.105(2)	0.144(3)	0.090(2)	0.010(2)	0.013(2)	-0.051(2)
O(3)	0.115(2)	0.0623(13)	0.0787(15)	0.0013(13)	0.0008(15)	-0.007(2)
O(4)	0.204(3)	0.070(2)	0.095(2)	-0.005(2)	-0.043(2)	-0.019(2)
O(5)	0.094(2)	0.100(2)	0.127(2)	-0.003(2)	0.018(2)	-0.005(2)
O(6)	0.115(2)	0.136(4)	0.143(3)	0.017(3)	0.002(2)	0.006(3)
N(1)	0.076(2)	0.082(2)	0.079(2)	0.003(2)	0.0040(14)	-0.005(2)
N(2)	0.083(2)	0.078(2)	0.073(2)	0.001(2)	0.0154(15)	-0.005(2)
N(3)	0.096(2)	0.077(2)	0.062(2)	-0.003(2)	-0.0008(15)	-0.005(2)
N(4)	0.0706(14)	0.079(2)	0.079(2)	-0.011(2)	0.0204(12)	-0.0014(15)
C(1)	0.080(2)	0.080(2)	0.082(2)	0.019(2)	0.002(2)	0.005(2)
C(2)	0.105(3)	0.081(2)	0.073(2)	0.001(2)	0.000(2)	0.012(2)
C(3)	0.101(3)	0.079(3)	0.110(3)	-0.011(3)	0.004(3)	-0.008(2)
C(4)	0.137(4)	0.074(2)	0.092(3)	-0.009(2)	-0.016(3)	-0.008(3)
C(5)	0.114(3)	0.073(2)	0.081(2)	0.001(2)	-0.002(2)	-0.020(2)
C(6)	0.112(3)	0.183(6)	0.100(3)	0.040(4)	-0.006(3)	-0.003(5)
C(7)	0.112(3)	0.130(4)	0.102(3)	-0.013(3)	-0.022(3)	-0.004(3)
C(8)	0.126(4)	0.141(5)	0.118(4)	0.019(4)	0.006(3)	0.025(4)
C(9)	0.202(5)	0.108(3)	0.144(4)	-0.039(3)	-0.063(4)	0.072(4)
C(10)	0.140(4)	0.100(4)	0.204(6)	0.024(4)	-0.070(4)	-0.018(4)
C(11)	0.079(2)	0.093(2)	0.076(2)	0.001(2)	0.009(2)	-0.001(2)
C(12)	0.092(2)	0.104(3)	0.093(3)	-0.017(2)	0.020(2)	-0.015(3)
C(13)	0.117(3)	0.111(3)	0.080(2)	0.010(3)	0.007(2)	-0.020(3)
C(14)	0.128(4)	0.126(4)	0.122(4)	0.006(4)	0.017(3)	-0.042(3)
C(15)	0.287(8)	0.220(6)	0.174(6)	0.089(5)	-0.025(6)	-0.145(6)
C(16)	0.238(7)	0.104(4)	0.092(3)	0.018(3)	0.028(4)	-0.026(5)
C(17)	0.095(2)	0.070(2)	0.069(2)	0.005(2)	0.019(2)	-0.015(2)
C(18)	0.077(2)	0.078(2)	0.072(2)	0.015(2)	0.018(2)	0.007(2)
C(19)	0.091(2)	0.098(3)	0.086(2)	0.014(2)	0.022(2)	0.007(2)
C(20)	0.081(2)	0.126(4)	0.089(2)	0.014(3)	0.027(2)	-0.001(3)
C(21)	0.090(2)	0.099(3)	0.071(2)	0.013(2)	0.015(2)	-0.014(2)
C(22)	0.115(3)	0.082(3)	0.127(4)	-0.001(3)	0.032(3)	0.005(3)
C(23)	0.079(2)	0.095(3)	0.085(2)	-0.010(2)	0.007(2)	-0.008(2)
C(24)	0.090(2)	0.098(3)	0.075(2)	0.005(2)	0.003(2)	0.012(2)
C(25)	0.106(3)	0.109(3)	0.072(2)	-0.006(2)	0.028(2)	-0.023(3)
C(26)	0.085(2)	0.133(4)	0.079(2)	0.014(3)	0.016(2)	0.026(3)
C(27)	0.106(2)	0.068(2)	0.074(2)	-0.008(2)	0.030(2)	0.013(2)
C(28)	0.091(2)	0.072(2)	0.079(2)	-0.012(2)	0.022(2)	-0.007(2)
C(29)	0.100(2)	0.076(2)	0.084(2)	-0.011(2)	0.029(2)	-0.009(2)
C(30)	0.085(2)	0.114(3)	0.092(3)	0.006(3)	0.010(2)	-0.025(3)
C(31)	0.131(4)	0.118(4)	0.108(3)	0.002(3)	0.003(3)	-0.047(3)
C(32)	0.120(3)	0.091(3)	0.083(2)	-0.005(2)	0.024(2)	-0.026(3)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	0.7111(5)	0.6282(4)	-0.1927(4)	0.080
H(4A)	0.5116(6)	0.5547(4)	-0.1088(4)	0.080
H(5A)	0.4675(5)	0.6628(4)	0.0470(4)	0.080
H(6A)	0.5224(6)	0.7902(7)	-0.3348(5)	0.080
H(7A)	0.3239(5)	0.7094(6)	-0.2662(4)	0.080
H(8A)	0.2691(6)	0.8034(7)	-0.1044(5)	0.080
H(9A)	0.4361(7)	0.9527(5)	-0.0805(5)	0.080
H(10A)	0.5955(7)	0.9376(6)	-0.2186(6)	0.080
H(11A)	0.8634(4)	0.8248(4)	-0.1372(3)	0.080
H(12A)	0.9724(5)	0.9610(4)	-0.0609(4)	0.080
H(12B)	0.9545(5)	0.9792(4)	0.0564(4)	0.080
H(13A)	0.7786(5)	1.0868(5)	0.0157(4)	0.080
H(14A)	1.0274(6)	1.1396(5)	-0.0317(5)	0.080
H(14B)	0.9302(6)	1.2063(5)	0.0291(5)	0.080
H(15A)	0.9707(9)	1.2451(8)	-0.1606(6)	0.080
H(15B)	0.8455(9)	1.2851(8)	-0.1107(6)	0.080
H(16A)	0.7477(9)	1.1919(5)	-0.2236(5)	0.080
H(16B)	0.8714(9)	1.1279(5)	-0.2464(5)	0.080
H(19A)	1.1633(4)	0.6550(4)	0.5050(3)	0.080
H(20A)	1.2471(4)	0.8428(5)	0.4976(3)	0.080
H(21A)	1.0711(4)	0.9522(4)	0.4047(3)	0.080
H(22A)	0.9034(5)	0.9885(5)	0.6255(4)	0.080
H(23A)	1.1048(4)	0.9137(4)	0.7167(3)	0.080
H(24A)	1.0725(5)	0.7202(4)	0.7315(3)	0.080
H(25A)	0.8442(5)	0.6747(5)	0.6504(3)	0.080
H(26A)	0.7427(4)	0.8444(5)	0.5830(3)	0.080
H(27A)	0.8921(4)	0.5692(3)	0.4375(3)	0.080
H(28A)	0.6844(4)	0.5335(3)	0.3641(3)	0.080
H(28B)	0.6109(4)	0.6195(3)	0.2992(3)	0.080
H(29A)	0.5569(4)	0.6999(4)	0.4529(3)	0.080
H(30A)	0.4218(5)	0.5390(4)	0.3745(4)	0.080
H(30B)	0.3708(5)	0.6057(4)	0.4646(4)	0.080
H(31A)	0.5157(6)	0.4217(5)	0.4877(5)	0.080
H(31B)	0.3962(6)	0.4535(5)	0.5503(5)	0.080
H(32A)	0.5162(5)	0.5590(4)	0.6505(4)	0.080
H(32B)	0.6210(5)	0.4744(4)	0.6322(4)	0.080

Table for *syn*-(+)-(R_p,R,R,R_p)-7a·½CH₂Cl₂

Table 1. Atomic coordinates [$\times 10^5$ for Pd, Fe; $\times 10^4$ for other atoms] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.32083(2)	0.20170(3)	0.23261(3)	0.06966(12)
Pd(2)	0.35791(2)	0.44392(3)	0.55743(3)	0.06416(11)
Fe(1)	0.32085(4)	0.22784(8)	-0.00364(6)	0.0780(3)
Fe(2)	0.47879(4)	0.56923(7)	0.73925(6)	0.0726(2)
S(1)	0.25725(8)	0.35487(13)	0.23195(11)	0.0803(5)
S(2)	0.42301(8)	0.29408(12)	0.55662(11)	0.0848(5)
O(1)	0.5145(2)	0.0421(5)	0.2111(3)	0.104(2)
O(2)	0.3441(2)	0.7825(4)	0.4909(3)	0.100(2)
N(1)	0.3683(2)	0.0644(4)	0.2058(4)	0.082(2)
N(2)	0.3110(2)	0.5837(4)	0.5836(4)	0.077(2)
N(3)	0.3044(2)	0.4300(4)	0.4174(3)	0.0784(15)
N(4)	0.3749(2)	0.2173(4)	0.3724(4)	0.088(2)
C(1)	0.2768(2)	0.1823(5)	0.1006(4)	0.083(2)
C(2)	0.3006(3)	0.0925(5)	0.0549(5)	0.088(2)
C(3)	0.2688(4)	0.0894(7)	-0.0407(5)	0.106(3)
C(4)	0.2268(3)	0.1780(7)	-0.0594(5)	0.110(3)
C(5)	0.2281(3)	0.2361(7)	0.0247(5)	0.094(2)
C(6)	0.3818(2)	0.3525(4)	0.0514(3)	0.161(4)
C(7)	0.4208(2)	0.2613(4)	0.0422(4)	0.129(3)
C(8)	0.4056(3)	0.2318(5)	-0.0543(4)	0.123(3)
C(9)	0.3572(3)	0.3048(6)	-0.1047(3)	0.143(4)
C(10)	0.3425(2)	0.3794(5)	-0.0394(3)	0.148(3)
C(11)	0.3498(3)	0.0324(5)	0.1192(5)	0.083(2)
C(12)	0.4209(3)	0.0075(5)	0.2741(5)	0.082(2)
C(13)	0.4879(3)	0.0603(5)	0.2902(4)	0.086(2)
C(14)	0.5396(4)	0.0114(6)	0.3739(5)	0.102(3)
C(15)	0.6009(4)	0.0028(10)	0.3387(7)	0.138(4)
C(16)	0.5829(4)	0.0306(13)	0.2405(7)	0.211(7)
C(17)	0.4031(3)	0.4637(4)	0.6904(4)	0.068(2)
C(18)	0.3802(3)	0.5530(5)	0.7304(4)	0.076(2)
C(19)	0.4160(3)	0.5663(5)	0.8269(4)	0.087(2)
C(20)	0.4626(3)	0.4771(5)	0.8471(4)	0.084(2)
C(21)	0.4531(3)	0.4156(5)	0.7616(4)	0.080(2)
C(22)	0.5358(2)	0.5819(5)	0.6448(3)	0.128(3)
C(23)	0.4952(3)	0.6743(5)	0.6416(4)	0.144(4)
C(24)	0.5121(4)	0.7232(6)	0.7318(5)	0.163(4)
C(25)	0.5632(3)	0.6611(7)	0.7906(4)	0.156(4)
C(26)	0.5779(2)	0.5738(6)	0.7369(4)	0.143(3)
C(27)	0.3311(3)	0.6200(5)	0.6678(4)	0.074(2)
C(28)	0.2676(3)	0.6437(5)	0.5107(5)	0.079(2)
C(29)	0.3051(3)	0.6943(5)	0.4436(4)	0.076(2)
C(30)	0.2613(4)	0.7405(6)	0.3554(5)	0.099(2)
C(31)	0.2979(4)	0.8378(7)	0.3376(5)	0.117(3)
C(32)	0.3415(5)	0.8640(7)	0.4279(5)	0.165(4)
C(33)	0.2852(3)	0.4011(4)	0.3414(4)	0.067(2)
C(34)	0.3940(3)	0.2450(4)	0.4479(4)	0.073(2)
Cl(1)	0.07076(13)	0.3455(3)	0.0312(3)	0.1915(13)
C(1W)	0.5000	-0.0724(13)	0.0000	0.119(5)

