

Supplementary Data

Cyclic Ether-Induced Asymmetric Cyclopalladation: Synthesis and Structural Characterization of Enantiopure Di- μ -acetato-bridged Dimers of Planar Chiral Cyclopalladated Ferrocenylimines and Their Derivatives

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Summary of crystal data for *syn*-(*-*)-(S_p,S,S,S_p)-2a: C₃₆H₄₂Fe₂N₂O₆Pd₂, red block, orthorhombic, space group P2₁2₁2₁, $a = 11.461(1)$ Å, $b = 20.724(4)$ Å, $c = 11.474(1)$ Å, $Z = 4$, $\rho = 1.659$ g cm⁻³. Of the 6077 reflections collected, 5314 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 5.31\%$, wR2 = 11.28%, and GOF = 1.079, absolute structure parameter: 0.45(2). For *syn*-(+)-(R_p,S,S,R_p)-2a·CH₂Cl₂:C₃₇H₄₄Cl₂Fe₂N₂O₆Pd₂, red prism, hexagonal, space group P3₂, $a = 11.026(1)$ Å, $b = 11.026(1)$ Å, $c = 27.253(2)$ Å, $\gamma = 120$, $Z = 3$, $\rho = 1.750$ g cm⁻³. Of the 7423 reflections collected, 5046 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 3.79\%$, wR2 = 6.50%, and GOF = 0.877, absolute structure parameter: 0.04(1). For *syn*-(+)-(R_p,R,R,R_p)-2b: C₃₈H₄₆Fe₂N₂O₆Pd₂, red block, orthorhombic, space group P2₁2₁2₁, $a = 11.754(1)$ Å, $b = 25.115(2)$ Å, $c = 30.107(1)$ Å, $Z = 4$, $\rho = 1.419$ g cm⁻³. Of the 12245 reflections collected, 9029 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 6.83\%$, wR2 = 14.19%, and GOF = 1.040, absolute structure parameter: 0.46(1). For *syn*-(*-*)-(R_p,S,S,S_p)-3: C₃₄H₃₉ClFe₂N₂O₄Pd₂, red prism, monoclinic, space group P2₁, $a = 11.959(2)$ Å, $b = 22.106(3)$ Å, $c = 13.080(2)$ Å, $\beta = 104.76(1)$, $Z = 4$, $\rho = 1.787$ g cm⁻³. Of the 35046 reflections collected, 16115 reflections ($F > 4\sigma(F_o)$) were

used for the refinement. The final residuals were $R1 = 3.95\%$, $wR2 = 7.44\%$, and $GOF = 0.880$, absolute structure parameter: $0.07(2)$. For *syn*-(+)-(R_p,R,R,R_p)-4a: C₃₂H₃₆Cl₂Fe₂N₂O₂Pd₂, red prism, monoclinic, space group P2₁, $a = 10.690(1)$ Å, $b = 11.908(2)$ Å, $c = 12.645(1)$ Å, $\beta = 97.52(6)$, $Z = 2$, $\rho = 1.823$ g cm⁻³. Of the 2886 reflections collected, 2574 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 5.21\%$, $wR2 = 13.05\%$, and $GOF = 1.071$, absolute structure parameter: $0.36(2)$. For *syn*-(+)-(S_p,S,S,S_p)-4a: C₃₂H₃₆Cl₂Fe₂N₂O₂Pd₂, red prism, monoclinic, space group P2₁, $a = 10.707(1)$ Å, $b = 11.896(2)$ Å, $c = 12.643(1)$ Å, $\beta = 97.45(1)$, $Z = 2$, $\rho = 1.822$ g cm⁻³. Of the 2988 reflections collected, 2779 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 3.84\%$, $wR2 = 9.30\%$, and $GOF = 1.069$, absolute structure parameter: $0.50(2)$. For *syn*-(+)-(R_p,R,R,R_p)-4b: C₃₂H₃₆Br₂Fe₂N₂O₂Pd₂, red prism, monoclinic, space group P2₁, $a = 10.605(2)$ Å, $b = 12.071(2)$ Å, $c = 12.881(3)$ Å, $\beta = 97.67(3)$, $Z = 2$, $\rho = 1.961$ g cm⁻³. Of the 2938 reflections collected, 2639 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 4.64\%$, $wR2 = 10.71\%$, and $GOF = 1.041$, absolute structure parameter: $0.52(1)$. For *syn*-(+)-(R_p,R,R,R_p)-5a: C₃₄H₄₀Cl₂Fe₂N₂O₂Pd₂, red prism, hexagonal, space group P6, $a = 24.414(1)$ Å, $b = 24.414(1)$ Å, $c = 10.506(1)$ Å, $\gamma = 120$, $Z = 6$, $\rho = 1.661$ g cm⁻³. Of the 6402 reflections collected, 6037 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 5.36\%$, $wR2 = 13.85\%$, and $GOF = 1.067$, absolute structure parameter: $0.50(2)$. For *syn*-(+)-(S_p,S,S,S_p)-5a: C₃₄H₄₀Cl₂Fe₂N₂O₂Pd₂, red prism, hexagonal, space group P6, $a = 24.427(4)$ Å, $b = 24.427(4)$ Å, $c = 10.514(2)$ Å, $\gamma = 120$, $Z = 6$, $\rho = 1.658$ g cm⁻³. Of the 6068 reflections collected, 5204 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 5.05\%$, $wR2 = 12.06\%$, and $GOF = 1.073$, absolute structure parameter: $0.47(4)$. For *syn*-(+)-(R_p,R,R,R_p)-6a: C₃₂H₃₆Fe₂N₄O₆Pd₂, red prism, monoclinic, space group P2₁, $a = 10.217(1)$ Å, $b = 12.940(1)$ Å, $c = 12.906(1)$ Å, $\beta = 93.81(1)$, $Z = 2$, $\rho = 1.750$ g cm⁻³. Of the 5676 reflections collected, 5502 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 6.19\%$, $wR2$

= 17.50%, and GOF = 1.091, absolute structure parameter: 0.33(2). For *syn*-(+)-(R_p,R,R,R_p)-7a·½CH₂Cl₂: C_{34.5}H₃₆ClFe₂N₄O₂Pd₂S₂, red prism, monoclinic, space group C2, $a = 20.670(4)$ Å, $b = 12.477(3)$ Å, $c = 14.661(3)$ Å, $\beta = 104.11(3)$, $Z = 4$, $\rho = 1.744$ g cm⁻³. Of the 5332 reflections collected, 4663 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 6.15\%$, $wR2 = 16.34\%$, and GOF = 1.078, absolute structure parameter: 0.46(3). For *syn*-(+)-(S_p,S,S,S_p)-7a·½CH₂Cl₂: C_{34.5}H₃₆ClFe₂N₄O₂Pd₂S₂, red prism, monoclinic, space group C2, $a = 20.649(4)$ Å, $b = 12.472(2)$ Å, $c = 14.664(3)$ Å, $\beta = 104.15(3)$, $Z = 4$, $\rho = 1.746$ g cm⁻³. Of the 5607 reflections collected, 5037 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 5.31\%$, $wR2 = 13.81\%$, and GOF = 1.035, absolute structure parameter: 0.51(2). For (+)-(R_p,R)-8: C₄₄H₃₈FeINOPd, red prism, orthorhombic, space group P2₁2₁2₁, $a = 10.407(2)$ Å, $b = 17.177(3)$ Å, $c = 20.811(4)$ Å, $Z = 4$, $\rho = 1.582$ g cm⁻³. Of the 5734 reflections collected, 4887 reflections ($F > 4\sigma(F_o)$) were used for the refinement. The final residuals were $R1 = 6.17\%$, $wR2 = 14.01\%$, and GOF = 1.017, absolute structure parameter: 0.44(2).

Crystallographic Studies. Crystallographic data of *syn*-(+)-(S_p,S,S,S_p)-2a, *syn*-(+)-(R_p,R,R,R_p)-2b, *syn*-(+)-(R_p,R,R,R_p)-4a, *syn*-(+)-(S_p,S,S,S_p)-4a, *syn*-(+)-(R_p,R,R,R_p)-4b, *syn*-(+)-(R_p,R,R,R_p)-5a, *syn*-(+)-(S_p,S,S,S_p)-5a, *syn*-(+)-(R_p,R,R,R_p)-6a, *syn*-(+)-(R_p,R,R,R_p)-7a·½CH₂Cl₂, *syn*-(+)-(S_p,S,S,S_p)-7a·½CH₂Cl₂, (+)-(R_p,R)-8 measured on a MSC/Rigaku RAXIS IIC imaging-plate diffractometer are summarised in Table 1 and 2. Intensities were collected at 294K using graphite-monochromatized Mo-K_α radiation ($\lambda = 0.71073$ Å) from a rotating-anode generator operating at 50 kV and 90 mA ($2\theta_{min} = 3^\circ$, $2\theta_{max} = 55^\circ$, $2 - 5^\circ$ oscillation frames in the range of 0-180°, exposure 8 min. per frame).³⁰ A self-consistent semi-empirical absorption correction based on Fourier coefficient fitting of symmetry-equivalent reflections was applied using the ABSCOR program.³¹ Crystallographic data of *syn*-(+)-(R_p,S,S,R_p)-2a·CH₂Cl₂ and *syn*-(+)-(R_p,S,S,S_p)-3 measured on a Bruker SMART-CCD diffractometer [ω -scans with 0.3° per frame, $4.26 < 2\theta < 52.04$ for *syn*-(+)-(R_p,S,S,R_p)-2a·CH₂Cl₂ and $3.52 < 2\theta < 56.72$ for *syn*-(+)-(R_p,S,S,S_p)-3] using

graphite-monochromatized Mo- K_{α} radiation ($\lambda = 0.71073 \text{ \AA}$). A self-consistent semi-empirical absorption correction was applied. The crystal structures were determined by the direct method, which yielded the positions of all non-hydrogen atoms, which were refined anisotropically. Refinement of weighted *R*-index $wR2$ was based on F^2 for all reflections except for *n* with very negative F^2 or flagged for potential systematic errors. A conventional *R*-factor *R**I* based on observed F greater than $4\sigma(F_o)$ is also calculated for comparison.

Tables for *syn*-(-)(S_p,S,S,S_p)-2aTable 1. Atomic coordinates [x 10⁵ for Pd, Fe; x 10⁴ for other atoms] and equivalent isotropic displacement parameters [Å² x 10⁴ for Pd, Fe; Å x 10³ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.75484(2)	0.54255(3)	0.826511(8)	0.05565(8)
Pd(2)	0.70755(2)	0.49521(2)	0.923577(8)	0.05572(8)
Fe(1)	0.55501(4)	0.57704(5)	0.73001(2)	0.0619(2)
Fe(2)	0.67324(5)	0.69513(5)	1.02010(2)	0.0618(2)
O(1)	0.8390(3)	0.8462(4)	0.75455(10)	0.1324(14)
O(2)	0.4043(3)	0.4100(3)	0.99573(10)	0.1272(13)
O(3)	0.7754(2)	0.3663(2)	0.82218(8)	0.0683(8)
O(4)	0.6984(2)	0.3223(2)	0.89304(8)	0.0696(8)
O(5)	0.9277(2)	0.5508(3)	0.85715(8)	0.0720(9)
O(6)	0.8832(2)	0.4749(3)	0.92788(8)	0.0701(8)
N(1)	0.7227(2)	0.7177(3)	0.82459(9)	0.0556(8)
N(2)	0.5328(2)	0.5289(3)	0.92546(9)	0.0586(9)
C(1)	0.6005(3)	0.5395(4)	0.79950(11)	0.0576(10)
C(2)	0.5466(3)	0.6520(3)	0.79517(11)	0.0568(10)
C(3)	0.4341(3)	0.6430(4)	0.77552(12)	0.0660(12)
C(4)	0.4131(3)	0.5228(4)	0.76754(13)	0.0677(12)
C(5)	0.5154(3)	0.4574(4)	0.78163(11)	0.0627(11)
C(6)	0.6393(4)	0.4880(5)	0.67753(13)	0.112(2)
C(7)	0.7087(4)	0.5815(5)	0.69417(13)	0.106(2)
C(8)	0.6485(4)	0.6831(5)	0.68620(14)	0.090(2)
C(9)	0.5434(4)	0.6559(4)	0.66530(13)	0.0782(14)
C(10)	0.5350(4)	0.5382(5)	0.65973(13)	0.086(2)
C(11)	0.6229(3)	0.7472(4)	0.80852(11)	0.0621(11)
C(12)	0.8097(3)	0.8051(4)	0.83596(13)	0.0701(12)
C(13)	0.8988(3)	0.8117(5)	0.79649(13)	0.0793(14)
C(14)	0.9942(4)	0.8997(4)	0.8031(2)	0.090(2)
C(15)	1.0004(5)	0.9632(6)	0.7578(2)	0.135(2)
C(16)	0.9173(4)	0.9074(6)	0.7263(2)	0.144(2)
C(17)	0.7099(3)	0.6507(3)	0.95031(11)	0.0593(11)
C(18)	0.5985(3)	0.7042(4)	0.95504(11)	0.0582(11)
C(19)	0.6085(3)	0.8173(4)	0.97421(12)	0.0644(12)
C(20)	0.7303(3)	0.8360(4)	0.98235(13)	0.0696(12)
C(21)	0.7921(3)	0.7344(4)	0.96806(12)	0.0652(12)
C(22)	0.6692(5)	0.5407(5)	1.05665(15)	0.112(2)
C(23)	0.5647(4)	0.6033(5)	1.06373(13)	0.086(2)
C(24)	0.5935(4)	0.7091(5)	1.08483(12)	0.082(2)
C(25)	0.7119(4)	0.7144(5)	1.09124(13)	0.088(2)
C(26)	0.7626(4)	0.6144(5)	1.07299(14)	0.107(2)
C(27)	0.5030(3)	0.6268(4)	0.94135(12)	0.0647(12)
C(28)	0.4441(3)	0.4406(4)	0.91467(13)	0.0717(13)
C(29)	0.4389(4)	0.3497(4)	0.95380(13)	0.0758(14)
C(30)	0.3480(4)	0.2566(4)	0.9473(2)	0.092(2)
C(31)	0.2852(5)	0.2511(5)	0.9925(2)	0.121(2)
C(32)	0.3428(6)	0.3295(5)	1.0246(2)	0.144(2)
C(33)	0.7708(4)	0.1695(4)	0.8448(2)	0.0850(15)
C(34)	0.7450(3)	0.2963(3)	0.85461(13)	0.0613(11)
C(35)	1.0803(3)	0.4780(4)	0.90485(15)	0.084(2)
C(36)	0.9531(3)	0.5052(4)	0.89581(13)	0.0634(11)

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

Table 2. Bond lengths (\AA) and angles (deg.).

Pd(1)-C(1)	1.926(3)	C(14)-C(15)	1.469(7)	C(9)-Fe(1)-C(8)	39.5(2)
Pd(1)-O(3)	2.040(3)	C(15)-C(16)	1.449(7)	C(2)-Fe(1)-C(6)	152.8(2)
Pd(1)-N(1)	2.044(3)	C(17)-C(18)	1.423(5)	C(7)-Fe(1)-C(6)	40.7(2)
Pd(1)-O(5)	2.162(2)	C(17)-C(21)	1.435(5)	C(3)-Fe(1)-C(6)	164.9(2)
Pd(1)-Pd(2)	2.8340(4)	C(18)-C(19)	1.409(6)	C(4)-Fe(1)-C(6)	126.9(2)
Pd(2)-C(17)	1.936(4)	C(18)-C(27)	1.461(5)	C(9)-Fe(1)-C(6)	66.9(2)
Pd(2)-O(6)	2.030(2)	C(19)-C(20)	1.431(5)	C(8)-Fe(1)-C(6)	67.2(2)
Pd(2)-N(2)	2.040(3)	C(20)-C(21)	1.423(6)	C(2)-Fe(1)-C(10)	164.6(2)
Pd(2)-O(4)	2.165(3)	C(22)-C(23)	1.410(7)	C(7)-Fe(1)-C(10)	67.8(2)
Fe(1)-C(2)	2.026(3)	C(22)-C(26)	1.439(7)	C(3)-Fe(1)-C(10)	127.9(2)
Fe(1)-C(7)	2.030(4)	C(23)-C(24)	1.391(7)	C(4)-Fe(1)-C(10)	110.2(2)
Fe(1)-C(3)	2.032(4)	C(24)-C(25)	1.370(6)	C(9)-Fe(1)-C(10)	39.1(2)
Fe(1)-C(4)	2.035(4)	C(25)-C(26)	1.386(7)	C(8)-Fe(1)-C(10)	66.7(2)
Fe(1)-C(9)	2.036(4)	C(28)-C(29)	1.517(6)	C(6)-Fe(1)-C(10)	40.7(2)
Fe(1)-C(8)	2.036(5)	C(29)-C(30)	1.503(6)	C(2)-Fe(1)-C(5)	68.51(15)
Fe(1)-C(6)	2.038(4)	C(30)-C(31)	1.463(7)	C(7)-Fe(1)-C(5)	124.1(2)
Fe(1)-C(10)	2.038(4)	C(31)-C(32)	1.434(8)	C(3)-Fe(1)-C(5)	69.7(2)
Fe(1)-C(5)	2.048(4)	C(33)-C(34)	1.509(6)	C(4)-Fe(1)-C(5)	41.51(15)
Fe(1)-C(1)	2.067(3)	C(35)-C(36)	1.513(5)	C(9)-Fe(1)-C(5)	156.4(2)
Fe(2)-C(18)	2.022(3)			C(8)-Fe(1)-C(5)	161.0(2)
Fe(2)-C(26)	2.029(4)	C(1)-Pd(1)-O(3)	93.72(14)	C(6)-Fe(1)-C(5)	106.4(2)
Fe(2)-C(23)	2.040(5)	C(1)-Pd(1)-N(1)	80.89(14)	C(10)-Fe(1)-C(5)	121.0(2)
Fe(2)-C(20)	2.042(4)	O(3)-Pd(1)-N(1)	173.81(10)	C(2)-Fe(1)-C(1)	41.06(15)
Fe(2)-C(24)	2.042(4)	C(1)-Pd(1)-O(5)	178.49(15)	C(7)-Fe(1)-C(1)	104.80(15)
Fe(2)-C(19)	2.044(4)	O(3)-Pd(1)-O(5)	87.79(11)	C(3)-Fe(1)-C(1)	69.80(14)
Fe(2)-C(22)	2.048(5)	N(1)-Pd(1)-O(5)	97.61(11)	C(4)-Fe(1)-C(1)	69.39(14)
Fe(2)-C(21)	2.049(4)	C(1)-Pd(1)-Pd(2)	101.56(9)	C(9)-Fe(1)-C(1)	162.4(2)
Fe(2)-C(25)	2.060(4)	O(3)-Pd(1)-Pd(2)	83.66(6)	C(8)-Fe(1)-C(1)	124.3(2)
Fe(2)-C(17)	2.070(3)	N(1)-Pd(1)-Pd(2)	100.33(7)	C(6)-Fe(1)-C(1)	117.4(2)
O(1)-C(16)	1.390(6)	O(5)-Pd(1)-Pd(2)	78.48(6)	C(10)-Fe(1)-C(1)	154.0(2)
O(1)-C(13)	1.420(5)	C(17)-Pd(2)-O(6)	93.96(13)	C(5)-Fe(1)-C(1)	41.14(14)
O(2)-C(32)	1.419(6)	C(17)-Pd(2)-N(2)	80.17(13)	C(18)-Fe(2)-C(26)	154.1(2)
O(2)-C(29)	1.423(5)	O(6)-Pd(2)-N(2)	173.49(11)	C(18)-Fe(2)-C(23)	108.2(2)
O(3)-C(34)	1.264(4)	C(17)-Pd(2)-O(4)	177.93(13)	C(26)-Fe(2)-C(23)	68.4(2)
O(4)-C(34)	1.242(4)	O(6)-Pd(2)-O(4)	88.07(11)	C(18)-Fe(2)-C(20)	68.0(2)
O(5)-C(36)	1.241(4)	N(2)-Pd(2)-O(4)	97.82(11)	C(26)-Fe(2)-C(20)	125.5(2)
O(6)-C(36)	1.255(4)	C(17)-Pd(2)-Pd(1)	101.20(10)	C(23)-Fe(2)-C(20)	156.5(2)
N(1)-C(11)	1.276(4)	O(6)-Pd(2)-Pd(1)	83.67(6)	C(18)-Fe(2)-C(24)	127.7(2)
N(1)-C(12)	1.450(5)	N(2)-Pd(2)-Pd(1)	100.16(7)	C(26)-Fe(2)-C(24)	67.0(2)
N(2)-C(27)	1.257(5)	O(4)-Pd(2)-Pd(1)	78.66(6)	C(23)-Fe(2)-C(24)	39.8(2)
N(2)-C(28)	1.467(5)	C(2)-Fe(1)-C(7)	118.6(2)	C(20)-Fe(2)-C(24)	123.0(2)
C(1)-C(2)	1.436(5)	C(2)-Fe(1)-C(3)	40.58(14)	C(18)-Fe(2)-C(19)	40.6(2)
C(1)-C(5)	1.446(5)	C(7)-Fe(1)-C(3)	153.5(2)	C(26)-Fe(2)-C(19)	163.4(2)
C(2)-C(3)	1.407(5)	C(2)-Fe(1)-C(4)	67.87(15)	C(23)-Fe(2)-C(19)	120.8(2)
C(2)-C(11)	1.449(5)	C(7)-Fe(1)-C(4)	163.3(2)	C(20)-Fe(2)-C(19)	41.01(15)
C(3)-C(4)	1.417(6)	C(3)-Fe(1)-C(4)	40.8(2)	C(24)-Fe(2)-C(19)	110.2(2)
C(4)-C(5)	1.447(5)	C(2)-Fe(1)-C(9)	128.0(2)	C(18)-Fe(2)-C(22)	119.2(2)
C(6)-C(7)	1.414(7)	C(7)-Fe(1)-C(9)	66.6(2)	C(26)-Fe(2)-C(22)	41.3(2)
C(6)-C(10)	1.418(6)	C(3)-Fe(1)-C(9)	110.6(2)	C(23)-Fe(2)-C(22)	40.4(2)
C(7)-C(8)	1.373(8)	C(4)-Fe(1)-C(9)	123.1(2)	C(20)-Fe(2)-C(22)	162.3(2)
C(8)-C(9)	1.376(6)	C(2)-Fe(1)-C(8)	108.5(2)	C(24)-Fe(2)-C(22)	67.1(2)
C(9)-C(10)	1.363(7)	C(7)-Fe(1)-C(8)	39.5(2)	C(19)-Fe(2)-C(22)	154.3(2)
C(12)-C(13)	1.510(5)	C(3)-Fe(1)-C(8)	121.1(2)	C(18)-Fe(2)-C(21)	67.97(14)
C(13)-C(14)	1.500(6)	C(4)-Fe(1)-C(8)	156.4(2)	C(26)-Fe(2)-C(21)	106.7(2)

