Open Clamshell Dinuclear Palladium(II) Complexes Possessing Out-of-Plane Anisotropy

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Supporting Information

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1. General Information

Reagents and solvents for syntheses were commercially purchased. TLC analysis was performed using Merck Silica gel 60 F_{254}. Silica gel chromatography was performed on Kanto 60 silica gel using a preparative medium pressure liquid chromatography system. Melting points were determined on a melting-point apparatus RFS-10 instrument (Sanyo Rikagaku Co., Ltd). IR spectra were recorded on a JASCO FT/IR-460plus spectrometer (JASCO, Tokyo, Japan). The ^{1}H and ^{13}C NMR spectra were measured on a BRUKER Biospin AVANCE III HD 500 spectrometer at 500 and 125 MHz, respectively. ^{1}H-NMR shifts in deuterated solvents were relative to the residual solvent signals: CD_2Cl_2 (δ 5.32 ppm), and DMSO-d_6 (δ 2.50 ppm). ^{13}C-NMR shifts were referenced to the solvent of CD_2Cl_2 (δ 53.8 ppm), and DMSO-d_6 (δ 39.5 ppm). Multiplicity was indicated by s (singlet), d (doublet), t (triplet), m (multiplet), or br (broaded). The coupling constant *J* was reported in Hz. High resolution (HR) and low resolution (LR) mass spectra (MS) were measured on a BRUKER micrOTOFII spectrometer using electrospray ionization time-of-flight (ESI-TOF) method, which were measured by National University Corporation, Tokyo Institute of Technology Center for Advanced Material Analysis. UV-vis spectra were measured on a JASCO V-550 UV-vis spectrometer. Fluorescence spectra were measured on a JASCO FP6500 spectrofluorometer. Elemental analyses were performed on a J-SCIENCE LAB MICRO CORDER JM10.

2. Supporting Figures, and Tables

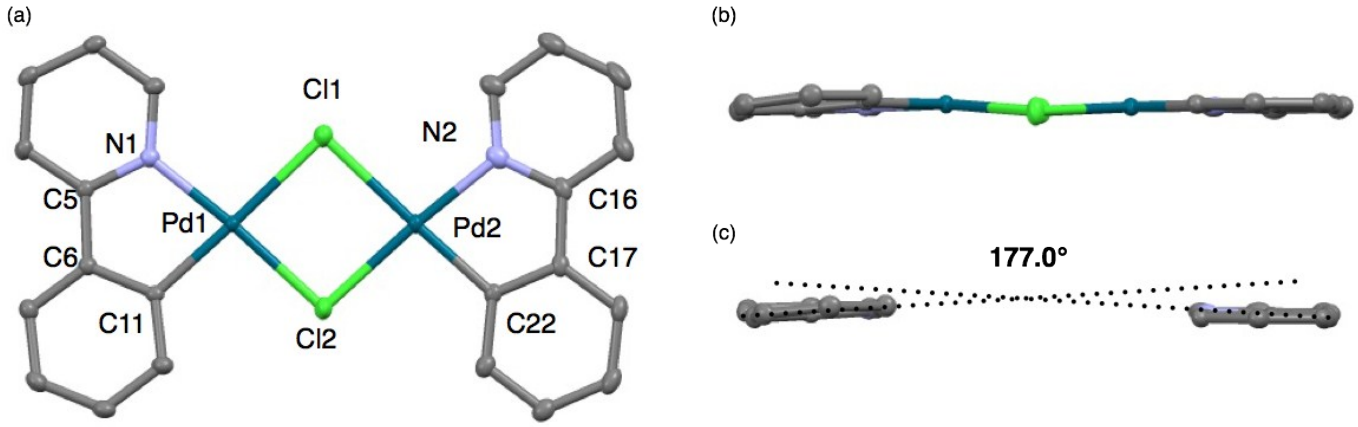


Figure S1. Crystal structure of **Pd_2-(μ-Cl)$_2$**[1] (a–c). Hydrogen atoms are omitted for clarity. Palladium and chlorine atoms are also omitted for clarity (c).

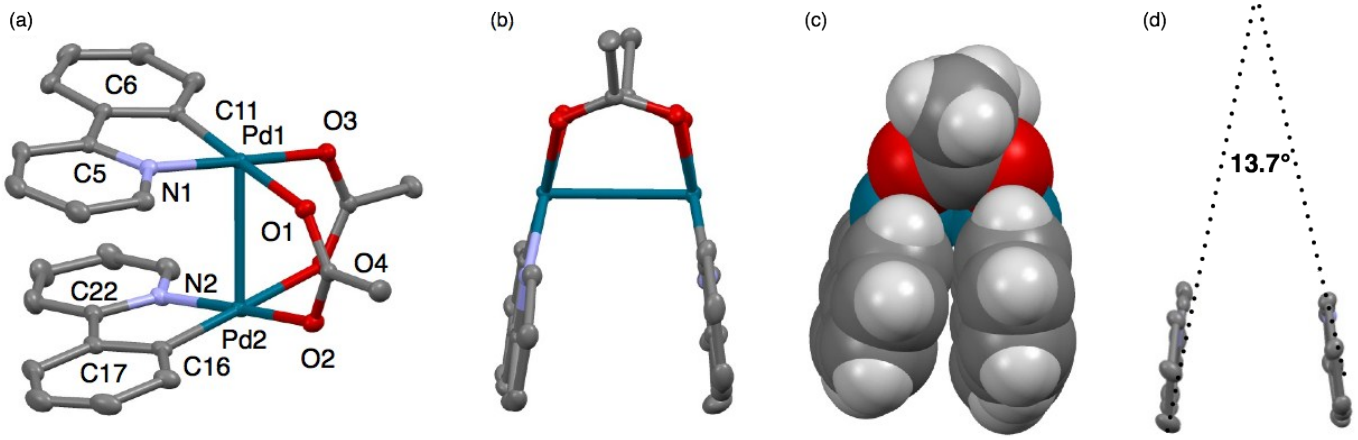


Figure S2. Crystal structure of **Pd_2-(μ-OAc)$_2$**[1] (a–d). Hydrogen atoms are omitted for clarity (a, b and d). Palladium atoms and acetate groups are also omitted for clarity (d).

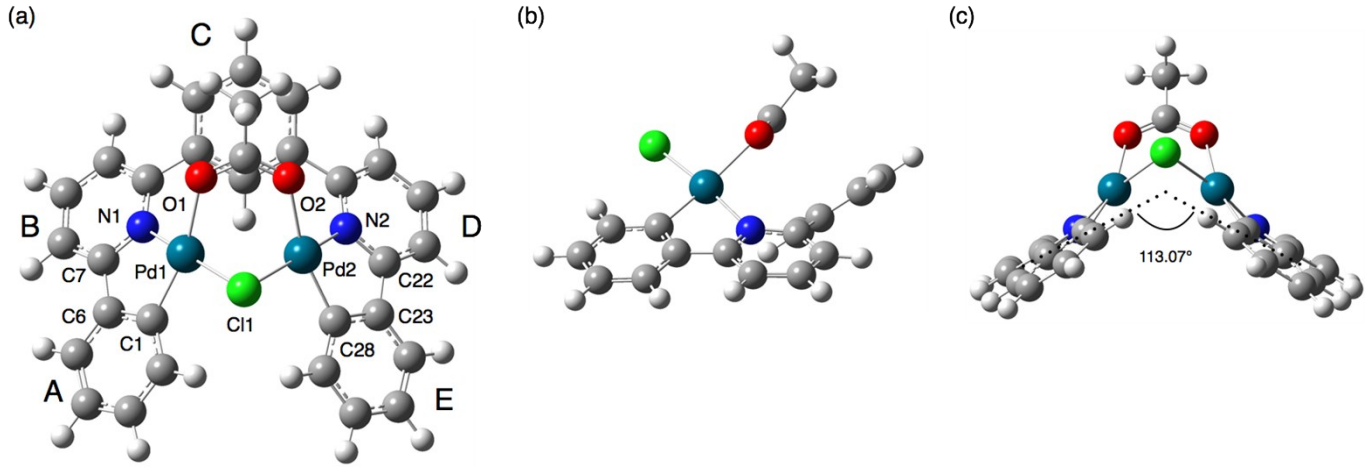


Figure S3. Calculated structures (ωB97XD/6-311G(d,p) for C, H, N, O, Cl atoms, and SDD+f for Pd atom) of **Pd_2** (a–c). C ring was omitted for clarity (c).

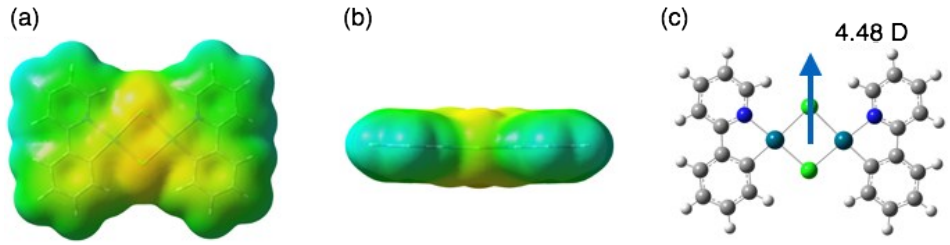


Figure S4. Electrostatic potential surfaces (a and b) and dipole moment (c) of **Pd_2-(μ-Cl)$_2$** calculated at the ωB97XD/6-311G(d,p) for C, H, N, Cl atoms, and SDD+f for Pd atom (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

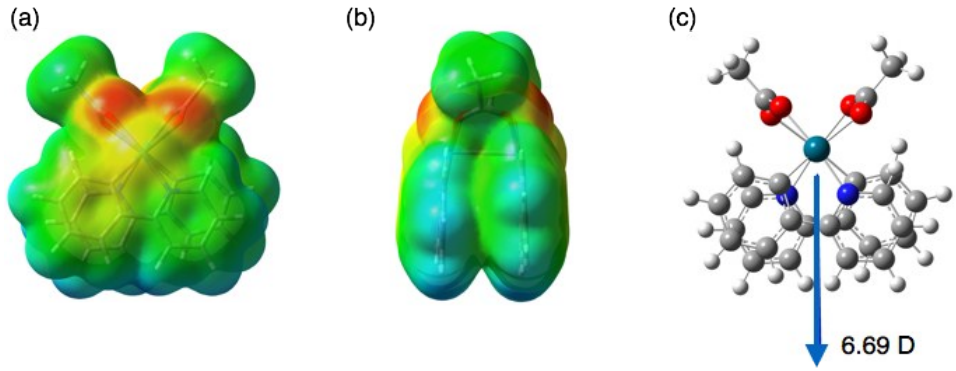


Figure S5. Electrostatic potential surfaces (a and b) and dipole moment (c) of **Pd_2-(μ-OAc)$_2$** calculated at the ωB97XD/6-311G(d,p) for C, H, N, O atoms, and SDD+f for Pd atom (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

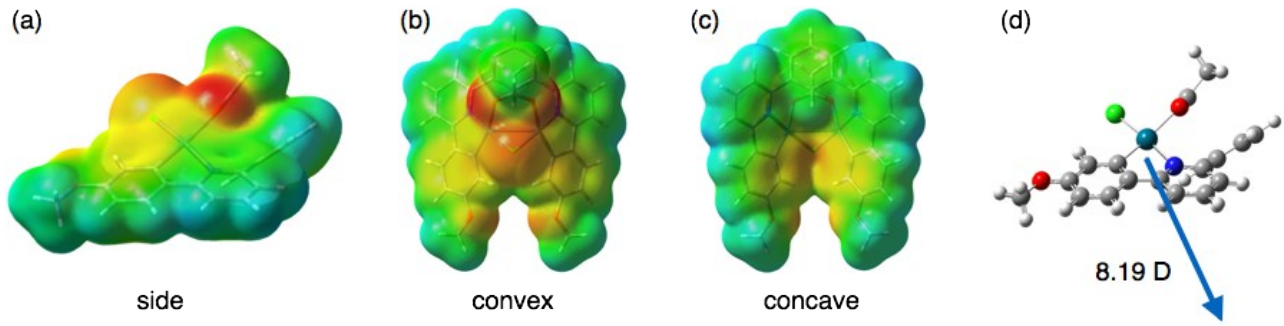


Figure S6. Electrostatic potential surfaces (a–c) and dipole moment (d) of **Pd_2-Me** calculated at the ωB97XD/6-311G(d,p) for C, H, N, O, Cl atoms, and SDD+f for Pd atom (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