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.942(6)	C(14)-C(15)	1.485(13)	C(1)-Fe(1)-C(9)	168.0(3)
Pd(1)-N(1)	2.060(5)	C(15)-C(16)	1.439(14)	C(2)-Fe(1)-C(7)	109.5(2)
Pd(1)-N(4)	2.090(5)	C(17)-C(18)	1.394(8)	C(4)-Fe(1)-C(7)	171.8(3)
Pd(1)-S(1)	2.318(2)	C(17)-C(21)	1.410(8)	C(3)-Fe(1)-C(7)	133.1(3)
Pd(2)-C(17)	1.962(6)	C(18)-C(19)	1.439(8)	C(10)-Fe(1)-C(7)	68.26(14)
Pd(2)-N(2)	2.075(5)	C(18)-C(27)	1.455(8)	C(6)-Fe(1)-C(7)	40.58(8)
Pd(2)-N(3)	2.089(5)	C(19)-C(20)	1.454(9)	C(1)-Fe(1)-C(7)	114.1(2)
Pd(2)-S(2)	2.305(2)	C(20)-C(21)	1.442(9)	C(9)-Fe(1)-C(7)	68.0(2)
Fe(1)-C(2)	1.984(7)	C(22)-C(23)	1.42	C(2)-Fe(1)-C(5)	69.6(3)
Fe(1)-C(4)	2.015(6)	C(22)-C(26)	1.42	C(4)-Fe(1)-C(5)	40.9(3)
Fe(1)-C(3)	2.038(8)	C(23)-C(24)	1.42	C(3)-Fe(1)-C(5)	68.9(3)
Fe(1)-C(10)	2.041(6)	C(24)-C(25)	1.42	C(10)-Fe(1)-C(5)	106.1(3)
Fe(1)-C(6)	2.041(4)	C(25)-C(26)	1.42	C(6)-Fe(1)-C(5)	113.4(3)
Fe(1)-C(1)	2.042(6)	C(28)-C(29)	1.530(9)	C(1)-Fe(1)-C(5)	42.0(2)
Fe(1)-C(9)	2.054(6)	C(29)-C(30)	1.501(8)	C(9)-Fe(1)-C(5)	130.0(3)
Fe(1)-C(7)	2.054(5)	C(30)-C(31)	1.486(12)	C(7)-Fe(1)-C(5)	146.6(2)
Fe(1)-C(5)	2.062(6)	C(31)-C(32)	1.444(10)	C(2)-Fe(1)-C(8)	117.6(3)
Fe(1)-C(8)	2.063(6)	Cl(1)-C(1W)#1	1.752(10)	C(4)-Fe(1)-C(8)	133.0(3)
Fe(2)-C(18)	2.020(6)	C(1W)-Cl(1)#2	1.752(10)	C(3)-Fe(1)-C(8)	111.3(3)
Fe(2)-C(23)	2.030(6)	C(1W)-Cl(1)#3	1.752(10)	C(10)-Fe(1)-C(8)	68.1(2)
Fe(2)-C(22)	2.033(5)			C(6)-Fe(1)-C(8)	68.10(14)
Fe(2)-C(17)	2.036(5)	C(1)-Pd(1)-N(1)	80.5(2)	C(1)-Fe(1)-C(8)	148.1(2)
Fe(2)-C(21)	2.037(6)	C(1)-Pd(1)-N(4)	175.5(2)	C(9)-Fe(1)-C(8)	40.35(12)
Fe(2)-C(19)	2.037(7)	N(1)-Pd(1)-N(4)	95.7(2)	C(7)-Fe(1)-C(8)	40.35(11)
Fe(2)-C(20)	2.048(6)	C(1)-Pd(1)-S(1)	88.4(2)	C(5)-Fe(1)-C(8)	169.9(3)
Fe(2)-C(24)	2.053(7)	N(1)-Pd(1)-S(1)	168.87(14)	C(18)-Fe(2)-C(23)	111.0(2)
Fe(2)-C(26)	2.058(5)	N(4)-Pd(1)-S(1)	95.40(14)	C(18)-Fe(2)-C(22)	135.0(2)
Fe(2)-C(25)	2.071(6)	C(17)-Pd(2)-N(2)	80.9(2)	C(23)-Fe(2)-C(22)	40.92(10)
S(1)-C(33)	1.670(6)	C(17)-Pd(2)-N(3)	175.9(2)	C(18)-Fe(2)-C(17)	40.2(2)
S(2)-C(34)	1.676(6)	N(2)-Pd(2)-N(3)	95.3(2)	C(23)-Fe(2)-C(17)	114.6(2)
O(1)-C(16)	1.381(9)	C(17)-Pd(2)-S(2)	88.3(2)	C(22)-Fe(2)-C(17)	109.5(2)
O(1)-C(13)	1.418(8)	N(2)-Pd(2)-S(2)	169.05(13)	C(18)-Fe(2)-C(21)	67.5(2)
O(2)-C(32)	1.366(9)	N(3)-Pd(2)-S(2)	95.59(14)	C(23)-Fe(2)-C(21)	144.7(3)
O(2)-C(29)	1.439(7)	C(2)-Fe(1)-C(4)	68.2(3)	C(22)-Fe(2)-C(21)	113.6(3)
N(1)-C(11)	1.296(8)	C(2)-Fe(1)-C(3)	40.6(3)	C(17)-Fe(2)-C(21)	40.5(2)
N(1)-C(12)	1.469(7)	C(4)-Fe(1)-C(3)	40.2(3)	C(18)-Fe(2)-C(19)	41.5(2)
N(2)-C(27)	1.286(7)	C(2)-Fe(1)-C(10)	169.1(3)	C(23)-Fe(2)-C(19)	134.3(2)
N(2)-C(28)	1.428(7)	C(4)-Fe(1)-C(10)	115.6(3)	C(22)-Fe(2)-C(19)	174.9(2)
N(3)-C(33)	1.146(7)	C(3)-Fe(1)-C(10)	148.4(2)	C(17)-Fe(2)-C(19)	70.0(2)
N(4)-C(34)	1.135(7)	C(2)-Fe(1)-C(6)	130.8(2)	C(21)-Fe(2)-C(19)	69.5(3)
C(1)-C(2)	1.452(9)	C(4)-Fe(1)-C(6)	146.9(3)	C(18)-Fe(2)-C(20)	69.0(3)
C(1)-C(5)	1.470(8)	C(3)-Fe(1)-C(6)	170.7(2)	C(23)-Fe(2)-C(20)	173.9(3)
C(2)-C(3)	1.396(9)	C(10)-Fe(1)-C(6)	40.72(10)	C(22)-Fe(2)-C(20)	143.3(2)
C(2)-C(11)	1.421(8)	C(2)-Fe(1)-C(1)	42.2(3)	C(17)-Fe(2)-C(20)	69.6(2)
C(3)-C(4)	1.392(11)	C(4)-Fe(1)-C(1)	69.8(3)	C(21)-Fe(2)-C(20)	41.3(2)
C(4)-C(5)	1.425(10)	C(3)-Fe(1)-C(1)	70.2(3)	C(19)-Fe(2)-C(20)	41.7(3)
C(6)-C(7)	1.42	C(10)-Fe(1)-C(1)	128.0(3)	C(18)-Fe(2)-C(24)	115.9(3)
C(6)-C(10)	1.42	C(6)-Fe(1)-C(1)	105.2(2)	C(23)-Fe(2)-C(24)	40.70(13)
C(7)-C(8)	1.42	C(2)-Fe(1)-C(9)	149.5(3)	C(22)-Fe(2)-C(24)	68.4(2)
C(8)-C(9)	1.42	C(4)-Fe(1)-C(9)	109.7(3)	C(17)-Fe(2)-C(24)	145.6(3)
C(9)-C(10)	1.42	C(3)-Fe(1)-C(9)	117.8(3)	C(21)-Fe(2)-C(24)	173.4(3)
C(12)-C(13)	1.500(9)	C(10)-Fe(1)-C(9)	40.58(12)	C(19)-Fe(2)-C(24)	108.9(3)
C(13)-C(14)	1.542(9)	C(6)-Fe(1)-C(9)	68.3(2)	C(20)-Fe(2)-C(24)	133.4(3)