C(23)-Fe(2)-C(21)	161.4(2)	C(3)-C(2)-Fe(1)	70.0(2)	C(17)-C(18)-C(27)	112.7(4)
C(20)-Fe(2)-C(21)	40.7(2)	C(1)-C(2)-Fe(1)	71.0(2)	C(19)-C(18)-Fe(2)	70.6(2)
C(24)-Fe(2)-C(21)	156.4(2)	C(11)-C(2)-Fe(1)	121.7(2)	C(17)-C(18)-Fe(2)	71.5(2)
C(19)-Fe(2)-C(21)	68.9(2)	C(2)-C(3)-C(4)	106.8(3)	C(27)-C(18)-Fe(2)	121.6(3)
C(22)-Fe(2)-C(21)	124.3(2)	C(2)-C(3)-Fe(1)	69.5(2)	C(18)-C(19)-C(20)	106.2(3)
C(18)-Fe(2)-C(25)	164.4(2)	C(4)-C(3)-Fe(1)	69.7(2)	C(18)-C(19)-Fe(2)	68.9(2)
C(26)-Fe(2)-C(25)	39.6(2)	C(3)-C(4)-C(5)	108.9(3)	C(20)-C(19)-Fe(2)	69.4(2)
C(23)-Fe(2)-C(25)	66.6(2)	C(3)-C(4)-Fe(1)	69.5(2)	C(21)-C(20)-C(19)	108.5(4)
C(20)-Fe(2)-C(25)	110.5(2)	C(5)-C(4)-Fe(1)	69.7(2)	C(21)-C(20)-Fe(2)	69.9(2)
C(24)-Fe(2)-C(25)	39.0(2)	C(1)-C(5)-C(4)	107.6(4)	C(19)-C(20)-Fe(2)	69.6(2)
C(19)-Fe(2)-C(25)	128.1(2)	C(1)-C(5)-Fe(1)	70.1(2)	C(20)-C(21)-C(17)	108.6(3)
C(22)-Fe(2)-C(25)	67.1(2)	C(4)-C(5)-Fe(1)	68.8(2)	C(20)-C(21)-Fe(2)	69.4(2)
C(21)-Fe(2)-C(25)	121.8(2)	C(7)-C(6)-C(10)	106.4(5)	C(17)-C(21)-Fe(2)	70.4(2)
C(18)-Fe(2)-C(17)	40.68(14)	C(7)-C(6)-Fe(1)	69.3(3)	C(23)-C(22)-C(26)	106.7(5)
C(26)-Fe(2)-C(17)	118.6(2)	C(10)-C(6)-Fe(1)	69.6(2)	C(23)-C(22)-Fe(2)	69.5(3)
C(23)-Fe(2)-C(17)	124.5(2)	C(8)-C(7)-C(6)	107.9(4)	C(26)-C(22)-Fe(2)	68.6(3)
C(20)-Fe(2)-C(17)	68.7(2)	C(8)-C(7)-Fe(1)	70.5(3)	C(24)-C(23)-C(22)	107.7(4)
C(24)-Fe(2)-C(17)	162.6(2)	C(6)-C(7)-Fe(1)	70.0(2)	C(24)-C(23)-Fe(2)	70.2(3)
C(19)-Fe(2)-C(17)	69.18(15)	C(7)-C(8)-C(9)	108.5(5)	C(22)-C(23)-Fe(2)	70.1(3)
C(22)-Fe(2)-C(17)	105.5(2)	C(7)-C(8)-Fe(1)	70.0(3)	C(25)-C(24)-C(23)	109.2(5)
C(21)-Fe(2)-C(17)	40.77(14)	C(9)-C(8)-Fe(1)	70.2(3)	C(25)-C(24)-Fe(2)	71.2(2)
C(25)-Fe(2)-C(17)	154.5(2)	C(10)-C(9)-C(8)	109.6(4)	C(23)-C(24)-Fe(2)	70.0(2)
C(16)-O(1)-C(13)	107.7(3)	C(10)-C(9)-Fe(1)	70.5(2)	C(24)-C(25)-C(26)	109.3(5)
C(32)-O(2)-C(29)	107.2(4)	C(8)-C(9)-Fe(1)	70.3(2)	C(24)-C(25)-Fe(2)	69.8(2)
C(34)-O(3)-Pd(1)	123.7(2)	C(9)-C(10)-C(6)	107.6(4)	C(26)-C(25)-Fe(2)	69.0(2)
C(34)-O(4)-Pd(2)	123.0(2)	C(9)-C(10)-Fe(1)	70.4(2)	C(25)-C(26)-C(22)	107.0(4)
C(36)-O(5)-Pd(1)	123.0(2)	C(6)-C(10)-Fe(1)	69.6(2)	C(25)-C(26)-Fe(2)	71.4(3)
C(36)-O(6)-Pd(2)	123.9(2)	N(1)-C(11)-C(2)	115.6(4)	C(22)-C(26)-Fe(2)	70.0(3)
C(11)-N(1)-C(12)	120.7(3)	N(1)-C(12)-C(13)	109.8(3)	N(2)-C(27)-C(18)	115.7(3)
C(11)-N(1)-Pd(1)	115.6(3)	O(1)-C(13)-C(14)	105.5(4)	N(2)-C(28)-C(29)	110.6(3)
C(12)-N(1)-Pd(1)	123.4(2)	O(1)-C(13)-C(12)	107.3(3)	O(2)-C(29)-C(30)	104.7(4)
C(27)-N(2)-C(28)	120.1(3)	C(14)-C(13)-C(12)	115.9(4)	O(2)-C(29)-C(28)	106.0(3)
C(27)-N(2)-Pd(2)	116.4(3)	C(15)-C(14)-C(13)	105.2(4)	C(30)-C(29)-C(28)	115.3(4)
C(28)-N(2)-Pd(2)	123.0(2)	C(16)-C(15)-C(14)	106.2(5)	C(31)-C(30)-C(29)	105.4(4)
C(2)-C(1)-C(5)	105.5(3)	O(1)-C(16)-C(15)	107.3(4)	C(32)-C(31)-C(30)	107.1(5)
C(2)-C(1)-Pd(1)	114.3(3)	C(18)-C(17)-C(21)	105.6(3)	O(2)-C(32)-C(31)	106.1(4)
C(5)-C(1)-Pd(1)	140.2(3)	C(18)-C(17)-Pd(2)	114.9(3)	O(4)-C(34)-O(3)	126.4(4)
C(2)-C(1)-Fe(1)	67.9(2)	C(21)-C(17)-Pd(2)	139.5(3)	O(4)-C(34)-C(33)	118.4(3)
C(5)-C(1)-Fe(1)	68.8(2)	C(18)-C(17)-Fe(2)	67.9(2)	O(3)-C(34)-C(33)	115.2(3)
Pd(1)-C(1)-Fe(1)	126.9(2)	C(21)-C(17)-Fe(2)	68.8(2)	O(5)-C(36)-O(6)	126.6(3)
C(3)-C(2)-C(1)	111.2(3)	Pd(2)-C(17)-Fe(2)	126.3(2)	O(5)-C(36)-C(35)	117.4(3)
C(3)-C(2)-C(11)	135.2(4)	C(19)-C(18)-C(17)	111.1(3)	O(6)-C(36)-C(35)	115.9(3)
C(1)-C(2)-C(11)	113.4(3)	C(19)-C(18)-C(27)	136.2(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)	0.06150(13)	0.0592(2)	0.04627(12)	0.00358(12)	0.00168(12)	0.00470(13)
Pd(2)	0.05604(12)	0.0646(2)	0.04648(12)	0.00158(13)	0.00377(11)	0.00452(14)
Fe(1)	0.0680(3)	0.0696(4)	0.0482(2)	0.0037(3)	-0.0022(2)	0.0110(3)
Fe(2)	0.0663(3)	0.0711(4)	0.0481(2)	-0.0032(3)	0.0023(2)	0.0101(3)
O(1)	0.099(2)	0.216(4)	0.082(2)	0.054(2)	-0.017(2)	-0.070(2)
O(2)	0.202(3)	0.104(2)	0.075(2)	-0.029(2)	0.045(2)	-0.076(2)
O(3)	0.083(2)	0.066(2)	0.0564(12)	-0.0017(12)	0.0037(13)	0.0144(13)
O(4)	0.078(2)	0.062(2)	0.0687(14)	-0.0019(13)	0.0017(14)	0.0008(14)
O(5)	0.0596(12)	0.090(2)	0.0667(13)	0.006(2)	0.0075(12)	0.0097(14)
O(6)	0.0608(12)	0.088(2)	0.0610(13)	0.0128(15)	-0.0013(11)	0.0102(14)
N(1)	0.0592(15)	0.055(2)	0.0524(14)	0.0045(13)	-0.0017(14)	-0.0023(13)
N(2)	0.067(2)	0.054(2)	0.0552(14)	-0.006(2)	0.0083(13)	-0.0043(14)
C(1)	0.071(2)	0.058(2)	0.044(2)	0.004(2)	0.004(2)	-0.004(2)
C(2)	0.068(2)	0.051(2)	0.051(2)	0.003(2)	0.001(2)	0.005(2)
C(3)	0.059(2)	0.074(3)	0.065(2)	-0.003(2)	0.000(2)	0.003(2)
C(4)	0.061(2)	0.074(3)	0.068(2)	-0.008(2)	0.006(2)	-0.006(2)
C(5)	0.078(2)	0.055(2)	0.055(2)	-0.001(2)	0.004(2)	-0.006(2)
C(6)	0.159(3)	0.118(4)	0.058(2)	0.000(3)	0.021(2)	0.076(3)
C(7)	0.070(2)	0.192(6)	0.055(2)	0.004(3)	0.007(2)	0.036(3)
C(8)	0.078(2)	0.121(4)	0.070(2)	0.006(3)	0.005(2)	-0.002(3)
C(9)	0.091(3)	0.079(3)	0.065(2)	0.012(2)	-0.006(2)	0.002(2)
C(10)	0.111(3)	0.088(3)	0.060(2)	-0.013(2)	-0.007(2)	-0.010(3)
C(11)	0.080(2)	0.056(2)	0.051(2)	-0.001(2)	0.005(2)	0.003(2)
C(12)	0.075(2)	0.071(3)	0.064(2)	-0.001(2)	-0.006(2)	-0.010(2)
C(13)	0.071(2)	0.089(3)	0.077(2)	0.017(3)	-0.009(2)	-0.020(2)
C(14)	0.078(2)	0.104(4)	0.087(3)	0.016(3)	-0.007(2)	-0.030(3)
C(15)	0.144(4)	0.176(6)	0.085(3)	0.028(4)	0.011(3)	-0.061(4)
C(16)	0.107(3)	0.234(7)	0.090(3)	0.072(4)	-0.010(3)	-0.061(4)
C(17)	0.057(2)	0.074(3)	0.048(2)	0.004(2)	-0.001(2)	-0.008(2)
C(18)	0.061(2)	0.070(3)	0.044(2)	0.004(2)	0.002(2)	0.005(2)
C(19)	0.072(2)	0.057(2)	0.065(2)	0.006(2)	-0.002(2)	0.005(2)
C(20)	0.071(2)	0.070(3)	0.068(2)	-0.005(2)	-0.015(2)	-0.012(2)
C(21)	0.067(2)	0.070(3)	0.058(2)	-0.007(2)	-0.006(2)	-0.008(2)
C(22)	0.177(5)	0.089(3)	0.069(2)	0.027(3)	0.027(3)	0.028(4)
C(23)	0.100(3)	0.098(4)	0.061(2)	0.000(2)	0.010(2)	-0.008(3)
C(24)	0.090(3)	0.097(4)	0.058(2)	-0.004(2)	0.010(2)	-0.007(3)
C(25)	0.079(3)	0.130(4)	0.056(2)	-0.013(2)	-0.007(2)	-0.002(3)
C(26)	0.094(3)	0.155(4)	0.072(2)	0.045(3)	0.010(2)	0.048(3)
C(27)	0.058(2)	0.080(3)	0.055(2)	0.005(2)	-0.002(2)	-0.001(2)
C(28)	0.062(2)	0.079(3)	0.074(2)	-0.010(2)	-0.003(2)	-0.011(2)
C(29)	0.094(3)	0.063(3)	0.071(2)	-0.006(2)	0.019(2)	-0.016(2)
C(30)	0.105(3)	0.074(3)	0.099(3)	-0.017(3)	0.022(3)	-0.030(3)
C(31)	0.150(4)	0.122(4)	0.089(3)	0.010(3)	0.013(3)	-0.057(4)
C(32)	0.238(6)	0.107(4)	0.086(3)	0.004(3)	0.060(4)	-0.072(4)
C(33)	0.108(3)	0.055(2)	0.092(3)	-0.018(2)	-0.020(3)	0.015(2)
C(34)	0.059(2)	0.060(2)	0.065(2)	-0.009(2)	-0.014(2)	0.009(2)
C(35)	0.062(2)	0.105(4)	0.085(2)	-0.020(3)	-0.009(2)	0.011(2)
C(36)	0.058(2)	0.067(3)	0.065(2)	-0.010(2)	-0.010(2)	0.010(2)

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[(ha^*)^2U_{11} + \dots + 2hka^*b^*U_{12}]$$

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

	x	y	z	U(eq)
H(3A)	0.3808(3)	0.7054(4)	0.76886(12)	0.080
H(4A)	0.3440(3)	0.4909(4)	0.75332(13)	0.080
H(5A)	0.5248(3)	0.3744(4)	0.77945(11)	0.080
H(6A)	0.6606(4)	0.4071(5)	0.67798(13)	0.080
H(7A)	0.7844(4)	0.5757(5)	0.70862(13)	0.080
H(8A)	0.6748(4)	0.7602(5)	0.69406(14)	0.080
H(9A)	0.4842(4)	0.7115(4)	0.65696(13)	0.080
H(10A)	0.4701(4)	0.4974(5)	0.64595(13)	0.080
H(11A)	0.5998(3)	0.8274(4)	0.80591(11)	0.080
H(12A)	0.7728(3)	0.8798(4)	0.83892(13)	0.080
H(12B)	0.8470(3)	0.7867(4)	0.86562(13)	0.080
H(13A)	0.9335(3)	0.7362(5)	0.79238(13)	0.080
H(14A)	0.9735(4)	0.9515(4)	0.8285(2)	0.080
H(14B)	1.0681(4)	0.8643(4)	0.8102(2)	0.080
H(15A)	0.9778(5)	1.0431(6)	0.7620(2)	0.080
H(15B)	1.0782(5)	0.9613(6)	0.7451(2)	0.080
H(16A)	0.9586(4)	0.8556(6)	0.7054(2)	0.080
H(16B)	0.8754(4)	0.9631(6)	0.7074(2)	0.080
H(19A)	0.5465(3)	0.8712(4)	0.98073(12)	0.080
H(20A)	0.7639(3)	0.9047(4)	0.99628(13)	0.080
H(21A)	0.8750(3)	0.7234(4)	0.97025(12)	0.080
H(22A)	0.6756(5)	0.4643(5)	1.04305(15)	0.080
H(23A)	0.4877(4)	0.5777(5)	1.05528(13)	0.080
H(24A)	0.5375(4)	0.7679(5)	1.09309(12)	0.080
H(25A)	0.7532(4)	0.7793(5)	1.10473(13)	0.080
H(26A)	0.8442(4)	0.5954(5)	1.07225(14)	0.080
H(27A)	0.4226(3)	0.6490(4)	0.94460(12)	0.080
H(28A)	0.3692(3)	0.4776(4)	0.91209(13)	0.080
H(28B)	0.4617(3)	0.4043(4)	0.88477(13)	0.080
H(29A)	0.5146(4)	0.3154(4)	0.95805(13)	0.080
H(30A)	0.2962(4)	0.2770(4)	0.9218(2)	0.080
H(30B)	0.3836(4)	0.1828(4)	0.9402(2)	0.080
H(31A)	0.2059(5)	0.2759(5)	0.9884(2)	0.080
H(31B)	0.2849(5)	0.1730(5)	1.0048(2)	0.080
H(32A)	0.3969(6)	0.2869(5)	1.0441(2)	0.080
H(32B)	0.2884(6)	0.3693(5)	1.0449(2)	0.080
H(33A)	0.8055(4)	0.1619(4)	0.8139(2)	0.080
H(33B)	0.7001(4)	0.1247(4)	0.8460(2)	0.080
H(33C)	0.8241(4)	0.1415(4)	0.8685(2)	0.080
H(35A)	1.1269(3)	0.5050(4)	0.87869(15)	0.080
H(35B)	1.0882(3)	0.3950(4)	0.90779(15)	0.080
H(35C)	1.1061(3)	0.5147(4)	0.93368(15)	0.080

Tables for *syn*-(+)-(R_p,S,S,R_p)-2a·CH₂Cl₂Table 1. Atomic coordinates [x 10⁵ for Pd, Fe; x 10⁴ for other atoms] and equivalent isotropic displacement parameters [Å² x 10⁴ for Pd, Fe; Å x 10³ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.291688(14)	0.820302(14)	0.005618(6)	0.03884(5)
Pd(2)	0.138067(14)	0.512915(15)	0.014060(6)	0.03858(5)
Fe(1)	0.29246(3)	1.10622(3)	0.069541(12)	0.04393(11)
Fe(2)	-0.14719(3)	0.22687(3)	-0.049734(12)	0.04395(11)
O(1)	0.16686(13)	1.05213(13)	-0.10991(6)	0.0612(6)
O(2)	-0.21814(13)	0.28214(14)	0.12936(6)	0.0645(6)
O(3)	0.35051(12)	0.74588(12)	-0.05780(5)	0.0496(5)
O(4)	0.29326(12)	0.53149(12)	-0.03155(6)	0.0529(5)
O(5)	0.42874(12)	0.80157(12)	0.05037(6)	0.0502(5)
O(6)	0.27099(12)	0.58599(13)	0.07730(5)	0.0495(5)
N(1)	0.15004(14)	0.85075(15)	-0.03109(6)	0.0412(6)
N(2)	-0.03497(14)	0.48090(14)	0.05062(7)	0.0450(6)
C(1)	0.2360(2)	0.8996(2)	0.05936(8)	0.0396(7)
C(2)	0.1258(2)	0.9254(2)	0.04501(9)	0.0465(8)
C(3)	0.0895(2)	0.9805(2)	0.08667(9)	0.0610(9)
C(4)	0.1754(2)	0.9850(2)	0.12564(9)	0.0594(9)
C(5)	0.2630(2)	0.9357(2)	0.10928(8)	0.0498(8)
C(6)	0.4086(3)	1.3061(2)	0.09437(11)	0.0854(12)
C(7)	0.3288(2)	1.3041(2)	0.05627(11)	0.0792(11)
C(8)	0.3618(2)	1.2496(2)	0.01487(9)	0.0736(11)
C(9)	0.4673(2)	1.2225(2)	0.02896(11)	0.0752(11)
C(10)	0.4953(2)	1.2577(2)	0.07762(10)	0.0714(10)
C(11)	0.0851(2)	0.8983(2)	-0.00541(8)	0.0440(7)
C(12)	0.1204(2)	0.8249(2)	-0.08444(8)	0.0492(8)
C(13)	0.2091(2)	0.9497(2)	-0.11654(8)	0.0495(8)
C(14)	0.3653(2)	1.0288(2)	-0.10846(9)	0.0612(9)
C(15)	0.2761(2)	1.1780(2)	-0.12955(11)	0.0867(12)
C(16)	0.4070(2)	1.1710(2)	-0.12848(12)	0.1007(12)
C(17)	0.0023(2)	0.4344(2)	-0.03918(8)	0.0441(8)
C(18)	-0.1344(2)	0.4075(2)	-0.02656(9)	0.0464(8)
C(19)	-0.2248(2)	0.3530(2)	-0.06693(9)	0.0568(8)
C(20)	-0.1427(2)	0.3493(2)	-0.10632(9)	0.0650(10)
C(21)	-0.0057(2)	0.3967(2)	-0.08954(8)	0.0489(8)
C(22)	-0.2254(2)	0.0818(2)	0.00429(10)	0.0708(10)
C(23)	-0.3089(2)	0.0323(2)	-0.03594(13)	0.0903(13)
C(24)	-0.2300(3)	0.0276(2)	-0.07483(10)	0.0827(12)
C(25)	-0.0957(2)	0.0767(2)	-0.05838(11)	0.0726(10)
C(26)	-0.0940(2)	0.1094(2)	-0.00834(10)	0.0725(10)
C(27)	-0.1475(2)	0.4338(2)	0.02505(9)	0.0453(8)
C(28)	-0.0381(2)	0.5096(2)	0.10369(8)	0.0479(8)
C(29)	-0.0750(2)	0.3842(2)	0.13579(8)	0.0466(8)
C(30)	0.0025(2)	0.3058(2)	0.12798(9)	0.0624(9)
C(31)	-0.2359(2)	0.1543(2)	0.14907(10)	0.0812(11)
C(32)	-0.0978(2)	0.1623(2)	0.14905(12)	0.1016(11)
C(33)	0.4238(2)	0.6157(2)	-0.10452(9)	0.0808(10)
C(34)	0.3495(2)	0.6355(2)	-0.06105(8)	0.0463(8)
C(35)	0.4756(2)	0.7200(3)	0.12444(10)	0.0832(11)
C(36)	0.3831(2)	0.6989(2)	0.08055(8)	0.0487(8)
C(1W)	-0.3577(2)	0.6662(3)	0.00948(14)	0.1039(12)
Cl(1)	-0.28704(8)	0.63025(9)	-0.04051(4)	0.1280(4)
Cl(2)	-0.25054(8)	0.70338(9)	0.06031(4)	0.1302(4)

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

Table 2. Bond lengths (\AA) and angles (deg.).

Pd(1)-C(1)	1.955(2)	C(13)-C(14)	1.508(3)	C(3)-Fe(1)-C(6)	123.42(11)
Pd(1)-N(1)	2.019(2)	C(14)-C(16)	1.499(3)	C(4)-Fe(1)-C(6)	108.28(10)
Pd(1)-O(5)	2.0311(15)	C(15)-C(16)	1.483(4)	C(8)-Fe(1)-C(6)	67.10(10)
Pd(1)-O(3)	2.1480(15)	C(17)-C(21)	1.424(3)	C(10)-Fe(1)-C(6)	39.87(11)
Pd(1)-Pd(2)	2.9442(2)	C(17)-C(18)	1.425(3)	C(9)-Fe(1)-C(6)	67.15(11)
Pd(2)-C(17)	1.949(2)	C(18)-C(19)	1.403(3)	C(3)-Fe(1)-C(2)	41.58(9)
Pd(2)-N(2)	2.021(2)	C(18)-C(27)	1.458(3)	C(4)-Fe(1)-C(2)	68.55(9)
Pd(2)-O(4)	2.0408(14)	C(19)-C(20)	1.418(4)	C(8)-Fe(1)-C(2)	109.10(9)
Pd(2)-O(6)	2.1417(13)	C(20)-C(21)	1.406(3)	C(10)-Fe(1)-C(2)	158.12(11)
Fe(1)-C(3)	2.011(2)	C(22)-C(23)	1.358(4)	C(9)-Fe(1)-C(2)	123.22(10)
Fe(1)-C(4)	2.016(2)	C(22)-C(26)	1.367(4)	C(6)-Fe(1)-C(2)	160.57(11)
Fe(1)-C(8)	2.024(2)	C(23)-C(24)	1.388(4)	C(3)-Fe(1)-C(7)	109.49(10)
Fe(1)-C(10)	2.026(2)	C(24)-C(25)	1.373(4)	C(4)-Fe(1)-C(7)	124.09(11)
Fe(1)-C(9)	2.028(2)	C(25)-C(26)	1.408(4)	C(8)-Fe(1)-C(7)	40.51(11)
Fe(1)-C(6)	2.033(2)	C(28)-C(29)	1.510(3)	C(10)-Fe(1)-C(7)	65.95(10)
Fe(1)-C(2)	2.034(2)	C(29)-C(30)	1.503(3)	C(9)-Fe(1)-C(7)	67.14(11)
Fe(1)-C(7)	2.044(3)	C(30)-C(32)	1.519(3)	C(6)-Fe(1)-C(7)	38.79(11)
Fe(1)-C(5)	2.050(2)	C(31)-C(32)	1.482(4)	C(2)-Fe(1)-C(7)	125.98(10)
Fe(1)-C(1)	2.058(2)	C(33)-C(34)	1.517(3)	C(3)-Fe(1)-C(5)	68.52(10)
Fe(2)-C(26)	2.014(3)	C(35)-C(36)	1.513(3)	C(4)-Fe(1)-C(5)	40.19(10)
Fe(2)-C(25)	2.014(3)	C(1W)-Cl(1)	1.712(4)	C(8)-Fe(1)-C(5)	158.49(11)
Fe(2)-C(19)	2.019(3)	C(1W)-Cl(2)	1.732(3)	C(10)-Fe(1)-C(5)	107.59(10)
Fe(2)-C(22)	2.023(2)			C(9)-Fe(1)-C(5)	122.19(11)
Fe(2)-C(23)	2.024(2)	C(1)-Pd(1)-N(1)	81.66(8)	C(6)-Fe(1)-C(5)	122.91(10)
Fe(2)-C(18)	2.026(2)	C(1)-Pd(1)-O(5)	90.66(8)	C(2)-Fe(1)-C(5)	67.87(9)
Fe(2)-C(24)	2.030(2)	N(1)-Pd(1)-O(5)	172.31(7)	C(7)-Fe(1)-C(5)	158.28(11)
Fe(2)-C(20)	2.034(3)	C(1)-Pd(1)-O(3)	174.79(8)	C(3)-Fe(1)-C(1)	69.64(9)
Fe(2)-C(21)	2.049(2)	N(1)-Pd(1)-O(3)	94.09(6)	C(4)-Fe(1)-C(1)	68.26(9)
Fe(2)-C(17)	2.065(2)	O(5)-Pd(1)-O(3)	93.57(6)	C(8)-Fe(1)-C(1)	123.55(10)
O(1)-C(15)	1.411(2)	C(1)-Pd(1)-Pd(2)	109.13(5)	C(10)-Fe(1)-C(1)	121.70(10)
O(1)-C(13)	1.432(3)	N(1)-Pd(1)-Pd(2)	100.52(4)	C(9)-Fe(1)-C(1)	106.97(9)
O(2)-C(29)	1.419(2)	O(5)-Pd(1)-Pd(2)	82.24(3)	C(6)-Fe(1)-C(1)	157.33(11)
O(2)-C(31)	1.427(3)	O(3)-Pd(1)-Pd(2)	74.51(3)	C(2)-Fe(1)-C(1)	41.01(9)
O(3)-C(34)	1.214(3)	C(17)-Pd(2)-N(2)	80.85(8)	C(7)-Fe(1)-C(1)	161.28(10)
O(4)-C(34)	1.279(2)	C(17)-Pd(2)-O(4)	90.60(8)	C(5)-Fe(1)-C(1)	40.06(8)
O(5)-C(36)	1.281(2)	N(2)-Pd(2)-O(4)	171.43(6)	C(26)-Fe(2)-C(25)	40.93(11)
O(6)-C(36)	1.244(2)	C(17)-Pd(2)-O(6)	174.39(6)	C(26)-Fe(2)-C(19)	158.96(11)
N(1)-C(11)	1.286(3)	N(2)-Pd(2)-O(6)	94.45(6)	C(25)-Fe(2)-C(19)	158.36(10)
N(1)-C(12)	1.486(3)	O(4)-Pd(2)-O(6)	94.05(5)	C(26)-Fe(2)-C(22)	39.59(10)
N(2)-C(27)	1.285(2)	C(17)-Pd(2)-Pd(1)	108.96(6)	C(25)-Fe(2)-C(22)	67.60(11)
N(2)-C(28)	1.485(3)	N(2)-Pd(2)-Pd(1)	100.90(4)	C(19)-Fe(2)-C(22)	123.64(10)
C(1)-C(5)	1.407(3)	O(4)-Pd(2)-Pd(1)	82.30(4)	C(26)-Fe(2)-C(23)	66.39(10)
C(1)-C(2)	1.434(3)	O(6)-Pd(2)-Pd(1)	74.82(4)	C(25)-Fe(2)-C(23)	67.12(10)
C(2)-C(11)	1.430(3)	C(3)-Fe(1)-C(4)	40.90(10)	C(19)-Fe(2)-C(23)	108.73(10)
C(2)-C(3)	1.436(3)	C(3)-Fe(1)-C(8)	124.38(11)	C(22)-Fe(2)-C(23)	39.22(11)
C(3)-C(4)	1.407(3)	C(4)-Fe(1)-C(8)	160.50(12)	C(26)-Fe(2)-C(18)	123.93(10)
C(4)-C(5)	1.397(4)	C(3)-Fe(1)-C(10)	158.77(11)	C(25)-Fe(2)-C(18)	159.18(9)
C(6)-C(7)	1.354(4)	C(4)-Fe(1)-C(10)	122.76(10)	C(19)-Fe(2)-C(18)	40.57(9)
C(6)-C(10)	1.384(4)	C(8)-Fe(1)-C(10)	66.79(10)	C(22)-Fe(2)-C(18)	110.07(10)
C(7)-C(8)	1.409(4)	C(3)-Fe(1)-C(9)	160.18(11)	C(23)-Fe(2)-C(18)	125.14(11)
C(8)-C(9)	1.392(4)	C(4)-Fe(1)-C(9)	157.51(11)	C(26)-Fe(2)-C(24)	67.09(11)
C(9)-C(10)	1.373(4)	C(8)-Fe(1)-C(9)	40.20(11)	C(25)-Fe(2)-C(24)	39.68(10)
C(12)-C(13)	1.506(3)	C(10)-Fe(1)-C(9)	39.60(11)	C(19)-Fe(2)-C(24)	123.42(10)