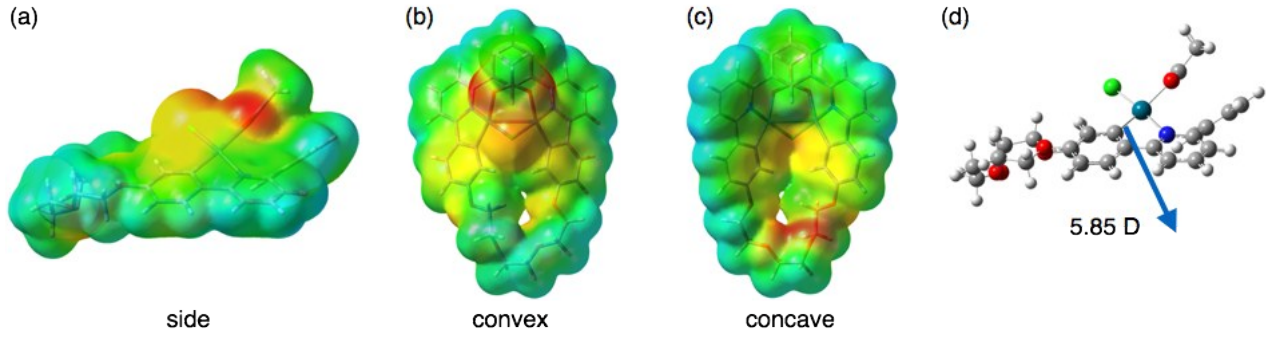


Figure S7. Electrostatic potential surfaces (a–c) and dipole moment (d) of **Pd_2-27** calculated at the ωB97XD/6-311G(d,p) for C, H, N, O, Cl atoms, and SDD+f for Pd atom (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

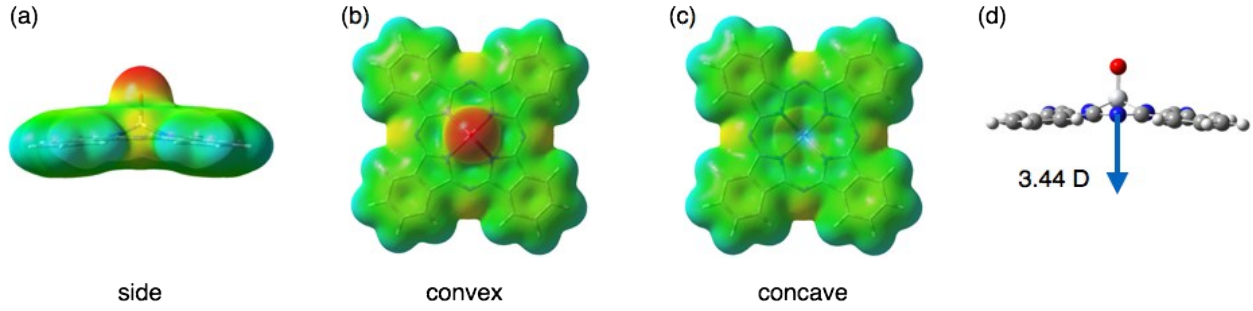


Figure S8. Electrostatic potential surfaces (a–c) and dipole moment (d) of TiOPc calculated at the ωB97XD/6-311G(d,p) for C, H, N, O atoms, and SDD+f for Ti atom (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

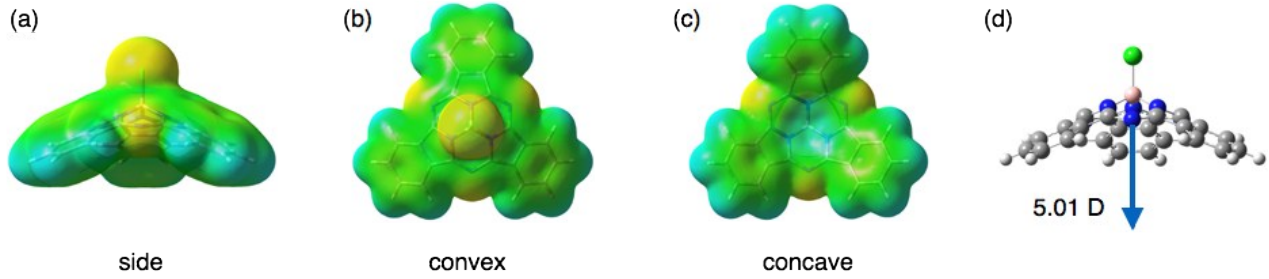


Figure S9. Electrostatic potential surfaces (a–c) and dipole moment (d) of SubPc calculated at the ωB97XD/6-311G(d,p) (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

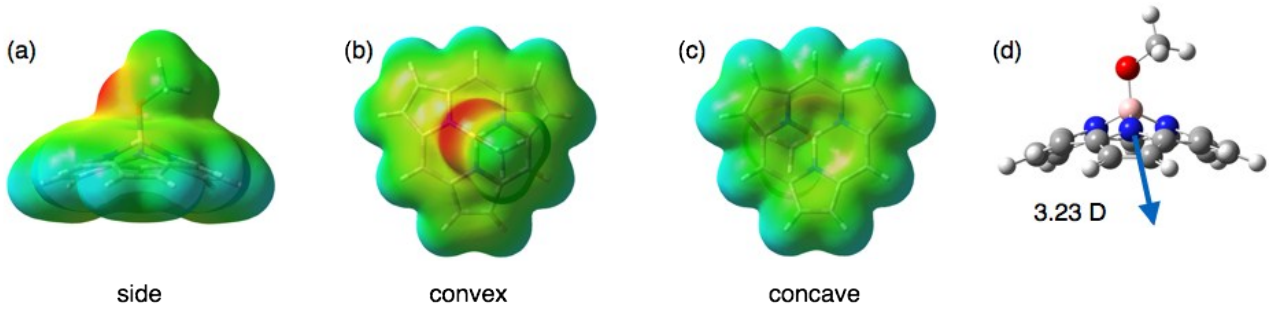


Figure S10. Electrostatic potential surfaces (a–c) and dipole moment (d) of subporphyrin calculated at the ωB97XD/6-311G(d,p) (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

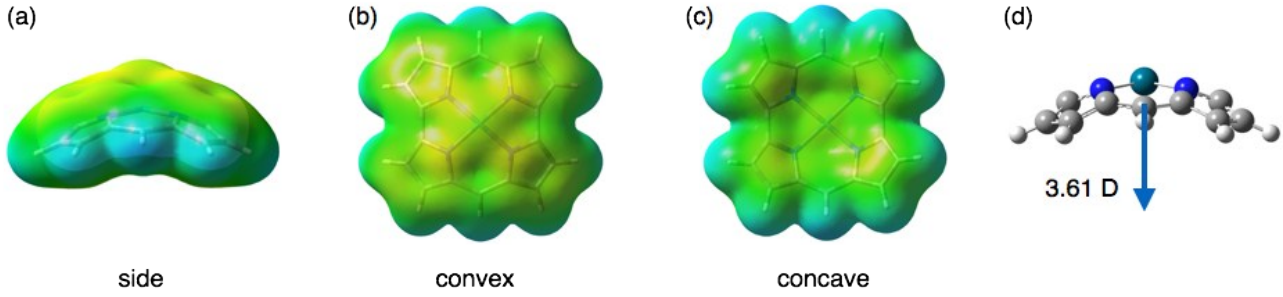


Figure S11. Electrostatic potential surfaces (a–c) and dipole moment (d) of Pd-coordinated norcorrole calculated at the ωB97XD/6-311G(d,p) for C, H, N atoms, and SDD+f for Pd atom (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

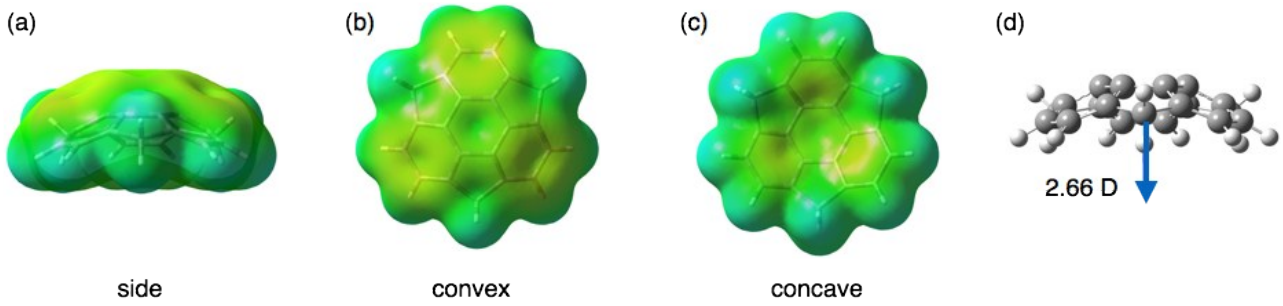


Figure S12. Electrostatic potential surfaces (a–c) and dipole moment (d) of sumanene calculated at the ωB97XD/6-311G(d,p) (color code: red = −49.7 kcal/mol, blue = 49.7 kcal/mol).

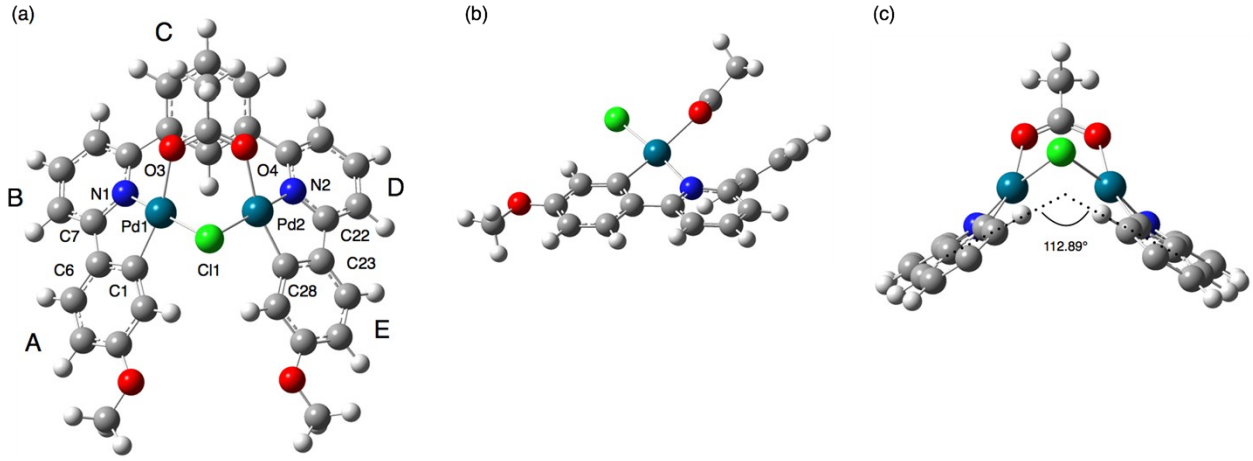


Figure S13. Calculated structures (ωB97XD/6-311G(d,p) for C, H, N, O, Cl atoms, and SDD+f for Pd atom) of **Pd_2-Me** (a–c). C ring and methoxy groups were omitted for clarity (c).