C(18)-Fe(2)-C(26)	173.8(3)	C(4)-C(3)-C(2)	107.1(7)	C(17)-C(18)-Fe(2)	70.5(3)
C(23)-Fe(2)-C(26)	68.4(2)	C(4)-C(3)-Fe(1)	69.1(4)	C(19)-C(18)-Fe(2)	69.9(4)
C(22)-Fe(2)-C(26)	40.62(10)	C(2)-C(3)-Fe(1)	67.6(4)	C(27)-C(18)-Fe(2)	121.4(4)
C(17)-Fe(2)-C(26)	134.0(3)	C(3)-C(4)-C(5)	110.8(6)	C(18)-C(19)-C(20)	105.6(5)
C(21)-Fe(2)-C(26)	109.2(3)	C(3)-C(4)-Fe(1)	70.8(4)	C(18)-C(19)-Fe(2)	68.6(4)
C(19)-Fe(2)-C(26)	143.2(2)	C(5)-C(4)-Fe(1)	71.3(4)	C(20)-C(19)-Fe(2)	69.5(4)
C(20)-Fe(2)-C(26)	112.3(2)	C(4)-C(5)-C(1)	106.7(6)	C(21)-C(20)-C(19)	106.7(5)
C(24)-Fe(2)-C(26)	68.0(2)	C(4)-C(5)-Fe(1)	67.8(4)	C(21)-C(20)-Fe(2)	68.9(4)
C(18)-Fe(2)-C(25)	145.8(3)	C(1)-C(5)-Fe(1)	68.3(3)	C(19)-C(20)-Fe(2)	68.8(4)
C(23)-Fe(2)-C(25)	68.2(2)	C(7)-C(6)-C(10)	108.0	C(17)-C(21)-C(20)	109.7(5)
C(22)-Fe(2)-C(25)	68.1(2)	C(7)-C(6)-Fe(1)	70.2(2)	C(17)-C(21)-Fe(2)	69.7(3)
C(17)-Fe(2)-C(25)	173.2(3)	C(10)-C(6)-Fe(1)	69.6(2)	C(20)-C(21)-Fe(2)	69.7(4)
C(21)-Fe(2)-C(25)	133.8(3)	C(8)-C(7)-C(6)	108.0	C(23)-C(22)-C(26)	108.0
C(19)-Fe(2)-C(25)	113.0(2)	C(8)-C(7)-Fe(1)	70.1(2)	C(23)-C(22)-Fe(2)	69.4(2)
C(20)-Fe(2)-C(25)	108.2(3)	C(6)-C(7)-Fe(1)	69.2(2)	C(26)-C(22)-Fe(2)	70.7(2)
C(24)-Fe(2)-C(25)	40.28(13)	C(9)-C(8)-C(7)	108.0	C(24)-C(23)-C(22)	108.0
C(26)-Fe(2)-C(25)	40.23(11)	C(9)-C(8)-Fe(1)	69.5(2)	C(24)-C(23)-Fe(2)	70.5(2)
C(33)-S(1)-Pd(1)	102.6(2)	C(7)-C(8)-Fe(1)	69.5(2)	C(22)-C(23)-Fe(2)	69.7(2)
C(34)-S(2)-Pd(2)	103.1(2)	C(8)-C(9)-C(10)	108.0	C(23)-C(24)-C(25)	108.0
C(16)-O(1)-C(13)	109.4(6)	C(8)-C(9)-Fe(1)	70.1(2)	C(23)-C(24)-Fe(2)	68.8(2)
C(32)-O(2)-C(29)	108.5(5)	C(10)-C(9)-Fe(1)	69.2(2)	C(25)-C(24)-Fe(2)	70.5(2)
C(11)-N(1)-C(12)	120.8(5)	C(9)-C(10)-C(6)	108.0	C(24)-C(25)-C(26)	108.0
C(11)-N(1)-Pd(1)	113.7(4)	C(9)-C(10)-Fe(1)	70.2(2)	C(24)-C(25)-Fe(2)	69.2(2)
C(12)-N(1)-Pd(1)	125.5(4)	C(6)-C(10)-Fe(1)	69.6(2)	C(26)-C(25)-Fe(2)	69.4(2)
C(27)-N(2)-C(28)	122.0(5)	N(1)-C(11)-C(2)	118.7(6)	C(25)-C(26)-C(22)	108.0
C(27)-N(2)-Pd(2)	114.7(4)	N(1)-C(12)-C(13)	113.4(5)	C(25)-C(26)-Fe(2)	70.4(2)
C(28)-N(2)-Pd(2)	122.6(4)	O(1)-C(13)-C(12)	109.2(5)	C(22)-C(26)-Fe(2)	68.7(2)
C(33)-N(3)-Pd(2)	163.1(5)	O(1)-C(13)-C(14)	104.9(6)	N(2)-C(27)-C(18)	114.5(5)
C(34)-N(4)-Pd(1)	163.9(5)	C(12)-C(13)-C(14)	112.7(6)	N(2)-C(28)-C(29)	111.9(5)
C(2)-C(1)-C(5)	104.5(5)	C(15)-C(14)-C(13)	103.7(6)	O(2)-C(29)-C(30)	105.6(5)
C(2)-C(1)-Pd(1)	115.3(4)	C(16)-C(15)-C(14)	107.2(7)	O(2)-C(29)-C(28)	108.5(5)
C(5)-C(1)-Pd(1)	140.0(5)	O(1)-C(16)-C(15)	109.5(8)	C(30)-C(29)-C(28)	114.8(5)
C(2)-C(1)-Fe(1)	66.7(4)	C(18)-C(17)-C(21)	107.0(5)	C(31)-C(30)-C(29)	103.9(5)
C(5)-C(1)-Fe(1)	69.8(4)	C(18)-C(17)-Pd(2)	112.9(4)	C(32)-C(31)-C(30)	104.7(7)
Pd(1)-C(1)-Fe(1)	121.7(2)	C(21)-C(17)-Pd(2)	140.1(4)	O(2)-C(32)-C(31)	111.4(7)
C(3)-C(2)-C(11)	137.5(7)	C(18)-C(17)-Fe(2)	69.3(3)	N(3)-C(33)-S(1)	178.1(5)
C(3)-C(2)-C(1)	110.8(6)	C(21)-C(17)-Fe(2)	69.8(3)	N(4)-C(34)-S(2)	176.2(6)
C(11)-C(2)-C(1)	111.6(5)	Pd(2)-C(17)-Fe(2)	124.7(3)	Cl(1)#2-C(1W)-	108.5(9)
C(3)-C(2)-Fe(1)	71.8(4)	C(17)-C(18)-C(19)	111.1(5)	Cl(1)#3	
C(11)-C(2)-Fe(1)	123.0(4)	C(17)-C(18)-C(27)	116.8(5)		
C(1)-C(2)-Fe(1)	71.0(4)	C(19)-C(18)-C(27)	131.8(6)		

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.0661(2)	0.0697(2)	0.0750(2)	-0.0042(2)	0.0207(2)	-0.0002(2)
Pd(2)	0.0586(2)	0.0551(2)	0.0771(2)	-0.0021(2)	0.0131(2)	0.0041(2)
Fe(1)	0.0596(4)	0.0966(6)	0.0756(4)	-0.0171(4)	0.0119(3)	-0.0144(4)
Fe(2)	0.0628(4)	0.0715(4)	0.0785(5)	0.0032(4)	0.0076(4)	-0.0011(4)
S(1)	0.0842(9)	0.0774(8)	0.0739(8)	0.0055(7)	0.0092(7)	0.0127(8)
S(2)	0.0915(9)	0.0773(8)	0.0770(9)	-0.0045(7)	0.0039(8)	0.0307(8)
O(1)	0.071(2)	0.158(4)	0.079(3)	-0.006(3)	0.014(2)	-0.004(3)
O(2)	0.085(2)	0.089(3)	0.111(3)	0.001(2)	-0.008(2)	-0.022(2)
N(1)	0.069(2)	0.074(3)	0.109(3)	-0.006(3)	0.030(2)	-0.014(2)
N(2)	0.059(2)	0.070(3)	0.100(3)	0.009(3)	0.014(2)	0.012(2)
N(3)	0.080(3)	0.063(2)	0.090(3)	-0.006(2)	0.018(2)	0.005(2)
N(4)	0.090(3)	0.078(3)	0.092(3)	-0.014(3)	0.013(2)	0.036(2)
C(1)	0.039(2)	0.101(4)	0.106(4)	-0.026(3)	0.008(2)	-0.027(3)
C(2)	0.071(3)	0.082(3)	0.104(4)	-0.036(3)	0.011(3)	-0.005(3)
C(3)	0.102(4)	0.109(5)	0.099(4)	-0.027(4)	0.008(4)	-0.035(4)
C(4)	0.078(3)	0.153(6)	0.090(4)	-0.031(4)	0.003(3)	-0.043(4)
C(5)	0.058(3)	0.123(6)	0.099(4)	0.002(4)	0.020(3)	-0.006(3)
C(6)	0.130(5)	0.146(6)	0.226(8)	-0.076(6)	0.080(6)	-0.074(5)
C(7)	0.089(4)	0.203(8)	0.086(4)	0.004(5)	0.006(4)	-0.061(5)
C(8)	0.083(4)	0.133(6)	0.164(6)	-0.029(5)	0.054(4)	-0.023(4)
C(9)	0.084(4)	0.232(10)	0.114(6)	0.012(6)	0.027(4)	-0.049(6)
C(10)	0.107(4)	0.120(6)	0.248(8)	0.062(6)	0.099(5)	0.031(4)
C(11)	0.069(3)	0.070(3)	0.118(4)	-0.023(3)	0.040(3)	-0.029(3)
C(12)	0.086(3)	0.069(3)	0.098(4)	0.010(3)	0.038(3)	0.010(3)
C(13)	0.104(4)	0.065(3)	0.083(4)	-0.012(3)	0.011(3)	0.006(3)
C(14)	0.127(5)	0.075(4)	0.086(4)	-0.001(3)	-0.006(4)	-0.002(4)
C(15)	0.086(5)	0.163(8)	0.147(7)	-0.005(7)	-0.008(5)	0.014(5)
C(16)	0.069(5)	0.400(21)	0.151(8)	0.094(10)	0.004(5)	-0.003(8)
C(17)	0.065(3)	0.049(3)	0.094(3)	-0.005(2)	0.025(2)	0.002(2)
C(18)	0.075(3)	0.076(3)	0.078(3)	-0.002(3)	0.022(3)	0.000(3)
C(19)	0.102(4)	0.077(3)	0.077(4)	-0.013(3)	0.014(3)	0.001(4)
C(20)	0.098(4)	0.083(4)	0.068(3)	0.009(3)	0.014(3)	0.001(3)
C(21)	0.081(3)	0.076(4)	0.079(3)	0.002(3)	0.014(3)	0.002(3)
C(22)	0.120(4)	0.153(7)	0.137(5)	0.002(5)	0.079(4)	-0.030(5)
C(23)	0.101(5)	0.186(8)	0.140(6)	0.067(6)	0.022(4)	-0.024(6)
C(24)	0.105(4)	0.114(6)	0.291(10)	0.048(7)	0.089(5)	-0.017(4)
C(25)	0.115(5)	0.206(10)	0.154(7)	-0.041(7)	0.044(5)	-0.061(6)
C(26)	0.061(3)	0.214(8)	0.158(6)	0.093(6)	0.035(4)	0.008(5)
C(27)	0.062(3)	0.068(3)	0.095(4)	-0.012(3)	0.027(3)	0.004(3)
C(28)	0.059(3)	0.073(3)	0.099(4)	0.000(3)	0.004(3)	0.004(3)
C(29)	0.065(3)	0.065(3)	0.091(4)	-0.006(3)	0.005(3)	0.006(3)
C(30)	0.097(4)	0.086(4)	0.095(4)	-0.010(4)	-0.011(4)	0.008(4)
C(31)	0.143(6)	0.124(6)	0.072(4)	-0.001(4)	0.005(4)	-0.023(6)
C(32)	0.273(10)	0.117(5)	0.078(5)	0.013(4)	-0.004(6)	-0.103(6)
C(33)	0.059(3)	0.061(3)	0.078(3)	0.000(3)	0.014(2)	-0.004(2)
C(34)	0.063(3)	0.065(3)	0.093(4)	0.015(3)	0.025(3)	0.020(2)
Cl(1)	0.1227(15)	0.195(2)	0.275(3)	0.113(2)	0.083(2)	0.046(2)
C(1W)	0.082(6)	0.150(10)	0.123(8)	0.000	0.023(6)	0.000