C(22)-Fe(2)-C(24)	66.80(10)	C(11)-C(2)-C(1)	115.4(2)	C(19)-C(18)-C(27)	136.3(2)
C(23)-Fe(2)-C(24)	40.03(12)	C(11)-C(2)-C(3)	136.3(2)	C(17)-C(18)-C(27)	113.0(2)
C(18)-Fe(2)-C(24)	160.28(10)	C(1)-C(2)-C(3)	108.2(2)	C(19)-C(18)-Fe(2)	69.44(14)
C(26)-Fe(2)-C(20)	159.01(11)	C(11)-C(2)-Fe(1)	123.78(13)	C(17)-C(18)-Fe(2)	71.10(12)
C(25)-Fe(2)-C(20)	122.24(11)	C(1)-C(2)-Fe(1)	70.42(10)	C(27)-C(18)-Fe(2)	122.1(2)
C(19)-Fe(2)-C(20)	40.95(10)	C(3)-C(2)-Fe(1)	68.38(10)	C(18)-C(19)-C(20)	106.2(2)
C(22)-Fe(2)-C(20)	159.43(10)	C(4)-C(3)-C(2)	106.7(2)	C(18)-C(19)-Fe(2)	69.98(14)
C(23)-Fe(2)-C(20)	124.10(11)	C(4)-C(3)-Fe(1)	69.73(12)	C(20)-C(19)-Fe(2)	70.1(2)
C(18)-Fe(2)-C(20)	67.49(10)	C(2)-C(3)-Fe(1)	70.04(11)	C(21)-C(20)-C(19)	109.0(2)
C(24)-Fe(2)-C(20)	108.15(10)	C(5)-C(4)-C(3)	109.2(2)	C(21)-C(20)-Fe(2)	70.43(14)
C(26)-Fe(2)-C(21)	123.44(9)	C(5)-C(4)-Fe(1)	71.20(13)	C(19)-C(20)-Fe(2)	68.97(14)
C(25)-Fe(2)-C(21)	106.89(10)	C(3)-C(4)-Fe(1)	69.37(12)	C(20)-C(21)-C(17)	108.7(2)
C(19)-Fe(2)-C(21)	68.84(9)	C(4)-C(5)-C(1)	109.2(2)	C(20)-C(21)-Fe(2)	69.29(12)
C(22)-Fe(2)-C(21)	159.57(9)	C(4)-C(5)-Fe(1)	68.60(13)	C(17)-C(21)-Fe(2)	70.37(10)
C(23)-Fe(2)-C(21)	158.73(11)	C(1)-C(5)-Fe(1)	70.29(12)	C(23)-C(22)-C(26)	108.4(3)
C(18)-Fe(2)-C(21)	67.64(9)	C(7)-C(6)-C(10)	108.0(3)	C(23)-C(22)-Fe(2)	70.46(15)
C(24)-Fe(2)-C(21)	122.40(10)	C(7)-C(6)-Fe(1)	71.03(14)	C(26)-C(22)-Fe(2)	69.85(14)
C(20)-Fe(2)-C(21)	40.28(9)	C(10)-C(6)-Fe(1)	69.77(13)	C(22)-C(23)-C(24)	108.7(2)
C(26)-Fe(2)-C(17)	107.88(9)	C(6)-C(7)-C(8)	108.5(3)	C(22)-C(23)-Fe(2)	70.32(12)
C(25)-Fe(2)-C(17)	122.03(9)	C(6)-C(7)-Fe(1)	70.2(2)	C(24)-C(23)-Fe(2)	70.21(13)
C(19)-Fe(2)-C(17)	69.36(8)	C(8)-C(7)-Fe(1)	68.97(14)	C(25)-C(24)-C(23)	108.0(3)
C(22)-Fe(2)-C(17)	124.29(9)	C(9)-C(8)-C(7)	107.0(2)	C(25)-C(24)-Fe(2)	69.54(14)
C(23)-Fe(2)-C(17)	160.16(12)	C(9)-C(8)-Fe(1)	70.05(14)	C(23)-C(24)-Fe(2)	69.76(14)
C(18)-Fe(2)-C(17)	40.75(8)	C(7)-C(8)-Fe(1)	70.52(14)	C(24)-C(25)-C(26)	106.9(2)
C(24)-Fe(2)-C(17)	157.52(10)	C(10)-C(9)-C(8)	107.4(3)	C(24)-C(25)-Fe(2)	70.8(2)
C(20)-Fe(2)-C(17)	68.22(8)	C(10)-C(9)-Fe(1)	70.13(14)	C(26)-C(25)-Fe(2)	69.5(2)
C(21)-Fe(2)-C(17)	40.50(8)	C(8)-C(9)-Fe(1)	69.74(13)	C(22)-C(26)-C(25)	108.0(2)
C(15)-O(1)-C(13)	105.9(2)	C(9)-C(10)-C(6)	109.1(3)	C(22)-C(26)-Fe(2)	70.6(2)
C(29)-O(2)-C(31)	106.6(2)	C(9)-C(10)-Fe(1)	70.27(12)	C(25)-C(26)-Fe(2)	69.6(2)
C(34)-O(3)-Pd(1)	126.01(14)	C(6)-C(10)-Fe(1)	70.35(12)	N(2)-C(27)-C(18)	115.6(2)
C(34)-O(4)-Pd(2)	118.62(15)	N(1)-C(11)-C(2)	115.3(2)	N(2)-C(28)-C(29)	113.2(2)
C(36)-O(5)-Pd(1)	119.46(11)	N(1)-C(12)-C(13)	114.40(14)	O(2)-C(29)-C(30)	104.7(2)
C(36)-O(6)-Pd(2)	125.77(14)	O(1)-C(13)-C(12)	109.2(2)	O(2)-C(29)-C(28)	109.8(2)
C(11)-N(1)-C(12)	119.8(2)	O(1)-C(13)-C(14)	104.6(2)	C(30)-C(29)-C(28)	118.3(2)
C(11)-N(1)-Pd(1)	115.66(15)	C(12)-C(13)-C(14)	118.4(2)	C(29)-C(30)-C(32)	102.6(2)
C(12)-N(1)-Pd(1)	124.54(15)	C(16)-C(14)-C(13)	102.5(2)	O(2)-C(31)-C(32)	108.1(2)
C(27)-N(2)-C(28)	119.6(2)	O(1)-C(15)-C(16)	108.4(2)	C(31)-C(32)-C(30)	104.7(2)
C(27)-N(2)-Pd(2)	116.1(2)	C(15)-C(16)-C(14)	105.3(2)	O(3)-C(34)-O(4)	127.6(2)
C(28)-N(2)-Pd(2)	124.29(12)	C(21)-C(17)-C(18)	105.5(2)	O(3)-C(34)-C(33)	117.8(2)
C(5)-C(1)-C(2)	106.7(2)	C(21)-C(17)-Pd(2)	140.2(2)	O(4)-C(34)-C(33)	114.6(2)
C(5)-C(1)-Pd(1)	141.4(2)	C(18)-C(17)-Pd(2)	114.2(2)	O(6)-C(36)-O(5)	126.4(2)
C(2)-C(1)-Pd(1)	111.8(2)	C(21)-C(17)-Fe(2)	69.13(10)	O(6)-C(36)-C(35)	117.8(2)
C(5)-C(1)-Fe(1)	69.64(12)	C(18)-C(17)-Fe(2)	68.15(10)	O(5)-C(36)-C(35)	115.8(2)
C(2)-C(1)-Fe(1)	68.57(11)	Pd(2)-C(17)-Fe(2)	127.29(11)	Cl(1)-C(1W)-Cl(2)	110.8(2)
Pd(1)-C(1)-Fe(1)	127.39(9)	C(19)-C(18)-C(17)	110.6(2)		

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)	0.04139(6)	0.03754(6)	0.03808(9)	0.00098(8)	-0.00118(8)	0.02010(5)
Pd(2)	0.03871(6)	0.03786(7)	0.03683(9)	0.00083(8)	0.00175(8)	0.01738(5)
Fe(1)	0.04732(14)	0.04227(13)	0.0407(2)	-0.00115(14)	0.00196(15)	0.02131(10)
Fe(2)	0.04564(14)	0.04286(14)	0.0400(2)	-0.00203(14)	-0.00291(15)	0.01959(11)
O(1)	0.0641(7)	0.0713(7)	0.0588(11)	0.0121(8)	0.0045(8)	0.0419(5)
O(2)	0.0453(7)	0.0687(8)	0.0700(12)	0.0160(8)	0.0087(8)	0.0215(6)
O(3)	0.0568(7)	0.0446(6)	0.0498(10)	0.0005(7)	0.0092(7)	0.0271(5)
O(4)	0.0511(6)	0.0539(6)	0.0635(11)	0.0105(7)	0.0144(7)	0.0337(5)
O(5)	0.0409(6)	0.0476(7)	0.0573(10)	0.0076(7)	-0.0087(7)	0.0185(5)
O(6)	0.0465(7)	0.0514(7)	0.0455(10)	0.0030(7)	-0.0049(7)	0.0206(5)
N(1)	0.0414(7)	0.0469(8)	0.0326(10)	-0.0024(8)	-0.0037(8)	0.0200(6)
N(2)	0.0441(8)	0.0410(8)	0.0491(12)	0.0044(8)	0.0032(8)	0.0207(6)
C(1)	0.0359(9)	0.0353(9)	0.0405(13)	0.0044(9)	-0.0003(10)	0.0125(7)
C(2)	0.0427(10)	0.0448(10)	0.0495(15)	-0.0066(10)	-0.0009(10)	0.0200(7)
C(3)	0.0661(11)	0.0598(11)	0.062(2)	-0.0025(12)	0.0216(12)	0.0354(8)
C(4)	0.0715(12)	0.0623(12)	0.0373(14)	-0.0078(11)	0.0062(12)	0.0281(9)
C(5)	0.0498(11)	0.0328(10)	0.052(2)	-0.0022(11)	-0.0011(11)	0.0099(8)
C(6)	0.089(2)	0.0537(14)	0.084(2)	-0.0170(14)	0.021(2)	0.0129(12)
C(7)	0.0635(12)	0.0576(12)	0.123(3)	0.0093(15)	0.003(2)	0.0353(9)
C(8)	0.074(2)	0.0614(14)	0.051(2)	0.0142(14)	-0.0053(14)	0.0077(12)
C(9)	0.0635(13)	0.0567(13)	0.091(2)	0.0082(14)	0.0294(14)	0.0191(10)
C(10)	0.0501(12)	0.0631(13)	0.077(2)	0.0149(14)	-0.0188(13)	0.0106(10)
C(11)	0.0326(9)	0.0406(9)	0.0554(15)	-0.0013(10)	-0.0045(10)	0.0158(7)
C(12)	0.0519(10)	0.0443(10)	0.0516(15)	-0.0137(10)	-0.0195(11)	0.0242(7)
C(13)	0.0610(10)	0.0616(11)	0.0326(13)	0.0023(10)	-0.0077(10)	0.0356(8)
C(14)	0.0480(10)	0.0815(13)	0.056(2)	0.0029(13)	-0.0016(11)	0.0338(9)
C(15)	0.089(2)	0.0699(14)	0.085(2)	0.0270(15)	0.008(2)	0.0277(12)
C(16)	0.0547(13)	0.113(2)	0.115(2)	0.059(2)	-0.0128(15)	0.0273(12)
C(17)	0.0510(10)	0.0327(9)	0.0439(14)	0.0069(10)	0.0029(10)	0.0173(7)
C(18)	0.0450(10)	0.0499(10)	0.0433(14)	-0.0047(10)	-0.0093(10)	0.0229(7)
C(19)	0.0561(10)	0.0661(11)	0.055(2)	-0.0078(12)	-0.0189(11)	0.0360(8)
C(20)	0.0899(14)	0.0576(12)	0.046(2)	-0.0075(12)	-0.0211(13)	0.0354(10)
C(21)	0.0531(11)	0.0439(10)	0.0429(14)	-0.0066(10)	-0.0025(11)	0.0191(8)
C(22)	0.0772(13)	0.0607(12)	0.077(2)	0.0262(13)	0.0255(14)	0.0360(9)
C(23)	0.0509(13)	0.0638(14)	0.143(3)	0.020(2)	0.003(2)	0.0187(10)
C(24)	0.122(2)	0.0458(12)	0.061(2)	-0.0090(13)	-0.023(2)	0.0276(12)
C(25)	0.0757(12)	0.0624(11)	0.093(2)	0.0141(13)	0.0243(14)	0.0442(8)
C(26)	0.0899(14)	0.0513(11)	0.075(2)	0.0011(13)	-0.0241(14)	0.0344(10)
C(27)	0.0373(9)	0.0404(9)	0.060(2)	0.0011(11)	0.0030(10)	0.0205(7)
C(28)	0.0547(10)	0.0583(11)	0.0315(13)	-0.0127(10)	-0.0024(10)	0.0288(8)
C(29)	0.0436(9)	0.0648(11)	0.0317(13)	0.0021(10)	0.0042(10)	0.0274(8)
C(30)	0.0663(11)	0.0886(13)	0.046(2)	0.0132(12)	0.0083(12)	0.0493(8)
C(31)	0.097(2)	0.0788(14)	0.063(2)	0.0312(14)	0.0254(15)	0.0405(11)
C(32)	0.1185(13)	0.1058(13)	0.119(2)	0.0572(15)	0.067(2)	0.0847(9)
C(33)	0.0846(12)	0.1095(15)	0.063(2)	0.0087(14)	0.0353(13)	0.0597(10)
C(34)	0.0409(9)	0.0548(10)	0.0430(14)	0.0048(11)	0.0080(10)	0.0238(7)
C(35)	0.0600(13)	0.106(2)	0.070(2)	0.016(2)	-0.0172(14)	0.0314(11)
C(36)	0.0427(10)	0.0632(11)	0.0415(14)	-0.0067(11)	-0.0106(10)	0.0274(8)
C(1W)	0.0681(12)	0.123(2)	0.135(3)	-0.031(2)	-0.015(2)	0.0587(11)
Cl(1)	0.1175(4)	0.1577(5)	0.1352(9)	-0.0231(6)	0.0010(5)	0.0886(3)
Cl(2)	0.1001(4)	0.1604(6)	0.1361(9)	-0.0262(6)	-0.0255(5)	0.0695(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)	0.0168(2)	1.0069(2)	0.08799(9)	0.073
H(4A)	0.1743(2)	1.0180(2)	0.15894(9)	0.071
H(5A)	0.3346(2)	0.9309(2)	0.12908(8)	0.060
H(6A)	0.4071(3)	1.3386(2)	0.12773(11)	0.103
H(7A)	0.2586(2)	1.3338(2)	0.05747(11)	0.095
H(8A)	0.3210(2)	1.2370(2)	-0.01798(9)	0.088
H(9A)	0.5142(2)	1.1866(2)	0.00785(11)	0.090
H(10A)	0.5653(2)	1.2498(2)	0.09734(10)	0.086
H(11A)	0.0165(2)	0.9140(2)	-0.01870(8)	0.053
H(12A)	0.0226(2)	0.7953(2)	-0.09007(8)	0.059
H(12B)	0.1349(2)	0.7485(2)	-0.09424(8)	0.059
H(13A)	0.1915(2)	0.9187(2)	-0.15081(8)	0.059
H(14A)	0.3880(2)	1.0335(2)	-0.07388(9)	0.073
H(14B)	0.4106(2)	0.9862(2)	-0.12623(9)	0.073
H(15A)	0.2876(2)	1.2570(2)	-0.11028(11)	0.104
H(15B)	0.2541(2)	1.1900(2)	-0.16302(11)	0.104
H(16A)	0.4763(2)	1.2438(2)	-0.10750(12)	0.121
H(16B)	0.4457(2)	1.1822(2)	-0.16121(12)	0.121
H(19A)	-0.3237(2)	0.3271(2)	-0.06813(9)	0.068
H(20A)	-0.1767(2)	0.3166(2)	-0.13964(9)	0.078
H(21A)	0.0713(2)	0.4019(2)	-0.10913(8)	0.059
H(22A)	-0.2545(2)	0.0949(2)	0.03689(10)	0.085
H(23A)	-0.4084(2)	0.0040(2)	-0.03724(13)	0.108
H(24A)	-0.2641(3)	-0.0046(2)	-0.10819(10)	0.099
H(25A)	-0.0170(2)	0.0842(2)	-0.07750(11)	0.087
H(26A)	-0.0130(2)	0.1447(2)	0.01367(10)	0.087
H(27A)	-0.2317(2)	0.4176(2)	0.03857(9)	0.054
H(28A)	-0.1060(2)	0.5397(2)	0.10909(8)	0.058
H(28B)	0.0531(2)	0.5859(2)	0.11334(8)	0.058
H(29A)	-0.0617(2)	0.4153(2)	0.17005(8)	0.056
H(30A)	0.0911(2)	0.3498(2)	0.14542(9)	0.075
H(30B)	0.0197(2)	0.2999(2)	0.09340(9)	0.075
H(31A)	-0.3019(2)	0.0758(2)	0.12925(10)	0.097
H(31B)	-0.2722(2)	0.1410(2)	0.18226(10)	0.097
H(32A)	-0.0999(2)	0.0889(2)	0.12880(12)	0.122
H(32B)	-0.0705(2)	0.1534(2)	0.18210(12)	0.122
H(33A)	0.4153(2)	0.5248(2)	-0.10276(9)	0.121
H(33B)	0.5210(2)	0.6864(2)	-0.10389(9)	0.121
H(33C)	0.3821(2)	0.6234(2)	-0.13443(9)	0.121
H(35A)	0.5582(2)	0.8107(3)	0.12256(10)	0.125
H(35B)	0.5019(2)	0.6491(3)	0.12458(10)	0.125
H(35C)	0.4255(2)	0.7135(3)	0.15403(10)	0.125
H(1WA)	-0.4491(2)	0.5864(3)	0.01650(14)	0.125
H(1WB)	-0.3698(2)	0.7457(3)	0.00231(14)	0.125

Tables for *syn*-(+)-(R_p, R, R, R_p)-2bTable 1. Atomic coordinates [x 10⁵ for Pd, Fe; x 10⁴ for other atoms] and equivalent isotropic displacement parameters [Å² x 10⁴ for Pd, Fe; Å x 10³ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	-0.01098(2)	0.339920(11)	0.040891(8)	0.05900(7)
Pd(2)	0.06818(2)	0.394810(12)	0.117207(9)	0.06910(8)
Fe(1)	0.14885(4)	0.29438(2)	-0.053531(15)	0.0615(2)
Fe(2)	0.19874(5)	0.52359(3)	0.11221(2)	0.1005(2)
O(1)	-0.2062(2)	0.37253(11)	-0.06892(8)	0.0925(10)
O(2)	0.3953(2)	0.36830(13)	0.17707(10)	0.1219(12)
O(3)	0.0040(2)	0.27480(9)	0.08208(7)	0.0708(7)
O(4)	0.0327(2)	0.31886(10)	0.14636(7)	0.0769(8)
O(5)	-0.1660(2)	0.36197(9)	0.07496(6)	0.0685(8)
O(6)	-0.0977(2)	0.41516(10)	0.12932(8)	0.0857(9)
N(1)	-0.0222(2)	0.39783(11)	-0.00530(8)	0.0614(9)
N(2)	0.2347(2)	0.38083(12)	0.10233(8)	0.0684(10)
C(1)	0.1291(3)	0.32626(14)	0.00885(9)	0.0579(10)
C(2)	0.1522(3)	0.36697(14)	-0.02323(10)	0.0691(12)
C(3)	0.2612(3)	0.35387(15)	-0.04451(12)	0.0762(12)
C(4)	0.3022(3)	0.30662(15)	-0.02435(10)	0.0781(13)
C(5)	0.2210(3)	0.29077(15)	0.00719(11)	0.0730(13)
C(6)	0.1177(4)	0.2847(2)	-0.11950(12)	0.093(2)
C(7)	0.1709(3)	0.2401(2)	-0.10220(12)	0.0880(15)
C(8)	0.1060(4)	0.2194(2)	-0.06938(12)	0.096(2)
C(9)	0.0014(4)	0.2526(2)	-0.06400(13)	0.1007(15)
C(10)	0.0114(4)	0.2931(2)	-0.09665(14)	0.101(2)
C(11)	0.0643(3)	0.40477(12)	-0.03165(10)	0.0634(11)
C(12)	0.0690(4)	0.44389(15)	-0.06836(12)	0.0896(15)
C(13)	-0.1276(3)	0.42735(15)	-0.01073(13)	0.0808(13)
C(14)	-0.2242(3)	0.38719(14)	-0.02539(11)	0.0714(12)
C(15)	-0.3410(3)	0.4129(2)	-0.02243(13)	0.0872(15)
C(16)	-0.4025(4)	0.3786(2)	-0.05980(15)	0.114(2)
C(17)	-0.3102(3)	0.3642(2)	-0.0900(2)	0.130(2)
C(18)	0.1010(3)	0.46089(14)	0.08764(12)	0.0712(12)
C(19)	0.2150(3)	0.4597(2)	0.06912(11)	0.0848(13)
C(20)	0.2277(4)	0.5126(2)	0.04629(14)	0.113(2)
C(21)	0.1322(4)	0.5425(2)	0.0515(2)	0.124(2)
C(22)	0.0522(4)	0.5117(2)	0.07746(13)	0.100(2)
C(23)	0.3214(5)	0.5674(2)	0.1392(2)	0.181(2)
C(24)	0.3075(5)	0.5129(2)	0.16154(15)	0.173(2)
C(25)	0.1954(5)	0.5175(3)	0.17868(14)	0.172(2)
C(26)	0.1533(6)	0.5632(2)	0.1655(2)	0.193(3)
C(27)	0.2145(6)	0.5947(3)	0.1435(2)	0.191(3)
C(28)	0.2878(3)	0.4141(2)	0.08065(11)	0.0739(13)
C(29)	0.4042(3)	0.4111(2)	0.06346(14)	0.104(2)
C(30)	0.2898(3)	0.3325(2)	0.11739(11)	0.0795(12)
C(31)	0.3098(3)	0.3295(2)	0.16586(11)	0.0890(15)
C(32)	0.3435(4)	0.2786(2)	0.18213(15)	0.111(2)
C(33)	0.4380(5)	0.2886(3)	0.2133(2)	0.158(3)
C(34)	0.4779(4)	0.3387(2)	0.1987(2)	0.183(3)
C(35)	-0.0109(4)	0.2259(2)	0.14739(13)	0.113(2)
C(36)	0.0106(3)	0.27835(14)	0.12306(11)	0.0736(12)
C(37)	-0.2931(3)	0.4077(2)	0.12072(14)	0.096(2)

C(38)	-0.1763(3)	0.39351(14)	0.10627(11)	0.0645(11)
Pd(1')	-0.37985(3)	0.621385(14)	-0.131636(9)	0.08429(11)
Pd(2')	-0.29819(3)	0.515006(14)	-0.143745(9)	0.07994(10)
Fe(1')	-0.59045(6)	0.69646(3)	-0.19030(2)	0.1058(2)
Fe(2')	-0.09908(5)	0.45841(3)	-0.22052(2)	0.0935(2)
O(1')	-0.2087(4)	0.75750(14)	-0.1849(2)	0.181(2)
O(2')	-0.5040(3)	0.3983(2)	-0.21895(15)	0.181(2)
O(3')	-0.4809(3)	0.58880(11)	-0.08346(8)	0.1000(11)
O(4')	-0.4423(2)	0.50466(11)	-0.10123(8)	0.1016(11)
O(5')	-0.2306(2)	0.61776(11)	-0.09014(9)	0.0992(10)
O(6')	-0.1956(2)	0.52928(12)	-0.08997(9)	0.0979(10)
N(1')	-0.2961(3)	0.65113(13)	-0.18479(9)	0.0808(11)
N(2')	-0.3861(3)	0.50395(14)	-0.20037(9)	0.0879(12)
C(1')	-0.5072(3)	0.6262(2)	-0.17155(12)	0.0853(14)
C(2')	-0.4773(4)	0.6432(2)	-0.21614(12)	0.104(2)
C(3')	-0.5768(4)	0.6464(2)	-0.24197(14)	0.106(2)
C(4')	-0.6647(4)	0.6317(2)	-0.21630(14)	0.111(2)
C(5')	-0.6263(4)	0.6188(2)	-0.17345(14)	0.102(2)
C(6')	-0.6878(6)	0.7626(2)	-0.1902(2)	0.161(3)
C(7')	-0.6694(6)	0.7427(2)	-0.1471(2)	0.150(3)
C(8')	-0.5605(5)	0.7519(2)	-0.1405(2)	0.161(3)
C(9')	-0.5166(5)	0.7642(2)	-0.1812(2)	0.156(3)
C(10')	-0.5928(5)	0.7759(2)	-0.2108(2)	0.153(2)
C(11')	-0.3534(3)	0.6578(2)	-0.22099(12)	0.0925(15)
C(12')	-0.3091(4)	0.6770(2)	-0.26463(13)	0.132(2)
C(13')	-0.1768(3)	0.6668(2)	-0.18147(14)	0.100(2)
C(14')	-0.1586(4)	0.7138(2)	-0.1594(2)	0.106(2)
C(15')	-0.0393(5)	0.7301(2)	-0.1530(2)	0.140(2)
C(16')	-0.0365(5)	0.7855(2)	-0.1661(2)	0.217(3)
C(17')	-0.1385(5)	0.7938(2)	-0.1949(2)	0.189(3)
C(18')	-0.1747(3)	0.5208(2)	-0.18457(11)	0.0853(14)
C(19')	-0.2112(3)	0.5190(2)	-0.22931(13)	0.094(2)
C(20')	-0.1121(4)	0.5237(2)	-0.25915(14)	0.122(2)
C(21')	-0.0174(4)	0.5280(2)	-0.23201(14)	0.122(2)
C(22')	-0.0537(4)	0.5243(2)	-0.1853(2)	0.103(2)
C(23')	-0.1840(5)	0.3896(2)	-0.2220(2)	0.143(2)
C(24')	-0.1084(7)	0.3935(2)	-0.2593(2)	0.178(3)
C(25')	0.0018(5)	0.4004(2)	-0.2421(2)	0.145(2)
C(26')	-0.0026(5)	0.3983(2)	-0.1987(2)	0.143(2)
C(27')	-0.1161(5)	0.3917(2)	-0.1847(2)	0.138(2)
C(28')	-0.3304(3)	0.5086(2)	-0.23739(13)	0.098(2)
C(29')	-0.3818(4)	0.5051(2)	-0.28270(11)	0.122(2)
C(30')	-0.5079(3)	0.4935(2)	-0.19968(14)	0.101(2)
C(31')	-0.5336(4)	0.4356(2)	-0.1847(2)	0.112(2)
C(32')	-0.6627(4)	0.4224(2)	-0.1829(2)	0.158(3)
C(33')	-0.6933(5)	0.3858(2)	-0.2087(2)	0.250(4)
C(34')	-0.5983(5)	0.3699(2)	-0.23176(14)	0.155(2)
C(35')	-0.5827(4)	0.5212(2)	-0.04873(15)	0.141(2)
C(36')	-0.4972(4)	0.5400(2)	-0.08108(13)	0.098(2)
C(37')	-0.0922(5)	0.5831(2)	-0.0398(2)	0.153(2)
C(38')	-0.1833(4)	0.5750(2)	-0.07602(14)	0.100(2)

Table 2. Bond lengths (\AA) and angles (deg.).

