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Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1
Table 4. Anisotropic displacement parameters (Å² x 10^3) for yu1. The anisotropic displacement factor exponent takes the form: -2π²[a²U₁₁ + ... + 2hkab U₁₂]

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The anisotropic refinements were failed for the other atoms, possibly due to the data collected at room temperature, not low temperature.
Spectroscopic data and Elemental Analysis of (1)*2 complex:
$^1$H NMR (500 MHz, D$_2$O, 50 mM, 60°C) δ = 10.30 (br, 8 H, PyHa), 9.62 (br, 4 H, PyHa'), 9.21 (br, 8 H, PyHb), 9.10 (br, 4 H, PyHb'), 8.81 (br, 12 H, PyHd+d'), 7.78 (br, 12 H, PyHc+c'), 6.09 (br, 4H, m-Terphenyl, Δδ = -1.2), 5.89 (br, 8 H, m-Terphenyl, Δδ = -1.6), 5.45 (br, 8 H, m-Terphenyl, Δδ = -2.2), 5.39 (br d, 4 H, m-Terphenyl, Δδ = -2.2), 5.26 (br s, 2 H, m-Terphenyl, Δδ = -2.5), 5.20 (br d, 2 H, m-Terphenyl, Δδ = -2.3), 2.92 (m, 24 H, NCH$_2$CH$_2$N). Anal. Calcd for C$_{120}$H$_{124}$N$_{48}$O$_{36}$Pd$_6$ •16H$_2$O: C, 38.52; H, 4.20; N, 17.97. Found: C, 38.40; H, 3.77; N, 18.12.

Spectroscopic data and Elemental Analysis of 1*3 complex:
$^1$H NMR (500 MHz, D$_2$O, 50 mM, 60°C) δ = 10.29 (s, 8 H, PyHa), 9.38 (s, 4 H, PyHa'), 9.23 (d, 8 H, J = 5.80 Hz, PyHb), 9.14 (d, 4 H, J = 5.5 Hz, PyHb'), 8.94 (d, 4 H, J = 7.35 Hz, PyHd'), 8.77 (d, 8 H, J = 7.9 Hz, PyHd), 7.91 (t, 4 H, J = 6.85 Hz, PyHc'), 7.85 (t, 8 H, J = 6.85 Hz, PyHc), 5.63 (br, 2 H, o-Terphenyl, Δδ = -1.8), 5.32 (br, 2 H, o-Terphenyl, Δδ = -2.1), 5.19 (br, 2 H, o-Terphenyl, Δδ = -2.0), 5.04 (br d, 4 H, o-Terphenyl, Δδ = -2.2), 4.80 (d, 4 H, J = 7.3 Hz, o-Terphenyl, Δδ = -2.3), 2.94 (m, 24 H, NCH$_2$CH$_2$N). Anal. Calcd for C$_{120}$H$_{124}$N$_{48}$O$_{36}$Pd$_6$ •16H$_2$O: C, 38.52; H, 4.20; N, 17.97. Found: C, 38.28; H, 3.69; N, 17.95.