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3)	0.2746(4)	0.0378(7)	-0.0838(5)	0.127
H(4)	0.2013(3)	0.1968(7)	-0.1187(5)	0.132
H(5)	0.2029(3)	0.2965(7)	0.0304(5)	0.112
H(6)	0.3820(2)	0.3884(4)	0.1070(3)	0.193
H(7)	0.4511(3)	0.2270(5)	0.0908(5)	0.154
H(8)	0.4241(4)	0.1747(6)	-0.0799(6)	0.147
H(9)	0.3383(4)	0.3038(8)	-0.1691(3)	0.171
H(10)	0.3124(3)	0.4359(6)	-0.0536(5)	0.178
H(11)	0.3684(3)	-0.0287(5)	0.0996(5)	0.099
H(12A)	0.4243(3)	-0.0651(5)	0.2519(5)	0.098
H(12B)	0.4083(3)	0.0030(5)	0.3335(5)	0.098
H(13)	0.4837(3)	0.1374(5)	0.3000(4)	0.103
H(14A)	0.5468(4)	0.0577(6)	0.4286(5)	0.122
H(14B)	0.5253(4)	-0.0585(6)	0.3903(5)	0.122
H(15A)	0.6349(4)	0.0513(10)	0.3730(7)	0.166
H(15B)	0.6183(4)	-0.0697(10)	0.3469(7)	0.166
H(16A)	0.6045(4)	0.0971(13)	0.2306(7)	0.253
H(16B)	0.5977(4)	-0.0251(13)	0.2041(7)	0.253
H(19)	0.4106(3)	0.6205(5)	0.8679(4)	0.104
H(20)	0.4927(3)	0.4625(5)	0.9041(4)	0.101
H(21)	0.4763(3)	0.3536(5)	0.7544(4)	0.095
H(22)	0.5351(2)	0.5350(5)	0.5952(3)	0.154
H(23)	0.4631(3)	0.6985(6)	0.5896(5)	0.172
H(24)	0.4931(5)	0.7851(6)	0.7492(7)	0.195
H(25)	0.5835(5)	0.6752(9)	0.8534(4)	0.188
H(26)	0.6095(3)	0.5206(7)	0.7582(5)	0.172
H(27)	0.3155(3)	0.6839(5)	0.6872(4)	0.088
H(28A)	0.2462(3)	0.6997(5)	0.5387(5)	0.095
H(28B)	0.2330(3)	0.5968(5)	0.4755(5)	0.095
H(29)	0.3350(3)	0.6408(5)	0.4268(4)	0.092
H(30A)	0.2558(4)	0.6903(6)	0.3036(5)	0.118
H(30B)	0.2178(4)	0.7591(6)	0.3645(5)	0.118
H(31A)	0.3235(4)	0.8232(7)	0.2917(5)	0.140
H(31B)	0.2672(4)	0.8962(7)	0.3148(5)	0.140
H(32A)	0.3860(5)	0.8781(7)	0.4202(5)	0.197
H(32B)	0.3255(5)	0.9285(7)	0.4521(5)	0.197

Tables for *syn*-($-$)-(S_p,S,S,S_p)-7a·½CH₂Cl₂Table 1. Atomic coordinates [$\times 10^5$ for Pd, Fe; $\times 10^4$ for other atoms] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.142067(11)	0.43200(2)	0.94272(2)	0.06073(7)
Pd(2)	0.179263(12)	0.67401(2)	1.26771(2)	0.06593(8)
Fe(1)	0.02090(2)	0.30641(4)	0.76050(4)	0.0699(2)
Fe(2)	0.17916(2)	0.64731(5)	1.50374(4)	0.0741(2)
S(1)	0.24316(5)	0.52113(8)	1.26817(7)	0.0765(3)
S(2)	0.07673(5)	0.58205(8)	0.94384(8)	0.0831(3)
O(1)	0.15698(14)	0.0933(2)	1.0086(2)	0.0990(11)
O(2)	-0.01412(12)	0.8313(3)	1.2908(2)	0.0979(11)
N(1)	0.18884(12)	0.2928(2)	0.9165(2)	0.0666(9)
N(2)	0.13150(14)	0.8115(2)	1.2964(2)	0.0748(9)
N(3)	0.19551(14)	0.4473(2)	1.0836(2)	0.0719(9)
N(4)	0.1252(2)	0.6617(3)	1.1262(2)	0.0843(11)
C(1)	0.09704(15)	0.4118(2)	0.8100(2)	0.0594(10)
C(2)	0.1192(2)	0.3205(3)	0.7684(3)	0.0724(11)
C(3)	0.0842(2)	0.3104(3)	0.6724(3)	0.0809(12)
C(4)	0.0383(2)	0.3968(3)	0.6530(3)	0.0794(13)
C(5)	0.0452(2)	0.4598(3)	0.7353(3)	0.0742(12)
C(6)	-0.0138(3)	0.1537(5)	0.7661(5)	0.161(3)
C(7)	-0.0606(2)	0.2179(7)	0.7154(4)	0.159(3)
C(8)	-0.0770(2)	0.2988(5)	0.7645(4)	0.132(2)
C(9)	-0.0358(2)	0.2885(5)	0.8547(4)	0.138(2)
C(10)	0.0023(2)	0.1963(5)	0.8505(4)	0.128(2)
C(11)	0.1678(2)	0.2558(3)	0.8343(3)	0.0718(11)
C(12)	0.2328(2)	0.2293(3)	0.9887(3)	0.0715(12)
C(13)	0.1946(2)	0.1810(3)	1.0564(3)	0.0775(12)
C(14)	0.2392(2)	0.1350(3)	1.1466(3)	0.0867(14)
C(15)	0.2025(3)	0.0362(4)	1.1624(3)	0.111(2)
C(16)	0.1587(3)	0.0120(4)	1.0708(4)	0.155(2)
C(17)	0.2247(2)	0.6921(3)	1.4011(3)	0.0748(12)
C(18)	0.1998(2)	0.7846(3)	1.4418(3)	0.0769(12)
C(19)	0.2314(2)	0.7858(4)	1.5404(3)	0.107(2)
C(20)	0.2738(2)	0.6973(4)	1.5609(3)	0.104(2)
C(21)	0.2706(2)	0.6394(4)	1.4753(3)	0.092(2)
C(22)	0.1576(2)	0.4962(5)	1.5379(5)	0.158(3)
C(23)	0.1410(2)	0.5681(6)	1.5989(4)	0.136(2)
C(24)	0.0964(2)	0.6419(4)	1.5546(4)	0.109(2)
C(25)	0.0818(2)	0.6100(5)	1.4633(4)	0.117(2)
C(26)	0.1161(2)	0.5279(4)	1.4505(4)	0.155(2)
C(27)	0.1490(2)	0.8461(3)	1.3801(3)	0.0826(13)
C(28)	0.0780(2)	0.8676(3)	1.2247(3)	0.0790(13)
C(29)	0.0133(2)	0.8153(3)	1.2107(3)	0.0748(12)
C(30)	-0.0386(2)	0.8660(4)	1.1258(3)	0.097(2)
C(31)	-0.1007(3)	0.8694(5)	1.1593(4)	0.134(2)
C(32)	-0.0811(2)	0.8414(7)	1.2567(4)	0.180(4)
C(33)	0.2155(2)	0.4762(3)	1.1599(3)	0.0656(10)
C(34)	0.1054(2)	0.6298(3)	1.0510(3)	0.0682(11)
Cl(1)	0.42899(7)	0.5304(2)	1.46881(15)	0.1825(8)
C(35)	0.5000	0.4479(7)	1.5000	0.113(3)