Pd(1)-C(1)	1.940(3)	C(14)-C(15)	1.520(5)	O(3')-C(36')	1.243(5)
Pd(1)-N(1)	2.019(3)	C(15)-C(16)	1.593(6)	O(4')-C(36')	1.255(5)
Pd(1)-O(3)	2.061(2)	C(16)-C(17)	1.463(6)	O(5')-C(38')	1.283(5)
Pd(1)-O(5)	2.164(2)	C(18)-C(22)	1.432(6)	O(6')-C(38')	1.231(5)
Pd(1)-Pd(2)	2.8402(4)	C(18)-C(19)	1.451(5)	N(1')-C(11')	1.294(5)
Pd(2)-C(18)	1.923(4)	C(19)-C(28)	1.471(5)	N(1')-C(13')	1.460(5)
Pd(2)-N(2)	2.038(3)	C(19)-C(20)	1.503(6)	N(2')-C(28')	1.300(5)
Pd(2)-O(6)	2.048(2)	C(20)-C(21)	1.360(7)	N(2')-C(30')	1.456(5)
Pd(2)-O(4)	2.141(2)	C(21)-C(22)	1.449(6)	C(1')-C(5')	1.414(6)
Fe(1)-C(8)	2.008(4)	C(23)-C(27)	1.438(9)	C(1')-C(2')	1.455(5)
Fe(1)-C(3)	2.012(4)	C(23)-C(24)	1.533(8)	C(2')-C(3')	1.408(6)
Fe(1)-C(7)	2.020(4)	C(24)-C(25)	1.420(8)	C(2')-C(11')	1.508(6)
Fe(1)-C(5)	2.021(3)	C(25)-C(26)	1.312(9)	C(3')-C(4')	1.343(6)
Fe(1)-C(4)	2.029(4)	C(26)-C(27)	1.261(9)	C(4')-C(5')	1.407(6)
Fe(1)-C(6)	2.038(4)	C(28)-C(29)	1.466(5)	C(6')-C(10')	1.321(8)
Fe(1)-C(2)	2.040(4)	C(30)-C(31)	1.483(5)	C(6')-C(7')	1.408(8)
Fe(1)-C(9)	2.051(4)	C(31)-C(32)	1.424(6)	C(6')-C(9')	2.031(9)
Fe(1)-C(1)	2.058(3)	C(32)-C(33)	1.476(7)	C(7')-C(8')	1.315(9)
Fe(1)-C(10)	2.075(4)	C(33)-C(34)	1.413(8)	C(8')-C(9')	1.368(9)
Fe(2)-C(26)	1.965(6)	C(35)-C(36)	1.528(5)	C(9')-C(10')	1.297(8)
Fe(2)-C(24)	1.980(5)	C(37)-C(38)	1.484(5)	C(11')-C(12')	1.495(6)
Fe(2)-C(23)	1.987(5)	Pd(1')-C(1')	1.924(4)	C(13')-C(14')	1.372(6)
Fe(2)-C(25)	2.011(4)	Pd(1')-N(1')	2.025(3)	C(14')-C(15')	1.474(7)
Fe(2)-C(27)	2.029(6)	Pd(1')-O(3')	2.048(3)	C(15')-C(16')	1.445(7)
Fe(2)-C(20)	2.036(4)	Pd(1')-O(5')	2.158(3)	C(16')-C(17')	1.495(9)
Fe(2)-C(22)	2.039(4)	Pd(1')-Pd(2')	2.8623(5)	C(18')-C(19')	1.417(5)
Fe(2)-C(21)	2.048(5)	Pd(2')-C(18')	1.909(4)	C(18')-C(22')	1.425(6)
Fe(2)-C(19)	2.073(4)	Pd(2')-N(2')	2.016(3)	C(19')-C(28')	1.445(6)
Fe(2)-C(18)	2.085(4)	Pd(2')-O(6')	2.053(3)	C(19')-C(20')	1.477(6)
O(1)-C(14)	1.380(4)	Pd(2')-O(4')	2.140(3)	C(20')-C(21')	1.386(7)
O(1)-C(17)	1.394(5)	Fe(1')-C(9')	1.928(6)	C(21')-C(22')	1.477(6)
O(2)-C(34)	1.388(6)	Fe(1')-C(7')	1.976(6)	C(23')-C(27')	1.381(8)
O(2)-C(31)	1.439(5)	Fe(1')-C(4')	2.005(5)	C(23')-C(24')	1.436(9)
O(3)-C(36)	1.242(4)	Fe(1')-C(3')	2.009(4)	C(24')-C(25')	1.407(9)
O(4)-C(36)	1.264(4)	Fe(1')-C(6')	2.017(5)	C(25')-C(26')	1.313(7)
O(5)-C(38)	1.239(4)	Fe(1')-C(2')	2.041(4)	C(26')-C(27')	1.409(8)
O(6)-C(38)	1.278(4)	Fe(1')-C(5')	2.059(4)	C(28')-C(29')	1.497(5)
N(1)-C(11)	1.303(4)	Fe(1')-C(8')	2.078(6)	C(30')-C(31')	1.553(6)
N(1)-C(13)	1.453(4)	Fe(1')-C(10')	2.088(6)	C(31')-C(32')	1.553(7)
N(2)-C(28)	1.232(4)	Fe(1')-C(1')	2.097(4)	C(32')-C(33')	1.257(9)
N(2)-C(30)	1.449(5)	Fe(2')-C(25')	1.988(6)	C(33')-C(34')	1.375(8)
C(1)-C(5)	1.402(5)	Fe(2')-C(23')	1.996(5)	C(35')-C(36')	1.478(6)
C(1)-C(2)	1.434(5)	Fe(2')-C(26')	2.000(5)	C(37')-C(38')	1.544(7)
C(2)-C(11)	1.425(5)	Fe(2')-C(27')	2.002(5)	C(1)-Pd(1)-N(1)	80.74(12)
C(2)-C(3)	1.470(5)	Fe(2')-C(24')	2.009(6)	C(1)-Pd(1)-O(3)	95.02(11)
C(3)-C(4)	1.418(5)	Fe(2')-C(20')	2.018(5)	N(1)-Pd(1)-O(3)	173.37(9)
C(4)-C(5)	1.404(5)	Fe(2')-C(21')	2.023(5)	C(1)-Pd(1)-O(5)	175.26(12)
C(6)-C(7)	1.384(6)	Fe(2')-C(19')	2.031(4)	N(1)-Pd(1)-O(5)	95.07(9)
C(6)-C(10)	1.443(6)	Fe(2')-C(22')	2.039(5)	O(3)-Pd(1)-O(5)	89.35(9)
C(7)-C(8)	1.354(6)	Fe(2')-C(18')	2.102(4)	C(1)-Pd(1)-Pd(2)	102.23(9)
C(8)-C(9)	1.494(6)	O(1')-C(17')	1.267(7)	N(1)-Pd(1)-Pd(2)	103.38(7)
C(9)-C(10)	1.422(6)	O(1')-C(14')	1.464(6)	O(3)-Pd(1)-Pd(2)	82.44(6)
C(11)-C(12)	1.481(5)	O(2')-C(34')	1.374(7)	O(5)-Pd(1)-Pd(2)	76.50(6)
C(13)-C(14)	1.581(5)	O(2')-C(31')	1.437(6)	C(18)-Pd(2)-N(2)	81.59(13)

C(18)-Pd(2)-O(6)	93.35(12)	C(24)-Fe(2)-C(23)	45.5(2)	C(5)-C(1)-Pd(1)	141.7(2)
N(2)-Pd(2)-O(6)	174.94(11)	C(26)-Fe(2)-C(25)	38.5(2)	C(2)-C(1)-Pd(1)	111.8(2)
C(18)-Pd(2)-O(4)	176.55(12)	C(24)-Fe(2)-C(25)	41.7(2)	C(5)-C(1)-Fe(1)	68.5(2)
N(2)-Pd(2)-O(4)	97.12(10)	C(23)-Fe(2)-C(25)	69.4(2)	C(2)-C(1)-Fe(1)	68.8(2)
O(6)-Pd(2)-O(4)	87.92(10)	C(26)-Fe(2)-C(27)	36.8(3)	Pd(1)-C(1)-Fe(1)	128.3(2)
C(18)-Pd(2)-Pd(1)	96.24(11)	C(24)-Fe(2)-C(27)	73.2(3)	C(11)-C(2)-C(1)	117.3(3)
N(2)-Pd(2)-Pd(1)	93.01(7)	C(23)-Fe(2)-C(27)	41.9(2)	C(11)-C(2)-C(3)	134.6(3)
O(6)-Pd(2)-Pd(1)	87.36(7)	C(25)-Fe(2)-C(27)	66.8(3)	C(1)-C(2)-C(3)	107.5(3)
O(4)-Pd(2)-Pd(1)	80.61(6)	C(26)-Fe(2)-C(20)	156.0(2)	C(11)-C(2)-Fe(1)	120.1(2)
C(8)-Fe(1)-C(3)	153.3(2)	C(24)-Fe(2)-C(20)	127.4(2)	C(1)-C(2)-Fe(1)	70.2(2)
C(8)-Fe(1)-C(7)	39.3(2)	C(23)-Fe(2)-C(20)	110.7(2)	C(3)-C(2)-Fe(1)	67.7(2)
C(3)-Fe(1)-C(7)	121.0(2)	C(25)-Fe(2)-C(20)	165.1(2)	C(4)-C(3)-C(2)	107.2(3)
C(8)-Fe(1)-C(5)	106.2(2)	C(27)-Fe(2)-C(20)	123.9(2)	C(4)-C(3)-Fe(1)	70.1(2)
C(3)-Fe(1)-C(5)	68.61(15)	C(26)-Fe(2)-C(22)	105.4(2)	C(2)-C(3)-Fe(1)	69.7(2)
C(7)-Fe(1)-C(5)	125.1(2)	C(24)-Fe(2)-C(22)	155.8(2)	C(5)-C(4)-C(3)	107.3(3)
C(8)-Fe(1)-C(4)	117.9(2)	C(23)-Fe(2)-C(22)	154.8(2)	C(5)-C(4)-Fe(1)	69.4(2)
C(3)-Fe(1)-C(4)	41.08(14)	C(25)-Fe(2)-C(22)	119.0(2)	C(3)-C(4)-Fe(1)	68.8(2)
C(7)-Fe(1)-C(4)	107.7(2)	C(27)-Fe(2)-C(22)	116.5(2)	C(1)-C(5)-C(4)	111.6(3)
C(5)-Fe(1)-C(4)	40.58(14)	C(20)-Fe(2)-C(22)	67.6(2)	C(1)-C(5)-Fe(1)	71.3(2)
C(8)-Fe(1)-C(6)	67.1(2)	C(26)-Fe(2)-C(21)	120.7(2)	C(4)-C(5)-Fe(1)	70.0(2)
C(3)-Fe(1)-C(6)	109.8(2)	C(24)-Fe(2)-C(21)	161.9(2)	C(7)-C(6)-C(10)	109.3(4)
C(7)-Fe(1)-C(6)	39.9(2)	C(23)-Fe(2)-C(21)	121.0(2)	C(7)-C(6)-Fe(1)	69.4(2)
C(5)-Fe(1)-C(6)	162.8(2)	C(25)-Fe(2)-C(21)	154.4(2)	C(10)-C(6)-Fe(1)	70.8(2)
C(4)-Fe(1)-C(6)	127.0(2)	C(27)-Fe(2)-C(21)	104.2(2)	C(8)-C(7)-C(6)	109.4(4)
C(8)-Fe(1)-C(2)	161.8(2)	C(20)-Fe(2)-C(21)	38.9(2)	C(8)-C(7)-Fe(1)	69.9(2)
C(3)-Fe(1)-C(2)	42.54(14)	C(22)-Fe(2)-C(21)	41.5(2)	C(6)-C(7)-Fe(1)	70.8(2)
C(7)-Fe(1)-C(2)	157.86(15)	C(26)-Fe(2)-C(19)	158.4(2)	C(7)-C(8)-C(9)	109.2(4)
C(5)-Fe(1)-C(2)	68.03(14)	C(24)-Fe(2)-C(19)	107.9(2)	C(7)-C(8)-Fe(1)	70.8(2)
C(4)-Fe(1)-C(2)	69.71(14)	C(23)-Fe(2)-C(19)	128.2(2)	C(9)-C(8)-Fe(1)	69.9(2)
C(6)-Fe(1)-C(2)	123.23(14)	C(25)-Fe(2)-C(19)	124.6(2)	C(10)-C(9)-C(8)	104.9(3)
C(8)-Fe(1)-C(9)	43.2(2)	C(27)-Fe(2)-C(19)	164.6(2)	C(10)-C(9)-Fe(1)	70.7(2)
C(3)-Fe(1)-C(9)	162.8(2)	C(20)-Fe(2)-C(19)	42.9(2)	C(8)-C(9)-Fe(1)	66.9(2)
C(7)-Fe(1)-C(9)	69.6(2)	C(22)-Fe(2)-C(19)	69.0(2)	C(9)-C(10)-C(6)	107.3(4)
C(5)-Fe(1)-C(9)	118.1(2)	C(21)-Fe(2)-C(19)	69.7(2)	C(9)-C(10)-Fe(1)	69.0(2)
C(4)-Fe(1)-C(9)	153.5(2)	C(26)-Fe(2)-C(18)	121.6(2)	C(6)-C(10)-Fe(1)	68.1(2)
C(6)-Fe(1)-C(9)	68.7(2)	C(24)-Fe(2)-C(18)	121.4(2)	N(1)-C(11)-C(2)	111.6(3)
C(2)-Fe(1)-C(9)	122.9(2)	C(23)-Fe(2)-C(18)	164.4(2)	N(1)-C(11)-C(12)	125.0(3)
C(8)-Fe(1)-C(1)	123.66(14)	C(25)-Fe(2)-C(18)	106.6(2)	C(2)-C(11)-C(12)	123.3(3)
C(3)-Fe(1)-C(1)	70.22(14)	C(27)-Fe(2)-C(18)	151.7(2)	N(1)-C(13)-C(14)	108.5(3)
C(7)-Fe(1)-C(1)	160.30(15)	C(20)-Fe(2)-C(18)	69.0(2)	O(1)-C(14)-C(15)	107.9(3)
C(5)-Fe(1)-C(1)	40.19(14)	C(22)-Fe(2)-C(18)	40.6(2)	O(1)-C(14)-C(13)	109.1(3)
C(4)-Fe(1)-C(1)	69.18(13)	C(21)-Fe(2)-C(18)	69.3(2)	C(15)-C(14)-C(13)	111.1(3)
C(6)-Fe(1)-C(1)	156.79(15)	C(19)-Fe(2)-C(18)	40.85(14)	C(14)-C(15)-C(16)	98.0(3)
C(2)-Fe(1)-C(1)	40.96(13)	C(14)-O(1)-C(17)	109.9(3)	C(17)-C(16)-C(15)	103.8(3)
C(9)-Fe(1)-C(1)	104.15(14)	C(34)-O(2)-C(31)	103.7(4)	O(1)-C(17)-C(16)	109.3(4)
C(8)-Fe(1)-C(10)	69.0(2)	C(36)-O(3)-Pd(1)	123.3(2)	C(22)-C(18)-C(19)	107.8(3)
C(3)-Fe(1)-C(10)	127.4(2)	C(36)-O(4)-Pd(2)	121.9(2)	C(22)-C(18)-Pd(2)	142.0(3)
C(7)-Fe(1)-C(10)	68.5(2)	C(38)-O(5)-Pd(1)	127.4(2)	C(19)-C(18)-Pd(2)	110.3(3)
C(5)-Fe(1)-C(10)	153.5(2)	C(38)-O(6)-Pd(2)	119.0(2)	C(22)-C(18)-Fe(2)	68.0(2)
C(4)-Fe(1)-C(10)	165.0(2)	C(11)-N(1)-C(13)	121.9(3)	C(19)-C(18)-Fe(2)	69.1(2)
C(6)-Fe(1)-C(10)	41.1(2)	C(11)-N(1)-Pd(1)	117.8(2)	Pd(2)-C(18)-Fe(2)	126.7(2)
C(2)-Fe(1)-C(10)	108.0(2)	C(13)-N(1)-Pd(1)	120.1(2)	C(18)-C(19)-C(28)	117.5(3)
C(9)-Fe(1)-C(10)	40.3(2)	C(28)-N(2)-C(30)	120.6(3)	C(18)-C(19)-C(20)	104.5(3)
C(1)-Fe(1)-C(10)	119.42(15)	C(28)-N(2)-Pd(2)	119.1(2)	C(28)-C(19)-C(20)	137.5(3)
C(26)-Fe(2)-C(24)	68.2(3)	C(30)-N(2)-Pd(2)	120.3(2)	C(18)-C(19)-Fe(2)	70.0(2)
C(26)-Fe(2)-C(23)	65.3(3)	C(5)-C(1)-C(2)	106.5(3)	C(28)-C(19)-Fe(2)	120.5(2)

C(20)-C(19)-Fe(2)	67.2(2)	O(6')-Pd(2')-O(4')	90.72(11)	C(25')-Fe(2')-C(24')	41.2(3)
C(21)-C(20)-C(19)	110.7(4)	C(18')-Pd(2')-Pd(1')	105.45(13)	C(23')-Fe(2')-C(24')	42.0(2)
C(21)-C(20)-Fe(2)	71.0(3)	N(2')-Pd(2')-Pd(1')	93.72(10)	C(26')-Fe(2')-C(24')	67.1(2)
C(19)-C(20)-Fe(2)	69.9(2)	O(6')-Pd(2')-Pd(1')	86.17(8)	C(27')-Fe(2')-C(24')	68.3(2)
C(20)-C(21)-C(22)	107.6(4)	O(4')-Pd(2')-Pd(1')	76.79(8)	C(25')-Fe(2')-C(20')	116.8(2)
C(20)-C(21)-Fe(2)	70.1(3)	C(9')-Fe(1')-C(7')	66.4(3)	C(23')-Fe(2')-C(20')	130.7(2)
C(22)-C(21)-Fe(2)	68.9(3)	C(9')-Fe(1')-C(4')	165.1(2)	C(26')-Fe(2')-C(20')	147.9(2)
C(18)-C(22)-C(21)	109.4(4)	C(7')-Fe(1')-C(4')	122.0(2)	C(27')-Fe(2')-C(20')	169.6(2)
C(18)-C(22)-Fe(2)	71.4(2)	C(9')-Fe(1')-C(3')	128.7(2)	C(24')-Fe(2')-C(20')	108.6(2)
C(21)-C(22)-Fe(2)	69.6(3)	C(7')-Fe(1')-C(3')	156.4(2)	C(25')-Fe(2')-C(21')	107.0(2)
C(27)-C(23)-C(24)	107.1(5)	C(4')-Fe(1')-C(3')	39.1(2)	C(23')-Fe(2')-C(21')	168.8(2)
C(27)-C(23)-Fe(2)	70.6(3)	C(9')-Fe(1')-C(6')	61.9(2)	C(26')-Fe(2')-C(21')	116.0(2)
C(24)-C(23)-Fe(2)	67.0(3)	C(7')-Fe(1')-C(6')	41.3(2)	C(27')-Fe(2')-C(21')	149.5(2)
C(25)-C(24)-C(23)	100.8(5)	C(4')-Fe(1')-C(6')	114.9(2)	C(24')-Fe(2')-C(21')	128.8(2)
C(25)-C(24)-Fe(2)	70.4(3)	C(3')-Fe(1')-C(6')	124.2(2)	C(20')-Fe(2')-C(21')	40.1(2)
C(23)-C(24)-Fe(2)	67.5(3)	C(9')-Fe(1')-C(2')	109.8(2)	C(25')-Fe(2')-C(19')	153.3(2)
C(26)-C(25)-C(24)	108.1(5)	C(7')-Fe(1')-C(2')	160.5(2)	C(23')-Fe(2')-C(19')	108.8(2)
C(26)-C(25)-Fe(2)	68.8(3)	C(4')-Fe(1')-C(2')	66.6(2)	C(26')-Fe(2')-C(19')	167.7(2)
C(24)-C(25)-Fe(2)	68.0(3)	C(3')-Fe(1')-C(2')	40.7(2)	C(27')-Fe(2')-C(19')	129.2(2)
C(27)-C(26)-C(25)	119.6(7)	C(6')-Fe(1')-C(2')	155.5(2)	C(24')-Fe(2')-C(19')	119.7(2)
C(27)-C(26)-Fe(2)	74.4(4)	C(9')-Fe(1')-C(5')	153.2(2)	C(20')-Fe(2')-C(19')	42.8(2)
C(25)-C(26)-Fe(2)	72.7(3)	C(7')-Fe(1')-C(5')	107.3(2)	C(21')-Fe(2')-C(19')	68.8(2)
C(26)-C(27)-C(23)	104.2(6)	C(4')-Fe(1')-C(5')	40.5(2)	C(25')-Fe(2')-C(22')	127.6(2)
C(26)-C(27)-Fe(2)	68.9(4)	C(3')-Fe(1')-C(5')	67.4(2)	C(23')-Fe(2')-C(22')	147.7(2)
C(23)-C(27)-Fe(2)	67.5(3)	C(6')-Fe(1')-C(5')	131.5(2)	C(26')-Fe(2')-C(22')	107.0(2)
N(2)-C(28)-C(29)	128.8(4)	C(2')-Fe(1')-C(5')	66.9(2)	C(27')-Fe(2')-C(22')	115.0(2)
N(2)-C(28)-C(19)	111.0(3)	C(9')-Fe(1')-C(8')	39.7(2)	C(24')-Fe(2')-C(22')	167.6(3)
C(29)-C(28)-C(19)	120.0(3)	C(7')-Fe(1')-C(8')	37.8(2)	C(20')-Fe(2')-C(22')	70.2(2)
N(2)-C(30)-C(31)	115.0(3)	C(4')-Fe(1')-C(8')	154.1(2)	C(21')-Fe(2')-C(22')	42.6(2)
C(32)-C(31)-O(2)	109.4(3)	C(3')-Fe(1')-C(8')	165.2(2)	C(19')-Fe(2')-C(22')	68.3(2)
C(32)-C(31)-C(30)	115.5(4)	C(6')-Fe(1')-C(8')	62.8(2)	C(25')-Fe(2')-C(18')	165.3(2)
O(2)-C(31)-C(30)	107.9(3)	C(2')-Fe(1')-C(8')	127.2(2)	C(23')-Fe(2')-C(18')	116.5(2)
C(31)-C(32)-C(33)	106.1(4)	C(5')-Fe(1')-C(8')	119.4(2)	C(26')-Fe(2')-C(18')	129.2(2)
C(34)-C(33)-C(32)	101.7(4)	C(9')-Fe(1')-C(10')	37.4(2)	C(27')-Fe(2')-C(18')	107.6(2)
O(2)-C(34)-C(33)	113.0(5)	C(7')-Fe(1')-C(10')	68.1(2)	C(24')-Fe(2')-C(18')	151.8(2)
O(3)-C(36)-O(4)	128.6(3)	C(4')-Fe(1')-C(10')	130.7(2)	C(20')-Fe(2')-C(18')	70.1(2)
O(3)-C(36)-C(35)	114.0(3)	C(3')-Fe(1')-C(10')	111.6(2)	C(21')-Fe(2')-C(18')	69.2(2)
O(4)-C(36)-C(35)	117.4(3)	C(6')-Fe(1')-C(10')	37.5(2)	C(19')-Fe(2')-C(18')	40.05(15)
O(5)-C(38)-O(6)	128.1(3)	C(2')-Fe(1')-C(10')	121.4(2)	C(22')-Fe(2')-C(18')	40.2(2)
O(5)-C(38)-C(37)	117.9(3)	C(5')-Fe(1')-C(10')	167.2(2)	C(17')-O(1')-C(14')	113.7(4)
O(6)-C(38)-C(37)	114.0(3)	C(8')-Fe(1')-C(10')	64.9(2)	C(34')-O(2')-C(31')	110.2(4)
C(1')-Pd(1')-N(1')	81.92(14)	C(9')-Fe(1')-C(1')	119.6(2)	C(36')-O(3')-Pd(1')	121.7(3)
C(1')-Pd(1')-O(3')	91.03(14)	C(7')-Fe(1')-C(1')	122.4(2)	C(36')-O(4')-Pd(2')	127.7(3)
N(1')-Pd(1')-O(3')	172.63(12)	C(4')-Fe(1')-C(1')	68.0(2)	C(38')-O(5')-Pd(1')	125.5(3)
C(1')-Pd(1')-O(5')	176.49(14)	C(3')-Fe(1')-C(1')	69.2(2)	C(38')-O(6')-Pd(2')	120.1(3)
N(1')-Pd(1')-O(5')	94.57(11)	C(6')-Fe(1')-C(1')	163.3(2)	C(11')-N(1')-C(13')	121.5(3)
O(3')-Pd(1')-O(5')	92.47(11)	C(2')-Fe(1')-C(1')	41.1(2)	C(11')-N(1')-Pd(1')	117.6(3)
C(1')-Pd(1')-Pd(2')	103.83(12)	C(5')-Fe(1')-C(1')	39.8(2)	C(13')-N(1')-Pd(1')	120.8(2)
N(1')-Pd(1')-Pd(2')	94.60(9)	C(8')-Fe(1')-C(1')	106.9(2)	C(28')-N(2')-C(30')	121.6(3)
O(3')-Pd(1')-Pd(2')	84.95(8)	C(10')-Fe(1')-C(1')	152.9(2)	C(28')-N(2')-Pd(2')	117.2(3)
O(5')-Pd(1')-Pd(2')	76.23(7)	C(25')-Fe(2')-C(23')	69.9(2)	C(30')-N(2')-Pd(2')	121.1(2)
C(18')-Pd(2')-N(2')	81.58(14)	C(25')-Fe(2')-C(26')	38.4(2)	C(5')-C(1')-C(2')	103.9(3)
C(18')-Pd(2')-O(6')	92.86(13)	C(23')-Fe(2')-C(26')	68.7(2)	C(5')-C(1')-Pd(1')	142.0(3)
N(2')-Pd(2')-O(6')	174.20(12)	C(25')-Fe(2')-C(27')	67.9(2)	C(2')-C(1')-Pd(1')	114.2(3)
C(18')-Pd(2')-O(4')	175.89(14)	C(23')-Fe(2')-C(27')	40.4(2)	C(5')-C(1')-Fe(1')	68.7(2)
N(2')-Pd(2')-O(4')	94.90(11)	C(26')-Fe(2')-C(27')	41.2(2)	C(2')-C(1')-Fe(1')	67.4(2)