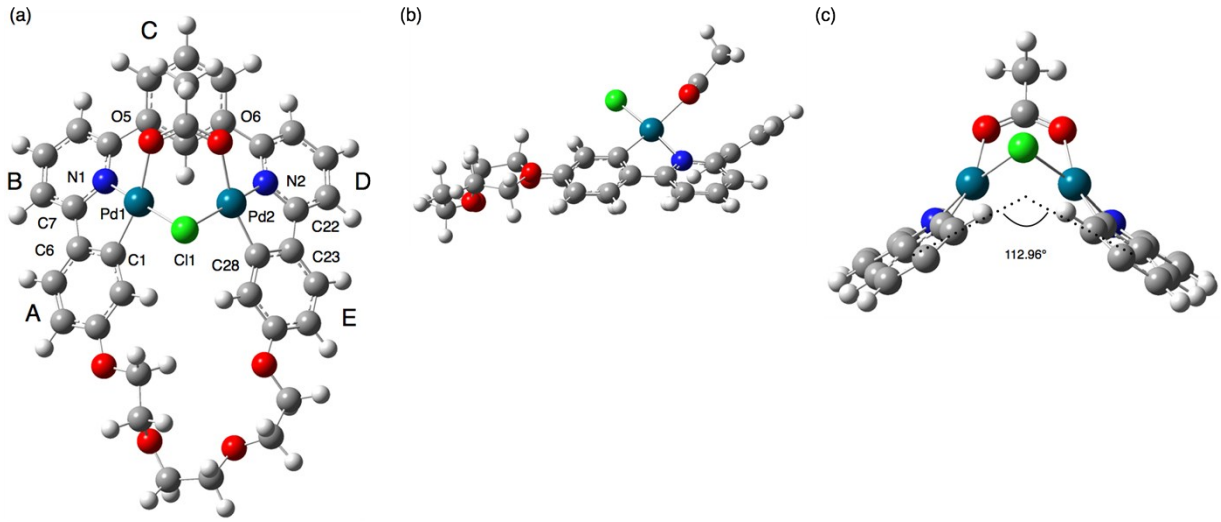


Figure S14. Calculated structures (ωB97XD/6-311G(d,p) for C, H, N, O, Cl atoms, and SDD+f for Pd atom) of **Pd_2-27** (a–c). C ring and tether chains were omitted for clarity (c).

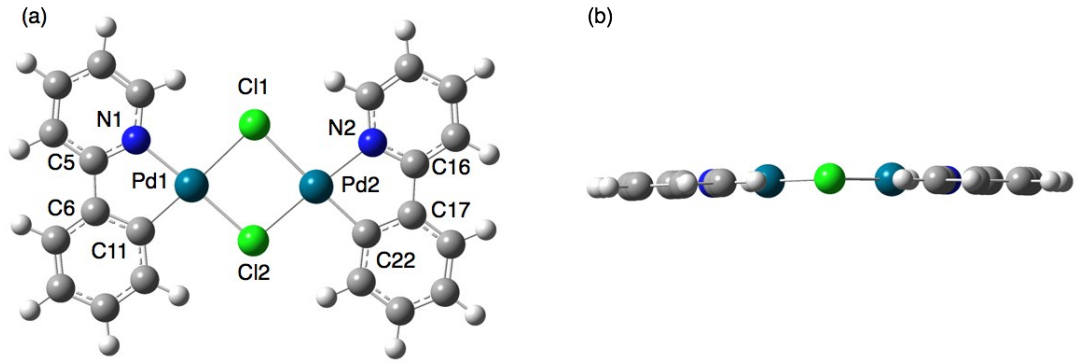


Figure S15. Calculated structures (ωB97XD/6-311G(d,p) for C, H, N, Cl atoms, and SDD+f for Pd atom) of **Pd_2-(μ-Cl)$_2$** (a and b).

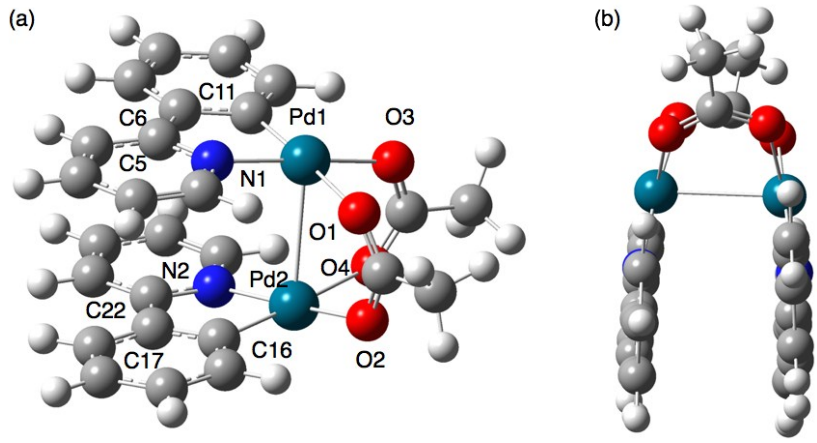


Figure S16. Calculated structures (ωB97XD/6-311G(d,p) for C, H, N, O atoms, and SDD+f for Pd atom) of **Pd_2-(μ-OAc)$_2$** (a and b).

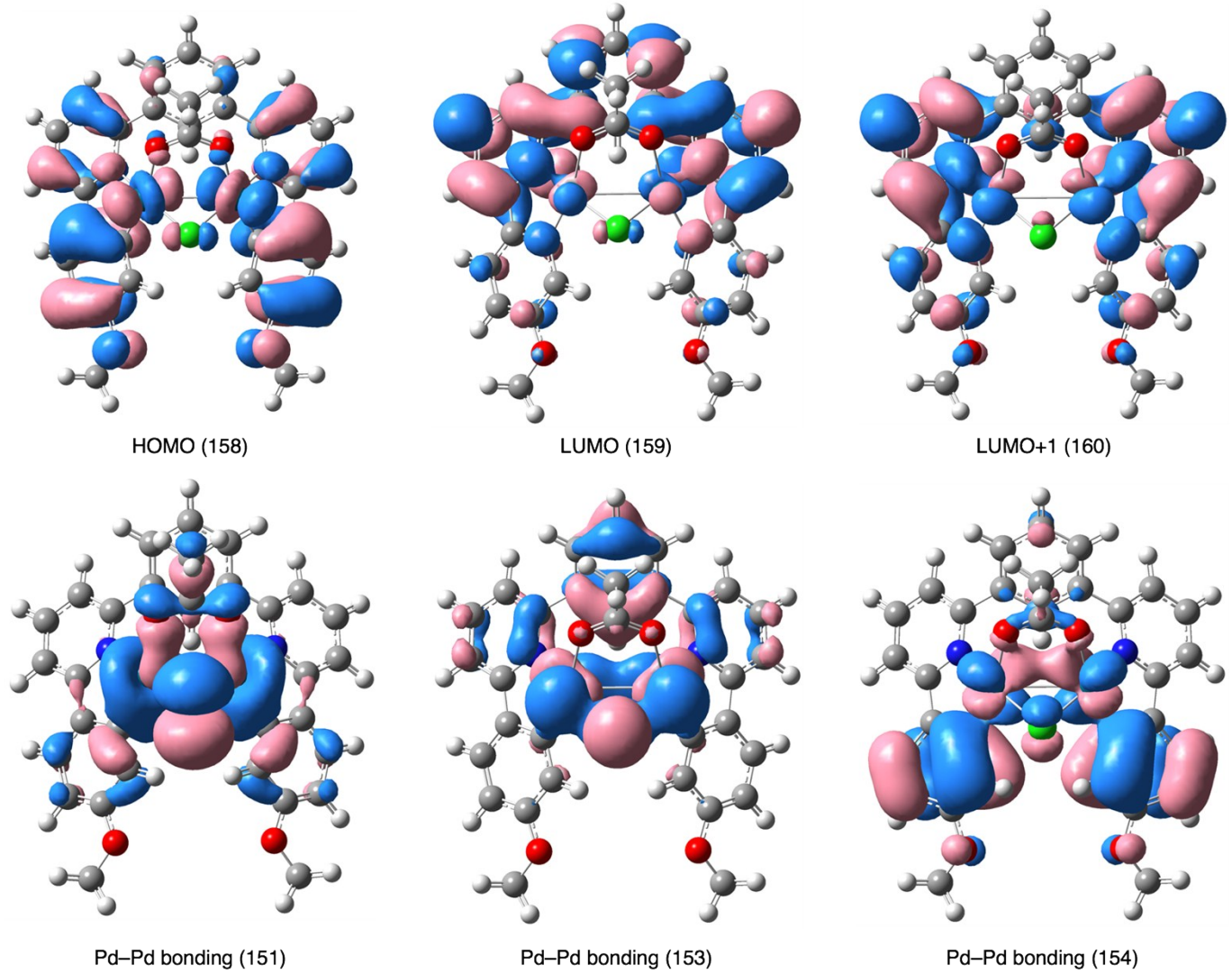


Figure S17. Selected molecular orbitals of **Pd_2-Me**.

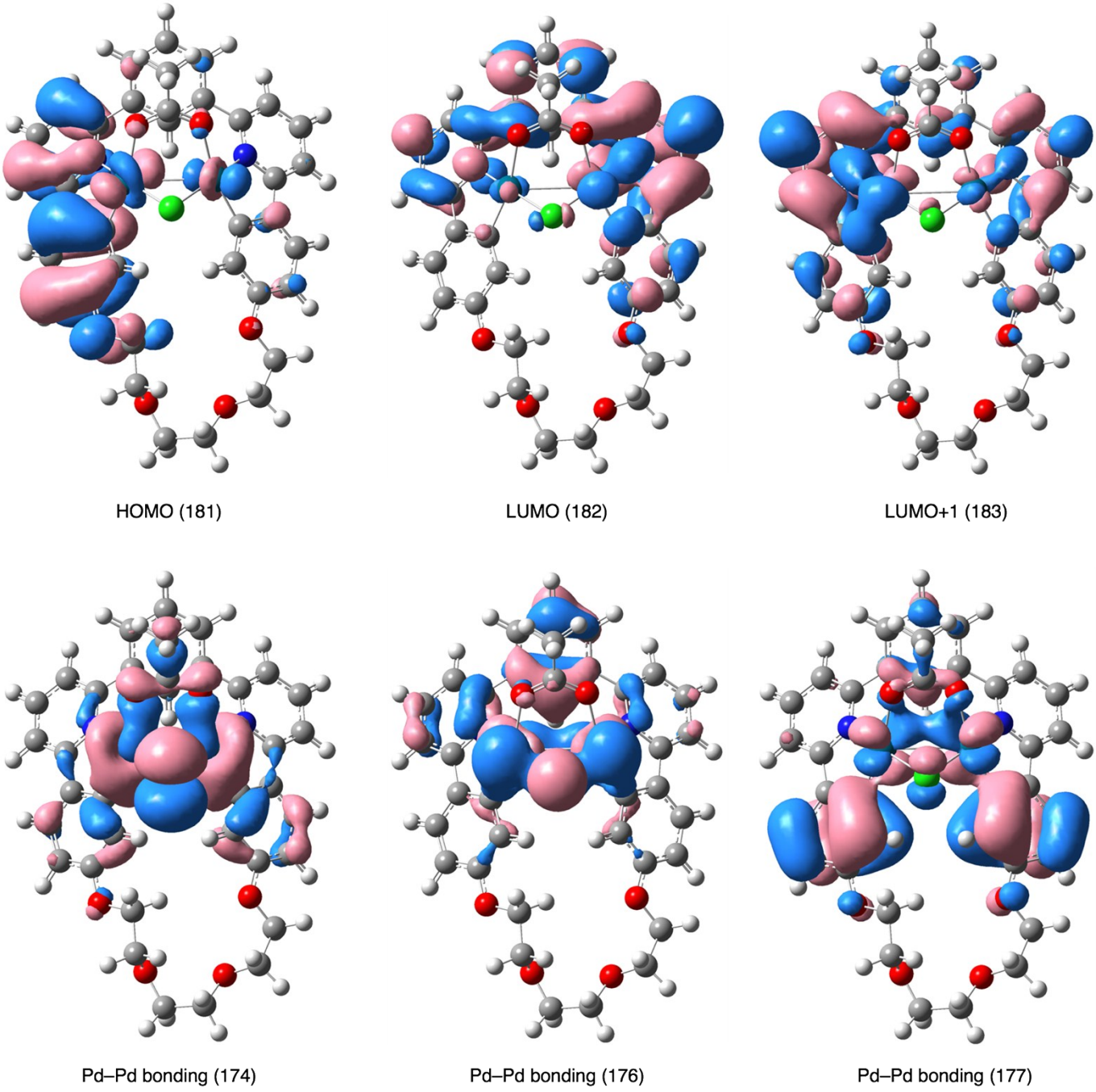


Figure S18. Selected molecular orbitals of **Pd_2-27**.