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(1)	1.957(3)	C(14)-C(15)	1.493(7)	C(7)-Fe(1)-C(1)	173.0(2)
Pd(1)-N(1)	2.068(3)	C(15)-C(16)	1.456(7)	C(10)-Fe(1)-C(1)	117.5(2)
Pd(1)-N(3)	2.099(3)	C(17)-C(21)	1.418(5)	C(2)-Fe(1)-C(1)	41.00(14)
Pd(1)-S(2)	2.3093(11)	C(17)-C(18)	1.450(6)	C(9)-Fe(1)-C(1)	110.5(2)
Pd(2)-C(17)	1.965(4)	C(18)-C(27)	1.430(5)	C(5)-Fe(1)-C(1)	41.98(13)
Pd(2)-N(2)	2.072(3)	C(18)-C(19)	1.434(6)	C(8)-Fe(1)-C(1)	134.6(2)
Pd(2)-N(4)	2.108(3)	C(19)-C(20)	1.395(7)	C(4)-Fe(1)-C(1)	69.72(14)
Pd(2)-S(1)	2.3177(11)	C(20)-C(21)	1.436(7)	C(7)-Fe(1)-C(6)	38.6(3)
Fe(1)-C(7)	1.986(6)	C(22)-C(23)	1.368(9)	C(10)-Fe(1)-C(6)	37.8(3)
Fe(1)-C(10)	2.005(6)	C(22)-C(26)	1.413(8)	C(2)-Fe(1)-C(6)	116.0(2)
Fe(1)-C(2)	2.013(4)	C(23)-C(24)	1.351(7)	C(9)-Fe(1)-C(6)	66.7(3)
Fe(1)-C(9)	2.029(6)	C(24)-C(25)	1.359(7)	C(5)-Fe(1)-C(6)	171.2(2)
Fe(1)-C(5)	2.035(4)	C(25)-C(26)	1.284(8)	C(8)-Fe(1)-C(6)	66.1(3)
Fe(1)-C(8)	2.038(5)	C(28)-C(29)	1.455(5)	C(4)-Fe(1)-C(6)	132.5(2)
Fe(1)-C(4)	2.041(4)	C(29)-C(30)	1.564(5)	C(1)-Fe(1)-C(6)	146.4(2)
Fe(1)-C(1)	2.042(3)	C(30)-C(31)	1.480(8)	C(7)-Fe(1)-C(3)	114.9(2)
Fe(1)-C(6)	2.044(6)	C(31)-C(32)	1.428(9)	C(10)-Fe(1)-C(3)	133.2(2)
Fe(1)-C(3)	2.051(4)	Cl(1)-C(35)	1.758(5)	C(2)-Fe(1)-C(3)	40.97(14)
Fe(2)-C(25)	2.006(4)	C(35)-Cl(1)#1	1.758(5)	C(9)-Fe(1)-C(3)	173.7(2)
Fe(2)-C(26)	2.006(5)			C(5)-Fe(1)-C(3)	68.9(2)
Fe(2)-C(23)	2.021(6)	C(1)-Pd(1)-N(1)	80.60(12)	C(8)-Fe(1)-C(3)	143.9(2)
Fe(2)-C(24)	2.026(5)	C(1)-Pd(1)-N(3)	176.21(12)	C(4)-Fe(1)-C(3)	40.5(2)
Fe(2)-C(22)	2.027(7)	N(1)-Pd(1)-N(3)	95.87(11)	C(1)-Fe(1)-C(3)	69.81(14)
Fe(2)-C(20)	2.028(4)	C(1)-Pd(1)-S(2)	88.58(10)	C(6)-Fe(1)-C(3)	109.4(2)
Fe(2)-C(18)	2.031(4)	N(1)-Pd(1)-S(2)	169.06(8)	C(25)-Fe(2)-C(26)	37.3(2)
Fe(2)-C(21)	2.034(4)	N(3)-Pd(1)-S(2)	94.99(9)	C(25)-Fe(2)-C(23)	63.8(2)
Fe(2)-C(17)	2.038(4)	C(17)-Pd(2)-N(2)	80.67(14)	C(26)-Fe(2)-C(23)	65.2(2)
Fe(2)-C(19)	2.038(5)	C(17)-Pd(2)-N(4)	176.01(14)	C(25)-Fe(2)-C(24)	39.4(2)
S(1)-C(33)	1.648(4)	N(2)-Pd(2)-N(4)	95.54(12)	C(26)-Fe(2)-C(24)	66.0(2)
S(2)-C(34)	1.649(4)	C(17)-Pd(2)-S(1)	87.63(12)	C(23)-Fe(2)-C(24)	39.0(2)
O(1)-C(16)	1.358(6)	N(2)-Pd(2)-S(1)	168.27(8)	C(25)-Fe(2)-C(22)	66.0(2)
O(1)-C(13)	1.423(5)	N(4)-Pd(2)-S(1)	96.14(9)	C(26)-Fe(2)-C(22)	41.0(2)
O(2)-C(32)	1.357(5)	C(7)-Fe(1)-C(10)	63.6(2)	C(23)-Fe(2)-C(22)	39.5(3)
O(2)-C(29)	1.437(5)	C(7)-Fe(1)-C(2)	145.9(2)	C(24)-Fe(2)-C(22)	67.8(2)
N(1)-C(11)	1.264(5)	C(10)-Fe(1)-C(2)	112.0(2)	C(25)-Fe(2)-C(20)	171.3(2)
N(1)-C(12)	1.450(4)	C(7)-Fe(1)-C(9)	65.4(2)	C(26)-Fe(2)-C(20)	149.0(2)
N(2)-C(27)	1.267(5)	C(10)-Fe(1)-C(9)	40.7(2)	C(23)-Fe(2)-C(20)	111.4(2)
N(2)-C(28)	1.499(5)	C(2)-Fe(1)-C(9)	135.4(2)	C(24)-Fe(2)-C(20)	132.3(2)
N(3)-C(33)	1.152(4)	C(7)-Fe(1)-C(5)	133.6(2)	C(22)-Fe(2)-C(20)	115.6(2)
N(4)-C(34)	1.150(5)	C(10)-Fe(1)-C(5)	149.2(2)	C(25)-Fe(2)-C(18)	111.6(2)
C(1)-C(2)	1.420(5)	C(2)-Fe(1)-C(5)	68.79(15)	C(26)-Fe(2)-C(18)	129.7(2)
C(1)-C(5)	1.460(4)	C(9)-Fe(1)-C(5)	115.9(2)	C(23)-Fe(2)-C(18)	151.7(2)
C(2)-C(3)	1.423(5)	C(7)-Fe(1)-C(8)	38.6(3)	C(24)-Fe(2)-C(18)	118.7(2)
C(2)-C(11)	1.456(5)	C(10)-Fe(1)-C(8)	66.3(2)	C(22)-Fe(2)-C(18)	167.6(2)
C(3)-C(4)	1.417(5)	C(2)-Fe(1)-C(8)	174.7(2)	C(20)-Fe(2)-C(18)	68.9(2)
C(4)-C(5)	1.418(5)	C(9)-Fe(1)-C(8)	40.1(2)	C(25)-Fe(2)-C(21)	147.3(2)
C(6)-C(10)	1.313(9)	C(5)-Fe(1)-C(8)	109.8(2)	C(26)-Fe(2)-C(21)	115.5(2)
C(6)-C(7)	1.332(9)	C(7)-Fe(1)-C(4)	110.2(2)	C(23)-Fe(2)-C(21)	131.1(2)
C(7)-C(8)	1.331(10)	C(10)-Fe(1)-C(4)	170.1(2)	C(24)-Fe(2)-C(21)	169.5(2)
C(8)-C(9)	1.393(7)	C(2)-Fe(1)-C(4)	68.3(2)	C(22)-Fe(2)-C(21)	106.1(2)
C(9)-C(10)	1.403(8)	C(9)-Fe(1)-C(4)	145.8(2)	C(20)-Fe(2)-C(21)	41.4(2)
C(12)-C(13)	1.534(6)	C(5)-Fe(1)-C(4)	40.7(2)	C(18)-Fe(2)-C(21)	69.1(2)
C(13)-C(14)	1.527(5)	C(8)-Fe(1)-C(4)	114.3(2)	C(25)-Fe(2)-C(17)	117.1(2)

C(26)-Fe(2)-C(17)	106.8(2)	C(4)-C(3)-C(2)	106.5(3)	C(19)-C(18)-C(17)	107.7(3)
C(23)-Fe(2)-C(17)	166.5(2)	C(4)-C(3)-Fe(1)	69.4(2)	C(27)-C(18)-Fe(2)	122.3(3)
C(24)-Fe(2)-C(17)	149.8(2)	C(2)-C(3)-Fe(1)	68.1(2)	C(19)-C(18)-Fe(2)	69.6(3)
C(22)-Fe(2)-C(17)	127.3(2)	C(3)-C(4)-C(5)	109.1(3)	C(17)-C(18)-Fe(2)	69.4(2)
C(20)-Fe(2)-C(17)	69.4(2)	C(3)-C(4)-Fe(1)	70.1(2)	C(20)-C(19)-C(18)	108.4(4)
C(18)-Fe(2)-C(17)	41.7(2)	C(5)-C(4)-Fe(1)	69.4(2)	C(20)-C(19)-Fe(2)	69.5(3)
C(21)-Fe(2)-C(17)	40.8(2)	C(4)-C(5)-C(1)	108.3(3)	C(18)-C(19)-Fe(2)	69.1(2)
C(25)-Fe(2)-C(19)	134.6(2)	C(4)-C(5)-Fe(1)	69.8(2)	C(19)-C(20)-C(21)	108.5(4)
C(26)-Fe(2)-C(19)	169.4(2)	C(1)-C(5)-Fe(1)	69.2(2)	C(19)-C(20)-Fe(2)	70.4(3)
C(23)-Fe(2)-C(19)	120.2(2)	C(10)-C(6)-C(7)	105.4(6)	C(21)-C(20)-Fe(2)	69.5(2)
C(24)-Fe(2)-C(19)	111.8(2)	C(10)-C(6)-Fe(1)	69.5(4)	C(17)-C(21)-C(20)	108.5(4)
C(22)-Fe(2)-C(19)	149.0(2)	C(7)-C(6)-Fe(1)	68.4(4)	C(17)-C(21)-Fe(2)	69.8(2)
C(20)-Fe(2)-C(19)	40.1(2)	C(8)-C(7)-C(6)	113.5(6)	C(20)-C(21)-Fe(2)	69.1(2)
C(18)-Fe(2)-C(19)	41.3(2)	C(8)-C(7)-Fe(1)	72.8(4)	C(23)-C(22)-C(26)	102.5(5)
C(21)-Fe(2)-C(19)	68.7(2)	C(6)-C(7)-Fe(1)	73.1(3)	C(23)-C(22)-Fe(2)	70.0(4)
C(17)-Fe(2)-C(19)	69.6(2)	C(7)-C(8)-C(9)	105.5(5)	C(26)-C(22)-Fe(2)	68.7(4)
C(33)-S(1)-Pd(2)	102.37(13)	C(7)-C(8)-Fe(1)	68.6(3)	C(24)-C(23)-C(22)	112.5(5)
C(34)-S(2)-Pd(1)	103.04(12)	C(9)-C(8)-Fe(1)	69.6(3)	C(24)-C(23)-Fe(2)	70.7(3)
C(16)-O(1)-C(13)	108.8(3)	C(8)-C(9)-C(10)	104.6(5)	C(22)-C(23)-Fe(2)	70.5(4)
C(32)-O(2)-C(29)	106.4(4)	C(8)-C(9)-Fe(1)	70.3(3)	C(23)-C(24)-C(25)	103.6(5)
C(11)-N(1)-C(12)	120.3(3)	C(10)-C(9)-Fe(1)	68.8(3)	C(23)-C(24)-Fe(2)	70.3(3)
C(11)-N(1)-Pd(1)	114.7(2)	C(6)-C(10)-C(9)	110.9(5)	C(25)-C(24)-Fe(2)	69.5(3)
C(12)-N(1)-Pd(1)	124.1(2)	C(6)-C(10)-Fe(1)	72.7(4)	C(26)-C(25)-C(24)	112.4(5)
C(27)-N(2)-C(28)	120.4(3)	C(9)-C(10)-Fe(1)	70.5(3)	C(26)-C(25)-Fe(2)	71.3(3)
C(27)-N(2)-Pd(2)	116.2(2)	N(1)-C(11)-C(2)	116.8(3)	C(24)-C(25)-Fe(2)	71.1(3)
C(28)-N(2)-Pd(2)	123.3(2)	N(1)-C(12)-C(13)	111.0(3)	C(25)-C(26)-C(22)	108.9(6)
C(33)-N(3)-Pd(1)	164.1(3)	O(1)-C(13)-C(14)	106.2(3)	C(25)-C(26)-Fe(2)	71.3(3)
C(34)-N(4)-Pd(2)	161.5(3)	O(1)-C(13)-C(12)	106.8(3)	C(22)-C(26)-Fe(2)	70.3(3)
C(2)-C(1)-C(5)	105.1(3)	C(14)-C(13)-C(12)	114.3(3)	N(2)-C(27)-C(18)	114.9(4)
C(2)-C(1)-Pd(1)	114.0(2)	C(15)-C(14)-C(13)	102.9(3)	C(29)-C(28)-N(2)	112.6(3)
C(5)-C(1)-Pd(1)	140.9(3)	C(16)-C(15)-C(14)	104.6(4)	O(2)-C(29)-C(28)	110.7(3)
C(2)-C(1)-Fe(1)	68.4(2)	O(1)-C(16)-C(15)	111.9(4)	O(2)-C(29)-C(30)	105.3(3)
C(5)-C(1)-Fe(1)	68.8(2)	C(21)-C(17)-C(18)	106.9(3)	C(28)-C(29)-C(30)	111.0(3)
Pd(1)-C(1)-Fe(1)	125.0(2)	C(21)-C(17)-Pd(2)	141.0(3)	C(31)-C(30)-C(29)	103.2(4)
C(1)-C(2)-C(3)	110.9(3)	C(18)-C(17)-Pd(2)	111.7(2)	C(32)-C(31)-C(30)	105.6(4)
C(1)-C(2)-C(11)	113.7(3)	C(21)-C(17)-Fe(2)	69.5(2)	O(2)-C(32)-C(31)	113.9(5)
C(3)-C(2)-C(11)	135.2(4)	C(18)-C(17)-Fe(2)	68.9(2)	N(3)-C(33)-S(1)	178.3(3)
C(1)-C(2)-Fe(1)	70.6(2)	Pd(2)-C(17)-Fe(2)	120.6(2)	N(4)-C(34)-S(2)	179.1(3)
C(3)-C(2)-Fe(1)	70.9(2)	C(27)-C(18)-C(19)	135.7(4)	Cl(1)#1-C(35)-Cl(1)	108.4(5)
C(11)-C(2)-Fe(1)	120.8(3)	C(27)-C(18)-C(17)	116.4(3)		