Pd(1')-C(1')-Fe(1')	125.8(2)	Fe(1')-C(9')-C(6')	61.2(2)	C(18')-C(22')-Fe(2')	72.3(2)
C(3')-C(2')-C(1')	109.1(4)	C(9')-C(10')-C(6')	101.7(5)	C(21')-C(22')-Fe(2')	68.1(3)
C(3')-C(2')-C(11')	137.3(4)	C(9')-C(10')-Fe(1')	64.6(3)	C(27')-C(23')-C(24')	106.2(6)
C(1')-C(2')-C(11')	113.2(3)	C(6')-C(10')-Fe(1')	68.3(3)	C(27')-C(23')-Fe(2')	70.0(3)
C(3')-C(2')-Fe(1')	68.4(3)	N(1')-C(11')-C(12')	127.1(4)	C(24')-C(23')-Fe(2')	69.5(3)
C(1')-C(2')-Fe(1')	71.5(2)	N(1')-C(11')-C(2')	112.9(3)	C(25')-C(24')-C(23')	106.8(5)
C(11')-C(2')-Fe(1')	120.5(3)	C(12')-C(11')-C(2')	120.0(3)	C(25')-C(24')-Fe(2')	68.6(3)
C(4')-C(3')-C(2')	107.7(4)	C(14')-C(13')-N(1')	114.5(4)	C(23')-C(24')-Fe(2')	68.5(3)
C(4')-C(3')-Fe(1')	70.3(3)	C(13')-C(14')-O(1')	109.2(4)	C(26')-C(25')-C(24')	109.1(5)
C(2')-C(3')-Fe(1')	70.9(3)	C(13')-C(14')-C(15')	116.8(4)	C(26')-C(25')-Fe(2')	71.3(3)
C(3')-C(4')-C(5')	110.3(4)	O(1')-C(14')-C(15')	104.1(4)	C(24')-C(25')-Fe(2')	70.2(3)
C(3')-C(4')-Fe(1')	70.6(3)	C(16')-C(15')-C(14')	104.7(4)	C(25')-C(26')-C(27')	109.9(5)
C(5')-C(4')-Fe(1')	71.8(3)	C(15')-C(16')-C(17')	106.0(5)	C(25')-C(26')-Fe(2')	70.3(3)
C(4')-C(5')-C(1')	109.0(4)	O(1')-C(17')-C(16')	106.4(5)	C(27')-C(26')-Fe(2')	69.5(3)
C(4')-C(5')-Fe(1')	67.7(3)	C(19')-C(18')-C(22')	106.9(3)	C(23')-C(27')-C(26')	107.9(5)
C(1')-C(5')-Fe(1')	71.6(2)	C(19')-C(18')-Pd(2')	112.4(3)	C(23')-C(27')-Fe(2')	69.6(3)
C(10')-C(6')-C(7')	113.1(6)	C(22')-C(18')-Pd(2')	140.6(3)	C(26')-C(27')-Fe(2')	69.3(3)
C(10')-C(6')-Fe(1')	74.2(4)	C(19')-C(18')-Fe(2')	67.2(2)	N(2')-C(28')-C(19')	111.1(3)
C(7')-C(6')-Fe(1')	67.8(3)	C(22')-C(18')-Fe(2')	67.5(2)	N(2')-C(28')-C(29')	125.1(4)
C(10')-C(6')-C(9')	38.7(3)	Pd(2')-C(18')-Fe(2')	126.7(2)	C(19')-C(28')-C(29')	123.8(4)
C(7')-C(6')-C(9')	74.4(4)	C(18')-C(19')-C(28')	117.4(3)	N(2')-C(30')-C(31')	111.3(3)
Fe(1')-C(6')-C(9')	56.9(2)	C(18')-C(19')-C(20')	109.8(3)	O(2')-C(31')-C(30')	110.8(4)
C(8')-C(7')-C(6')	103.2(5)	C(28')-C(19')-C(20')	132.5(4)	O(2')-C(31')-C(32')	97.1(4)
C(8')-C(7')-Fe(1')	75.4(4)	C(18')-C(19')-Fe(2')	72.7(2)	C(30')-C(31')-C(32')	113.5(4)
C(6')-C(7')-Fe(1')	70.9(3)	C(28')-C(19')-Fe(2')	121.1(3)	C(33')-C(32')-C(31')	114.4(5)
C(7')-C(8')-C(9')	105.6(5)	C(20')-C(19')-Fe(2')	68.1(3)	C(32')-C(33')-C(34')	107.1(5)
C(7')-C(8')-Fe(1')	66.9(4)	C(21')-C(20')-C(19')	106.2(4)	O(2')-C(34')-C(33')	111.2(4)
C(9')-C(8')-Fe(1')	64.2(3)	C(21')-C(20')-Fe(2')	70.2(3)	O(3')-C(36')-O(4')	126.1(4)
C(10')-C(9')-C(8')	114.1(5)	C(19')-C(20')-Fe(2')	69.1(3)	O(3')-C(36')-C(35')	117.2(4)
C(10')-C(9')-Fe(1')	78.0(4)	C(20')-C(21')-C(22')	109.1(4)	O(4')-C(36')-C(35')	116.4(4)
C(8')-C(9')-Fe(1')	76.1(4)	C(20')-C(21')-Fe(2')	69.7(3)	O(6')-C(38')-O(5')	128.1(4)
C(10')-C(9')-C(6')	39.6(3)	C(22')-C(21')-Fe(2')	69.2(3)	O(6')-C(38')-C(37')	116.6(4)
C(8')-C(9')-C(6')	75.0(4)	C(18')-C(22')-C(21')	107.8(4)	O(5')-C(38')-C(37')	115.1(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)	0.05041(13)	0.07149(15)	0.05509(12)	-0.00436(13)	0.00184(12)	-0.00021(14)
Pd(2)	0.04965(13)	0.0917(2)	0.06598(14)	-0.01746(15)	0.00057(13)	-0.0039(2)
Fe(1)	0.0504(3)	0.0748(3)	0.0592(2)	-0.0040(3)	0.0009(2)	0.0022(3)
Fe(2)	0.0940(4)	0.1136(4)	0.0940(4)	-0.0275(4)	0.0145(3)	-0.0385(4)
O(1)	0.0643(15)	0.129(2)	0.0844(15)	-0.020(2)	-0.0101(13)	0.006(2)
O(2)	0.094(2)	0.145(3)	0.126(2)	0.005(2)	-0.053(2)	-0.004(2)
O(3)	0.0676(14)	0.0862(15)	0.0587(11)	0.0103(12)	-0.0002(12)	-0.0088(14)
O(4)	0.076(2)	0.098(2)	0.0561(12)	0.0038(13)	-0.0012(11)	-0.0176(14)
O(5)	0.0613(14)	0.090(2)	0.0542(11)	-0.0071(12)	0.0066(10)	-0.0002(13)
O(6)	0.0552(14)	0.108(2)	0.094(2)	-0.0269(14)	0.0139(13)	-0.0006(14)
N(1)	0.054(2)	0.075(2)	0.0545(13)	0.0025(14)	-0.0025(12)	0.007(2)
N(2)	0.050(2)	0.090(2)	0.0653(15)	-0.018(2)	0.0070(13)	0.003(2)
C(1)	0.054(2)	0.080(2)	0.0395(14)	0.007(2)	0.0051(14)	0.005(2)
C(2)	0.060(2)	0.084(2)	0.063(2)	-0.010(2)	-0.007(2)	-0.013(2)
C(3)	0.053(2)	0.096(3)	0.080(2)	-0.011(2)	0.021(2)	-0.015(2)
C(4)	0.085(2)	0.086(2)	0.063(2)	0.008(2)	-0.008(2)	0.017(2)
C(5)	0.084(3)	0.074(2)	0.061(2)	-0.003(2)	0.007(2)	-0.006(2)
C(6)	0.126(3)	0.078(2)	0.075(2)	0.007(2)	0.012(3)	-0.009(3)
C(7)	0.076(3)	0.104(3)	0.084(2)	-0.007(2)	0.012(2)	0.014(2)
C(8)	0.113(3)	0.092(3)	0.083(2)	-0.017(2)	-0.026(2)	-0.019(3)
C(9)	0.074(2)	0.134(3)	0.094(2)	-0.033(2)	0.010(2)	-0.049(2)
C(10)	0.069(2)	0.107(3)	0.127(3)	-0.042(2)	-0.020(2)	0.019(3)
C(11)	0.079(2)	0.052(2)	0.059(2)	0.002(2)	-0.004(2)	-0.016(2)
C(12)	0.087(3)	0.088(3)	0.094(3)	0.002(2)	0.007(2)	-0.012(2)
C(13)	0.065(2)	0.084(2)	0.093(2)	-0.014(2)	0.013(2)	0.016(2)
C(14)	0.059(2)	0.072(2)	0.083(2)	0.013(2)	0.002(2)	0.015(2)
C(15)	0.052(2)	0.108(3)	0.102(3)	0.003(2)	-0.002(2)	0.008(2)
C(16)	0.078(3)	0.136(4)	0.127(3)	0.030(3)	-0.031(2)	-0.012(3)
C(17)	0.072(3)	0.191(5)	0.125(3)	-0.042(3)	0.013(3)	-0.022(3)
C(18)	0.049(2)	0.080(2)	0.084(2)	-0.019(2)	-0.007(2)	-0.006(2)
C(19)	0.074(2)	0.125(3)	0.056(2)	-0.019(2)	0.018(2)	-0.039(2)
C(20)	0.104(3)	0.138(4)	0.097(3)	-0.020(3)	0.026(2)	-0.037(3)
C(21)	0.114(4)	0.117(4)	0.139(4)	0.027(3)	0.016(3)	-0.003(3)
C(22)	0.078(3)	0.115(3)	0.106(3)	-0.033(3)	-0.021(2)	0.011(3)
C(23)	0.157(4)	0.218(4)	0.167(4)	-0.092(3)	0.022(3)	-0.130(3)
C(24)	0.194(5)	0.195(5)	0.130(3)	-0.071(3)	-0.083(3)	-0.024(4)
C(25)	0.201(5)	0.230(5)	0.086(3)	-0.067(3)	0.064(3)	-0.097(5)
C(26)	0.172(5)	0.203(5)	0.204(5)	-0.105(4)	0.077(4)	-0.096(4)
C(27)	0.179(6)	0.150(4)	0.244(6)	-0.091(4)	-0.005(5)	-0.035(5)
C(28)	0.057(2)	0.098(3)	0.067(2)	-0.017(2)	0.002(2)	0.007(2)
C(29)	0.046(2)	0.146(4)	0.119(3)	0.007(3)	0.013(2)	-0.010(3)
C(30)	0.049(2)	0.104(3)	0.085(2)	-0.035(2)	0.016(2)	0.003(2)
C(31)	0.063(2)	0.134(3)	0.070(2)	-0.015(2)	-0.009(2)	0.029(2)
C(32)	0.087(3)	0.146(4)	0.101(3)	-0.002(3)	0.000(2)	0.017(3)
C(33)	0.137(4)	0.220(6)	0.118(4)	-0.003(4)	-0.025(3)	0.037(5)
C(34)	0.109(4)	0.291(7)	0.149(4)	0.072(5)	-0.047(3)	-0.065(5)
C(35)	0.131(4)	0.128(3)	0.081(2)	0.036(3)	0.014(3)	0.000(3)
C(36)	0.061(2)	0.087(2)	0.073(2)	0.027(2)	0.000(2)	0.012(2)
C(37)	0.084(3)	0.088(3)	0.117(3)	-0.032(2)	-0.009(3)	-0.001(2)
C(38)	0.040(2)	0.068(2)	0.085(2)	0.005(2)	0.001(2)	-0.007(2)
Pd(1')	0.0779(2)	0.1027(2)	0.0722(2)	0.0166(2)	0.00301(15)	0.0175(2)
Pd(2')	0.0705(2)	0.0997(2)	0.0696(2)	0.0053(2)	-0.00200(15)	0.0068(2)
Fe(1')	0.0838(4)	0.1386(5)	0.0949(4)	0.0231(4)	0.0020(3)	0.0335(4)

Fe(2')	0.0793(4)	0.1189(5)	0.0822(3)	0.0070(3)	0.0054(3)	0.0215(4)
O(1')	0.136(3)	0.112(2)	0.297(5)	0.072(3)	0.009(3)	0.002(3)
O(2')	0.107(2)	0.209(4)	0.226(4)	-0.068(3)	0.029(3)	-0.029(3)
O(3')	0.117(2)	0.103(2)	0.080(2)	0.0171(15)	0.007(2)	0.009(2)
O(4')	0.101(2)	0.113(2)	0.090(2)	0.008(2)	0.018(2)	0.001(2)
O(5')	0.101(2)	0.098(2)	0.099(2)	0.002(2)	-0.015(2)	0.004(2)
O(6')	0.089(2)	0.113(2)	0.092(2)	-0.001(2)	-0.020(2)	-0.003(2)
N(1')	0.069(2)	0.096(2)	0.078(2)	0.007(2)	0.002(2)	0.012(2)
N(2')	0.078(2)	0.120(3)	0.065(2)	0.008(2)	0.003(2)	0.009(2)
C(1')	0.062(2)	0.109(3)	0.085(2)	0.021(2)	-0.004(2)	0.016(2)
C(2')	0.089(3)	0.154(4)	0.070(2)	0.008(3)	0.014(2)	0.034(3)
C(3')	0.082(3)	0.148(4)	0.087(3)	0.010(3)	-0.019(2)	0.021(3)
C(4')	0.091(3)	0.144(4)	0.096(3)	0.013(3)	-0.009(2)	0.031(3)
C(5')	0.078(3)	0.126(3)	0.102(3)	0.026(3)	0.024(2)	0.006(3)
C(6')	0.172(5)	0.134(4)	0.177(5)	-0.017(4)	-0.045(4)	0.084(4)
C(7')	0.185(6)	0.149(5)	0.116(3)	0.009(4)	0.030(4)	0.014(5)
C(8')	0.177(5)	0.156(4)	0.149(4)	0.004(4)	-0.032(4)	0.074(4)
C(9')	0.076(3)	0.158(5)	0.234(6)	0.024(5)	-0.005(4)	0.022(4)
C(10')	0.123(4)	0.193(5)	0.141(4)	0.063(4)	0.040(3)	0.042(4)
C(11')	0.081(3)	0.124(3)	0.072(2)	0.012(2)	0.007(2)	0.017(3)
C(12')	0.096(3)	0.210(5)	0.090(3)	0.054(3)	0.015(2)	0.037(3)
C(13')	0.065(2)	0.131(4)	0.105(3)	0.008(3)	0.004(2)	0.003(3)
C(14')	0.088(3)	0.098(3)	0.131(3)	-0.002(3)	-0.006(3)	-0.009(3)
C(15')	0.132(5)	0.136(4)	0.151(4)	-0.030(4)	-0.001(4)	0.013(4)
C(16')	0.171(4)	0.118(3)	0.363(7)	-0.089(4)	0.144(4)	-0.098(3)
C(17')	0.119(4)	0.167(5)	0.281(7)	0.037(6)	0.058(5)	0.064(4)
C(18')	0.077(3)	0.115(3)	0.063(2)	-0.006(2)	-0.003(2)	0.001(3)
C(19')	0.067(2)	0.125(3)	0.090(2)	0.026(3)	0.014(2)	0.000(3)
C(20')	0.113(3)	0.170(4)	0.082(2)	0.039(3)	0.022(2)	0.028(4)
C(21')	0.082(3)	0.173(4)	0.112(3)	0.030(3)	0.026(3)	0.002(3)
C(22')	0.079(3)	0.115(3)	0.115(3)	0.008(3)	-0.002(2)	0.003(3)
C(23')	0.142(5)	0.094(3)	0.194(5)	-0.006(4)	-0.025(4)	0.002(4)
C(24')	0.285(8)	0.159(5)	0.090(3)	-0.039(3)	-0.033(4)	0.050(6)
C(25')	0.130(4)	0.185(5)	0.119(4)	-0.010(4)	0.023(3)	0.035(4)
C(26')	0.137(4)	0.170(4)	0.121(4)	0.021(4)	-0.005(3)	0.065(4)
C(27')	0.181(5)	0.120(4)	0.114(3)	-0.010(3)	0.045(3)	-0.005(4)
C(28')	0.072(3)	0.135(4)	0.086(2)	0.020(3)	-0.005(2)	0.009(3)
C(29')	0.091(3)	0.211(5)	0.066(2)	0.007(3)	0.011(2)	-0.019(4)
C(30')	0.063(2)	0.155(4)	0.085(2)	-0.014(3)	0.005(2)	0.001(3)
C(31')	0.081(3)	0.144(4)	0.112(3)	-0.011(3)	0.005(3)	-0.015(3)
C(32')	0.090(4)	0.203(6)	0.182(5)	-0.003(5)	0.038(3)	-0.028(4)
C(33')	0.089(4)	0.226(5)	0.435(9)	-0.192(5)	0.020(5)	-0.037(4)
C(34')	0.271(6)	0.094(3)	0.099(3)	0.048(2)	-0.084(3)	-0.020(4)
C(35')	0.134(4)	0.157(4)	0.132(3)	0.050(3)	0.055(3)	0.005(4)
C(36')	0.086(3)	0.118(3)	0.089(2)	0.022(3)	0.015(2)	-0.008(3)
C(37')	0.174(5)	0.102(3)	0.182(4)	-0.035(3)	-0.087(4)	0.023(4)
C(38')	0.084(3)	0.120(3)	0.094(3)	-0.003(3)	-0.028(2)	0.002(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)	0.2973(3)	0.37464(15)	-0.06722(12)	0.080
H(4A)	0.3716(3)	0.28846(15)	-0.03160(10)	0.080
H(5A)	0.2257(3)	0.25917(15)	0.02500(11)	0.080
H(6A)	0.1462(4)	0.3070(2)	-0.14282(12)	0.080
H(7A)	0.2436(3)	0.2265(2)	-0.11119(12)	0.080
H(8A)	0.1234(4)	0.1883(2)	-0.05215(12)	0.080
H(9A)	-0.0605(4)	0.2477(2)	-0.04365(13)	0.080
H(10A)	-0.0406(4)	0.3223(2)	-0.10039(14)	0.080
H(12A)	0.0010(4)	0.46510(15)	-0.06805(12)	0.080
H(12B)	0.0747(4)	0.42552(15)	-0.09618(12)	0.080
H(12C)	0.1341(4)	0.46652(15)	-0.06455(12)	0.080
H(13A)	-0.1487(3)	0.44511(15)	0.01623(13)	0.080
H(13B)	-0.1175(3)	0.45351(15)	-0.03360(13)	0.080
H(14A)	-0.2204(3)	0.35643(14)	-0.00655(11)	0.080
H(15A)	-0.3740(3)	0.4087(2)	0.00645(13)	0.080
H(15B)	-0.3386(3)	0.4500(2)	-0.03017(13)	0.080
H(16A)	-0.4361(4)	0.3475(2)	-0.04671(15)	0.080
H(16B)	-0.4611(4)	0.3989(2)	-0.07416(15)	0.080
H(17A)	-0.3150(3)	0.3854(2)	-0.1164(2)	0.080
H(17B)	-0.3161(3)	0.3273(2)	-0.0980(2)	0.080
H(20A)	0.2943(4)	0.5235(2)	0.03028(14)	0.080
H(21A)	0.1187(4)	0.5779(2)	0.0406(2)	0.080
H(22A)	-0.0223(4)	0.5228(2)	0.08674(13)	0.080
H(23A)	0.3859(5)	0.5803(2)	0.1229(2)	0.080
H(24A)	0.3654(5)	0.4862(2)	0.16453(15)	0.080
H(25A)	0.1574(5)	0.4901(3)	0.19525(14)	0.080
H(26A)	0.0737(6)	0.5684(2)	0.1711(2)	0.080
H(27A)	0.1932(6)	0.6299(3)	0.1342(2)	0.080
H(29A)	0.4382(3)	0.3792(2)	0.07498(14)	0.080
H(29B)	0.4463(3)	0.4415(2)	0.07369(14)	0.080
H(29C)	0.4056(3)	0.4101(2)	0.03164(14)	0.080
H(30A)	0.2447(3)	0.3026(2)	0.10816(11)	0.080
H(30B)	0.3627(3)	0.3295(2)	0.10328(11)	0.080
H(31A)	0.2406(3)	0.3404(2)	0.18009(11)	0.080
H(32A)	0.2812(4)	0.2630(2)	0.19808(15)	0.080
H(32B)	0.3638(4)	0.2552(2)	0.15824(15)	0.080
H(33A)	0.4148(5)	0.2910(3)	0.2437(2)	0.080
H(33B)	0.4929(5)	0.2605(3)	0.2101(2)	0.080
H(34A)	0.5382(4)	0.3317(2)	0.1780(2)	0.080
H(34B)	0.5097(4)	0.3582(2)	0.2231(2)	0.080
H(35A)	-0.0079(4)	0.2315(2)	0.17885(13)	0.080
H(35B)	0.0476(4)	0.2013(2)	0.13880(13)	0.080
H(35C)	-0.0839(4)	0.2117(2)	0.13948(13)	0.080
H(37A)	-0.3494(3)	0.3904(2)	0.10269(14)	0.080
H(37B)	-0.3016(3)	0.4456(2)	0.11831(14)	0.080
H(37C)	-0.3029(3)	0.3971(2)	0.15107(14)	0.080
H(3'A)	-0.5791(4)	0.6557(2)	-0.27283(14)	0.080
H(4'A)	-0.7422(4)	0.6306(2)	-0.22630(14)	0.080
H(5'A)	-0.6738(4)	0.6078(2)	-0.14924(14)	0.080
H(6'A)	-0.7614(6)	0.7628(2)	-0.2040(2)	0.080
H(7'A)	-0.7238(6)	0.7319(2)	-0.1252(2)	0.080
H(8'A)	-0.5200(5)	0.7448(2)	-0.1135(2)	0.080
H(9'A)	-0.4374(5)	0.7717(2)	-0.1858(2)	0.080

H(10B)	-0.5849(5)	0.7881(2)	-0.2408(2)	0.080
H(12D)	-0.2292(4)	0.6844(2)	-0.26230(13)	0.080
H(12E)	-0.3489(4)	0.7089(2)	-0.27286(13)	0.080
H(12F)	-0.3213(4)	0.6501(2)	-0.28678(13)	0.080
H(13C)	-0.1348(3)	0.6385(2)	-0.16761(14)	0.080
H(13D)	-0.1477(3)	0.6716(2)	-0.21093(14)	0.080
H(14B)	-0.1974(4)	0.7118(2)	-0.1315(2)	0.080
H(15C)	-0.0138(5)	0.7222(2)	-0.1235(2)	0.080
H(15D)	0.0086(5)	0.7119(2)	-0.1738(2)	0.080
H(16C)	-0.0569(5)	0.8048(2)	-0.1399(2)	0.080
H(16D)	0.0372(5)	0.7970(2)	-0.1759(2)	0.080
H(17C)	-0.1077(5)	0.7870(2)	-0.2238(2)	0.080
H(17D)	-0.1717(5)	0.8288(2)	-0.1942(2)	0.080
H(20B)	-0.1143(4)	0.5244(2)	-0.29096(14)	0.080
H(21B)	0.0602(4)	0.5313(2)	-0.24161(14)	0.080
H(22B)	-0.0057(4)	0.5249(2)	-0.1595(2)	0.080
H(23B)	-0.2655(5)	0.3878(2)	-0.2217(2)	0.080
H(24B)	-0.1338(7)	0.3933(2)	-0.2896(2)	0.080
H(25B)	0.0690(5)	0.4047(2)	-0.2599(2)	0.080
H(26B)	0.0624(5)	0.4023(2)	-0.1797(2)	0.080
H(27B)	-0.1408(5)	0.3906(2)	-0.1544(2)	0.080
H(29D)	-0.4612(4)	0.4966(2)	-0.28037(11)	0.080
H(29E)	-0.3434(4)	0.4773(2)	-0.29869(11)	0.080
H(29F)	-0.3729(4)	0.5382(2)	-0.29819(11)	0.080
H(30C)	-0.5450(3)	0.5179(2)	-0.17985(14)	0.080
H(30D)	-0.5389(3)	0.4988(2)	-0.22881(14)	0.080
H(31B)	-0.4934(4)	0.4281(2)	-0.1577(2)	0.080
H(32C)	-0.6758(4)	0.4079(2)	-0.1539(2)	0.080
H(32D)	-0.7049(4)	0.4550(2)	-0.1852(2)	0.080
H(33C)	-0.7342(5)	0.3570(2)	-0.1952(2)	0.080
H(33D)	-0.7419(5)	0.4032(2)	-0.2298(2)	0.080
H(34C)	-0.6035(5)	0.3734(2)	-0.26338(14)	0.080
H(34D)	-0.5854(5)	0.3331(2)	-0.22472(14)	0.080
H(35D)	-0.5861(4)	0.4831(2)	-0.05033(15)	0.080
H(35E)	-0.6543(4)	0.5360(2)	-0.05801(15)	0.080
H(35F)	-0.5673(4)	0.5319(2)	-0.01877(15)	0.080
H(37D)	-0.0591(5)	0.5493(2)	-0.0324(2)	0.080
H(37E)	-0.1283(5)	0.5979(2)	-0.0140(2)	0.080
H(37F)	-0.0338(5)	0.6069(2)	-0.0499(2)	0.080

Tables for *syn*-(-)-(R_p,S,S,S_p)-3Table 1. Atomic coordinates and equivalent isotropic displacement parameters (Å²).

atom	x	y	z	U(eq)
Pd(1)	0.13292(3)	-0.07519(2)	-0.33351(3)	0.05177(13)
Pd(2)	0.32629(3)	-0.10050(2)	-0.11779(3)	0.05338(13)
Fe(1)	-0.10265(6)	-0.16529(3)	-0.47851(6)	0.0620(3)
Fe(2)	0.42539(7)	-0.23612(4)	0.02778(7)	0.0839(3)
Cl(1)	0.27776(10)	-0.14689(6)	-0.28252(11)	0.0648(5)
O(1)	-0.0367(4)	0.0419(2)	-0.5913(3)	0.121(2)
O(2)	0.5695(3)	0.0558(2)	0.1071(5)	0.167(3)
O(3)	0.2513(2)	-0.00436(13)	-0.3342(2)	0.0578(11)
O(4)	0.3653(3)	-0.01353(14)	-0.1727(3)	0.0677(12)
N(1)	-0.0068(3)	-0.0181(2)	-0.3748(3)	0.0475(13)
N(2)	0.3734(3)	-0.0691(2)	0.0300(3)	0.076(2)
C(1)	-0.0005(2)	-0.13213(12)	-0.3414(2)	0.056(2)
C(2)	-0.1103(2)	-0.10344(14)	-0.3635(3)	0.051(2)
C(3)	-0.1953(2)	-0.1488(2)	-0.3669(3)	0.078(2)
C(4)	-0.1381(3)	-0.2054(2)	-0.3468(3)	0.085(2)
C(5)	-0.0177(3)	-0.19517(12)	-0.3311(3)	0.082(2)
C(6)	-0.1769(3)	-0.21781(14)	-0.6036(2)	0.086(2)
C(7)	-0.2146(3)	-0.15674(15)	-0.6175(3)	0.096(3)
C(8)	-0.1160(4)	-0.11971(15)	-0.6110(4)	0.141(3)
C(9)	-0.0174(3)	-0.1579(2)	-0.5931(4)	0.084(2)
C(10)	-0.0551(3)	-0.2185(2)	-0.5885(3)	0.085(2)
C(11)	-0.1090(4)	-0.0380(2)	-0.3916(4)	0.065(2)
C(12)	0.0095(5)	0.0457(3)	-0.3933(5)	0.101(3)
C(13)	0.0465(5)	0.0544(2)	-0.5033(4)	0.078(2)
C(14)	0.1026(5)	0.1148(3)	-0.5102(4)	0.124(3)
C(15)	0.0625(6)	0.1279(3)	-0.6147(5)	0.143(3)
C(16)	-0.0503(5)	0.0953(4)	-0.6479(5)	0.203(4)
C(17)	0.2932(2)	-0.17686(13)	-0.0479(2)	0.064(2)
C(18)	0.3233(3)	-0.1689(2)	0.0635(2)	0.097(3)
C(19)	0.3025(4)	-0.2244(2)	0.1103(3)	0.104(2)
C(20)	0.2595(4)	-0.2666(2)	0.0278(4)	0.140(3)
C(21)	0.2537(3)	-0.23721(14)	-0.0699(3)	0.101(3)
C(22)	0.5306(2)	-0.31047(13)	0.0594(3)	0.110(3)
C(23)	0.5256(3)	-0.2876(2)	-0.0431(3)	0.096(2)
C(24)	0.5641(4)	-0.2266(2)	-0.0323(4)	0.113(3)
C(25)	0.5929(3)	-0.21180(14)	0.0770(5)	0.112(3)
C(26)	0.5722(3)	-0.2636(2)	0.1336(3)	0.095(3)
C(27)	0.3670(4)	-0.1088(3)	0.0986(5)	0.086(2)
C(28)	0.4110(4)	-0.0107(2)	0.0720(4)	0.080(2)
C(29)	0.5355(4)	-0.0041(2)	0.0711(5)	0.104(3)
C(30)	0.6327(4)	-0.0456(3)	0.1058(6)	0.144(4)
C(31)	0.7278(6)	0.0028(3)	0.1209(7)	0.183(4)
C(32)	0.6864(4)	0.0674(3)	0.1126(6)	0.137(3)
C(33)	0.4073(4)	0.0646(2)	-0.2689(4)	0.068(2)
C(34)	0.3325(4)	0.0092(2)	-0.2652(4)	0.053(2)
Pd(1')	0.67016(3)	0.07102(2)	-0.37998(3)	0.05546(13)
Pd(2')	0.85697(3)	0.04681(2)	-0.16071(3)	0.05326(13)
Fe(1')	0.57907(6)	0.20307(4)	-0.53074(7)	0.0748(3)
Fe(2')	1.09741(6)	0.13400(3)	-0.02016(6)	0.0634(3)
Cl(1')	0.71610(11)	0.12108(6)	-0.21756(11)	0.0668(5)
O(1')	0.3870(4)	0.0031(2)	-0.6387(4)	0.169(3)