Spectroscopic data and Elemental Analysis of (1)*5 complex (n = 1-3 depending on the concentrations):
$^1$H NMR (500 MHz, D$_2$O, 100 mM, 60°C) δ = 10.27 (br, 8 H, PyHa), 9.38 (s, 4 H, PyHa'), 9.21 (br, 8 H, PyHb), 9.15 (br, 4 H, PyHb'), 8.94 (br, 4 H, PyHd'), 8.69 (br, 8 H, PyHd), 7.98 (br, 4 H, PyHc'), 7.83 (br, 8 H, PyHc), 6.6-5.9 (br m, one cis-Stilbene), 5.37, 5.30, 5.04, 4.48 (br q, two cis-Stilbene, Δδ = -1.8, -1.9, -2.2, -2.1,
resp.), 2.90 (br, 24 H, NCH₂CH₂N). 1•(5)₂ complex: ¹H NMR (500 MHz, D₂O, saturated solution (ca. 40 mM), 60°C) δ = 10.28 (s, 8 H, PyHa), 9.41 (s, 4 H, PyHa'), 9.23 (d, 8 H, J = 5.35 Hz, PyHb), 9.16 (d, 4 H, J = 5.35 Hz, PyHb'), 8.94 (d, 4 H, J = 8.05 Hz, PyHd'), 8.72 (d, 8 H, J = 7.80 Hz, PyHd), 7.97 (t, 4 H, J = 7.60, 5.85 Hz, PyHc'), 7.84 (t, 8 H, J = 7.55, 6.10 Hz, PyHc), 5.38 (br d, 4 H, J = 7.3 Hz, cis-Stilbene, Δδ = -1.8), 5.29 (t, 8 H, J = 7.3 Hz, cis-Stilbene, Δδ = -1.9), 5.05 (d, 8 H, J = 7.55 Hz, cis-Stilbene, Δδ = -2.2), 4.49 (s, 4 H, cis-Stilbene, Δδ = -2.1), 2.92–2.83 (br m, 24 H, NCH₂CH₂N). Anal. Calcd for C₁₁₂H₁₂₀N₄₈O₃₆Pd₆ •12H₂O: C, 37.69; H, 4.07; N, 18.84. Found: C, 37.77; H, 3.66; N, 18.89. 1•(5) complex: ¹H NMR (500 MHz, D₂O, 20 mM, 60°C) δ = 10.26 (s, 8 H, PyHa), 9.33 (s, 4 H, PyHa'), 9.21 (d, 8 H, J = 5.2 Hz, PyHb), 9.13 (br, 4 H, PyHb'), 8.99 (d, 4 H, J = 8.25 Hz, PyHd'), 8.68 (d, 8 H, J = 7.6 Hz, PyHd), 7.99 (br, 4 H, PyHc'), 7.84 (t, 8 H, J = 7.35, 6.10 Hz, PyHc), 5.33 (br, 2 H, cis-Stilbene, Δδ = -1.9), 5.24 (br, 4 H, cis-Stilbene, Δδ = -2.0), 5.01 (d, 4 H, J = 7.3 Hz, cis-Stilbene, Δδ = -2.2), 4.40 (s, 2H, cis-Stilbene, Δδ = -2.2), 2.90 (m, 24 H, NCH₂CH₂N).
N(31C)-Pd(4)-N(31D)  90.1(5)
N(31C)-Pd(4)-N(1D)  91.8(8)
N(31D)-Pd(4)-N(1D)  177.2(9)
N(31C)-Pd(4)-N(2D)  174.9(7)
N(31D)-Pd(4)-N(2D)  93.6(6)
N(1D)-Pd(4)-N(2D)  84.4(9)
N(21D)-Pd(5)-N(31A)  92.2(5)
N(21D)-Pd(5)-N(2E)  176.8(8)
N(31A)-Pd(5)-N(2E)  90.8(7)
N(21D)-Pd(5)-N(1E)  95.4(9)
N(31A)-Pd(5)-N(1E)  172.2(9)
N(2E)-Pd(5)-N(1E)  81.6(11)
N(1F)-Pd(6)-N(41A)  173.8(9)
N(1F)-Pd(6)-N(2F)  83.1(11)
N(41A)-Pd(6)-N(2F)  91.8(9)
N(1F)-Pd(6)-N(41D)  94.1(8)
N(41A)-Pd(6)-N(41D)  91.0(5)
N(2F)-Pd(6)-N(41D)  177.0(10)
C(12A)-N(11A)-C(11A)  115.1(12)
C(12A)-N(12A)-C(13A)  114.9(12)
C(13A)-N(13A)-C(11A)  114.2(11)
N(11A)-C(11A)-N(13A)  125.6(12)
N(11A)-C(11A)-C(31A)  117.8(12)
N(13A)-C(11A)-C(31A)  116.3(12)
N(11A)-C(12A)-N(12A)  125.4(12)
N(11A)-C(12A)-C(41A)  116.2(12)
N(12A)-C(12A)-C(41A)  118.4(13)
N(13A)-C(13A)-N(12A)  124.5(12)