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.05896(10)	0.05228(10)	0.07031(14)	-0.00084(12)	0.01459(10)	0.00404(11)
Pd(2)	0.06672(12)	0.06596(14)	0.06775(14)	-0.00316(12)	0.02153(10)	0.00050(12)
Fe(1)	0.0634(2)	0.0676(3)	0.0751(3)	0.0049(3)	0.0100(2)	-0.0027(2)
Fe(2)	0.0613(2)	0.0915(3)	0.0685(3)	-0.0147(3)	0.0138(2)	-0.0151(3)
S(1)	0.0846(5)	0.0768(5)	0.0664(5)	0.0020(5)	0.0152(4)	0.0117(5)
S(2)	0.0894(5)	0.0774(5)	0.0749(6)	-0.0078(5)	0.0053(5)	0.0310(5)
O(1)	0.096(2)	0.083(2)	0.099(2)	-0.0045(15)	-0.012(2)	-0.020(2)
O(2)	0.0686(13)	0.139(2)	0.081(2)	0.014(2)	0.0094(13)	0.001(2)
N(1)	0.0567(12)	0.0583(14)	0.087(2)	-0.0032(14)	0.0210(12)	-0.0076(12)
N(2)	0.0804(15)	0.068(2)	0.082(2)	-0.0180(15)	0.0324(13)	-0.0135(15)
N(3)	0.0725(14)	0.061(2)	0.079(2)	0.0039(14)	0.0126(13)	0.0101(14)
N(4)	0.097(2)	0.063(2)	0.092(2)	-0.012(2)	0.023(2)	0.016(2)
C(1)	0.0625(14)	0.054(2)	0.062(2)	0.0027(14)	0.0148(13)	-0.0013(14)
C(2)	0.076(2)	0.067(2)	0.078(2)	-0.009(2)	0.027(2)	-0.005(2)
C(3)	0.097(2)	0.072(2)	0.077(2)	-0.021(2)	0.028(2)	-0.016(2)
C(4)	0.090(2)	0.075(2)	0.073(2)	-0.004(2)	0.019(2)	-0.001(2)
C(5)	0.080(2)	0.066(2)	0.073(2)	0.016(2)	0.011(2)	0.004(2)
C(6)	0.135(4)	0.098(3)	0.258(7)	-0.011(4)	0.062(4)	-0.044(3)
C(7)	0.094(3)	0.254(8)	0.127(4)	-0.031(5)	0.023(3)	-0.066(4)
C(8)	0.074(2)	0.189(5)	0.139(4)	0.064(4)	0.041(2)	0.015(3)
C(9)	0.157(3)	0.162(4)	0.120(3)	-0.032(3)	0.083(2)	-0.077(3)
C(10)	0.069(2)	0.137(4)	0.159(4)	0.068(3)	-0.007(2)	-0.031(2)
C(11)	0.060(2)	0.067(2)	0.089(2)	0.004(2)	0.020(2)	0.020(2)
C(12)	0.066(2)	0.056(2)	0.084(2)	-0.001(2)	0.002(2)	0.005(2)
C(13)	0.068(2)	0.072(2)	0.085(2)	-0.002(2)	0.003(2)	-0.001(2)
C(14)	0.092(2)	0.081(2)	0.079(2)	0.007(2)	0.006(2)	0.008(2)
C(15)	0.135(4)	0.098(3)	0.089(3)	0.017(3)	0.009(3)	-0.021(3)
C(16)	0.225(5)	0.115(3)	0.094(3)	0.028(3)	-0.025(3)	-0.093(3)
C(17)	0.0581(15)	0.085(2)	0.082(2)	-0.006(2)	0.0181(15)	-0.023(2)
C(18)	0.072(2)	0.089(2)	0.070(2)	-0.022(2)	0.016(2)	-0.022(2)
C(19)	0.114(3)	0.113(3)	0.093(3)	-0.026(3)	0.023(2)	-0.040(3)
C(20)	0.093(2)	0.127(4)	0.086(3)	-0.019(3)	0.013(2)	-0.030(3)
C(21)	0.056(2)	0.123(4)	0.093(3)	0.000(3)	0.010(2)	-0.011(2)
C(22)	0.097(2)	0.124(4)	0.271(6)	0.056(4)	0.081(3)	0.018(3)
C(23)	0.098(3)	0.198(5)	0.112(4)	0.045(3)	0.026(3)	-0.048(3)
C(24)	0.087(2)	0.109(3)	0.145(3)	-0.051(3)	0.056(2)	-0.025(2)
C(25)	0.072(2)	0.155(4)	0.114(4)	-0.002(3)	0.005(2)	-0.045(3)
C(26)	0.151(3)	0.147(3)	0.205(4)	-0.103(3)	0.117(2)	-0.089(3)
C(27)	0.081(2)	0.074(2)	0.096(3)	-0.017(2)	0.029(2)	-0.011(2)
C(28)	0.092(2)	0.066(2)	0.083(2)	-0.002(2)	0.029(2)	0.004(2)
C(29)	0.081(2)	0.056(2)	0.081(2)	-0.006(2)	0.007(2)	0.000(2)
C(30)	0.107(3)	0.072(2)	0.097(3)	-0.008(2)	-0.005(3)	-0.008(2)
C(31)	0.099(3)	0.120(4)	0.165(5)	0.021(4)	-0.003(3)	0.012(3)
C(32)	0.075(2)	0.314(11)	0.154(5)	0.053(6)	0.032(3)	0.006(5)
C(33)	0.068(2)	0.062(2)	0.064(2)	0.004(2)	0.010(2)	0.011(2)
C(34)	0.076(2)	0.058(2)	0.072(2)	-0.004(2)	0.020(2)	0.019(2)
Cl(1)	0.1185(8)	0.1995(15)	0.245(2)	0.1096(12)	0.0737(9)	0.0419(10)
C(35)	0.073(3)	0.117(5)	0.145(6)	0.000	0.019(3)	0.000

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	0.0903(2)	0.2551(3)	0.6297(3)	0.080
H(4A)	0.0068(2)	0.4090(3)	0.5939(3)	0.080
H(5A)	0.0195(2)	0.5225(3)	0.7408(3)	0.080
H(6A)	0.0036(3)	0.0897(5)	0.7445(5)	0.080
H(7A)	-0.0809(2)	0.2071(7)	0.6498(4)	0.080
H(8A)	-0.1109(2)	0.3519(5)	0.7430(4)	0.080
H(9A)	-0.0349(2)	0.3325(5)	0.9087(4)	0.080
H(10A)	0.0355(2)	0.1669(5)	0.9021(4)	0.080
H(11A)	0.1834(2)	0.1883(3)	0.8165(3)	0.080
H(12A)	0.2677(2)	0.2746(3)	1.0237(3)	0.080
H(12B)	0.2530(2)	0.1731(3)	0.9604(3)	0.080
H(13A)	0.1644(2)	0.2333(3)	1.0707(3)	0.080
H(14A)	0.2426(2)	0.1847(3)	1.1976(3)	0.080
H(14B)	0.2831(2)	0.1189(3)	1.1393(3)	0.080
H(15A)	0.1761(3)	0.0486(4)	1.2068(3)	0.080
H(15B)	0.2334(3)	-0.0210(4)	1.1850(3)	0.080
H(16A)	0.1757(3)	-0.0505(4)	1.0463(4)	0.080
H(16B)	0.1142(3)	-0.0037(4)	1.0761(4)	0.080
H(19A)	0.2240(2)	0.8386(4)	1.5845(3)	0.080
H(20A)	0.2994(2)	0.6767(4)	1.6222(3)	0.080
H(21A)	0.2946(2)	0.5750(4)	1.4689(3)	0.080
H(22A)	0.1871(2)	0.4355(5)	1.5501(5)	0.080
H(23A)	0.1610(2)	0.5689(6)	1.6653(4)	0.080
H(24A)	0.0764(2)	0.7003(4)	1.5806(4)	0.080
H(25A)	0.0521(2)	0.6480(5)	1.4131(4)	0.080
H(26A)	0.1135(2)	0.4956(4)	1.3903(4)	0.080
H(27A)	0.1299(2)	0.9093(3)	1.4002(3)	0.080
H(28A)	0.0906(2)	0.8699(3)	1.1659(3)	0.080
H(28B)	0.0740(2)	0.9400(3)	1.2447(3)	0.080
H(29A)	0.0175(2)	0.7400(3)	1.2000(3)	0.080
H(30A)	-0.0452(2)	0.8234(4)	1.0698(3)	0.080
H(30B)	-0.0248(2)	0.9368(4)	1.1133(3)	0.080
H(31A)	-0.1333(3)	0.8202(5)	1.1247(4)	0.080
H(31B)	-0.1196(3)	0.9401(5)	1.1524(4)	0.080
H(32A)	-0.0969(2)	0.8948(7)	1.2932(4)	0.080
H(32B)	-0.1016(2)	0.7743(7)	1.2651(4)	0.080

Table 2. Bond lengths (Å) and angles (deg.).