O(2')	0.9477(8)	-0.1556(2)	0.0211(4)	0.316(5)
O(3')	0.6261(3)	-0.01358(14)	-0.3261(2)	0.0704(12)
O(4')	0.7257(3)	-0.0177(2)	-0.1564(3)	0.0776(13)
N(1')	0.6260(3)	0.0409(2)	-0.5389(3)	0.0624(14)
N(2')	0.9830(3)	-0.0155(2)	-0.1131(3)	0.0558(14)
C(1')	0.6959(2)	0.14288(12)	-0.4572(2)	0.060(2)
C(2')	0.6756(3)	0.1361(2)	-0.5684(2)	0.057(2)
C(3')	0.7013(3)	0.1921(2)	-0.6106(3)	0.103(3)
C(4')	0.7376(3)	0.23342(13)	-0.5255(3)	0.071(2)
C(5')	0.7342(2)	0.20302(12)	-0.4307(3)	0.064(2)
C(6')	0.4234(2)	0.1789(2)	-0.5013(3)	0.129(3)
C(7')	0.4662(3)	0.2318(2)	-0.4427(4)	0.163(3)
C(8')	0.4809(4)	0.2771(2)	-0.5152(5)	0.134(3)
C(9')	0.4471(4)	0.2522(2)	-0.6186(5)	0.155(4)
C(10')	0.4116(4)	0.1915(2)	-0.6100(3)	0.153(4)
C(11')	0.6344(4)	0.0811(3)	-0.6076(4)	0.091(2)
C(12')	0.5730(4)	-0.0226(2)	-0.5620(4)	0.086(2)
C(13')	0.4369(7)	-0.0206(2)	-0.5428(4)	0.140(3)
C(14')	0.4057(5)	-0.0840(3)	-0.5697(6)	0.214(4)
C(15')	0.2834(5)	-0.0738(3)	-0.5924(5)	0.150(3)
C(16')	0.2699(5)	-0.0209(4)	-0.6593(6)	0.161(4)
C(17')	0.9831(2)	0.10021(12)	-0.1560(2)	0.053(2)
C(18')	1.0901(2)	0.06888(14)	-0.1265(3)	0.054(2)
C(19')	1.1800(2)	0.1113(2)	-0.1239(3)	0.073(2)
C(20')	1.1284(3)	0.1688(2)	-0.1517(3)	0.090(2)
C(21')	1.0067(3)	0.16199(12)	-0.1716(3)	0.064(2)
C(22')	1.0172(3)	0.1217(2)	0.0992(2)	0.128(3)
C(23')	1.1250(3)	0.0910(2)	0.1218(3)	0.086(2)
C(24')	1.2133(3)	0.1347(2)	0.1273(3)	0.101(3)
C(25')	1.1601(4)	0.1925(2)	0.1081(4)	0.097(2)
C(26')	1.0389(3)	0.18445(15)	0.0907(3)	0.097(3)
C(27')	1.0857(4)	0.0085(2)	-0.1121(3)	0.055(2)
C(28')	0.9726(4)	-0.0766(2)	-0.0914(3)	0.055(2)
C(29')	0.9492(7)	-0.0883(3)	-0.0061(6)	0.173(4)
C(30')	1.0575(5)	-0.0777(3)	0.0745(5)	0.142(3)
C(31')	1.0262(6)	-0.1019(3)	0.1667(5)	0.180(4)
C(32')	0.9873(7)	-0.1663(2)	0.1280(4)	0.152(3)
C(33')	0.6052(4)	-0.1002(2)	-0.2118(4)	0.071(2)
C(34')	0.6515(4)	-0.0400(2)	-0.2416(4)	0.071(2)

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

Pd(1)-C(1)	2.014(2)	C(17)-C(18)	1.42	N(2')-C(28')	1.392(5)
Pd(1)-N(1)	2.053(3)	C(17)-C(21)	1.42	C(1')-C(2')	1.42
Pd(1)-O(3)	2.112(3)	C(18)-C(19)	1.42	C(1')-C(5')	1.42
Pd(1)-Cl(1)	2.3171(13)	C(18)-C(27)	1.459(6)	C(2')-C(11')	1.364(6)
Pd(1)-Pd(2)	3.2090(6)	C(19)-C(20)	1.42	C(2')-C(3')	1.42
Pd(2)-N(2)	1.995(4)	C(20)-C(21)	1.42	C(3')-C(4')	1.42
Pd(2)-C(17)	2.007(3)	C(22)-C(26)	1.42	C(4')-C(5')	1.42
Pd(2)-O(4)	2.145(3)	C(22)-C(23)	1.42	C(6')-C(7')	1.42
Pd(2)-Cl(1)	2.3226(15)	C(23)-C(24)	1.42	C(6')-C(10')	1.42
Fe(1)-C(8)	1.975(4)	C(24)-C(25)	1.42	C(7')-C(8')	1.42
Fe(1)-C(7)	1.973(4)	C(25)-C(26)	1.42	C(8')-C(9')	1.42
Fe(1)-C(9)	2.022(4)	C(28)-C(29)	1.499(7)	C(9')-C(10')	1.42
Fe(1)-C(6)	2.018(3)	C(29)-C(30)	1.460(7)	C(12')-C(13')	1.710(9)
Fe(1)-C(1)	2.032(2)	C(30)-C(31)	1.536(8)	C(13')-C(14')	1.469(8)
Fe(1)-C(10)	2.048(4)	C(31)-C(32)	1.507(9)	C(14')-C(15')	1.434(8)
Fe(1)-C(5)	2.047(3)	C(33)-C(34)	1.524(6)	C(15')-C(16')	1.443(9)
Fe(1)-C(2)	2.052(3)	Pd(1')-C(1')	1.949(3)	C(17')-C(18')	1.42
Fe(1)-C(4)	2.075(4)	Pd(1')-O(3')	2.112(3)	C(17')-C(21')	1.42
Fe(1)-C(3)	2.078(4)	Pd(1')-N(1')	2.117(4)	C(18')-C(27')	1.352(6)
Fe(2)-C(25)	2.015(4)	Pd(1')-Cl(1')	2.3336(14)	C(18')-C(19')	1.42
Fe(2)-C(24)	2.019(4)	Pd(1')-Pd(2')	3.1997(6)	C(19')-C(20')	1.42
Fe(2)-C(26)	2.032(4)	Pd(2')-C(17')	1.903(2)	C(20')-C(21')	1.42
Fe(2)-C(23)	2.039(4)	Pd(2')-N(2')	2.019(4)	C(22')-C(23')	1.42
Fe(2)-C(19)	2.050(4)	Pd(2')-O(4')	2.132(3)	C(22')-C(26')	1.42
Fe(2)-C(22)	2.047(3)	Pd(2')-Cl(1')	2.3341(13)	C(23')-C(24')	1.42
Fe(2)-C(18)	2.051(4)	Fe(1')-C(5')	1.979(3)	C(24')-C(25')	1.42
Fe(2)-C(20)	2.095(4)	Fe(1')-C(1')	1.991(2)	C(25')-C(26')	1.42
Fe(2)-C(17)	2.097(3)	Fe(1')-C(4')	1.995(3)	C(28')-C(29')	1.244(9)
Fe(2)-C(21)	2.124(3)	Fe(1')-C(2')	2.014(3)	C(29')-C(30')	1.467(8)
O(1)-C(13)	1.345(5)	Fe(1')-C(9')	2.016(5)	C(30')-C(31')	1.452(9)
O(1)-C(16)	1.381(8)	Fe(1')-C(3')	2.016(4)	C(31')-C(32')	1.543(9)
O(2)-C(32)	1.405(7)	Fe(1')-C(10')	2.023(4)	C(33')-C(34')	1.530(7)
O(2)-C(29)	1.428(7)	Fe(1')-C(8')	2.054(4)	C(1)-Pd(1)-N(1)	77.83(12)
O(3)-C(34)	1.184(5)	Fe(1')-C(6')	2.065(3)	C(1)-Pd(1)-O(3)	170.40(11)
O(4)-C(34)	1.276(5)	Fe(1')-C(7')	2.084(4)	N(1)-Pd(1)-O(3)	92.59(13)
N(1)-C(11)	1.264(5)	Fe(2')-C(19')	1.937(4)	C(1)-Pd(1)-Cl(1)	96.40(8)
N(1)-C(12)	1.453(7)	Fe(2')-C(18')	1.988(3)	N(1)-Pd(1)-Cl(1)	174.05(11)
N(2)-C(27)	1.270(7)	Fe(2')-C(20')	2.005(4)	O(3)-Pd(1)-Cl(1)	93.19(9)
N(2)-C(28)	1.430(6)	Fe(2')-C(23')	2.036(4)	C(1)-Pd(1)-Pd(2)	108.66(7)
C(1)-C(5)	1.42	Fe(2')-C(22')	2.048(3)	N(1)-Pd(1)-Pd(2)	133.96(10)
C(1)-C(2)	1.42	Fe(2')-C(24')	2.068(4)	O(3)-Pd(1)-Pd(2)	78.43(8)
C(2)-C(3)	1.42	Fe(2')-C(17')	2.085(2)	Cl(1)-Pd(1)-Pd(2)	46.31(4)
C(2)-C(11)	1.493(6)	Fe(2')-C(26')	2.087(4)	N(2)-Pd(2)-C(17)	83.7(2)
C(3)-C(4)	1.42	Fe(2')-C(21')	2.094(3)	N(2)-Pd(2)-O(4)	88.9(2)
C(4)-C(5)	1.42	Fe(2')-C(25')	2.099(4)	C(17)-Pd(2)-O(4)	172.56(12)
C(6)-C(7)	1.42	O(1')-C(13')	1.350(7)	N(2)-Pd(2)-Cl(1)	174.01(13)
C(6)-C(10)	1.42	O(1')-C(16')	1.458(7)	C(17)-Pd(2)-Cl(1)	91.13(9)
C(7)-C(8)	1.42	O(2')-C(32')	1.378(7)	O(4)-Pd(2)-Cl(1)	96.28(9)
C(8)-C(9)	1.42	O(2')-C(29')	1.530(7)	N(2)-Pd(2)-Pd(1)	138.91(12)
C(9)-C(10)	1.42	O(3')-C(34')	1.219(6)	C(17)-Pd(2)-Pd(1)	111.45(7)
C(12)-C(13)	1.622(8)	O(4')-C(34')	1.330(6)	O(4)-Pd(2)-Pd(1)	73.67(8)
C(13)-C(14)	1.506(7)	N(1')-C(11')	1.285(7)	Cl(1)-Pd(2)-Pd(1)	46.17(3)
C(14)-C(15)	1.359(7)	N(1')-C(12')	1.537(6)	C(8)-Fe(1)-C(7)	42.16(8)
C(15)-C(16)	1.493(9)	N(2')-C(27')	1.335(6)	C(8)-Fe(1)-C(9)	41.59(9)

C(7)-Fe(1)-C(9)	70.20(12)	C(23)-Fe(2)-C(22)	40.67(6)	C(2)-C(3)-Fe(1)	68.90(10)
C(8)-Fe(1)-C(6)	70.23(10)	C(19)-Fe(2)-C(22)	118.78(15)	C(4)-C(3)-Fe(1)	69.90(13)
C(7)-Fe(1)-C(6)	41.66(6)	C(25)-Fe(2)-C(18)	109.58(14)	C(3)-C(4)-C(5)	108.0
C(9)-Fe(1)-C(6)	69.31(10)	C(24)-Fe(2)-C(18)	127.5(2)	C(3)-C(4)-Fe(1)	70.11(12)
C(8)-Fe(1)-C(1)	119.09(14)	C(26)-Fe(2)-C(18)	121.50(14)	C(5)-C(4)-Fe(1)	68.80(9)
C(7)-Fe(1)-C(1)	153.22(13)	C(23)-Fe(2)-C(18)	163.9(2)	C(4)-C(5)-C(1)	108.0
C(9)-Fe(1)-C(1)	108.76(13)	C(19)-Fe(2)-C(18)	40.52(8)	C(4)-C(5)-Fe(1)	70.91(11)
C(6)-Fe(1)-C(1)	164.67(12)	C(22)-Fe(2)-C(18)	155.01(15)	C(1)-C(5)-Fe(1)	69.08(11)
C(8)-Fe(1)-C(10)	69.61(12)	C(25)-Fe(2)-C(20)	161.8(2)	C(7)-C(6)-C(10)	108.0
C(7)-Fe(1)-C(10)	69.66(9)	C(24)-Fe(2)-C(20)	154.9(2)	C(7)-C(6)-Fe(1)	67.45(14)
C(9)-Fe(1)-C(10)	40.83(8)	C(26)-Fe(2)-C(20)	123.9(2)	C(10)-C(6)-Fe(1)	70.70(14)
C(6)-Fe(1)-C(10)	40.86(6)	C(23)-Fe(2)-C(20)	119.1(2)	C(8)-C(7)-C(6)	108.0
C(1)-Fe(1)-C(10)	127.96(12)	C(19)-Fe(2)-C(20)	40.05(7)	C(8)-C(7)-Fe(1)	69.01(14)
C(8)-Fe(1)-C(5)	154.3(2)	C(22)-Fe(2)-C(20)	105.97(13)	C(6)-C(7)-Fe(1)	70.89(13)
C(7)-Fe(1)-C(5)	163.05(15)	C(18)-Fe(2)-C(20)	67.30(10)	C(7)-C(8)-C(9)	108.0
C(9)-Fe(1)-C(5)	120.1(2)	C(25)-Fe(2)-C(17)	123.56(14)	C(7)-C(8)-Fe(1)	68.83(12)
C(6)-Fe(1)-C(5)	126.07(12)	C(24)-Fe(2)-C(17)	110.30(14)	C(9)-C(8)-Fe(1)	70.97(15)
C(1)-Fe(1)-C(5)	40.7	C(26)-Fe(2)-C(17)	157.66(13)	C(10)-C(9)-C(8)	108.0
C(10)-Fe(1)-C(5)	108.46(14)	C(23)-Fe(2)-C(17)	126.43(14)	C(10)-C(9)-Fe(1)	70.57(12)
C(8)-Fe(1)-C(2)	107.11(15)	C(19)-Fe(2)-C(17)	67.28(9)	C(8)-C(9)-Fe(1)	67.43(14)
C(7)-Fe(1)-C(2)	117.71(12)	C(22)-Fe(2)-C(17)	161.36(13)	C(9)-C(10)-C(6)	108.0
C(9)-Fe(1)-C(2)	127.9(2)	C(18)-Fe(2)-C(17)	40.02(5)	C(9)-C(10)-Fe(1)	68.60(13)
C(6)-Fe(1)-C(2)	152.24(12)	C(20)-Fe(2)-C(17)	66.46(8)	C(6)-C(10)-Fe(1)	68.43(12)
C(1)-Fe(1)-C(2)	40.69(5)	C(25)-Fe(2)-C(21)	157.7(2)	N(1)-C(11)-C(2)	111.3(4)
C(10)-Fe(1)-C(2)	165.91(13)	C(24)-Fe(2)-C(21)	122.1(2)	N(1)-C(12)-C(13)	110.1(4)
C(5)-Fe(1)-C(2)	68.19(8)	C(26)-Fe(2)-C(21)	160.27(15)	O(1)-C(13)-C(14)	112.1(4)
C(8)-Fe(1)-C(4)	163.4(2)	C(23)-Fe(2)-C(21)	108.05(15)	O(1)-C(13)-C(12)	115.1(5)
C(7)-Fe(1)-C(4)	124.9(2)	C(19)-Fe(2)-C(21)	66.77(9)	C(14)-C(13)-C(12)	112.7(4)
C(9)-Fe(1)-C(4)	153.9(2)	C(22)-Fe(2)-C(21)	124.22(12)	C(15)-C(14)-C(13)	101.6(5)
C(6)-Fe(1)-C(4)	106.63(13)	C(18)-Fe(2)-C(21)	66.75(8)	C(14)-C(15)-C(16)	104.5(6)
C(1)-Fe(1)-C(4)	68.02(9)	C(20)-Fe(2)-C(21)	39.32(6)	O(1)-C(16)-C(15)	106.4(5)
C(10)-Fe(1)-C(4)	119.3(2)	C(17)-Fe(2)-C(21)	39.3	C(18)-C(17)-C(21)	108.0
C(5)-Fe(1)-C(4)	40.30(7)	Pd(1)-Cl(1)-Pd(2)	87.52(5)	C(18)-C(17)-Pd(2)	109.6(2)
C(2)-Fe(1)-C(4)	67.67(10)	C(13)-O(1)-C(16)	104.0(4)	C(21)-C(17)-Pd(2)	142.3(2)
C(8)-Fe(1)-C(3)	126.0(2)	C(32)-O(2)-C(29)	112.5(5)	C(18)-C(17)-Fe(2)	68.23(14)
C(7)-Fe(1)-C(3)	105.80(14)	C(34)-O(3)-Pd(1)	127.2(3)	C(21)-C(17)-Fe(2)	71.37(13)
C(9)-Fe(1)-C(3)	165.0(2)	C(34)-O(4)-Pd(2)	129.1(3)	Pd(2)-C(17)-Fe(2)	121.85(12)
C(6)-Fe(1)-C(3)	117.87(13)	C(11)-N(1)-C(12)	118.3(4)	C(19)-C(18)-C(17)	108.0
C(1)-Fe(1)-C(3)	67.96(9)	C(11)-N(1)-Pd(1)	121.2(3)	C(19)-C(18)-C(27)	137.7(3)
C(10)-Fe(1)-C(3)	152.6(2)	C(12)-N(1)-Pd(1)	120.3(3)	C(17)-C(18)-C(27)	114.3(3)
C(5)-Fe(1)-C(3)	67.70(10)	C(27)-N(2)-C(28)	114.9(5)	C(19)-C(18)-Fe(2)	69.69(12)
C(2)-Fe(1)-C(3)	40.22(7)	C(27)-N(2)-Pd(2)	113.1(4)	C(17)-C(18)-Fe(2)	71.75(12)
C(4)-Fe(1)-C(3)	39.99(7)	C(28)-N(2)-Pd(2)	132.0(4)	C(27)-C(18)-Fe(2)	123.1(3)
C(25)-Fe(2)-C(24)	41.22(7)	C(5)-C(1)-C(2)	108.0	C(20)-C(19)-C(18)	108.0
C(25)-Fe(2)-C(26)	41.08(7)	C(5)-C(1)-Pd(1)	137.76(13)	C(20)-C(19)-Fe(2)	71.71(13)
C(24)-Fe(2)-C(26)	69.10(9)	C(2)-C(1)-Pd(1)	114.24(13)	C(18)-C(19)-Fe(2)	69.79(11)
C(25)-Fe(2)-C(23)	69.05(10)	C(5)-C(1)-Fe(1)	70.18(13)	C(21)-C(20)-C(19)	108.0
C(24)-Fe(2)-C(23)	40.96(8)	C(2)-C(1)-Fe(1)	70.38(12)	C(21)-C(20)-Fe(2)	71.44(11)
C(26)-Fe(2)-C(23)	68.72(8)	Pd(1)-C(1)-Fe(1)	124.11(12)	C(19)-C(20)-Fe(2)	68.24(14)
C(25)-Fe(2)-C(19)	125.9(2)	C(3)-C(2)-C(1)	108.0	C(20)-C(21)-C(17)	108.0
C(24)-Fe(2)-C(19)	164.2(2)	C(3)-C(2)-C(11)	136.7(2)	C(20)-C(21)-Fe(2)	69.24(12)
C(26)-Fe(2)-C(19)	106.9(2)	C(1)-C(2)-C(11)	114.6(2)	C(17)-C(21)-Fe(2)	69.32(12)
C(23)-Fe(2)-C(19)	153.3(2)	C(3)-C(2)-Fe(1)	70.88(11)	C(26)-C(22)-C(23)	108.0
C(25)-Fe(2)-C(22)	68.89(9)	C(1)-C(2)-Fe(1)	68.93(10)	C(26)-C(22)-Fe(2)	69.06(14)
C(24)-Fe(2)-C(22)	68.81(9)	C(11)-C(2)-Fe(1)	117.4(3)	C(23)-C(22)-Fe(2)	69.4(2)
C(26)-Fe(2)-C(22)	40.74(6)	C(2)-C(3)-C(4)	108.0	C(24)-C(23)-C(22)	108.0

C(24)-C(23)-Fe(2)	68.77(11)	C(9')-Fe(1')-C(3')	109.6(2)	C(22')-Fe(2')-C(26')	40.16(6)
C(22)-C(23)-Fe(2)	69.96(13)	C(5')-Fe(1')-C(10')	167.8(2)	C(24')-Fe(2')-C(26')	67.14(10)
C(23)-C(24)-C(25)	108.0	C(1')-Fe(1')-C(10')	130.1(2)	C(17')-Fe(2')-C(26')	121.37(13)
C(23)-C(24)-Fe(2)	70.27(11)	C(4')-Fe(1')-C(10')	150.2(2)	C(19')-Fe(2')-C(21')	69.37(10)
C(25)-C(24)-Fe(2)	69.22(15)	C(2')-Fe(1')-C(10')	109.6(2)	C(18')-Fe(2')-C(21')	68.44(8)
C(26)-C(25)-C(24)	108.0	C(9')-Fe(1')-C(10')	41.16(8)	C(20')-Fe(2')-C(21')	40.46(7)
C(26)-C(25)-Fe(2)	70.11(12)	C(3')-Fe(1')-C(10')	118.2(2)	C(23')-Fe(2')-C(21')	157.59(14)
C(24)-C(25)-Fe(2)	69.6(2)	C(5')-Fe(1')-C(8')	113.5(2)	C(22')-Fe(2')-C(21')	121.98(12)
C(25)-C(26)-C(22)	108.0	C(1')-Fe(1')-C(8')	146.4(2)	C(24')-Fe(2')-C(21')	160.4(2)
C(25)-C(26)-Fe(2)	68.81(12)	C(4')-Fe(1')-C(8')	106.89(15)	C(17')-Fe(2')-C(21')	39.7
C(22)-C(26)-Fe(2)	70.19(12)	C(2')-Fe(1')-C(8')	170.9(2)	C(26')-Fe(2')-C(21')	108.36(14)
N(2)-C(27)-C(18)	119.2(5)	C(9')-Fe(1')-C(8')	40.82(8)	C(19')-Fe(2')-C(25')	125.26(15)
N(2)-C(28)-C(29)	107.5(4)	C(3')-Fe(1')-C(8')	130.9(2)	C(18')-Fe(2')-C(25')	161.4(2)
O(2)-C(29)-C(30)	110.0(4)	C(10')-Fe(1')-C(8')	68.59(11)	C(20')-Fe(2')-C(25')	110.06(15)
O(2)-C(29)-C(28)	106.7(4)	C(5')-Fe(1')-C(6')	127.9(2)	C(23')-Fe(2')-C(25')	67.48(9)
C(30)-C(29)-C(28)	130.6(5)	C(1')-Fe(1')-C(6')	107.01(12)	C(22')-Fe(2')-C(25')	67.27(10)
C(29)-C(30)-C(31)	96.2(5)	C(4')-Fe(1')-C(6')	167.0(2)	C(24')-Fe(2')-C(25')	39.83(7)
C(32)-C(31)-C(30)	115.5(5)	C(2')-Fe(1')-C(6')	117.12(14)	C(17')-Fe(2')-C(25')	157.6(2)
O(2)-C(32)-C(31)	97.8(5)	C(9')-Fe(1')-C(6')	68.52(10)	C(26')-Fe(2')-C(25')	39.66(7)
O(3)-C(34)-O(4)	128.1(4)	C(3')-Fe(1')-C(6')	150.8(2)	C(21')-Fe(2')-C(25')	124.6(2)
O(3)-C(34)-C(33)	123.5(4)	C(10')-Fe(1')-C(6')	40.64(6)	Pd(2')-Cl(1')-Pd(1')	86.55(5)
O(4)-C(34)-C(33)	107.8(4)	C(8')-Fe(1')-C(6')	67.81(10)	C(13')-O(1')-C(16')	101.9(5)
C(1')-Pd(1')-O(3')	168.69(11)	C(5')-Fe(1')-C(7')	105.37(15)	C(32')-O(2')-C(29')	112.5(5)
C(1')-Pd(1')-N(1')	77.30(13)	C(1')-Fe(1')-C(7')	114.3(2)	C(34')-O(3')-Pd(1')	134.5(3)
O(3')-Pd(1')-N(1')	91.61(13)	C(4')-Fe(1')-C(7')	128.4(2)	C(34')-O(4')-Pd(2')	124.4(3)
C(1')-Pd(1')-Cl(1')	93.08(9)	C(2')-Fe(1')-C(7')	148.4(2)	C(11')-N(1')-C(12')	126.4(4)
O(3')-Pd(1')-Cl(1')	97.88(9)	C(9')-Fe(1')-C(7')	68.14(11)	C(11')-N(1')-Pd(1')	115.2(3)
N(1')-Pd(1')-Cl(1')	170.01(11)	C(3')-Fe(1')-C(7')	168.5(2)	C(12')-N(1')-Pd(1')	117.9(3)
C(1')-Pd(1')-Pd(2')	115.75(7)	C(10')-Fe(1')-C(7')	68.02(9)	C(27')-N(2')-C(28')	120.8(4)
O(3')-Pd(1')-Pd(2')	74.31(8)	C(8')-Fe(1')-C(7')	40.13(8)	C(27')-N(2')-Pd(2')	110.2(3)
N(1')-Pd(1')-Pd(2')	140.36(10)	C(6')-Fe(1')-C(7')	40.03(7)	C(28')-N(2')-Pd(2')	128.8(3)
Cl(1')-Pd(1')-Pd(2')	46.73(3)	C(19')-Fe(2')-C(18')	42.40(7)	C(2')-C(1')-C(5')	108.0
C(17')-Pd(2')-N(2')	83.71(13)	C(19')-Fe(2')-C(20')	42.19(8)	C(2')-C(1')-Pd(1')	115.89(14)
C(17')-Pd(2')-O(4')	175.11(11)	C(18')-Fe(2')-C(20')	70.26(10)	C(5')-C(1')-Pd(1')	136.09(14)
N(2')-Pd(2')-O(4')	91.85(14)	C(19')-Fe(2')-C(23')	121.7(2)	C(2')-C(1')-Fe(1')	70.09(13)
C(17')-Pd(2')-Cl(1')	94.34(8)	C(18')-Fe(2')-C(23')	105.54(14)	C(5')-C(1')-Fe(1')	68.62(11)
N(2')-Pd(2')-Cl(1')	177.96(12)	C(20')-Fe(2')-C(23')	160.00(15)	Pd(1')-C(1')-Fe(1')	127.66(12)
O(4')-Pd(2')-Cl(1')	90.12(9)	C(19')-Fe(2')-C(22')	157.1(2)	C(11')-C(2')-C(1')	115.5(3)
C(17')-Pd(2')-Pd(1')	106.98(7)	C(18')-Fe(2')-C(22')	119.47(13)	C(11')-C(2')-C(3')	136.4(3)
N(2')-Pd(2')-Pd(1')	133.33(10)	C(20')-Fe(2')-C(22')	158.51(15)	C(1')-C(2')-C(3')	108.0
O(4')-Pd(2')-Pd(1')	77.58(9)	C(23')-Fe(2')-C(22')	40.69(6)	C(11')-C(2')-Fe(1')	125.0(3)
Cl(1')-Pd(2')-Pd(1')	46.72(3)	C(19')-Fe(2')-C(24')	108.36(14)	C(1')-C(2')-Fe(1')	68.37(11)
C(5')-Fe(1')-C(1')	41.91(5)	C(18')-Fe(2')-C(24')	123.9(2)	C(3')-C(2')-Fe(1')	69.47(11)
C(5')-Fe(1')-C(4')	41.86(6)	C(20')-Fe(2')-C(24')	124.81(14)	C(2')-C(3')-C(4')	108.0
C(1')-Fe(1')-C(4')	70.40(8)	C(23')-Fe(2')-C(24')	40.47(7)	C(2')-C(3')-Fe(1')	69.26(10)
C(5')-Fe(1')-C(2')	70.25(8)	C(22')-Fe(2')-C(24')	67.86(9)	C(4')-C(3')-Fe(1')	68.48(11)
C(1')-Fe(1')-C(2')	41.53(6)	C(19')-Fe(2')-C(17')	69.58(9)	C(5')-C(4')-C(3')	108.0
C(4')-Fe(1')-C(2')	69.94(10)	C(18')-Fe(2')-C(17')	40.72(5)	C(5')-C(4')-Fe(1')	68.47(10)
C(5')-Fe(1')-C(9')	147.4(2)	C(20')-Fe(2')-C(17')	68.34(9)	C(3')-C(4')-Fe(1')	70.06(12)
C(1')-Fe(1')-C(9')	170.5(2)	C(23')-Fe(2')-C(17')	121.88(13)	C(4')-C(5')-C(1')	108.0
C(4')-Fe(1')-C(9')	115.9(2)	C(22')-Fe(2')-C(17')	105.61(11)	C(4')-C(5')-Fe(1')	69.67(12)
C(2')-Fe(1')-C(9')	132.1(2)	C(24')-Fe(2')-C(17')	159.3(2)	C(1')-C(5')-Fe(1')	69.47(10)
C(5')-Fe(1')-C(3')	70.19(10)	C(19')-Fe(2')-C(26')	161.2(2)	C(7')-C(6')-C(10')	108.0
C(1')-Fe(1')-C(3')	69.97(9)	C(18')-Fe(2')-C(26')	155.59(14)	C(7')-C(6')-Fe(1')	70.7(2)
C(4')-Fe(1')-C(3')	41.46(7)	C(20')-Fe(2')-C(26')	124.0(2)	C(10')-C(6')-Fe(1')	68.1(2)
C(2')-Fe(1')-C(3')	41.26(7)	C(23')-Fe(2')-C(26')	67.72(9)	C(8')-C(7')-C(6')	108.0