Table S1. Selected Experimental Bond Length (Å) and Angles (degree) in **Pd_2-Me**

	Distance / Å			angle / °	
	molecule A	**molecule B**		**molecule A**	**molecule B**
Pd1–Pd2	2.955(2)	2.934(2)	N1–Pd1–C1	81.9(3)	80.7(3)
Pd1–Cl1	2.362(2)	2.375(2)	O3–Pd1–Cl1	89.3(1)	89.5(1)
Pd1–O3	2.142(5)	2.138(5)	N2–Pd2–C28	82.0(2)	81.4(2)
Pd2–Cl1	2.370(2)	2.355(2)	O4–Pd2–Cl1	89.7(1)	88.9(1)
Pd2–O4	2.169(5)	2.161(5)	N1–Pd1–Cl1	175.2(2)	174.6(2)
Pd1–N1	2.051(6)	2.033(6)	C1–Pd1–O3	163.5(3)	163.4(3)
Pd1–C1	1.980(7)	1.966(7)	N2–Pd2–Cl1	169.4(2)	175.5(2)
Pd2–N2	2.049(6)	2.040(6)	C28–Pd2–O4	157.7(2)	163.0(2)
Pd2–C28	1.977(7)	1.978(7)			
N1–C7	1.373(9)	1.366(9)			
C7–C6	1.45(1)	1.45(1)			
C6–C1	1.40(1)	1.42(1)			
N2–C22	1.364(9)	1.357(9)			
C22–C23	1.44(1)	1.44(1)			
C23–C28	1.401(9)	1.406(9)			

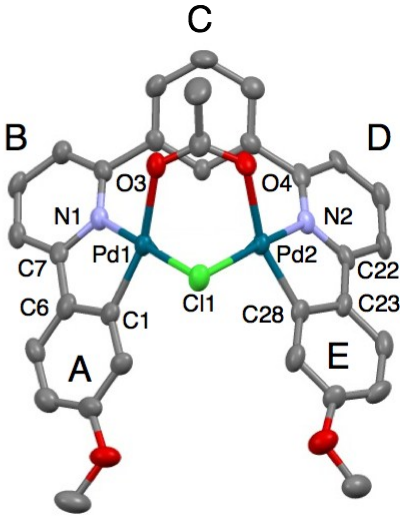


Table S2. Selected Experimental Bond Length (Å) and Angles (degree) in **Pd_2-27**

	Distance / Å			angle / °	
	molecule A	**molecule B**		**molecule A**	**molecule B**
Pd1–Pd2	2.9619(9)	2.943(1)	N1–Pd1–C1	81.0(2)	81.0(3)
Pd1–Cl1	2.382(2)	2.371(2)	O5–Pd1–Cl1	89.3(1)	89.5(2)
Pd1–O5	2.179(4)	2.141(8)	N2–Pd2–C28	81.3(2)	81.2(3)
Pd2–Cl1	2.369(1)	2.371(2)	O6–Pd2–Cl1	89.2(1)	88.4(1)
Pd2–O6	2.153(5)	2.152(6)	N1–Pd1–Cl1	169.0(2)	173.0(2)
Pd1–N1	2.071(6)	2.057(7)	C1–Pd1–O5	164.1(2)	161.4(3)
Pd1–C1	1.962(6)	1.941(9)	N2–Pd2–Cl1	174.3(2)	173.2(2)
Pd2–N2	2.053(5)	2.052(5)	C28–Pd2–O6	159.4(2)	164.9(2)
Pd2–C28	1.977(8)	1.945(9)			
N1–C7	1.361(8)	1.37(1)			
C7–C6	1.45(1)	1.44(2)			
C6–C1	1.41(1)	1.42(1)			
N2–C22	1.35(1)	1.38(1)			
C22–C23	1.47(1)	1.46(1)			
C23–C28	1.414(9)	1.426(8)			

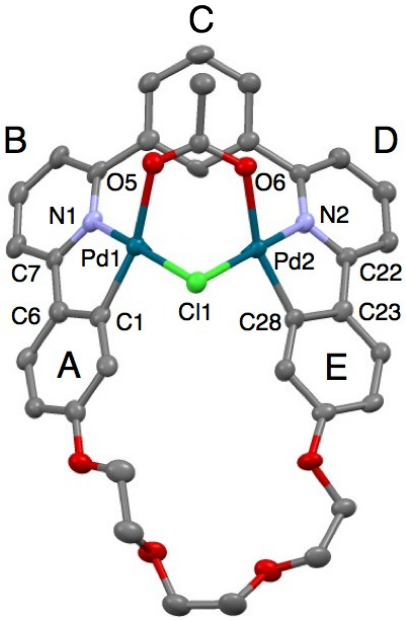


Table S3. Selected Experimental Bond Length (Å) and Angles (degree) in **Pd_2-(μ-Cl)$_2$**[1]

	Distance / Å		Angle / °
Pd1–Pd2	3.4938(2)	N1–Pd1–C11	81.22(4)
Pd1–Cl1	2.4232(3)	Cl1–Pd1–Cl2	86.30(1)
Pd1–Cl2	2.3633(3)	N2–Pd2–C22	81.25(4)
Pd2–Cl1	2.4271(3)	Cl1–Pd2–Cl2	86.00(1)
Pd2–Cl2	2.3725(3)	N1–Pd1–Cl2	173.98(3)
Pd1–N1	2.0134(9)	C11–Pd1–Cl1	177.08(3)
Pd1–C11	1.987(1)	N2–Pd2–Cl2	176.34(3)
Pd2–N2	2.015(1)	C22–Pd2–Cl1	178.32(3)
Pd2–C22	1.987(1)		
N1–C5	1.372(2)		
C5–C6	1.458(1)		
C6–C11	1.393(1)		
N2–C16	1.374(1)		
C16–C17	1.455(2)		
C17–C22	1.394(2)		

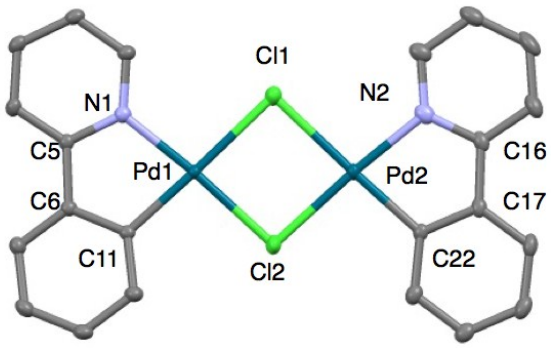


Table S4. Selected Experimental Bond Length (Å) and Angles (degree) in **Pd_2-(μ-OAc)$_2$**[1]

	Distance / Å		Angle / °
Pd1–Pd2	2.8621(1)	N1–Pd1–C11	81.84(3)
Pd1–O1	2.1429(6)	O1–Pd1–O3	89.76(2)
Pd1–O3	2.0473(6)	N2–Pd2–C22	81.68(3)
Pd2–O2	2.0520(6)	O2–Pd2–O4	89.76(2)
Pd2–O4	2.1562(6)	N1–Pd1–O3	174.98(2)
Pd1–N1	2.0116(7)	C11–Pd1–O1	175.60(3)
Pd1–C11	1.9566(7)	N2–Pd2–O2	174.30(2)
Pd2–N2	2.0052(6)	C22–Pd2–O4	176.94(3)
Pd2–C22	1.9616(8)		
N1–C5	1.360(1)		
C5–C6	1.461(1)		
C6–C11	1.419(1)		
N2–C16	1.367(1)		
C16–C17	1.455(1)		
C17–C22	1.409(1)		

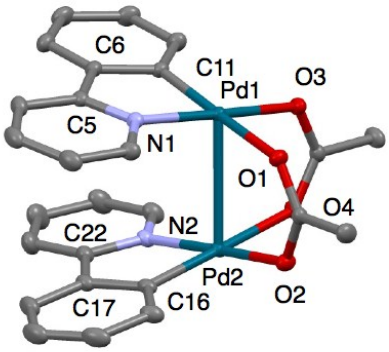


Table S5. Selected Calculated Bond Length (Å) and Angles (deg) in **Pd_2**

	Distance / Å		angle / °
Pd1–Pd2	3.0008	N1–Pd1–C1	80.99
Pd1–Cl1	2.4007	O3–Pd1–Cl1	89.02
Pd1–O3	2.1435	N2–Pd2–C28	80.99
Pd2–Cl1	2.4007	O4–Pd2–Cl1	89.01
Pd2–O4	2.1435	N1–Pd1–Cl1	171.65
Pd1–N1	2.0745	C1–Pd1–O3	164.47
Pd1–C1	1.9598	N2–Pd2–Cl1	171.65
Pd2–N2	2.0745	C28–Pd2–O4	164.47
Pd2–C28	1.9598		
N1–C7	1.3539		
C7–C6	1.4657		
C6–C1	1.4106		
N2–C22	1.3539		
C22–C23	1.4657		
C23–C28	1.4106		

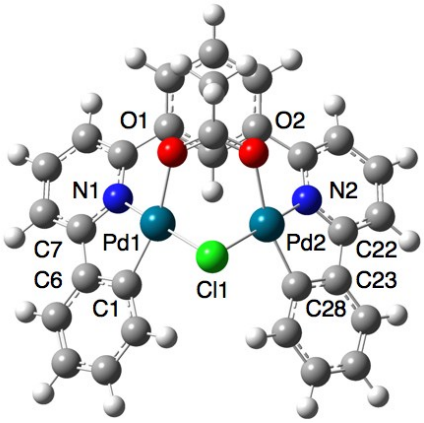


Table S6. Selected Calculated Bond Length (Å) and Angles (deg) in **Pd_2-Me**

	Distance / Å		angle / °
Pd1–Pd2	2.9973	N1–Pd1–C1	81.09
Pd1–Cl1	2.3990	O3–Pd1–Cl1	89.05
Pd1–O3	2.1433	N2–Pd2–C28	81.09
Pd2–Cl1	2.3991	O4–Pd2–Cl1	89.05
Pd2–O4	2.1433	N1–Pd1–Cl1	171.72
Pd1–N1	2.0747	C1–Pd1–O3	164.62
Pd1–C1	1.9595	N2–Pd2–Cl1	171.73
Pd2–N2	2.0747	C28–Pd2–O4	164.63
Pd2–C28	1.9595		
N1–C7	1.3548		
C7–C6	1.4596		
C6–C1	1.4169		
N2–C22	1.3548		
C22–C23	1.4596		
C23–C28	1.4169		

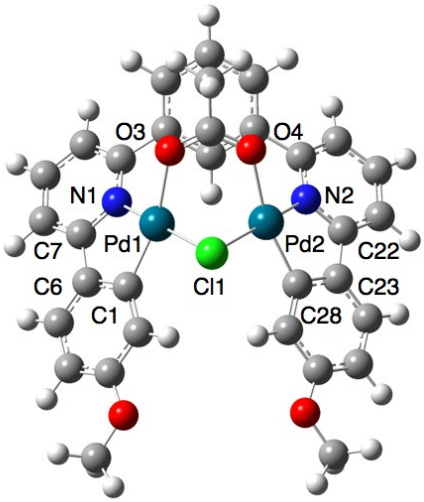


Table S7. Selected Calculated Bond Length (Å) and Angles (deg) in **Pd_2-27**

	Distance / Å		angle / °
Pd1–Pd2	2.9990	N1–Pd1–C1	80.82
Pd1–Cl1	2.4081	O5–Pd1–Cl1	88.84
Pd1–O5	2.1444	N2–Pd2–C28	81.24
Pd2–Cl1	2.3981	O6–Pd2–Cl1	89.09
Pd2–O6	2.1405	N1–Pd1–Cl1	172.13
Pd1–N1	2.0726	C1–Pd1–O5	164.88
Pd1–C1	1.9576	N2–Pd2–Cl1	171.42
Pd2–N2	2.0757	C28–Pd2–O6	164.07
Pd2–C28	1.9610		
N1–C7	1.3557		
C7–C6	1.4572		
C6–C1	1.4087		
N2–C22	1.3545		
C22–C23	1.4601		
C23–C28	1.4165		