Pd(1)-C(20)	1.974(4)	C(30)-C(31)	1.368(8)	C(8)-Fe(1)-C(3)	111.7(2)
Pd(1)-C(18)	2.148(4)	C(31)-C(32)	1.384(7)	C(4)-Fe(1)-C(3)	39.7(2)
Pd(1)-N(1)	2.162(4)	C(33)-C(34)	1.405(7)	C(6)-Fe(1)-C(3)	142.0(2)
Pd(1)-C(17)	2.205(4)	C(33)-C(38)	1.410(7)	C(1)-Fe(1)-C(3)	68.9(2)
Pd(1)-C(19)	2.572(4)	C(34)-C(35)	1.422(8)	C(2)-Fe(1)-C(3)	41.3(2)
Pd(1)-I(1)	2.6659(7)	C(35)-C(36)	1.358(8)	C(5)-Fe(1)-C(10)	115.0(2)
Fe(1)-C(5)	2.020(5)	C(36)-C(37)	1.353(8)	C(9)-Fe(1)-C(10)	40.5(2)
Fe(1)-C(9)	2.031(5)	C(37)-C(38)	1.376(7)	C(8)-Fe(1)-C(10)	66.9(2)
Fe(1)-C(8)	2.033(5)	C(39)-C(40)	1.366(8)	C(4)-Fe(1)-C(10)	143.3(2)
Fe(1)-C(4)	2.042(5)	C(39)-C(44)	1.385(8)	C(6)-Fe(1)-C(10)	40.6(2)
Fe(1)-C(6)	2.045(6)	C(40)-C(41)	1.366(9)	C(1)-Fe(1)-C(10)	110.6(2)
Fe(1)-C(1)	2.047(4)	C(41)-C(42)	1.389(11)	C(2)-Fe(1)-C(10)	136.4(2)
Fe(1)-C(2)	2.050(4)	C(42)-C(43)	1.345(10)	C(3)-Fe(1)-C(10)	176.8(2)
Fe(1)-C(3)	2.050(5)	C(43)-C(44)	1.401(8)	C(5)-Fe(1)-C(7)	130.2(2)
Fe(1)-C(10)	2.060(5)			C(9)-Fe(1)-C(7)	68.5(2)
Fe(1)-C(7)	2.060(5)	C(20)-Pd(1)-C(18)	66.3(2)	C(8)-Fe(1)-C(7)	41.0(2)
O(1)-C(13)	1.425(6)	C(20)-Pd(1)-N(1)	161.60(15)	C(4)-Fe(1)-C(7)	107.0(2)
O(1)-C(16)	1.439(7)	C(18)-Pd(1)-N(1)	100.29(15)	C(6)-Fe(1)-C(7)	39.6(2)
N(1)-C(11)	1.272(6)	C(20)-Pd(1)-C(17)	82.8(2)	C(1)-Fe(1)-C(7)	170.8(2)
N(1)-C(12)	1.477(6)	C(18)-Pd(1)-C(17)	38.28(15)	C(2)-Fe(1)-C(7)	146.2(2)
C(1)-C(11)	1.405(6)	N(1)-Pd(1)-C(17)	94.1(2)	C(3)-Fe(1)-C(7)	113.4(2)
C(1)-C(2)	1.435(7)	C(20)-Pd(1)-C(19)	30.3(2)	C(10)-Fe(1)-C(7)	67.6(2)
C(1)-C(5)	1.443(7)	C(18)-Pd(1)-C(19)	36.45(15)	C(13)-O(1)-C(16)	108.8(4)
C(2)-C(3)	1.446(6)	N(1)-Pd(1)-C(19)	133.84(14)	C(11)-N(1)-C(12)	118.7(4)
C(2)-C(17)	1.482(6)	C(17)-Pd(1)-C(19)	62.1(2)	C(11)-N(1)-Pd(1)	125.7(3)
C(3)-C(4)	1.388(8)	C(20)-Pd(1)-I(1)	100.45(12)	C(12)-N(1)-Pd(1)	115.6(3)
C(4)-C(5)	1.367(7)	C(18)-Pd(1)-I(1)	163.00(11)	C(11)-C(1)-C(2)	128.6(4)
C(6)-C(7)	1.390(8)	N(1)-Pd(1)-I(1)	94.86(9)	C(11)-C(1)-C(5)	125.5(5)
C(6)-C(10)	1.426(8)	C(17)-Pd(1)-I(1)	133.31(10)	C(2)-C(1)-C(5)	105.3(4)
C(7)-C(8)	1.435(8)	C(19)-Pd(1)-I(1)	130.68(10)	C(11)-C(1)-Fe(1)	119.9(3)
C(8)-C(9)	1.381(8)	C(5)-Fe(1)-C(9)	147.3(2)	C(2)-C(1)-Fe(1)	69.6(2)
C(9)-C(10)	1.416(8)	C(5)-Fe(1)-C(8)	170.6(2)	C(5)-C(1)-Fe(1)	68.3(3)
C(12)-C(13)	1.506(7)	C(9)-Fe(1)-C(8)	39.7(2)	C(1)-C(2)-C(3)	107.2(4)
C(13)-C(14)	1.544(7)	C(5)-Fe(1)-C(4)	39.3(2)	C(1)-C(2)-C(17)	129.5(4)
C(14)-C(15)	1.469(9)	C(9)-Fe(1)-C(4)	173.4(2)	C(3)-C(2)-C(17)	122.2(4)
C(15)-C(16)	1.483(10)	C(8)-Fe(1)-C(4)	133.8(2)	C(1)-C(2)-Fe(1)	69.4(3)
C(17)-C(18)	1.428(6)	C(5)-Fe(1)-C(6)	107.7(2)	C(3)-C(2)-Fe(1)	69.4(3)
C(17)-C(21)	1.509(6)	C(9)-Fe(1)-C(6)	68.3(2)	C(17)-C(2)-Fe(1)	135.5(3)
C(18)-C(27)	1.470(6)	C(8)-Fe(1)-C(6)	67.3(2)	C(4)-C(3)-C(2)	108.3(4)
C(18)-C(19)	1.530(6)	C(4)-Fe(1)-C(6)	111.6(2)	C(4)-C(3)-Fe(1)	69.8(3)
C(19)-C(20)	1.320(6)	C(5)-Fe(1)-C(1)	41.6(2)	C(2)-C(3)-Fe(1)	69.3(2)
C(19)-C(33)	1.460(6)	C(9)-Fe(1)-C(1)	116.5(2)	C(5)-C(4)-C(3)	109.0(4)
C(20)-C(39)	1.490(6)	C(8)-Fe(1)-C(1)	147.5(2)	C(5)-C(4)-Fe(1)	69.5(3)
C(21)-C(22)	1.375(6)	C(4)-Fe(1)-C(1)	68.7(2)	C(3)-C(4)-Fe(1)	70.5(3)
C(21)-C(26)	1.394(7)	C(6)-Fe(1)-C(1)	133.3(2)	C(4)-C(5)-C(1)	110.3(5)
C(22)-C(23)	1.375(7)	C(5)-Fe(1)-C(2)	68.4(2)	C(4)-C(5)-Fe(1)	71.2(3)
C(23)-C(24)	1.368(8)	C(9)-Fe(1)-C(2)	112.4(2)	C(1)-C(5)-Fe(1)	70.2(3)
C(24)-C(25)	1.371(8)	C(8)-Fe(1)-C(2)	117.2(2)	C(7)-C(6)-C(10)	109.1(5)
C(25)-C(26)	1.394(8)	C(4)-Fe(1)-C(2)	68.3(2)	C(7)-C(6)-Fe(1)	70.8(3)
C(27)-C(32)	1.388(6)	C(6)-Fe(1)-C(2)	174.3(2)	C(10)-C(6)-Fe(1)	70.2(3)
C(27)-C(28)	1.415(6)	C(1)-Fe(1)-C(2)	41.0(2)	C(6)-C(7)-C(8)	106.2(5)
C(28)-C(29)	1.369(7)	C(5)-Fe(1)-C(3)	66.9(2)	C(6)-C(7)-Fe(1)	69.6(3)
C(29)-C(30)	1.380(9)	C(9)-Fe(1)-C(3)	136.7(2)	C(8)-C(7)-Fe(1)	68.5(3)

C(9)-C(8)-C(7)	109.8(5)	C(17)-C(18)-C(19)	114.3(4)	C(28)-C(27)-C(18)	123.0(4)
C(9)-C(8)-Fe(1)	70.0(3)	C(27)-C(18)-C(19)	119.4(4)	C(29)-C(28)-C(27)	120.7(5)
C(7)-C(8)-Fe(1)	70.5(3)	C(17)-C(18)-Pd(1)	73.0(2)	C(28)-C(29)-C(30)	120.6(5)
C(8)-C(9)-C(10)	107.6(5)	C(27)-C(18)-Pd(1)	114.4(3)	C(31)-C(30)-C(29)	119.6(5)
C(8)-C(9)-Fe(1)	70.2(3)	C(19)-C(18)-Pd(1)	87.0(2)	C(30)-C(31)-C(32)	120.8(5)
C(10)-C(9)-Fe(1)	70.9(3)	C(20)-C(19)-C(33)	134.3(4)	C(31)-C(32)-C(27)	120.8(5)
C(9)-C(10)-C(6)	107.3(5)	C(20)-C(19)-C(18)	104.6(4)	C(34)-C(33)-C(38)	117.6(4)
C(9)-C(10)-Fe(1)	68.6(3)	C(33)-C(19)-C(18)	121.1(4)	C(34)-C(33)-C(19)	119.3(4)
C(6)-C(10)-Fe(1)	69.1(3)	C(20)-C(19)-Pd(1)	48.9(2)	C(38)-C(33)-C(19)	123.1(4)
N(1)-C(11)-C(1)	126.3(5)	C(33)-C(19)-Pd(1)	172.9(3)	C(33)-C(34)-C(35)	120.1(5)
N(1)-C(12)-C(13)	111.7(4)	C(18)-C(19)-Pd(1)	56.5(2)	C(36)-C(35)-C(34)	119.6(5)
O(1)-C(13)-C(12)	113.4(4)	C(19)-C(20)-C(39)	130.5(4)	C(37)-C(36)-C(35)	120.8(5)
O(1)-C(13)-C(14)	105.2(4)	C(19)-C(20)-Pd(1)	100.8(3)	C(36)-C(37)-C(38)	121.6(5)
C(12)-C(13)-C(14)	110.8(4)	C(39)-C(20)-Pd(1)	128.7(3)	C(37)-C(38)-C(33)	120.3(4)
C(15)-C(14)-C(13)	101.5(5)	C(22)-C(21)-C(26)	117.9(4)	C(40)-C(39)-C(44)	118.0(5)
C(14)-C(15)-C(16)	105.7(5)	C(22)-C(21)-C(17)	123.2(4)	C(40)-C(39)-C(20)	119.7(5)
O(1)-C(16)-C(15)	107.0(5)	C(26)-C(21)-C(17)	118.8(4)	C(44)-C(39)-C(20)	122.2(5)
C(18)-C(17)-C(2)	120.4(4)	C(23)-C(22)-C(21)	121.5(5)	C(41)-C(40)-C(39)	122.6(7)
C(18)-C(17)-C(21)	121.1(4)	C(24)-C(23)-C(22)	120.0(5)	C(40)-C(41)-C(42)	118.4(7)
C(2)-C(17)-C(21)	114.8(3)	C(23)-C(24)-C(25)	120.4(5)	C(43)-C(42)-C(41)	121.1(6)
C(18)-C(17)-Pd(1)	68.7(2)	C(24)-C(25)-C(26)	119.4(5)	C(42)-C(43)-C(44)	119.5(7)
C(2)-C(17)-Pd(1)	112.3(3)	C(21)-C(26)-C(25)	120.7(5)	C(39)-C(44)-C(43)	120.2(6)
C(21)-C(17)-Pd(1)	108.0(3)	C(32)-C(27)-C(28)	117.6(4)		
C(17)-C(18)-C(27)	126.0(4)	C(32)-C(27)-C(18)	119.5(4)		