C(8')-C(7')-Fe(1')	68.82(14)	C(18')-C(17')-Fe(2')	65.99(12)	C(24')-C(23')-Fe(2')	70.98(13)
C(6')-C(7')-Fe(1')	69.26(13)	C(21')-C(17')-Fe(2')	70.51(13)	C(22')-C(23')-Fe(2')	70.09(12)
C(7')-C(8')-C(9')	108.0	Pd(2')-C(17')-Fe(2')	126.32(13)	C(25')-C(24')-C(23')	108.0
C(7')-C(8')-Fe(1')	71.05(14)	C(27')-C(18')-C(17')	117.1(3)	C(25')-C(24')-Fe(2')	71.25(15)
C(9')-C(8')-Fe(1')	68.2(2)	C(27')-C(18')-C(19')	134.9(3)	C(23')-C(24')-Fe(2')	68.56(12)
C(8')-C(9')-C(10')	108.0	C(17')-C(18')-C(19')	108.0	C(24')-C(25')-C(26')	108.0
C(8')-C(9')-Fe(1')	71.0(2)	C(27')-C(18')-Fe(2')	127.9(3)	C(24')-C(25')-Fe(2')	68.92(13)
C(10')-C(9')-Fe(1')	69.66(12)	C(17')-C(18')-Fe(2')	73.29(10)	C(26')-C(25')-Fe(2')	69.70(11)
C(6')-C(10')-C(9')	108.0	C(19')-C(18')-Fe(2')	66.87(11)	C(22')-C(26')-C(25')	108.0
C(6')-C(10')-Fe(1')	71.3(2)	C(20')-C(19')-C(18')	108.0	C(22')-C(26')-Fe(2')	68.45(13)
C(9')-C(10')-Fe(1')	69.18(13)	C(20')-C(19')-Fe(2')	71.47(14)	C(25')-C(26')-Fe(2')	70.64(12)
N(1')-C(11')-C(2')	116.0(4)	C(18')-C(19')-Fe(2')	70.74(11)	N(2')-C(27')-C(18')	117.3(4)
N(1')-C(12')-C(13')	107.9(4)	C(21')-C(20')-C(19')	108.0	C(29')-C(28')-N(2')	115.9(5)
O(1')-C(13')-C(14')	97.1(5)	C(21')-C(20')-Fe(2')	73.17(9)	C(28')-C(29')-C(30')	104.6(6)
O(1')-C(13')-C(12')	94.8(5)	C(19')-C(20')-Fe(2')	66.34(13)	C(28')-C(29')-O(2')	115.4(6)
C(14')-C(13')-C(12')	97.7(5)	C(20')-C(21')-C(17')	108.0	C(30')-C(29')-O(2')	92.8(5)
C(15')-C(14')-C(13')	94.7(5)	C(20')-C(21')-Fe(2')	66.37(10)	C(31')-C(30')-C(29')	99.8(5)
C(14')-C(15')-C(16')	101.8(5)	C(17')-C(21')-Fe(2')	69.76(11)	C(30')-C(31')-C(32')	100.8(5)
C(15')-C(16')-O(1')	103.2(5)	C(23')-C(22')-C(26')	108.0	O(2')-C(32')-C(31')	99.8(5)
C(18')-C(17')-C(21')	108.0	C(23')-C(22')-Fe(2')	69.22(13)	O(3')-C(34')-O(4')	122.8(5)
C(18')-C(17')-Pd(2')	111.01(13)	C(26')-C(22')-Fe(2')	71.39(15)	O(3')-C(34')-C(33')	128.7(4)
C(21')-C(17')-Pd(2')	140.99(13)	C(24')-C(23')-C(22')	108.0	O(4')-C(34')-C(33')	108.5(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)	0.0460(2)	0.0505(2)	0.0510(2)	0.0044(2)	-0.0021(2)	-0.0015(2)
Pd(2)	0.0437(2)	0.0504(2)	0.0601(3)	0.0082(2)	0.0024(2)	0.0046(2)
Fe(1)	0.0492(4)	0.0671(5)	0.0659(5)	-0.0035(4)	0.0079(4)	-0.0112(4)
Fe(2)	0.0723(5)	0.0637(5)	0.1116(7)	0.0273(5)	0.0159(5)	0.0098(4)
Cl(1)	0.0536(8)	0.0513(8)	0.0833(10)	-0.0038(7)	0.0062(7)	0.0047(6)
O(1)	0.224(4)	0.097(3)	0.031(2)	-0.026(2)	0.011(3)	-0.081(3)
O(2)	0.079(3)	0.108(4)	0.316(6)	-0.057(4)	0.057(3)	-0.014(3)
O(3)	0.053(2)	0.050(2)	0.057(2)	-0.003(2)	-0.012(2)	-0.019(2)
O(4)	0.070(2)	0.058(2)	0.076(2)	-0.037(2)	0.021(2)	-0.024(2)
N(1)	0.051(2)	0.045(2)	0.049(2)	0.004(2)	0.017(2)	0.013(2)
N(2)	0.077(3)	0.080(3)	0.072(3)	0.030(3)	0.018(2)	0.009(2)
C(1)	0.065(3)	0.069(3)	0.035(3)	-0.003(3)	0.014(2)	-0.017(3)
C(2)	0.034(2)	0.062(3)	0.060(3)	-0.013(3)	0.015(2)	0.008(2)
C(3)	0.051(3)	0.107(4)	0.078(4)	-0.014(3)	0.023(3)	-0.046(3)
C(4)	0.029(3)	0.105(4)	0.114(5)	0.037(4)	0.007(3)	-0.011(3)
C(5)	0.127(5)	0.047(3)	0.062(4)	0.015(3)	0.007(3)	-0.027(3)
C(6)	0.076(4)	0.093(4)	0.077(4)	-0.059(3)	-0.003(3)	0.004(3)
C(7)	0.090(4)	0.099(5)	0.096(5)	-0.013(4)	0.019(4)	0.009(4)
C(8)	0.182(6)	0.163(8)	0.095(5)	0.025(5)	0.066(5)	0.006(6)
C(9)	0.072(4)	0.091(4)	0.085(4)	-0.025(4)	0.014(3)	-0.025(3)
C(10)	0.092(4)	0.067(4)	0.101(4)	-0.027(3)	0.033(3)	-0.006(3)
C(11)	0.035(3)	0.073(4)	0.079(4)	-0.019(3)	0.002(3)	0.005(3)
C(12)	0.083(4)	0.104(5)	0.118(5)	-0.018(4)	0.029(4)	0.014(4)
C(13)	0.102(4)	0.077(4)	0.036(3)	0.008(3)	-0.018(3)	-0.023(3)
C(14)	0.139(5)	0.116(5)	0.094(5)	0.054(4)	-0.011(4)	-0.066(4)
C(15)	0.238(7)	0.105(5)	0.109(5)	0.073(4)	0.088(5)	0.071(5)
C(16)	0.092(5)	0.398(12)	0.122(5)	0.145(6)	0.034(4)	0.034(7)
C(17)	0.044(3)	0.072(3)	0.066(3)	0.041(3)	0.000(3)	0.034(2)
C(18)	0.058(3)	0.099(5)	0.132(5)	-0.016(4)	0.023(4)	0.004(3)
C(19)	0.105(4)	0.067(4)	0.148(5)	0.051(4)	0.048(4)	-0.014(3)
C(20)	0.096(4)	0.138(5)	0.213(6)	0.119(4)	0.088(4)	0.011(4)
C(21)	0.033(3)	0.082(4)	0.179(6)	0.059(4)	0.011(4)	0.014(3)
C(22)	0.079(4)	0.093(4)	0.126(5)	0.031(4)	-0.031(4)	0.046(3)
C(23)	0.085(4)	0.091(4)	0.122(5)	0.070(3)	0.043(3)	0.041(3)
C(24)	0.081(3)	0.081(4)	0.205(6)	0.016(4)	0.086(4)	0.031(3)
C(25)	0.067(3)	0.103(5)	0.194(6)	0.012(5)	0.082(3)	0.011(3)
C(26)	0.054(4)	0.133(6)	0.088(5)	0.020(4)	-0.004(3)	0.012(4)
C(27)	0.042(3)	0.109(4)	0.113(4)	-0.067(3)	0.033(3)	-0.016(3)
C(28)	0.095(4)	0.046(3)	0.090(4)	0.027(3)	0.007(3)	-0.007(3)
C(29)	0.029(3)	0.104(5)	0.156(6)	-0.049(4)	-0.019(4)	0.009(3)
C(30)	0.066(4)	0.096(5)	0.216(8)	-0.036(5)	-0.066(5)	0.013(4)
C(31)	0.154(6)	0.164(8)	0.251(9)	-0.042(7)	0.089(6)	0.037(6)
C(32)	0.077(4)	0.154(7)	0.180(7)	-0.005(6)	0.030(5)	0.003(5)
C(33)	0.069(3)	0.063(3)	0.074(4)	0.029(3)	0.022(3)	0.023(3)
C(34)	0.074(3)	0.027(2)	0.059(3)	0.005(2)	0.017(3)	-0.026(2)
Pd(1')	0.0451(2)	0.0526(2)	0.0650(3)	-0.0035(2)	0.0073(2)	0.0026(2)
Pd(2')	0.0525(2)	0.0503(2)	0.0534(2)	-0.0009(2)	0.0069(2)	-0.0085(2)
Fe(1')	0.0539(5)	0.0786(6)	0.0884(6)	0.0268(5)	0.0116(4)	0.0082(4)
Fe(2')	0.0599(5)	0.0655(5)	0.0607(5)	-0.0119(4)	0.0078(4)	-0.0125(4)
Cl(1')	0.0664(8)	0.0587(9)	0.0660(9)	-0.0093(7)	-0.0004(7)	0.0014(7)
O(1')	0.213(5)	0.096(4)	0.197(5)	0.024(4)	0.048(4)	-0.037(4)
O(2')	0.718(13)	0.115(4)	0.118(4)	-0.023(4)	0.112(6)	-0.156(6)
O(3')	0.070(2)	0.064(2)	0.056(2)	0.038(2)	-0.023(2)	-0.004(2)

O(4')	0.066(2)	0.081(2)	0.089(3)	0.034(2)	0.027(2)	-0.008(2)
N(1')	0.029(2)	0.060(3)	0.093(3)	-0.037(2)	0.006(2)	-0.015(2)
N(2')	0.074(3)	0.040(2)	0.051(3)	0.001(2)	0.011(2)	-0.015(2)
C(1')	0.041(3)	0.049(3)	0.090(4)	-0.004(3)	0.020(3)	-0.016(2)
C(2')	0.079(3)	0.059(3)	0.039(3)	0.025(2)	0.026(2)	0.001(3)
C(3')	0.087(4)	0.137(6)	0.079(4)	0.026(4)	0.011(4)	0.011(4)
C(4')	0.043(3)	0.044(3)	0.112(5)	-0.003(3)	-0.005(3)	-0.010(2)
C(5')	0.081(3)	0.062(3)	0.051(3)	0.002(3)	0.017(3)	-0.024(3)
C(6')	0.119(4)	0.140(6)	0.164(5)	0.078(4)	0.101(3)	0.036(4)
C(7')	0.159(5)	0.202(7)	0.134(6)	0.042(5)	0.049(5)	0.131(5)
C(8')	0.071(4)	0.098(5)	0.217(8)	-0.050(5)	0.008(5)	0.015(4)
C(9')	0.117(5)	0.106(6)	0.230(9)	0.058(6)	0.019(6)	0.030(5)
C(10')	0.063(4)	0.151(7)	0.194(8)	0.011(6)	-0.057(5)	0.006(5)
C(11')	0.105(4)	0.108(4)	0.061(3)	0.064(3)	0.021(3)	0.041(4)
C(12')	0.065(3)	0.115(4)	0.081(4)	-0.069(3)	0.025(3)	-0.007(3)
C(13')	0.272(8)	0.049(4)	0.053(4)	0.016(3)	-0.044(5)	-0.055(4)
C(14')	0.139(5)	0.102(5)	0.292(8)	0.125(5)	-0.145(5)	-0.038(4)
C(15')	0.156(5)	0.156(5)	0.119(6)	0.041(5)	-0.001(5)	-0.105(4)
C(16')	0.049(4)	0.256(10)	0.143(7)	-0.014(7)	-0.039(5)	0.000(5)
C(17')	0.023(2)	0.050(3)	0.078(4)	0.002(3)	-0.005(3)	0.003(2)
C(18')	0.053(3)	0.073(3)	0.042(3)	0.012(3)	0.022(2)	-0.023(3)
C(19')	0.052(3)	0.090(4)	0.079(4)	0.028(3)	0.021(3)	-0.007(3)
C(20')	0.141(4)	0.056(3)	0.081(4)	-0.026(3)	0.042(3)	-0.060(3)
C(21')	0.015(2)	0.086(4)	0.085(4)	0.000(3)	0.001(3)	-0.004(2)
C(22')	0.138(5)	0.225(8)	0.037(3)	-0.008(4)	0.052(3)	-0.063(5)
C(23')	0.159(5)	0.045(3)	0.036(3)	-0.002(3)	-0.008(4)	-0.023(3)
C(24')	0.105(5)	0.127(5)	0.053(4)	-0.036(4)	-0.015(4)	0.008(4)
C(25')	0.091(4)	0.092(5)	0.110(5)	-0.026(4)	0.029(4)	-0.022(4)
C(26')	0.090(4)	0.136(6)	0.068(4)	0.001(4)	0.028(3)	0.012(4)
C(27')	0.045(3)	0.071(3)	0.043(3)	0.000(3)	0.000(3)	0.011(3)
C(28')	0.084(3)	0.029(2)	0.041(3)	0.007(2)	-0.005(3)	-0.015(3)
C(29')	0.217(8)	0.026(4)	0.260(10)	0.025(5)	0.034(7)	-0.023(4)
C(30')	0.079(5)	0.156(6)	0.162(6)	0.105(5)	-0.022(4)	0.022(4)
C(31')	0.163(6)	0.234(9)	0.137(7)	-0.059(6)	0.026(6)	-0.098(6)
C(32')	0.311(8)	0.056(4)	0.115(5)	0.057(3)	0.102(5)	0.060(5)
C(33')	0.077(3)	0.060(3)	0.082(4)	-0.009(3)	0.029(3)	-0.051(3)
C(34')	0.031(3)	0.097(4)	0.084(4)	-0.036(3)	0.013(3)	0.010(3)

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

	x	y	z	U(eq)
H(3A)	-0.2790(2)	-0.1421(3)	-0.3817(4)	0.093
H(4A)	-0.1753(4)	-0.2448(2)	-0.3452(5)	0.102
H(5A)	0.0430(4)	-0.22610(13)	-0.3152(4)	0.099
H(6A)	-0.2261(3)	-0.25313(14)	-0.6025(2)	0.103
H(7A)	-0.2946(4)	-0.1427(2)	-0.6299(4)	0.115
H(8A)	-0.1160(6)	-0.07557(15)	-0.6180(5)	0.169
H(9A)	0.0628(4)	-0.1446(3)	-0.5831(5)	0.101
H(10A)	-0.0052(3)	-0.2543(2)	-0.5736(4)	0.103
H(11)	-0.1750(4)	-0.0148(2)	-0.4180(4)	0.078
H(12A)	0.0692(5)	0.0621(3)	-0.3353(5)	0.121
H(12B)	-0.0617(5)	0.0675(3)	-0.3966(5)	0.121
H(13A)	0.1072(5)	0.0244(2)	-0.5014(4)	0.094
H(14A)	0.0783(5)	0.1448(3)	-0.4663(4)	0.149
H(14B)	0.1863(5)	0.1117(3)	-0.4899(4)	0.149
H(15A)	0.1158(6)	0.1137(3)	-0.6543(5)	0.171
H(15B)	0.0517(6)	0.1712(3)	-0.6254(5)	0.171
H(16A)	-0.1117(5)	0.1195(4)	-0.6322(5)	0.243
H(16B)	-0.0696(5)	0.0871(4)	-0.7232(5)	0.243
H(19A)	0.3130(5)	-0.2317(3)	0.1861(3)	0.124
H(20A)	0.2375(5)	-0.3086(2)	0.0368(5)	0.168
H(21A)	0.2286(4)	-0.2556(2)	-0.1402(4)	0.121
H(22A)	0.5075(2)	-0.35112(13)	0.0758(3)	0.132
H(23A)	0.4989(4)	-0.3098(3)	-0.1098(3)	0.116
H(24A)	0.5697(5)	-0.1995(2)	-0.0900(5)	0.136
H(25A)	0.6221(4)	-0.1727(2)	0.1078(6)	0.135
H(26A)	0.5836(4)	-0.2664(2)	0.2103(3)	0.115
H(27A)	0.3898(4)	-0.0996(3)	0.1702(5)	0.103
H(28A)	0.4027(4)	-0.0071(2)	0.1436(4)	0.096
H(28B)	0.3649(4)	0.0206(2)	0.0291(4)	0.096
H(29A)	0.5300(4)	-0.0008(2)	-0.0047(5)	0.125
H(30A)	0.6372(4)	-0.0750(3)	0.0520(6)	0.173
H(30B)	0.6321(4)	-0.0661(3)	0.1713(6)	0.173
H(31A)	0.7808(6)	-0.0030(3)	0.1899(7)	0.220
H(31B)	0.7711(6)	-0.0038(3)	0.0684(7)	0.220
H(32A)	0.7234(4)	0.0910(3)	0.1745(6)	0.165
H(32B)	0.6966(4)	0.0871(3)	0.0494(6)	0.165
H(33A)	0.4679(4)	0.0669(2)	-0.2049(4)	0.102
H(33B)	0.3604(4)	0.1004(2)	-0.2761(4)	0.102
H(33C)	0.4405(4)	0.0614(2)	-0.3282(4)	0.102
H(3'A)	0.6925(5)	0.2011(2)	-0.6856(3)	0.124
H(4'A)	0.7593(4)	0.27577(15)	-0.5314(5)	0.085
H(5'A)	0.7542(3)	0.2206(2)	-0.3596(3)	0.077
H(6'A)	0.4063(2)	0.1403(2)	-0.4718(3)	0.155
H(7'A)	0.4848(5)	0.2359(3)	-0.3656(4)	0.196
H(8'A)	0.5098(5)	0.3182(2)	-0.4970(7)	0.161
H(9'A)	0.4467(6)	0.2735(3)	-0.6845(5)	0.187
H(10B)	0.3827(5)	0.1635(3)	-0.6689(3)	0.183
H(11B)	0.6136(4)	0.0730(3)	-0.6798(4)	0.109
H(12C)	0.6201(4)	-0.0520(2)	-0.5151(4)	0.103
H(12D)	0.5695(4)	-0.0340(2)	-0.6344(4)	0.103
H(13B)	0.4234(7)	-0.0025(2)	-0.4786(4)	0.168
H(14C)	0.4303(5)	-0.0979(3)	-0.6309(6)	0.257
H(14D)	0.4335(5)	-0.1113(3)	-0.5106(6)	0.257

H(15C)	0.2591(5)	-0.0658(3)	-0.5284(5)	0.180
H(15D)	0.2403(5)	-0.1079(3)	-0.6292(5)	0.180
H(16C)	0.2178(5)	0.0081(4)	-0.6402(6)	0.193
H(16D)	0.2406(5)	-0.0318(4)	-0.7331(6)	0.193
H(19B)	1.2627(2)	0.1021(2)	-0.1093(4)	0.087
H(20B)	1.1696(4)	0.2067(2)	-0.1565(5)	0.108
H(21B)	0.9496(3)	0.19468(13)	-0.1877(4)	0.077
H(22B)	0.9413(3)	0.1031(2)	0.0922(2)	0.154
H(23B)	1.1365(4)	0.0474(2)	0.1337(4)	0.104
H(24B)	1.2964(3)	0.1265(3)	0.1421(4)	0.122
H(25B)	1.1999(5)	0.2310(2)	0.1058(5)	0.117
H(26B)	0.9804(4)	0.2165(2)	0.0750(4)	0.116
H(27B)	1.1516(4)	-0.0155(2)	-0.1019(3)	0.066
H(28C)	0.9129(4)	-0.0940(2)	-0.1482(3)	0.066
H(28D)	1.0448(4)	-0.0965(2)	-0.0917(3)	0.066
H(29B)	0.8832(7)	-0.0655(3)	0.0054(6)	0.207
H(30C)	1.1216(5)	-0.0996(3)	0.0593(5)	0.170
H(30D)	1.0764(5)	-0.0350(3)	0.0825(5)	0.170
H(31C)	0.9637(6)	-0.0791(3)	0.1830(5)	0.216
H(31D)	1.0918(6)	-0.1026(3)	0.2281(5)	0.216
H(32C)	1.0514(7)	-0.1946(2)	0.1434(4)	0.183
H(32D)	0.9263(7)	-0.1811(2)	0.1582(4)	0.183
H(33D)	0.6414(4)	-0.1094(2)	-0.1392(4)	0.107
H(33E)	0.6220(4)	-0.1318(2)	-0.2561(4)	0.107
H(33F)	0.5231(4)	-0.0973(2)	-0.2215(4)	0.107

Tables for *syn*-(+)-(R_p,R,R,R_p)-4aTable 1. Atomic coordinates [x 10⁵ for Pd, Fe; x 10⁴ for other atoms] and equivalent isotropic displacement parameters [Å² x 10⁴ for Pd, Fe; Å x 10³ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.67435(3)	0.39997(2)	0.75121(2)	0.06359(8)
Pd(2)	0.81671(3)	0.18771(3)	0.64058(2)	0.06700(9)
Fe(1)	0.43913(6)	0.46823(5)	0.90945(4)	0.0733(2)
Fe(2)	1.07104(6)	0.00439(5)	0.64272(5)	0.0752(2)
Cl(1)	0.89450(10)	0.34386(8)	0.74042(8)	0.0729(3)
Cl(2)	0.61593(11)	0.21498(8)	0.71437(9)	0.0838(4)
O(1)	0.8442(3)	0.6547(3)	0.9832(2)	0.0854(10)
O(2)	0.6736(3)	-0.1624(3)	0.6113(2)	0.0861(10)
N(1)	0.7053(3)	0.5662(3)	0.7796(2)	0.0706(10)
N(2)	0.7590(3)	0.0667(3)	0.5342(3)	0.0848(12)
C(1)	0.5018(4)	0.4480(3)	0.7624(3)	0.0721(13)
C(2)	0.4890(4)	0.5654(4)	0.7887(3)	0.0709(12)
C(3)	0.3603(4)	0.5852(4)	0.7995(3)	0.0835(14)
C(4)	0.2963(5)	0.4820(5)	0.7885(3)	0.096(2)
C(5)	0.3810(4)	0.3968(4)	0.7618(3)	0.0802(14)
C(6)	0.4428(6)	0.3460(5)	1.0202(4)	0.121(2)
C(7)	0.5661(5)	0.3879(5)	1.0185(3)	0.103(2)
C(8)	0.5620(5)	0.5046(5)	1.0444(3)	0.100(2)
C(9)	0.4403(5)	0.5301(5)	1.0614(3)	0.112(2)
C(10)	0.3644(6)	0.4388(6)	1.0479(4)	0.121(2)
C(11)	0.6075(4)	0.6258(4)	0.7991(3)	0.0769(14)
C(12)	0.8285(4)	0.6224(3)	0.7945(3)	0.0697(12)
C(13)	0.8978(4)	0.5979(4)	0.9011(3)	0.0782(14)
C(14)	1.0359(4)	0.6376(5)	0.9137(4)	0.096(2)
C(15)	1.0530(5)	0.7073(7)	1.0089(5)	0.150(3)
C(16)	0.9270(5)	0.7385(5)	1.0291(4)	0.132(2)
C(17)	0.9770(5)	0.1492(4)	0.5936(3)	0.0856(15)
C(18)	0.9705(5)	0.0688(4)	0.5135(4)	0.098(2)
C(19)	1.0932(5)	0.0355(5)	0.4928(4)	0.124(2)
C(20)	1.1788(5)	0.1021(5)	0.5607(5)	0.122(2)
C(21)	1.1105(4)	0.1742(5)	0.6259(4)	0.104(2)
C(22)	0.9797(4)	-0.0658(4)	0.7560(3)	0.092(2)
C(23)	0.9921(5)	-0.1474(4)	0.6750(4)	0.094(2)
C(24)	1.1157(5)	-0.1614(4)	0.6659(4)	0.098(2)
C(25)	1.1853(5)	-0.0904(5)	0.7438(4)	0.100(2)
C(26)	1.1016(4)	-0.0354(5)	0.8013(4)	0.096(2)
C(27)	0.8460(4)	0.0216(4)	0.4848(3)	0.091(2)
C(28)	0.6328(5)	0.0167(5)	0.5270(4)	0.124(2)
C(29)	0.6094(4)	-0.0586(4)	0.6150(5)	0.107(2)
C(30)	0.4689(5)	-0.0897(6)	0.6115(8)	0.198(4)
C(31)	0.4568(4)	-0.1982(4)	0.5843(4)	0.088(2)
C(32)	0.5822(4)	-0.2372(3)	0.5559(3)	0.0745(13)

Table 2. Bond lengths (\AA) and angles (deg.).