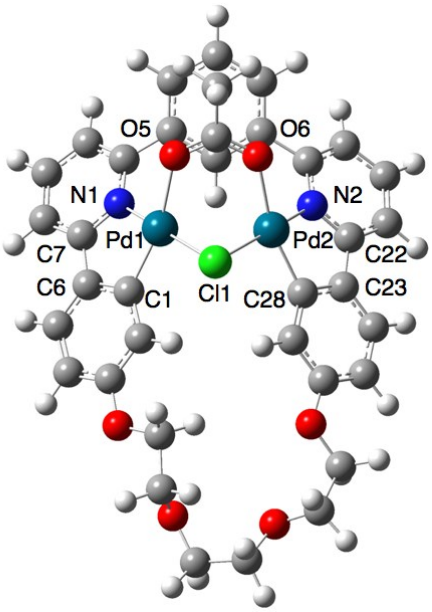


Table S8. Selected Calculated Bond Length (Å) and Angles (deg) in **Pd_2-(μ-Cl)$_2$**

	Distance / Å		Angle / °
Pd1–Pd2	3.5693	N1–Pd1–C11	81.07
Pd1–Cl1	2.3735	Cl1–Pd1–Cl2	85.73
Pd1–Cl2	2.5033	N2–Pd2–C22	81.07
Pd2–Cl1	2.3735	Cl1–Pd2–Cl2	85.73
Pd2–Cl2	2.5033	N1–Pd1–Cl2	177.37
Pd1–N1	2.0491	C11–Pd1–Cl1	177.97
Pd1–C11	1.9682	N2–Pd2–Cl2	177.37
Pd2–N2	2.0491	C22–Pd2–Cl1	177.97
Pd2–C22	1.9682		
N1–C5	1.3531		
C5–C6	1.4627		
C6–C11	1.4089		
N2–C16	1.3531		
C16–C17	1.4627		
C17–C22	1.4088		

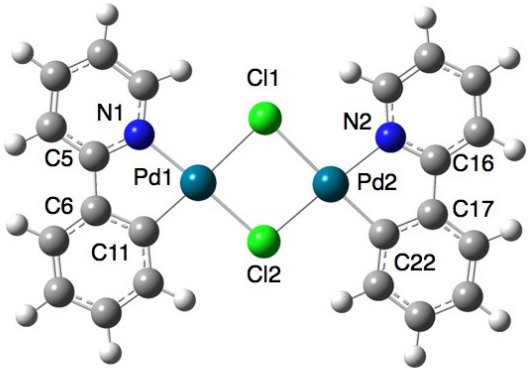
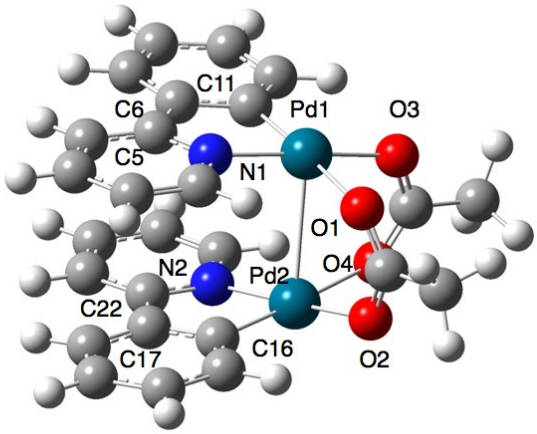


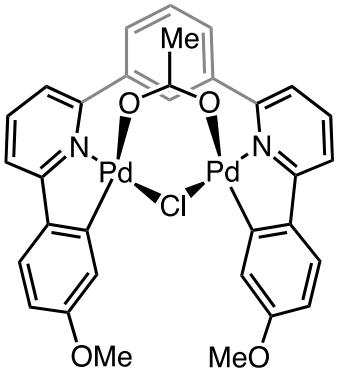
Table S9. Selected Calculated Bond Length (Å) and Angles (deg) in **Pd_2-(μ-OAc)$_2$**

	Distance / Å		Angle / °
Pd1–Pd2	2.9202	N1–Pd1–C11	81.29
Pd1–O1	2.1724	O1–Pd1–O3	90.31
Pd1–O3	2.0658	N2–Pd2–C22	81.29
Pd2–O2	2.0657	O2–Pd2–O4	90.30
Pd2–O4	2.1724	N1–Pd1–O3	172.92
Pd1–N1	2.0352	C11–Pd1–O1	176.23
Pd1–C11	1.9573	N2–Pd2–O2	172.91
Pd2–N2	2.0052	C22–Pd2–O4	176.24
Pd2–C22	2.0352		
N1–C5	1.3522		
C5–C6	1.4657		
C6–C11	1.4093		
N2–C16	1.3522		
C16–C17	1.4657		
C17–C22	1.4093		



3. Synthesis and Characterization Data

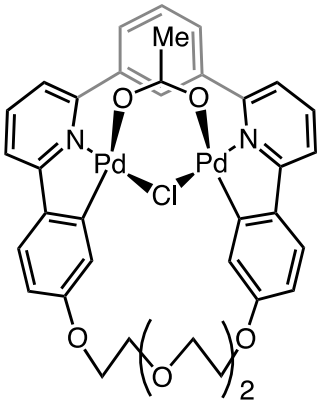
Pd_2-Me



The mixture of **1**[2] (50.0 mg, 0.112 mmol), potassium tetrachloropalladate (80.8 mg, 0.247 mmol, 220 mol%), and sodium hydrogen carbonate (94.1 mg, 1.12 mmol, 1000 mol%) in acetic acid (10 mL) and water (1 mL) was degassed by freeze-pump-thaw cycling in three times, and stirred at reflux temperature for 2 h under an Ar atomsphere. The mixture was cooled to room temperature, and the reaction was quenched by addition of water. The mixture was extracted with dichloromethane. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (CH_2Cl_2 -> CH_2Cl_2/MeOH = 100/1) to give **Pd_2-Me** (32.6 mg, 39% yield) as pale yellow solid.

Mp: 260 °C (decomp.) (crystals from CH_2Cl_2-MeOH). IR (KBr): ν 2929, 1583, 1556, 1458, 1427, 1338, 1302, 1269, 1223, 1209, 1176, 1036, 789 cm^{-1}. ^1H NMR (500 MHz, r.t., CD_2Cl_2): δ 9.73 (1H, t, *J* = 1.7 Hz), 7.89 (2H, t, *J* = 7.8 Hz), 7.73 (2H, dd, *J* = 7.7, 1.9 Hz), 7.60 (2H, dd, *J* = 8.1, 1.1 Hz), 7.58 (1H, t, *J* = 7.6 Hz), 7.41 (2H, d, *J* = 8.6 Hz), 7.31 (2H, dd, *J* = 7.6, 1.2 Hz), 7.28 (2H, d, *J* = 2.5 Hz), 6.70 (2H, dd, *J* = 8.4, 2.6 Hz), 3.88 (6H, s), 1.33 (3H, s) ppm. ^{13}C NMR (125 MHz, r.t., CD_2Cl_2): δ 177.3, 166.1, 160.3, 158.7, 153.1, 139.8, 139.2 (2 peaks), 131.5, 129.4, 127.6, 125.6, 122.4, 120.5, 116.8, 111.2, 55.7, 22.2 ppm (18 peaks). HRMS (ESI-TOF-MS, negative) (*m*/*z*) for $C_{32}H_{25}N_2O_4Cl_2Pd_2$ ([M+Cl]$^-$): Calculated 784.9273; Found 784.9236. Anal. Calcd. for $C_{32}H_{25}ClN_2O_4Pd_2$: C, 51.26; H, 3.36; N, 3.74, Found: C, 51.06; H, 3.57; N, 3.80.

Pd_2-27

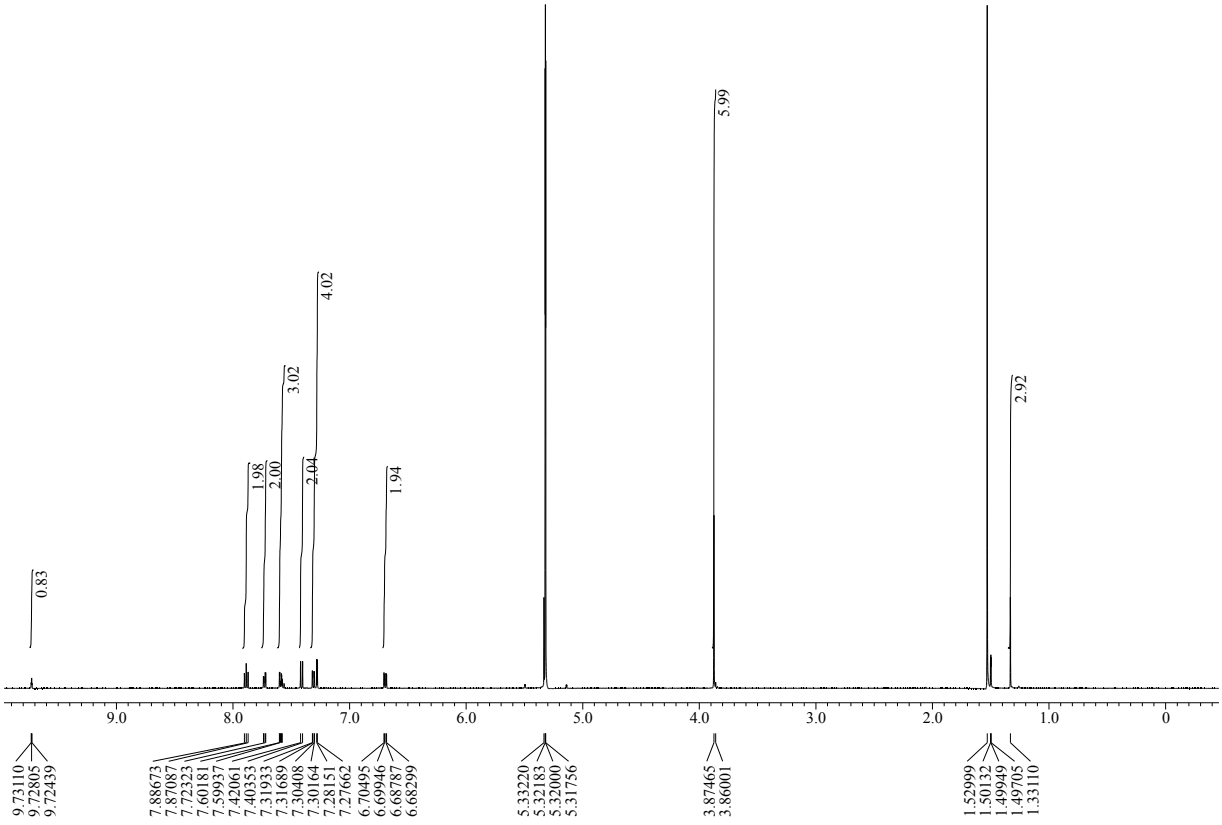


The mixture of **2**[2] (50.0 mg, 0.0942 mmol), potassium tetrachloropalladate (67.6 mg, 0.207 mmol, 220 mol%), and sodium hydrogen carbonate (79.1 mg, 0.942 mmol, 1000 mol%) in acetic acid (10 mL) and water (1 mL) was degassed by freeze-pump-thaw cycling in three times, and stirred at reflux temperature for 2 h under an Ar atomsphere. The mixture was cooled to room temperature, and the reaction was quenched by addition of water. The mixture was extracted with dichloromethane. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (CH_2Cl_2 -> CH_2Cl_2/MeOH = 50/1) to give **Pd_2-27** (33.4 mg, 42% yield) as pale yellow solid.