Symmetry transformations used to generate equivalent atoms:

Table 3.. Anisotropic displacement parameters [$\text{\AA} \times 10^4$ for Pd, Fe and I; $\text{\AA} \times 10^3$ for other atoms]

atom	U11	U22	U33	U23	U13	U12
Pd(1)	0.0482(2)	0.0629(2)	0.0498(2)	0.00403(14)	0.0024(2)	0.0002(2)
Fe(1)	0.0609(4)	0.0632(4)	0.0570(3)	-0.0017(3)	0.0067(3)	0.0070(3)
I(1)	0.0850(2)	0.1069(2)	0.05079(15)	0.0094(2)	0.0017(2)	-0.0183(2)
O(1)	0.056(2)	0.096(2)	0.074(2)	0.012(2)	0.011(2)	0.010(2)
N(1)	0.054(2)	0.063(2)	0.061(2)	-0.007(2)	0.002(2)	-0.003(2)
C(1)	0.058(3)	0.064(3)	0.055(2)	-0.007(2)	-0.006(2)	0.004(2)
C(2)	0.055(3)	0.057(2)	0.051(2)	-0.004(2)	-0.003(2)	0.007(2)
C(3)	0.073(3)	0.058(2)	0.052(2)	0.005(2)	0.011(2)	0.003(2)
C(4)	0.083(4)	0.070(3)	0.065(3)	0.007(2)	0.005(3)	0.022(3)
C(5)	0.056(3)	0.090(3)	0.062(3)	-0.002(2)	-0.001(2)	0.027(3)
C(6)	0.074(4)	0.092(4)	0.086(3)	-0.005(3)	0.024(3)	0.010(3)
C(7)	0.070(3)	0.077(3)	0.078(3)	-0.014(3)	0.013(3)	0.004(3)
C(8)	0.070(3)	0.089(3)	0.067(3)	-0.024(3)	0.022(3)	-0.015(3)
C(9)	0.087(4)	0.116(4)	0.053(3)	0.003(3)	0.007(3)	0.024(4)
C(10)	0.073(3)	0.087(4)	0.075(3)	0.009(3)	0.024(3)	0.002(3)
C(11)	0.047(3)	0.068(3)	0.071(3)	-0.010(2)	-0.004(2)	0.001(2)
C(12)	0.059(3)	0.073(3)	0.066(3)	-0.014(2)	0.011(3)	-0.011(2)
C(13)	0.055(3)	0.072(3)	0.069(3)	-0.003(2)	0.002(3)	-0.004(2)
C(14)	0.083(4)	0.082(3)	0.091(4)	-0.017(3)	0.018(3)	-0.030(3)
C(15)	0.156(7)	0.088(4)	0.095(4)	0.020(3)	0.031(5)	-0.003(5)
C(16)	0.112(5)	0.085(4)	0.095(4)	0.014(3)	0.026(4)	0.015(3)
C(17)	0.052(2)	0.052(2)	0.050(2)	-0.004(2)	0.002(2)	-0.002(2)
C(18)	0.036(2)	0.063(2)	0.044(2)	0.006(2)	0.005(2)	-0.003(2)
C(19)	0.046(2)	0.059(2)	0.061(2)	-0.007(2)	0.004(2)	-0.004(2)
C(20)	0.058(3)	0.057(3)	0.046(2)	0.001(2)	-0.016(2)	0.007(2)
C(21)	0.043(2)	0.061(2)	0.065(3)	0.001(2)	-0.002(2)	-0.002(2)
C(22)	0.054(3)	0.097(4)	0.050(3)	-0.011(2)	-0.001(2)	-0.010(3)
C(23)	0.056(3)	0.092(3)	0.074(3)	-0.023(3)	0.001(3)	-0.013(3)
C(24)	0.062(3)	0.096(4)	0.089(3)	-0.027(3)	-0.009(3)	-0.011(3)
C(25)	0.059(3)	0.084(3)	0.090(4)	-0.001(3)	0.000(3)	-0.016(3)
C(26)	0.080(4)	0.075(3)	0.062(3)	-0.007(2)	0.008(3)	-0.018(3)
C(27)	0.043(2)	0.070(2)	0.044(2)	-0.012(2)	0.007(2)	-0.004(2)
C(28)	0.067(3)	0.085(3)	0.050(2)	-0.001(2)	-0.009(2)	0.018(3)
C(29)	0.083(4)	0.120(4)	0.056(3)	-0.005(3)	-0.014(3)	0.021(3)
C(30)	0.063(3)	0.137(5)	0.068(3)	-0.038(3)	-0.003(3)	-0.007(3)
C(31)	0.075(3)	0.102(4)	0.080(3)	-0.031(3)	-0.001(3)	-0.019(3)
C(32)	0.068(3)	0.072(3)	0.062(2)	-0.008(2)	-0.003(3)	-0.002(3)
C(33)	0.056(3)	0.074(3)	0.053(2)	-0.012(2)	0.010(2)	0.008(3)
C(34)	0.060(3)	0.082(3)	0.069(3)	0.009(2)	0.014(3)	0.007(3)
C(35)	0.079(4)	0.103(4)	0.083(4)	0.026(3)	0.014(3)	0.017(3)
C(36)	0.072(3)	0.106(4)	0.080(3)	-0.002(3)	0.023(3)	0.000(3)
C(37)	0.041(2)	0.114(4)	0.080(3)	-0.014(3)	0.012(2)	0.014(3)
C(38)	0.045(3)	0.073(3)	0.066(3)	0.002(2)	-0.003(2)	-0.003(2)
C(39)	0.054(3)	0.090(3)	0.050(2)	0.006(2)	-0.002(2)	0.012(3)
C(40)	0.060(3)	0.125(5)	0.085(4)	0.016(3)	-0.010(3)	0.018(4)
C(41)	0.086(4)	0.176(6)	0.087(4)	0.024(4)	-0.017(4)	0.022(5)
C(42)	0.081(4)	0.239(8)	0.066(3)	0.034(4)	-0.012(4)	0.049(5)
C(43)	0.106(4)	0.157(4)	0.077(3)	0.067(3)	0.024(3)	0.072(4)
C(44)	0.097(4)	0.115(4)	0.075(3)	0.033(3)	0.025(3)	0.027(4)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
H(3A)	0.0172(5)	0.2744(3)	0.2335(2)	0.073
H(4A)	0.2412(6)	0.2328(3)	0.2663(2)	0.087
H(5A)	0.3928(5)	0.3432(3)	0.2479(2)	0.083
H(6A)	0.4290(6)	0.2310(3)	0.1200(3)	0.101
H(7A)	0.2131(5)	0.1613(3)	0.1171(2)	0.090
H(8A)	0.0494(5)	0.2572(3)	0.0672(2)	0.090
H(9A)	0.1629(6)	0.3825(4)	0.0393(2)	0.102
H(10A)	0.4015(6)	0.3668(3)	0.0696(3)	0.094
H(11A)	0.3775(5)	0.4841(3)	0.1952(2)	0.075
H(12A)	0.2944(5)	0.6143(3)	0.0983(2)	0.079
H(12B)	0.3972(5)	0.5946(3)	0.1511(2)	0.079
H(13A)	0.2830(5)	0.6669(3)	0.2270(2)	0.078
H(14A)	0.3548(6)	0.7852(3)	0.1938(3)	0.103
H(14B)	0.4290(6)	0.7331(3)	0.1432(3)	0.103
H(15A)	0.2834(8)	0.7537(4)	0.0671(3)	0.136
H(15B)	0.2745(8)	0.8342(4)	0.1032(3)	0.136
H(16A)	0.0894(6)	0.8053(3)	0.1470(3)	0.117
H(16B)	0.0786(6)	0.7453(3)	0.0900(3)	0.117
H(22A)	-0.0531(5)	0.4063(3)	0.0697(2)	0.080
H(23A)	-0.2025(5)	0.3311(3)	0.0175(3)	0.089
H(24A)	-0.3688(5)	0.2759(3)	0.0738(3)	0.099
H(25A)	-0.3804(5)	0.2897(3)	0.1837(3)	0.093
H(26A)	-0.2255(5)	0.3625(3)	0.2371(3)	0.087
H(28A)	0.0749(5)	0.4190(3)	0.3297(2)	0.081
H(29A)	0.1838(6)	0.4641(4)	0.4178(3)	0.104
H(30A)	0.2046(6)	0.5962(4)	0.4356(3)	0.108
H(31A)	0.1155(5)	0.6830(4)	0.3645(3)	0.102
H(32A)	0.0024(5)	0.6397(3)	0.2763(2)	0.080
H(34A)	-0.1981(5)	0.4688(3)	0.3298(2)	0.084
H(35A)	-0.3638(6)	0.4768(4)	0.4065(3)	0.106
H(36A)	-0.5427(6)	0.5495(3)	0.3850(3)	0.103
H(37A)	-0.5560(5)	0.6213(3)	0.2939(2)	0.094
H(38A)	-0.3953(4)	0.6197(3)	0.2186(2)	0.074
H(40A)	-0.3363(5)	0.4882(4)	0.0943(3)	0.108
H(41)	-0.4845(7)	0.5283(5)	0.0201(3)	0.139
H(42A)	-0.4992(7)	0.6600(5)	-0.0044(3)	0.155
H(43A)	-0.3657(6)	0.7476(4)	0.0429(3)	0.136
H(44A)	-0.2022(7)	0.7039(4)	0.1106(3)	0.115