N(13A)-C(13A)-C(21A)  119.0(11)
N(12A)-C(13A)-C(21A)  116.5(12)
C(22A)-N(21A)-C(23A)  117.3(12)
C(22A)-N(21A)-Pd(1)  121.1(10)
C(23A)-N(21A)-Pd(1)  121.4(9)
C(25A)-C(21A)-C(22A)  119.8(13)
C(25A)-C(21A)-C(13A)  122.7(12)
C(22A)-C(21A)-C(13A)  117.5(12)
N(21A)-C(22A)-C(21A)  124.4(13)
N(21A)-C(23A)-C(24A)  121.9(14)
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C(25B)-C(21B)-C(11B)  118.9(12)
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C(21B)-C(25B)-C(24B)  117.2(14)
C(33B)-N(31B)-C(32B)  112.9(11)
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C(12C)-N(13C)-C(11C)  115.1(11)
N(11C)-C(11C)-N(13C)  124.2(12)
N(11C)-C(11C)-C(21C)  116.9(11)
N(13C)-C(11C)-C(21C)  118.9(11)
N(12C)-C(12C)-N(13C)  125.2(12)
N(12C)-C(12C)-C(31C)  118.3(13)
N(13C)-C(12C)-C(31C)  116.4(13)
N(11C)-C(13C)-N(12C)  123.4(14)
N(11C)-C(13C)-C(41C)  121.5(12)
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N(12D)-C(13D)-C(41D)  115.2(14)
C(23D)-N(21D)-C(22D)  118.0(15)
C(23D)-N(21D)-Pd(5)   120.1(11)
C(22D)-N(21D)-Pd(5)   121.6(11)
C(22D)-C(21D)-C(25D)  118.9(16)
C(22D)-C(21D)-C(11D)  121.0(16)
C(25D)-C(21D)-C(11D)  119.8(14)
N(21D)-C(22D)-C(21D)  122.5(16)
N(21D)-C(23D)-C(24D)  121.3(16)
C(25D)-C(24D)-C(23D)  118.5(19)
C(24D)-C(25D)-C(21D)  120.4(18)
C(33D)-N(31D)-C(32D)  119.6(14)
C(33D)-N(31D)-Pd(4)   120.6(11)
C(32D)-N(31D)-Pd(4)   119.2(11)
C(32D)-C(31D)-C(35D)  116.8(15)
C(32D)-C(31D)-C(12D)  122.0(13)
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C(31D)-C(35D)-C(34D)  120.6(17)
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C(43D)-N(41D)-Pd(6)   121.6(12)
C(42D)-N(41D)-Pd(6)   123.0(11)
C(45D)-C(41D)-C(42D)  120.9(15)
C(45D)-C(41D)-C(13D)  120.8(16)
C(42D)-C(41D)-C(13D)  118.2(15)
N(41D)-C(42D)-C(41D)  122.6(15)
N(41D)-C(43D)-C(44D)  126.0(17)
C(43D)-C(44D)-C(45D)  118.3(17)
C(41D)-C(45D)-C(44D)  116.4(17)
C(1A)-N(1A)-Pd(1)    105.8(10)
C(2A)-N(2A)-Pd(1)    110.9(11)
C(2A)-C(1A)-N(1A)   110.5(17)
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C(1B)-N(1B)-Pd(2) 107.7(14)
C(2B)-N(2B)-Pd(2) 108.7(13)
N(1B)-C(1B)-C(2B) 117(2)
C(1B)-C(2B)-N(2B) 112.8(16)
C(1C)-N(1C)-Pd(3) 107.1(14)
C(2C)-N(2C)-Pd(3) 107.3(13)
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C(1C)-C(2C)-N(2C) 116(2)
C(1D)-N(1D)-Pd(4) 108.9(17)
C(2D)-N(2D)-Pd(4) 107.6(17)
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C(1F)-N(1F)-Pd(6) 115(3)
C(2F)-N(2F)-Pd(6) 107(3)
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C(103)-C(102)-C(101) 116(3)