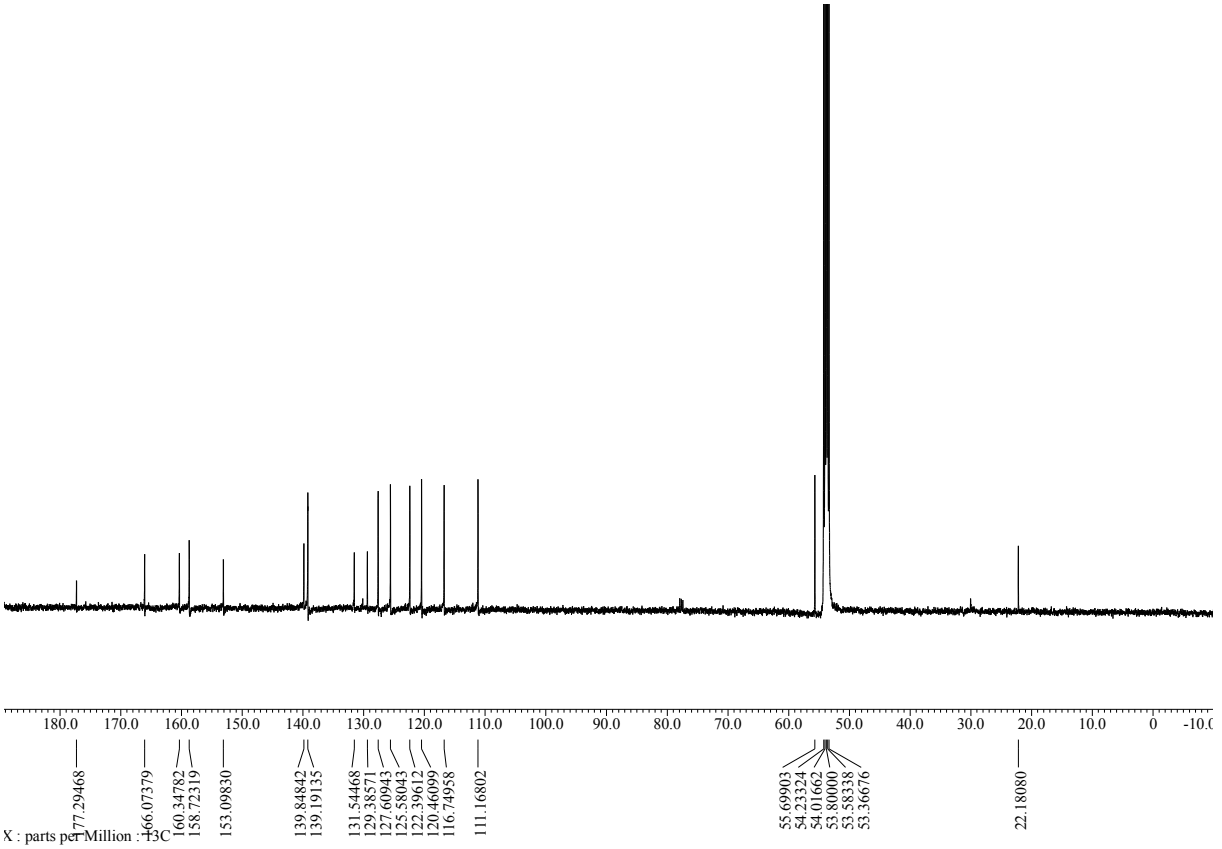
Mp: 260 °C (decomp.) (crystals from CH_2Cl_2-MeOH). IR (KBr): ν 2925, 1583, 1552, 1446, 1300, 1265, 1207, 1176, 1134, 1059, 945, 787 cm^{-1}. ^1H NMR (500 MHz, r.t., DMSO-d_6): δ 9.61 (1H, t, J = 1.7 Hz), 8.12 (2H, t, J = 7.8 Hz), 7.99 (2H, dd, J = 8.2, 1.9 Hz), 7.84 (2H, dd, J = 7.9, 1.8 Hz), 7.69 (2H, d, J = 8.8 Hz), 7.64 (1H, t, J = 7.8 Hz), 7.54 (2H, dd, J = 7.7, 1.3 Hz), 7.07 (2H, d, J = 2.8 Hz), 6.76 (2H, dd, J = 8.8, 2.5 Hz), 4.17-4.07 (4H, m), 3.88-3.81 (2H, m), 3.80-3.73 (2H, m), 3.63 (4H, s), 1.20 (3H, s) ppm. ^{13}C NMR (125 MHz, r.t., DMSO-d_6): δ 175.9, 172.0. 164.8, 159.3, 157.0, 151.9, 140.0, 138.8, 130.2, 129.2, 127.5, 126.2, 122.7, 121.1, 117.1, 109.7, 68.7, 68.1, 67.0, 54.9, 21.1 ppm (20 peaks). HRMS (ESI-TOF-MS, positive) (*m*/*z*) for $C_{36}H_{31}N_2O_6ClPd_2Na$ ($[M+Na]^+$): Calculated 858.9846; Found 858.9855. Anal. Calcd. for $C_{36}H_{31}ClN_2O_6Pd_2.H_2O$: C, 50.63; H, 3.90; N, 3.28, Found: C, 50.51; H, 3.93; N, 3.29.

4. ^{1}H and ^{13}C NMR Spectra

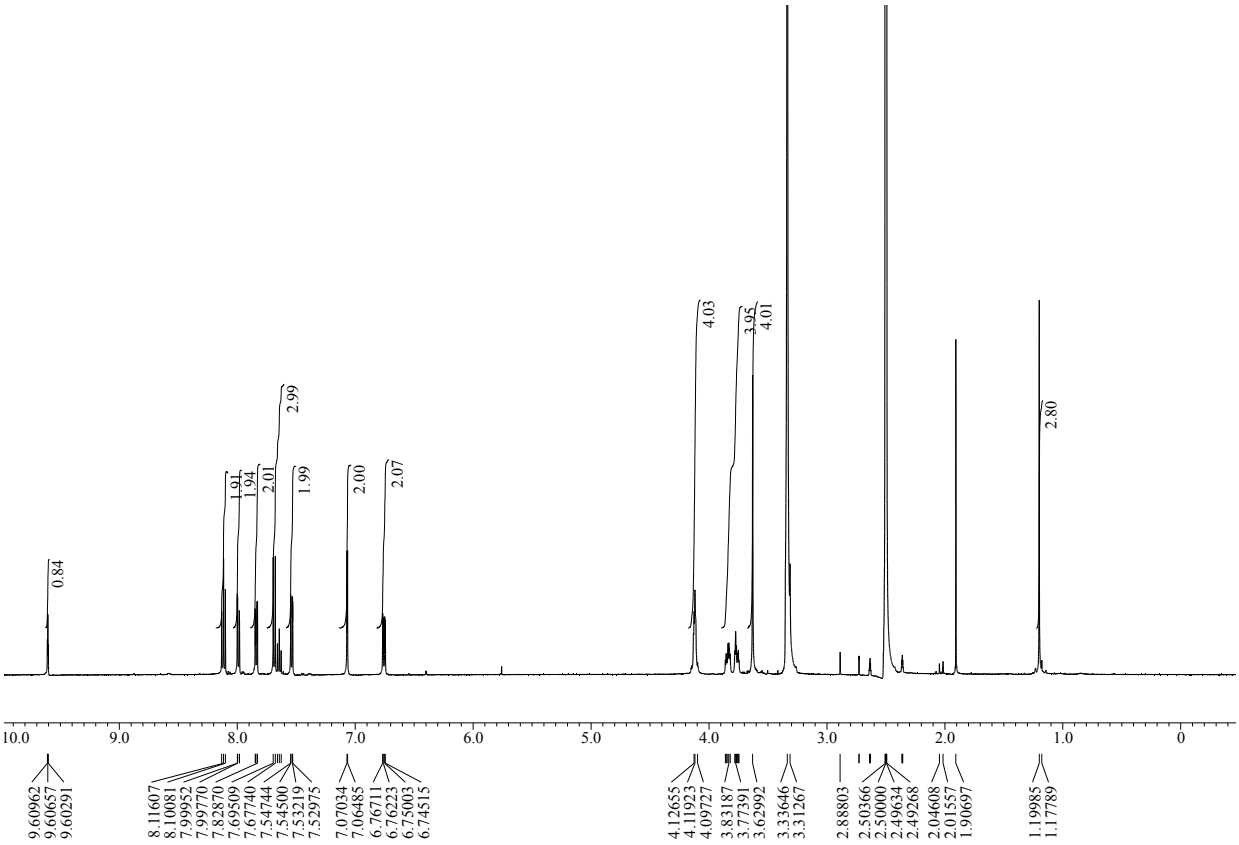
^{1}H-NMR (500 MHz, CD_2Cl_2) spectrum of **Pd_2-Me**.



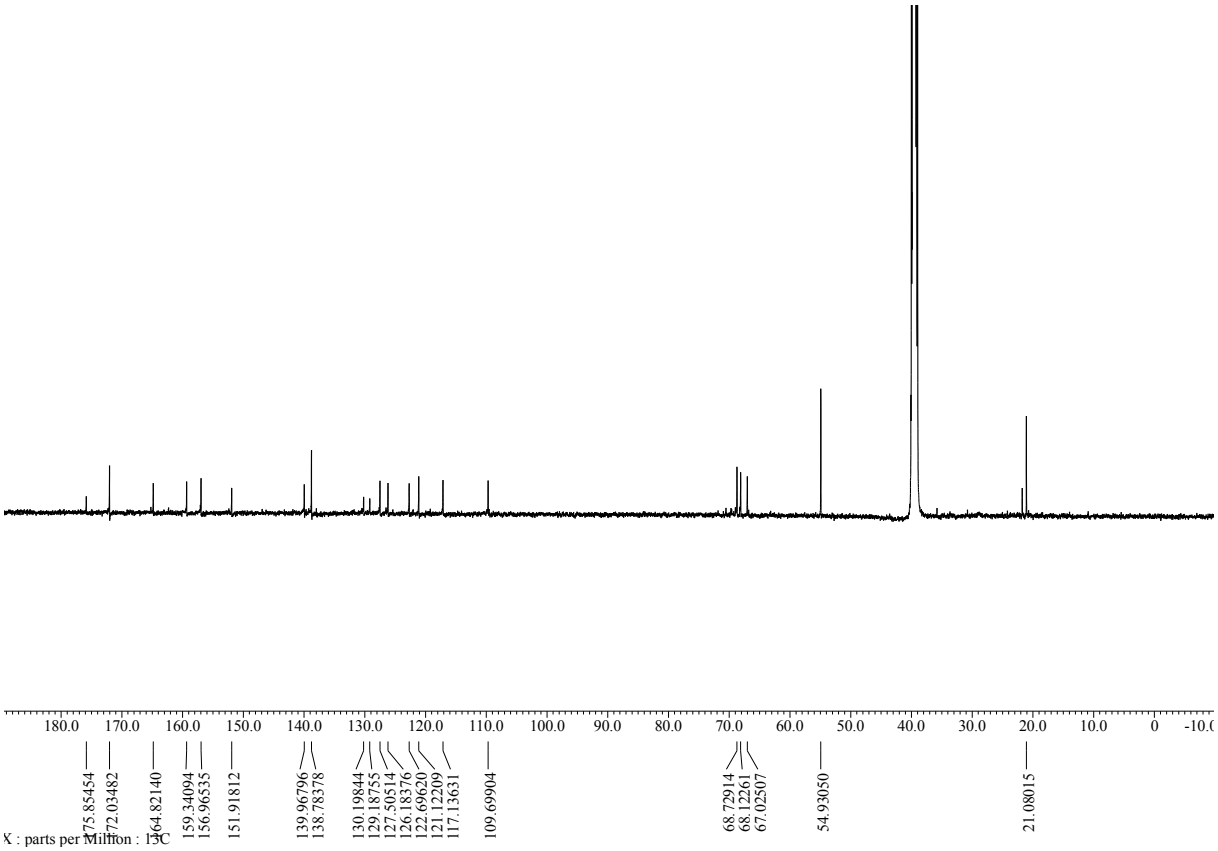
^{13}C-NMR (125 MHz, CD_2Cl_2) spectrum of **Pd_2-Me**.



^{1}H-NMR (500 MHz, DMSO-d_6) spectrum of **Pd_2-27**.