Pd(1)-C(1)	1.954(4)	C(18)-C(27)	1.446(7)	C(2)-Fe(1)-C(1)	41.2(2)
Pd(1)-N(1)	2.030(3)	C(19)-C(20)	1.413(8)	C(7)-Fe(1)-C(1)	106.7(2)
Pd(1)-Cl(2)	2.3203(11)	C(20)-C(21)	1.451(8)	C(10)-Fe(1)-C(1)	162.9(2)
Pd(1)-Cl(1)	2.4673(11)	C(22)-C(26)	1.400(6)	C(9)-Fe(1)-C(1)	156.5(2)
Pd(2)-C(17)	1.941(5)	C(22)-C(23)	1.430(7)	C(8)-Fe(1)-C(1)	121.5(2)
Pd(2)-N(2)	2.013(4)	C(23)-C(24)	1.352(7)	C(3)-Fe(1)-C(1)	68.0(2)
Pd(2)-Cl(1)	2.3384(12)	C(24)-C(25)	1.431(7)	C(6)-Fe(1)-C(5)	107.8(2)
Pd(2)-Cl(2)	2.4713(15)	C(25)-C(26)	1.389(7)	C(4)-Fe(1)-C(5)	40.9(2)
Fe(1)-C(6)	2.016(5)	C(28)-C(29)	1.475(8)	C(2)-Fe(1)-C(5)	68.6(2)
Fe(1)-C(4)	2.022(5)	C(29)-C(30)	1.542(7)	C(7)-Fe(1)-C(5)	120.7(2)
Fe(1)-C(2)	2.042(4)	C(30)-C(31)	1.339(9)	C(10)-Fe(1)-C(5)	126.6(2)
Fe(1)-C(7)	2.042(5)	C(31)-C(32)	1.506(6)	C(9)-Fe(1)-C(5)	162.5(2)
Fe(1)-C(10)	2.047(6)	C(1)-Pd(1)-N(1)	80.51(15)	C(8)-Fe(1)-C(5)	156.5(2)
Fe(1)-C(9)	2.056(5)	C(1)-Pd(1)-Cl(2)	93.50(12)	C(3)-Fe(1)-C(5)	67.8(2)
Fe(1)-C(8)	2.059(4)	N(1)-Pd(1)-Cl(2)	173.76(10)	C(1)-Fe(1)-C(5)	40.3(2)
Fe(1)-C(3)	2.068(4)	C(1)-Pd(1)-Cl(1)	178.34(11)	C(19)-Fe(2)-C(18)	42.2(2)
Fe(1)-C(1)	2.072(4)	N(1)-Pd(1)-Cl(1)	98.00(10)	C(19)-Fe(2)-C(25)	125.4(2)
Fe(1)-C(5)	2.071(4)	Cl(2)-Pd(1)-Cl(1)	88.02(4)	C(18)-Fe(2)-C(25)	164.4(2)
Fe(2)-C(19)	1.976(5)	C(17)-Pd(2)-N(2)	80.3(2)	C(19)-Fe(2)-C(22)	152.7(2)
Fe(2)-C(18)	1.988(5)	C(17)-Pd(2)-Cl(1)	95.02(13)	C(18)-Fe(2)-C(22)	118.9(2)
Fe(2)-C(25)	1.998(5)	N(2)-Pd(2)-Cl(1)	170.61(11)	C(25)-Fe(2)-C(22)	67.9(2)
Fe(2)-C(22)	2.017(5)	C(17)-Pd(2)-Cl(2)	172.73(13)	C(19)-Fe(2)-C(20)	41.4(2)
Fe(2)-C(20)	2.018(6)	N(2)-Pd(2)-Cl(2)	98.11(12)	C(18)-Fe(2)-C(20)	68.8(2)
Fe(2)-C(26)	2.044(5)	Cl(1)-Pd(2)-Cl(2)	87.52(4)	C(25)-Fe(2)-C(20)	108.2(2)
Fe(2)-C(24)	2.043(5)	C(6)-Fe(1)-C(4)	121.9(2)	C(22)-Fe(2)-C(20)	165.0(2)
Fe(2)-C(17)	2.051(4)	C(6)-Fe(1)-C(2)	161.0(2)	C(19)-Fe(2)-C(26)	163.8(2)
Fe(2)-C(23)	2.058(5)	C(4)-Fe(1)-C(2)	68.5(2)	C(18)-Fe(2)-C(26)	153.5(2)
Fe(2)-C(21)	2.082(6)	C(6)-Fe(1)-C(7)	40.7(2)	C(25)-Fe(2)-C(26)	40.2(2)
O(1)-C(16)	1.408(6)	C(4)-Fe(1)-C(7)	156.7(2)	C(22)-Fe(2)-C(26)	40.3(2)
O(1)-C(13)	1.422(5)	C(2)-Fe(1)-C(7)	123.7(2)	C(20)-Fe(2)-C(26)	127.5(2)
O(2)-C(29)	1.417(6)	C(6)-Fe(1)-C(10)	42.0(2)	C(19)-Fe(2)-C(24)	105.3(2)
O(2)-C(32)	1.436(5)	C(4)-Fe(1)-C(10)	108.7(2)	C(18)-Fe(2)-C(24)	125.6(2)
N(1)-C(11)	1.314(5)	C(2)-Fe(1)-C(10)	154.9(2)	C(25)-Fe(2)-C(24)	41.5(2)
N(1)-C(12)	1.468(5)	C(7)-Fe(1)-C(10)	69.0(2)	C(22)-Fe(2)-C(24)	67.9(2)
N(2)-C(27)	1.302(6)	C(6)-Fe(1)-C(9)	67.2(2)	C(20)-Fe(2)-C(24)	119.5(2)
N(2)-C(28)	1.466(6)	C(4)-Fe(1)-C(9)	126.1(2)	C(26)-Fe(2)-C(24)	68.4(2)
C(1)-C(5)	1.428(6)	C(2)-Fe(1)-C(9)	121.7(2)	C(19)-Fe(2)-C(17)	70.6(2)
C(1)-C(2)	1.447(6)	C(7)-Fe(1)-C(9)	67.3(2)	C(18)-Fe(2)-C(17)	40.2(2)
C(2)-C(3)	1.419(6)	C(10)-Fe(1)-C(9)	38.5(2)	C(25)-Fe(2)-C(17)	154.6(2)
C(2)-C(11)	1.448(6)	C(6)-Fe(1)-C(8)	67.9(2)	C(22)-Fe(2)-C(17)	107.5(2)
C(3)-C(4)	1.405(7)	C(4)-Fe(1)-C(8)	161.3(2)	C(20)-Fe(2)-C(17)	69.5(2)
C(4)-C(5)	1.430(7)	C(2)-Fe(1)-C(8)	107.5(2)	C(26)-Fe(2)-C(17)	120.1(2)
C(6)-C(7)	1.411(8)	C(7)-Fe(1)-C(8)	40.8(2)	C(24)-Fe(2)-C(17)	162.2(2)
C(6)-C(10)	1.456(9)	C(10)-Fe(1)-C(8)	66.8(2)	C(19)-Fe(2)-C(23)	117.3(2)
C(7)-C(8)	1.429(8)	C(9)-Fe(1)-C(8)	39.2(2)	C(18)-Fe(2)-C(23)	108.1(2)
C(8)-C(9)	1.380(8)	C(6)-Fe(1)-C(3)	157.3(2)	C(25)-Fe(2)-C(23)	67.0(2)
C(9)-C(10)	1.354(9)	C(4)-Fe(1)-C(3)	40.2(2)	C(22)-Fe(2)-C(23)	41.1(2)
C(12)-C(13)	1.479(5)	C(2)-Fe(1)-C(3)	40.4(2)	C(20)-Fe(2)-C(23)	152.2(2)
C(13)-C(14)	1.539(6)	C(7)-Fe(1)-C(3)	161.1(2)	C(26)-Fe(2)-C(23)	67.6(2)
C(14)-C(15)	1.454(8)	C(10)-Fe(1)-C(3)	121.4(2)	C(24)-Fe(2)-C(23)	38.5(2)
C(15)-C(16)	1.451(8)	C(9)-Fe(1)-C(3)	109.8(2)	C(17)-Fe(2)-C(23)	126.9(2)
C(17)-C(18)	1.388(6)	C(8)-Fe(1)-C(3)	125.1(2)	C(19)-Fe(2)-C(21)	70.6(2)
C(17)-C(21)	1.463(7)	C(6)-Fe(1)-C(1)	124.1(2)	C(18)-Fe(2)-C(21)	68.7(2)
C(18)-C(19)	1.428(8)	C(4)-Fe(1)-C(1)	68.4(2)	C(25)-Fe(2)-C(21)	119.9(2)

C(22)-Fe(2)-C(21)	126.8(2)	C(1)-C(5)-Fe(1)	69.9(2)	C(19)-C(18)-Fe(2)	68.4(3)
C(20)-Fe(2)-C(21)	41.4(2)	C(4)-C(5)-Fe(1)	67.7(2)	C(27)-C(18)-Fe(2)	115.9(3)
C(26)-Fe(2)-C(21)	108.5(2)	C(7)-C(6)-C(10)	107.7(5)	C(20)-C(19)-C(18)	105.7(5)
C(24)-Fe(2)-C(21)	155.0(2)	C(7)-C(6)-Fe(1)	70.6(3)	C(20)-C(19)-Fe(2)	70.9(3)
C(17)-Fe(2)-C(21)	41.5(2)	C(10)-C(6)-Fe(1)	70.1(3)	C(18)-C(19)-Fe(2)	69.4(3)
C(23)-Fe(2)-C(21)	165.2(2)	C(6)-C(7)-C(8)	106.5(5)	C(19)-C(20)-C(21)	110.1(5)
Pd(2)-Cl(1)-Pd(1)	88.33(5)	C(6)-C(7)-Fe(1)	68.7(3)	C(19)-C(20)-Fe(2)	67.7(3)
Pd(1)-Cl(2)-Pd(2)	88.64(4)	C(8)-C(7)-Fe(1)	70.2(3)	C(21)-C(20)-Fe(2)	71.6(3)
C(16)-O(1)-C(13)	110.3(4)	C(9)-C(8)-C(7)	107.8(5)	C(20)-C(21)-C(17)	105.4(4)
C(29)-O(2)-C(32)	104.8(3)	C(9)-C(8)-Fe(1)	70.3(3)	C(20)-C(21)-Fe(2)	66.9(3)
C(11)-N(1)-C(12)	116.8(3)	C(7)-C(8)-Fe(1)	69.0(2)	C(17)-C(21)-Fe(2)	68.1(3)
C(11)-N(1)-Pd(1)	116.5(3)	C(10)-C(9)-C(8)	111.5(6)	C(26)-C(22)-C(23)	107.5(4)
C(12)-N(1)-Pd(1)	126.2(3)	C(10)-C(9)-Fe(1)	70.4(3)	C(26)-C(22)-Fe(2)	70.9(3)
C(27)-N(2)-C(28)	120.8(4)	C(8)-C(9)-Fe(1)	70.5(3)	C(23)-C(22)-Fe(2)	71.0(3)
C(27)-N(2)-Pd(2)	116.1(3)	C(9)-C(10)-C(6)	106.5(5)	C(24)-C(23)-C(22)	109.1(4)
C(28)-N(2)-Pd(2)	122.1(3)	C(9)-C(10)-Fe(1)	71.1(3)	C(24)-C(23)-Fe(2)	70.2(3)
C(5)-C(1)-C(2)	107.5(4)	C(6)-C(10)-Fe(1)	67.9(3)	C(22)-C(23)-Fe(2)	67.9(3)
C(5)-C(1)-Pd(1)	137.4(3)	N(1)-C(11)-C(2)	115.0(4)	C(23)-C(24)-C(25)	107.2(5)
C(2)-C(1)-Pd(1)	114.8(3)	N(1)-C(12)-C(13)	111.2(3)	C(23)-C(24)-Fe(2)	71.4(3)
C(5)-C(1)-Fe(1)	69.8(2)	O(1)-C(13)-C(12)	111.7(3)	C(25)-C(24)-Fe(2)	67.6(3)
C(2)-C(1)-Fe(1)	68.3(2)	O(1)-C(13)-C(14)	104.5(3)	C(26)-C(25)-C(24)	109.0(4)
Pd(1)-C(1)-Fe(1)	121.2(2)	C(12)-C(13)-C(14)	113.2(4)	C(26)-C(25)-Fe(2)	71.7(3)
C(3)-C(2)-C(11)	139.1(4)	C(15)-C(14)-C(13)	106.0(4)	C(24)-C(25)-Fe(2)	70.9(3)
C(3)-C(2)-C(1)	107.7(4)	C(16)-C(15)-C(14)	105.8(4)	C(25)-C(26)-C(22)	107.0(4)
C(11)-C(2)-C(1)	113.1(4)	O(1)-C(16)-C(15)	107.1(5)	C(25)-C(26)-Fe(2)	68.1(3)
C(3)-C(2)-Fe(1)	70.8(2)	C(18)-C(17)-C(21)	107.3(4)	C(22)-C(26)-Fe(2)	68.8(3)
C(11)-C(2)-Fe(1)	121.6(3)	C(18)-C(17)-Pd(2)	115.1(4)	N(2)-C(27)-C(18)	114.3(4)
C(1)-C(2)-Fe(1)	70.5(2)	C(21)-C(17)-Pd(2)	137.3(3)	N(2)-C(28)-C(29)	116.5(4)
C(4)-C(3)-C(2)	108.1(4)	C(18)-C(17)-Fe(2)	67.5(3)	O(2)-C(29)-C(28)	112.0(5)
C(4)-C(3)-Fe(1)	68.2(3)	C(21)-C(17)-Fe(2)	70.4(3)	O(2)-C(29)-C(30)	105.3(4)
C(2)-C(3)-Fe(1)	68.8(2)	Pd(2)-C(17)-Fe(2)	121.6(2)	C(28)-C(29)-C(30)	112.7(5)
C(3)-C(4)-C(5)	109.2(4)	C(17)-C(18)-C(19)	111.4(5)	C(31)-C(30)-C(29)	107.5(5)
C(3)-C(4)-Fe(1)	71.7(2)	C(17)-C(18)-C(27)	114.1(5)	C(30)-C(31)-C(32)	107.5(4)
C(5)-C(4)-Fe(1)	71.4(2)	C(19)-C(18)-C(27)	133.1(5)	O(2)-C(32)-C(31)	105.1(3)
C(1)-C(5)-C(4)	107.2(4)	C(17)-C(18)-Fe(2)	72.3(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)	0.0700(2)	0.05843(13)	0.06343(13)	-0.00138(14)	0.01273(12)	0.0021(2)
Pd(2)	0.0750(2)	0.05616(13)	0.07044(15)	0.00014(14)	0.01176(14)	0.0036(2)
Fe(1)	0.0792(4)	0.0739(3)	0.0689(3)	-0.0016(3)	0.0172(3)	0.0033(3)
Fe(2)	0.0740(3)	0.0729(3)	0.0840(3)	0.0042(3)	0.0300(3)	0.0047(3)
Cl(1)	0.0731(6)	0.0599(5)	0.0847(5)	-0.0021(5)	0.0060(5)	0.0044(5)
Cl(2)	0.0769(6)	0.0624(5)	0.1155(7)	-0.0133(5)	0.0260(6)	-0.0057(5)
O(1)	0.083(2)	0.102(2)	0.0750(14)	-0.014(2)	0.0243(14)	-0.007(2)
O(2)	0.068(2)	0.078(2)	0.111(2)	0.000(2)	0.006(2)	0.001(2)
N(1)	0.082(2)	0.061(2)	0.069(2)	0.017(2)	0.011(2)	0.014(2)
N(2)	0.085(2)	0.083(2)	0.080(2)	0.001(2)	-0.009(2)	0.014(2)
C(1)	0.081(2)	0.064(2)	0.071(2)	0.021(2)	0.006(2)	0.012(2)
C(2)	0.071(2)	0.080(2)	0.062(2)	0.009(2)	0.011(2)	0.002(2)
C(3)	0.082(2)	0.100(3)	0.069(2)	-0.002(2)	0.011(2)	0.039(2)
C(4)	0.088(3)	0.108(3)	0.094(3)	-0.006(3)	0.026(2)	0.029(3)
C(5)	0.076(2)	0.077(2)	0.086(2)	-0.012(3)	0.001(2)	-0.007(3)
C(6)	0.180(6)	0.094(3)	0.084(3)	0.029(3)	-0.011(3)	-0.010(4)
C(7)	0.101(3)	0.143(4)	0.058(2)	0.035(3)	-0.016(2)	0.013(4)
C(8)	0.111(3)	0.116(3)	0.067(2)	-0.006(3)	-0.008(2)	-0.034(3)
C(9)	0.150(4)	0.107(3)	0.080(2)	-0.005(3)	0.021(3)	0.042(3)
C(10)	0.105(4)	0.163(5)	0.098(3)	0.029(4)	0.024(3)	-0.009(4)
C(11)	0.096(3)	0.064(2)	0.070(2)	0.008(2)	0.012(2)	0.020(2)
C(12)	0.082(2)	0.060(2)	0.070(2)	-0.013(2)	0.021(2)	-0.002(2)
C(13)	0.086(3)	0.081(3)	0.068(2)	0.002(2)	0.012(2)	0.001(3)
C(14)	0.077(3)	0.114(4)	0.102(3)	-0.006(3)	0.032(2)	-0.004(3)
C(15)	0.088(3)	0.219(7)	0.151(4)	-0.064(5)	0.040(3)	-0.037(5)
C(16)	0.137(5)	0.130(4)	0.123(3)	-0.071(3)	-0.008(3)	-0.008(4)
C(17)	0.122(3)	0.071(2)	0.073(2)	-0.010(2)	0.046(2)	0.013(2)
C(18)	0.126(4)	0.088(3)	0.089(2)	-0.005(3)	0.052(2)	0.013(3)
C(19)	0.156(4)	0.129(4)	0.103(3)	0.040(3)	0.075(3)	0.065(3)
C(20)	0.102(3)	0.104(3)	0.177(4)	0.045(3)	0.080(3)	0.035(3)
C(21)	0.085(3)	0.111(4)	0.120(3)	-0.004(4)	0.032(3)	-0.008(3)
C(22)	0.066(2)	0.120(4)	0.091(3)	0.039(3)	0.015(2)	0.012(3)
C(23)	0.097(3)	0.093(3)	0.086(2)	0.017(3)	-0.010(3)	-0.008(3)
C(24)	0.110(4)	0.070(3)	0.116(3)	0.006(3)	0.019(3)	0.016(3)
C(25)	0.084(3)	0.094(3)	0.123(3)	0.015(3)	0.014(3)	-0.006(3)
C(26)	0.094(3)	0.108(3)	0.088(3)	-0.005(3)	0.014(3)	0.006(3)
C(27)	0.132(4)	0.081(2)	0.052(2)	0.011(2)	-0.018(2)	0.025(3)
C(28)	0.104(3)	0.106(3)	0.148(4)	-0.048(3)	-0.040(3)	0.044(3)
C(29)	0.065(3)	0.078(3)	0.173(4)	-0.033(3)	0.002(3)	0.008(2)
C(30)	0.095(4)	0.124(5)	0.390(10)	-0.076(7)	0.085(5)	-0.023(4)
C(31)	0.076(3)	0.086(3)	0.100(3)	-0.007(3)	0.010(2)	0.011(3)
C(32)	0.086(3)	0.054(2)	0.082(2)	-0.002(2)	0.004(2)	0.006(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)	0.3249(4)	0.6566(4)	0.8144(3)	0.080
H(4A)	0.2085(5)	0.4716(5)	0.7948(3)	0.080
H(5A)	0.3606(4)	0.3192(4)	0.7485(3)	0.080
H(6A)	0.4148(6)	0.2704(5)	1.0052(4)	0.080
H(7A)	0.6381(5)	0.3451(5)	1.0044(3)	0.080
H(8A)	0.6313(5)	0.5563(5)	1.0480(3)	0.080
H(9A)	0.4116(5)	0.6038(5)	1.0773(3)	0.080
H(10A)	0.2763(6)	0.4346(6)	1.0553(4)	0.080
H(11A)	0.6138(4)	0.7038(4)	0.8184(3)	0.080
H(12A)	0.8767(4)	0.5967(3)	0.7404(3)	0.080
H(12B)	0.8172(4)	0.7021(3)	0.7866(3)	0.080
H(13A)	0.8960(4)	0.5185(4)	0.9140(3)	0.080
H(14A)	1.0931(4)	0.5752(5)	0.9172(4)	0.080
H(14B)	1.0485(4)	0.6836(5)	0.8536(4)	0.080
H(15A)	1.0902(5)	0.6619(7)	1.0675(5)	0.080
H(15B)	1.1066(5)	0.7709(7)	1.0018(5)	0.080
H(16A)	0.9065(5)	0.8090(5)	0.9943(4)	0.080
H(16B)	0.9204(5)	0.7464(5)	1.1037(4)	0.080
H(19A)	1.1134(5)	-0.0176(5)	0.4405(4)	0.080
H(20A)	1.2690(5)	0.0963(5)	0.5669(5)	0.080
H(21A)	1.1455(4)	0.2248(5)	0.6810(4)	0.080
H(22A)	0.9021(4)	-0.0396(4)	0.7778(3)	0.080
H(23A)	0.9235(5)	-0.1824(4)	0.6304(4)	0.080
H(24A)	1.1496(5)	-0.2098(4)	0.6160(4)	0.080
H(25A)	1.2757(5)	-0.0851(5)	0.7559(4)	0.080
H(26A)	1.1236(4)	0.0166(5)	0.8587(4)	0.080
H(27A)	0.8283(4)	-0.0382(4)	0.4342(3)	0.080
H(28A)	0.5728(5)	0.0770(5)	0.5192(4)	0.080
H(28B)	0.6203(5)	-0.0280(5)	0.4632(4)	0.080
H(29A)	0.6391(4)	-0.0204(4)	0.6803(5)	0.080
H(30A)	0.4422(5)	-0.0786(6)	0.6804(8)	0.080
H(30B)	0.4185(5)	-0.0428(6)	0.5609(8)	0.080
H(31A)	0.4333(4)	-0.2423(4)	0.6421(4)	0.080
H(31B)	0.3925(4)	-0.2059(4)	0.5243(4)	0.080
H(32A)	0.5840(4)	-0.2319(3)	0.4803(3)	0.080
H(32B)	0.5987(4)	-0.3136(3)	0.5778(3)	0.080

Tables for *syn*-(-)-(S_p,S,S,S_p)-4aTable 1. Atomic coordinates [x 10⁵ for Pd, Fe; x 10⁴ for other atoms] and equivalent isotropic displacement parameters [Å² x 10⁴ for Pd, Fe; Å x 10³ for other atoms]

atom	x	y	z	U(eq)
Pd(1)	0.18337(3)	0.10585(3)	0.35939(2)	0.06553(8)
Pd(2)	0.32564(3)	-0.10633(2)	0.24896(2)	0.06272(8)
Fe(1)	-0.07139(5)	0.28855(6)	0.35741(5)	0.0735(2)
Fe(2)	0.56091(6)	-0.17507(5)	0.09047(5)	0.0712(2)
Cl(1)	0.38377(10)	0.07903(9)	0.28525(10)	0.0825(3)
Cl(2)	0.10568(9)	-0.04989(9)	0.25981(9)	0.0744(3)
O(1)	0.3270(2)	0.4570(3)	0.3902(3)	0.0843(10)
O(2)	0.1568(3)	-0.3614(3)	0.0186(2)	0.0875(11)
N(1)	0.2420(4)	0.2304(3)	0.4642(3)	0.0828(12)
N(2)	0.2954(3)	-0.2735(3)	0.2195(2)	0.0645(9)
C(1)	0.0206(4)	0.1436(4)	0.4073(3)	0.0779(13)
C(2)	0.0304(4)	0.2267(4)	0.4877(3)	0.0838(15)
C(3)	-0.0926(5)	0.2564(5)	0.5103(4)	0.121(2)
C(4)	-0.1763(5)	0.1898(5)	0.4412(5)	0.113(2)
C(5)	-0.1062(4)	0.1195(5)	0.3783(4)	0.100(2)
C(6)	0.0122(4)	0.4399(5)	0.3266(4)	0.092(2)
C(7)	-0.1163(5)	0.4545(4)	0.3326(4)	0.092(2)
C(8)	-0.1852(4)	0.3879(6)	0.2538(4)	0.095(2)
C(9)	-0.1022(5)	0.3285(5)	0.1998(4)	0.101(2)
C(10)	0.0186(5)	0.3600(5)	0.2437(4)	0.100(2)
C(11)	0.1542(5)	0.2739(5)	0.5144(3)	0.098(2)
C(12)	0.3684(5)	0.2803(5)	0.4734(5)	0.126(2)
C(13)	0.3893(4)	0.3519(4)	0.3849(5)	0.099(2)
C(14)	0.5245(5)	0.3828(6)	0.3846(8)	0.203(4)
C(15)	0.5428(4)	0.4940(5)	0.4159(4)	0.092(2)
C(16)	0.4167(4)	0.5334(4)	0.4438(4)	0.0817(15)
C(17)	0.4986(4)	-0.1510(4)	0.2344(3)	0.0715(13)
C(18)	0.5091(4)	-0.2702(4)	0.2115(3)	0.0764(13)
C(19)	0.6387(4)	-0.2922(5)	0.1985(4)	0.089(2)
C(20)	0.7048(4)	-0.1879(5)	0.2120(4)	0.089(2)
C(21)	0.6157(4)	-0.1022(5)	0.2342(4)	0.0836(15)
C(22)	0.4365(5)	-0.2041(6)	-0.0432(4)	0.105(2)
C(23)	0.5545(5)	-0.2310(6)	-0.0639(4)	0.103(2)
C(24)	0.6345(5)	-0.1404(6)	-0.0466(4)	0.109(2)
C(25)	0.5630(6)	-0.0508(6)	-0.0185(5)	0.123(2)
C(26)	0.4429(6)	-0.0885(6)	-0.0175(4)	0.114(2)
C(27)	0.3950(4)	-0.3308(4)	0.2014(3)	0.0745(13)
C(28)	0.1718(4)	-0.3268(4)	0.2066(3)	0.0742(13)
C(29)	0.0976(4)	-0.3036(4)	0.0978(3)	0.0765(14)
C(30)	-0.0374(4)	-0.3442(5)	0.0863(4)	0.093(2)
C(31)	-0.0529(5)	-0.4161(7)	-0.0094(5)	0.138(3)
C(32)	0.0715(5)	-0.4411(6)	-0.0293(5)	0.132(2)