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C(105)-C(104)-C(103) 115(2)
C(106)-C(105)-C(104) 132(2)
C(105)-C(106)-C(101) 113(2)
C(108)-C(107)-C(101) 133(2)
C(107)-C(108)-C(109) 128(2)
C(114)-C(109)-C(110) 121(2)
C(114)-C(109)-C(108) 125.9(19)
C(110)-C(109)-C(108) 113(2)
C(109)-C(110)-C(111) 115(2)
C(112)-C(111)-C(110) 119(2)
C(113)-C(112)-C(111) 123(2)
C(112)-C(113)-C(114) 119(2)
C(109)-C(114)-C(113) 122(2)
C(202)-C(201)-C(206) 121(2)
C(202)-C(201)-C(207) 121.8(19)
C(206)-C(201)-C(207) 116.9(18)
C(201)-C(202)-C(203) 116(2)
C(204)-C(203)-C(202) 124(2)
C(203)-C(204)-C(205) 118(2)
C(206)-C(205)-C(204) 117(2)
C(205)-C(206)-C(201) 124(2)
C(208)-C(207)-C(201) 126(2)
C(207)-C(208)-C(209) 135(2)
C(214)-C(209)-C(210) 117.3(19)
C(214)-C(209)-C(208) 123(2)
C(210)-C(209)-C(208) 119.3(19)
C(209)-C(210)-C(211) 119(2)
C(210)-C(211)-C(212) 118(2)
C(213)-C(212)-C(211) 117(2)
C(212)-C(213)-C(214) 123(2)
C(209)-C(214)-C(213) 126(2)
C(306)-C(301)-C(302) 133(3)
C(306)-C(301)-C(307) 115(2)
C(302)-C(301)-C(307) 111(2)
C(303)-C(302)-C(301) 102(3)
C(304)-C(303)-C(302) 131(4)
C(303)-C(304)-C(305) 118(4)
C(304)-C(305)-C(306) 118(3)
C(301)-C(306)-C(305) 114(2)
C(308)-C(307)-C(301) 128(2)
C(307)-C(308)-C(309) 126(3)
C(310)-C(309)-C(314) 124(2)
C(310)-C(309)-C(308) 126(2)
C(314)-C(309)-C(308) 109(2)
C(309)-C(310)-C(311) 117(2)
C(312)-C(311)-C(310) 124(2)
C(311)-C(312)-C(313) 118(2)
C(314)-C(313)-C(312) 120(2)
C(313)-C(314)-C(309)  117(2)
O(202)-N(200)-O(203)  135(4)
O(202)-N(200)-O(201)  97.8(19)
O(203)-N(200)-O(201)  126(4)
C(426)-C(402)-C(437)  149(6)
C(426)-C(402)-C(425)  85(4)
C(437)-C(402)-C(425)  71(3)
C(438)-C(408)-C(409)  99(5)
C(408)-C(409)-C(438)  38(3)
C(416)-C(410)-C(434)  25.8(19)
C(427)-C(411)-C(428)  85(6)
C(427)-C(411)-C(433)  68(4)
C(428)-C(411)-C(433)  150(7)
C(427)-C(411)-C(449)  11(3)
C(428)-C(411)-C(449)  78(4)
C(433)-C(411)-C(449)  77(3)
C(434)-C(415)-C(436)  128(3)
C(434)-C(416)-C(410)  83(9)
C(443)-C(417)-C(418)  50(2)
C(443)-C(418)-C(417)  69(3)
C(422)-C(420)-C(421)  82(3)
C(422)-C(420)-C(444)  29(3)
C(421)-C(420)-C(444)  110(3)
C(440)-C(421)-C(420)  124(3)
C(440)-C(421)-C(435)  149(4)
C(420)-C(421)-C(435)  82(4)
C(440)-C(421)-C(422)  164(4)
C(420)-C(421)-C(422)  39(3)
C(435)-C(421)-C(422)  44.3(19)
C(444)-C(422)-C(420)  110(5)
C(444)-C(422)-C(435)  130(5)
C(420)-C(422)-C(435)  119(5)
C(444)-C(422)-C(421)  164(5)
C(420)-C(422)-C(421)  58(4)
C(435)-C(422)-C(421)  63(2)
C(437)-C(425)-C(402)  38.7(15)
C(437)-C(425)-C(426)  67(2)
C(402)-C(425)-C(426)  29.6(15)