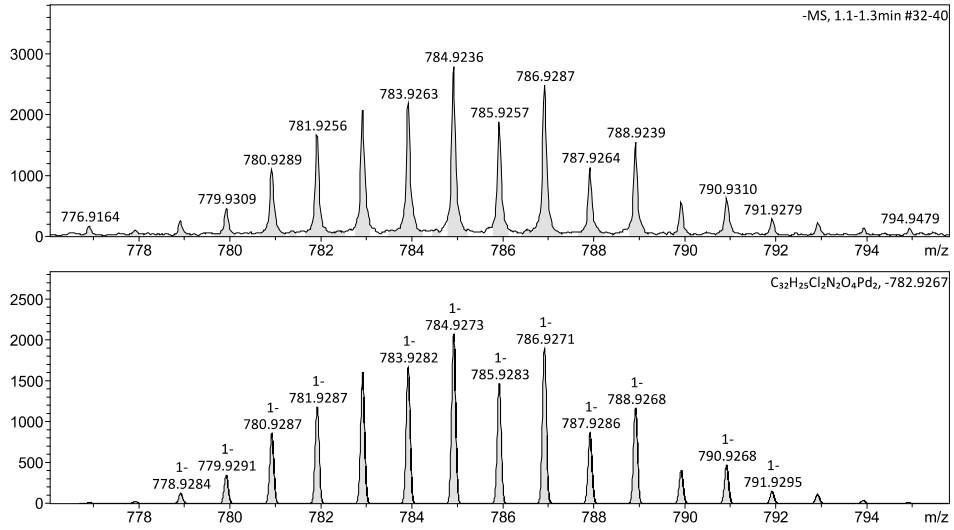


^{13}C-NMR (125 MHz, DMSO-d_6) spectrum of **Pd_2-27**.

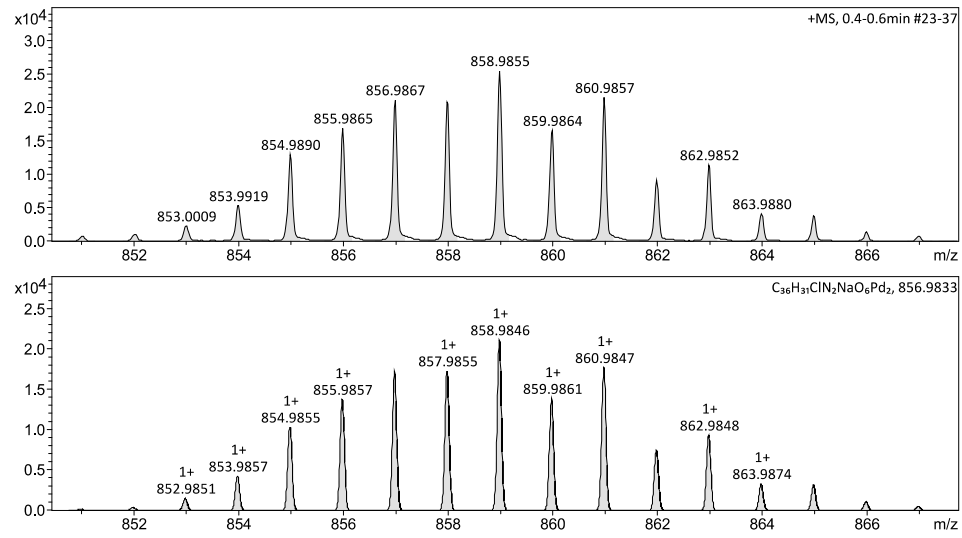


5. ESI-TOF-MS Spectra

ESI-TOF-MS spectrum (negative) (upper: found, bottom: calculated for $C_{32}H_{25}Cl_2N_2O_4Pd_2$ $[M+Cl]^-$) of **Pd_2-Me**.



ESI-TOF-MS spectrum (positive) (upper: found, bottom: calculated for $C_{36}H_{31}ClN_2O_6Pd_2Na$ $[M+Na]^+$) of **Pd_2-27**.



6. X-ray Crystallographic Analysis

Single crystals suitable for X-ray analyses were mounted on a fiber loop. Diffraction experiments were were performed on a Rigaku Saturn CCD area detector with graphite-monochromated Mo-□□ radiation (□□= 0.71073 Å). Intensidy data ($6° < 2\theta < 55°$) collected at 93 K were corrected by Lorentz polarization effects and absorption. Structure solution and refinements were carried out by using the CrystalStructure program package.[3] The heavy-atom positions were determined by a direct method program (SIR92[4]) and the remaining non-hydrogen atoms were found by subsequent Fourier syntheses and refined by full-matrix least-squares techniques against F^2 using the SHELXL-2014/7 program.[5] The co-crystalized THF molecule lying around the center of symmetry as well as the some carbon atoms in the polyether macrocycle in **Pd_2-27** was disordered and refined with restraint geometry. The hydrogen atoms were included in the refinements with a riding model. The absolute structure of **Pd_2-Me** was determined on the basis of the Flack absolute structure parameter.[6] Crystallographic data have been deposited with Cambridge Crystallographic Data Centre: Deposition number CCDC-1954907 (**Pd_2-Me**), CCDC-1954908 (**Pd_2-27**). Copies of the data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge, CB2 1EZ, UK; Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

The single crystal of **Pd_2-Me** was obtained by the slow vaporization from CH_2Cl_2/benzene solution.
Crystal data of **Pd_2-Me**: $C_{32}H_{25}ClN_2O_4Pd_2$-CH_2Cl_2, yellow prism, 0.24×0.24×0.20 mm^3, orthorhombic, space group $P2_12_12_1$ (No. 19), a = 17.065(11) Å, b = 17.488(11) Å, c = 20.605(12) Å, V = 6149(7) Å^3, ρ_{calcd} = 1.803 g/cm^3, Z = 8, 14102 reflections measured, R_1 = 0.0526 [$I > 2\sigma(I)$], and wR_2 = 0.1372 (all data), GOF=1.036.

The single crystal of **Pd_2- 27** was obtained by the slow vaporization from CH_2Cl_2/THF solution.
Crystal data of **Pd_2-27**: $C_{36}H_{31}ClN_2O_6Pd_2 \cdot (C_4H_8O)_{0.75}$, yellow prism, 0.17×0.09×0.03 mm^3, triclinic, space group $P\bar{1}$ (No. 2), a = 12.641(3) Å, b = 13.964(3) Å, c = 21.656(5) Å, α = 73.184(11)□, β = 76.622(12)□, γ = 74.112(12)□, V = 3470.9(13) Å^3, ρ_{calcd} = 1.703 g/cm^3, Z = 4, 15761 reflections measured, R_1 = 0.0557[$I > 2\sigma(I)$], and wR_2 = 0.1407 (all data), GOF=0.807.

7. Theoretical Calculations

DFT calculations were carried out by Gaussian09 program.[7] We employed the DFT calculations with the long-range and dispersion-corrected ωB97X-D functional.[5] The 6-311G(d,p) basis set[9-11] was employed for hydrogen, carbon, boron, nitrogen, oxygen, and chlorine atoms. The SDD basis set,[12] as an effective core potential basis set, was used for palladium atom. Additional f polarization functions were added to palladium and titanium atoms ($\zeta_{f(Pd)}$=1.472 and $\zeta_{f(Ti)}$=1.506).[13] The X-ray structures of **Pd_2-Me**, **Pd_2-27**, **Pd_2-(μ-Cl)$_2$**,[1] **Pd_2-(μ-OAc)$_2$**,[1] TiOPc,[14] SubPc derivative,[15] subporphyrin derivative,[16] Pd-coordinated norcorrle derivative,[17] and sumanene[18] were used as initial structures for the calculation. The X-ray structure of **Pd_2-Me** was used as initial structure for the calculation of model compound **Pd_2**. All of the structures were fully optimized without any symmetry restrictions. Frequency calculations were carried out to ensure that the structures obtained were a minimum.

Pd_2-Me

Electronic energy = −2360.90843535 hartree, ZPE = 0.503025 hartree
Charge = 0 Multiplicity = 1

Pd	10.9392	12.4974	9.9681
Pd	8.0211	12.1265	9.6891
Cl	9.7631	11.2642	8.3329
O	12.5155	7.3782	10.6878
O	7.1434	6.8903	9.1857

O	10.4318	14.3034	8.9343
O	8.2185	14.0464	8.6994
N	11.8465	13.5095	11.5038
N	6.727	12.7522	11.1494
C	11.9318	10.9772	10.7579
C	11.826	9.6411	10.4612
C	12.71	8.7108	11.0299
C	13.6998	9.1532	11.9179
C	13.8209	10.4648	12.1796
C	12.9404	11.4109	11.6336
C	12.9336	12.8222	11.9859
C	13.8585	13.506	12.7627
C	13.6622	14.8211	13.0862
C	12.483	15.4524	12.7092
C	11.5752	14.7511	11.9344
C	10.1998	15.3247	11.6398
C	10.0086	16.6521	11.4234
C	8.7441	17.1505	11.1988
C	7.6263	16.2988	11.2936
C	7.8362	14.9417	11.5182
C	9.1161	14.4591	11.7181
C	6.6724	14.0009	11.6913
C	5.6366	14.3699	12.5299
C	4.6775	13.4115	12.8472
C	4.7901	12.1087	12.3836
C	5.8243	11.7992	11.5182
C	6.07	10.5243	10.898
C	5.1912	9.405	10.9969
C	5.5239	8.1599	10.422
C	6.6827	8.0532	9.7317
C	7.5359	9.148	9.6184
C	7.2321	10.3686	10.1315
C	13.4302	6.4251	11.2359
C	6.4403	5.7046	9.4041
C	9.3107	14.6445	8.4975
C	9.2492	15.8546	7.6362
H	11.1651	9.347	9.8758
H	14.2853	8.5443	12.3057
H	14.496	10.7674	12.7436
H	14.609	13.0539	13.0743
H	14.3189	15.295	13.5424
H	12.2882	16.3202	12.982
H	10.74	17.2262	11.4073
H	8.62	18.0529	11.0103
H	6.7646	16.6367	11.1982
H	9.2518	13.559	11.9074

H	5.5804	15.2366	12.8606
H	3.9668	13.6452	13.3992
H	4.1789	11.4583	12.648
H	4.3959	9.4953	11.4714
H	4.9408	7.4396	10.4966
H	8.3472	9.0425	9.1771
H	13.3039	5.5698	10.8189
H	13.2887	6.3443	12.1815
H	14.3244	6.7331	11.0702
H	7.0182	4.9426	9.3234
H	5.7234	5.6301	8.7687
H	6.0782	5.7404	10.2918
H	9.9363	15.8245	6.9661
H	9.3885	16.6194	8.201
H	8.391	15.9228	7.2124

Pd_2-27

Electronic energy = −2667.36382066 hartree, ZPE = 0.607770 hartree

Charge = 0 Multiplicity = 1

Pd	8.1524	11.5739	0.5909
Pd	6.6966	9.1976	1.5941
Cl	5.8404	11.043	0.3793
O	7.219	11.3964	-4.7902
O	5.826	9.4218	-6.1784
O	4.401	7.0323	-5.5855
O	4.3229	7.0939	-2.7314
O	7.7943	12.1997	2.6476
O	6.6647	10.3973	3.3816
N	10.2202	11.6531	0.6829
N	7.5969	7.6013	2.5188
C	8.5451	11.5441	-1.331
C	7.6116	11.4322	-2.3634
C	8.0237	11.5534	-3.7005
C	9.3836	11.7949	-4.0092
C	10.2897	11.9371	-2.9952
C	9.8937	11.8241	-1.6519
C	10.8055	11.8973	-0.5213
C	12.1899	12.1664	-0.6113
C	12.9163	12.1727	0.5581
C	12.3463	11.8462	1.7664
C	10.9777	11.5436	1.8135
C	10.3948	10.8844	2.9911
C	10.6925	11.2592	4.2975
C	10.2267	10.4794	5.379
C	9.501	9.325	5.1603
C	9.1869	8.9515	3.8375

C	9.6239	9.7545	2.7846
C	8.4959	7.6683	3.5492
C	8.8896	6.5047	4.2055
C	8.3399	5.2898	3.8191
C	7.4769	5.2337	2.7519
C	7.1262	6.4114	2.0874
C	6.3218	6.4903	0.8607
C	5.7122	5.4123	0.2474
C	5.0024	5.5861	-0.9323
C	4.9423	6.8228	-1.5272
C	5.5291	7.9412	-0.9078
C	6.1977	7.7849	0.3046
C	5.8168	11.1466	-4.5796
C	5.238	10.6577	-5.8697
C	5.1252	8.6683	-7.1557
C	3.94	7.9412	-6.618
C	3.3497	6.5241	-4.8107
C	3.8839	5.977	-3.5063
C	7.2022	11.5487	3.5124
C	7.0178	12.1959	4.9149
H	6.715	11.2846	-2.1674
H	9.6557	11.8415	-4.8969
H	11.1806	12.1285	-3.181
H	12.5897	12.3373	-1.4336
H	13.8159	12.4044	0.5326
H	12.857	11.8279	2.5446
H	11.2003	12.0251	4.441
H	10.4227	10.7508	6.2477
H	9.2081	8.8021	5.8709
H	9.3834	9.533	1.9145
H	9.5199	6.5503	4.8884
H	8.5615	4.5144	4.283
H	7.1355	4.4188	2.4595
H	5.8022	4.5641	0.6187
H	4.5642	4.8679	-1.3267
H	5.4851	8.7739	-1.3197
H	5.7313	10.4766	-3.8839
H	5.416	11.9764	-4.276
H	5.4297	11.2629	-6.6025
H	4.2803	10.5143	-5.8145
H	4.8937	9.3133	-7.8414
H	5.7749	8.0446	-7.5145
H	3.4757	7.4224	-7.2919
H	3.3172	8.558	-6.2013
H	2.7558	7.2823	-4.6937
H	2.9136	5.8804	-5.3893

H	4.6584	5.4047	-3.6259
H	3.2233	5.5042	-2.9755
H	7.2193	11.5561	5.6017
H	7.6099	12.9466	4.993
H	6.1098	12.4931	5.012

Pd_2

Electronic energy = −2131.86952574 hartree, ZPE = 0.437835 hartree

Charge = 0 Multiplicity = 1

Pd	-1.30217	-0.65943	0.0000
Pd	-4.22027	-1.03033	-0.279
Cl	-2.47827	-1.89263	-1.6352
O	-1.80957	1.14657	-1.0338
O	-4.02287	0.88957	-1.2687
N	-0.39487	0.35267	1.5357
N	-5.51437	-0.40463	1.1813
C	-0.30957	-2.17963	0.7898
C	-0.41537	-3.51573	0.4931
C	0.46863	-4.44603	1.0618
C	1.45843	-4.00363	1.9498
C	1.57953	-2.69203	2.2115
C	0.69903	-1.74593	1.6655
C	0.69223	-0.33463	2.0178
C	1.61713	0.34917	2.7946
C	1.42083	1.66427	3.1181
C	0.24163	2.29557	2.7411
C	-0.66617	1.59427	1.9663
C	-2.04157	2.16787	1.6717
C	-2.23277	3.49527	1.4553
C	-3.49727	3.99367	1.2307
C	-4.61507	3.14197	1.3255
C	-4.40517	1.78487	1.5501
C	-3.12527	1.30227	1.75
C	-5.56897	0.84407	1.7232
C	-6.60477	1.21307	2.5618
C	-7.56387	0.25467	2.8791
C	-7.45127	-1.04813	2.4155
C	-6.41707	-1.35763	1.5501
C	-6.17137	-2.63253	0.9299
C	-7.05017	-3.75183	1.0288
C	-6.71747	-4.99693	0.4539
C	-5.55867	-5.10363	-0.2364
C	-4.70547	-4.00883	-0.3497
C	-5.00927	-2.78823	0.1634
C	-2.93067	1.48767	-1.4706
C	-2.99217	2.69777	-2.3319

H	-1.07627	-3.80983	-0.0923
H	2.04393	-4.61253	2.3376
H	2.25463	-2.38943	2.7755
H	2.36763	-0.10293	3.1062
H	2.07753	2.13817	3.5743
H	0.04683	3.16337	3.0139
H	-1.50137	4.06937	1.4392
H	-3.62137	4.89607	1.0422
H	-5.47677	3.47987	1.2301
H	-2.98957	0.40217	1.9393
H	-6.66097	2.07977	2.8925
H	-8.27457	0.48837	3.4311
H	-8.06247	-1.69853	2.6799
H	-7.84547	-3.66153	1.5033
H	-7.30057	-5.71723	0.5285
H	-3.89417	-4.11433	-0.791
H	-2.30507	2.66767	-3.002
H	-2.85287	3.46257	-1.7671
H	-3.85037	2.76597	-2.7557
H	0.38738	-5.48499	0.81917
H	-5.29672	-6.03312	-0.69719

Pd_2-(μ-Cl)$_2$

Electronic energy = −2133.79702495 hartree, ZPE = 0.326707 hartree

Charge = 0 Multiplicity = 1

Pd	0.8415	2.1438	0.3011
Pd	-0.5813	0.0164	2.6795
Cl	-1.3702	1.262	0.7515
Cl	1.5067	1.0781	2.3029
N	0.3435	3.232	-1.3179
N	-2.3226	-0.8941	3.1236
C	-0.8761	3.244	-1.9116
C	-1.1265	4.0195	-3.0316
C	-0.1019	4.7831	-3.5744
C	1.1435	4.7781	-2.967
C	1.3569	3.9989	-1.8358
C	2.6228	3.8744	-1.1236
C	3.7928	4.5542	-1.4621
C	4.9684	4.2854	-0.7781
C	4.9698	3.3322	0.2332
C	3.7908	2.6872	0.5896
C	2.614	2.9591	-0.0729
C	-3.4872	-0.7409	2.4364
C	-4.6516	-1.3824	2.8379
C	-4.6165	-2.2041	3.9569
C	-3.4439	-2.3616	4.6539

C	-2.2899	-1.6981	4.237
C	-0.9879	-1.7671	4.8828
C	-0.6998	-2.5222	6.0234
C	0.5726	-2.5181	6.5547
C	1.5735	-1.758	5.9524
C	1.2781	-1.0046	4.8219
C	0.0102	-1.0039	4.2786
H	-1.588	2.7344	-1.5382
H	-1.918	4.0084	-3.4155
H	-0.2448	5.3718	-4.3488
H	1.8069	5.3543	-3.3202
H	3.7511	5.2125	-2.1681
H	5.7492	4.6804	-1.0045
H	5.762	3.0801	0.6655
H	3.8484	2.0722	1.2745
H	-3.4746	-0.167	1.6711
H	-5.3677	-1.2254	2.4067
H	-5.355	-2.6004	4.2003
H	-3.3976	-2.8781	5.4538
H	-1.3856	-2.9927	6.4103
H	0.8044	-2.9947	7.3573
H	2.4499	-1.7517	6.2857
H	1.9169	-0.47	4.4315

Pd_2-(μ-OAc)$_2$

Electronic energy = −1670.32141216 hartree, ZPE = 0.429065 hartree

Charge = 0 Multiplicity = 1

Pd	-2.78313	1.3253	0.000
Pd	-4.41503	-0.6114	-1.3334
O	-4.46853	2.4811	-0.6445
O	-5.81143	0.8838	-1.4926
O	-3.81283	0.7781	1.6828
O	-4.96543	-0.9093	0.73
N	-1.66263	1.7278	-1.6214
N	-2.97113	-2.0026	-1.3471
C	-2.10053	2.4108	-2.6908
H	-2.95393	2.8249	-2.6541
C	-1.34393	2.5303	-3.8506
H	-1.67553	3.0101	-4.6011
C	-0.08943	1.9315	-3.8856
H	0.45297	2.0056	-4.6616
C	0.36457	1.2293	-2.7877
H	1.22357	0.8234	-2.8017
C	-0.44763	1.1188	-1.6546
C	-0.13393	0.3726	-0.4378
C	1.05247	-0.3219	-0.2287

H	1.72827	-0.3195	-0.8963
C	1.24797	-1.0176	0.9546
H	2.05147	-1.5036	1.0948
C	0.25707	-1.0004	1.941
H	0.39467	-1.468	2.7568
C	-0.93193	-0.3023	1.7365
H	-1.59563	-0.2952	2.4163
C	-1.15673	0.3842	0.5455
C	-2.62763	-2.7567	-0.2904
H	-3.13983	-2.6895	0.5072
C	-1.55213	-3.6289	-0.3243
H	-1.33183	-4.1598	0.4328
C	-0.80063	-3.7101	-1.4945
H	-0.04973	-4.2889	-1.5419
C	-1.15593	-2.9437	-2.5809
H	-0.65043	-2.9963	-3.383
C	-2.25433	-2.0919	-2.5074
C	-2.76643	-1.2363	-3.5672
C	-2.25653	-1.208	-4.8702
H	-1.51913	-1.758	-5.1068
C	-2.83283	-0.3756	-5.8097
H	-2.48933	-0.3532	-6.6956
C	-3.91063	0.4278	-5.4672
H	-4.29603	1.003	-6.1181
C	-4.43343	0.3956	-4.1696
H	-5.17653	0.9431	-3.9441
C	-3.86833	-0.4345	-3.209
C	-5.54103	2.0752	-1.1553
C	-6.62343	3.0898	-1.4094
H	-6.34063	3.9622	-1.0653
H	-7.44653	2.81	-0.9556
H	-6.78883	3.1579	-2.3729
C	-4.63853	-0.1843	1.6997
C	-5.25703	-0.4849	3.0493
H	-6.15733	-0.8507	2.922
H	-5.31113	0.3408	3.5752
H	-4.70263	-1.1388	3.5247

TiOPc

Electronic energy = −1800.65696660 hartree, ZPE = 0.421515 hartree

Charge = 0 Multiplicity = 1

Ti	4.7311	5.0363	9.057
O	4.6848	5.0168	10.6844
N	5.9586	3.5078	8.4761
N	6.308	6.2598	8.4827
N	3.5239	6.5577	8.3689

N	3.2056	3.8002	8.3518
N	8.1227	4.6729	8.3845
N	5.146	8.3826	8.2472
N	1.3847	5.401	8.2276
N	4.3584	1.6718	8.3034
C	5.6201	2.166	8.344
C	6.8015	1.353	8.2393
C	7.0205	-0.0153	8.1321
C	8.2853	-0.4719	8.0483
C	9.4014	0.4176	7.9607
C	9.1516	1.7678	8.0876
C	7.9071	2.2509	8.2315
C	7.3384	3.5468	8.378
C	7.5868	5.8798	8.3963
C	8.4316	7.1034	8.2276
C	9.794	7.2259	8.0405
C	10.2731	8.5524	7.8076
C	9.3829	9.6159	7.7618
C	8.0129	9.474	7.9358
C	7.5669	8.1585	8.1569
C	6.1861	7.6393	8.3257
C	3.8863	7.908	8.2485
C	2.7409	8.7097	8.0915
C	2.5748	10.0795	7.9201
C	1.3169	10.5764	7.7828
C	0.1726	9.7217	7.8403
C	0.3543	8.3311	7.9659
C	1.601	7.8467	8.1059
C	2.168	6.5034	8.2642
C	1.9124	4.208	8.2537
C	1.089	2.9761	8.136
C	-0.3234	2.8188	8.0261
C	-0.7885	1.4825	8.0091
C	0.0699	0.4218	8.0666
C	1.4558	0.5679	8.153
C	1.9472	1.8889	8.1726
C	3.2984	2.4374	8.2995
H	3.42283	10.73157	7.89666
H	1.1809	11.6265	7.62888
H	-0.81304	10.13488	7.78837
H	-0.48676	7.66983	7.95019
H	-0.98752	3.65521	7.96082
H	-1.84081	1.29812	7.94961
H	-0.33854	-0.56693	8.04441
H	2.10979	-0.27758	8.20172
H	6.19579	-0.69685	8.11634

H	8.45912	-1.52769	8.04727
H	10.39348	0.04926	7.80257
H	9.97462	2.45136	8.07088
H	10.45	6.38103	8.06809
H	11.31978	8.72555	7.66837
H	9.77264	10.59624	7.58309
H	7.34277	10.30755	7.90392

SubPc

Electronic energy = −1735.35744551 hartree, ZPE = 0.321853 hartree

Charge = 0 Multiplicity = 1

B	5.1095	2.835	5.0072
Cl	4.7454	1.0532	5.4282
C	5.3459	3.2888	2.5433
C	6.4679	3.4277	1.6177
C	6.5611	3.68	0.2526
C	7.7959	3.75	-0.331
C	8.9672	3.6037	0.4126
C	8.9017	3.4425	1.7834
C	7.6613	3.3312	2.3894
C	7.2676	3.169	3.7777
C	7.2311	3.7277	5.9963
C	7.5708	4.5664	7.1371
C	8.7811	5.0498	7.594
C	8.7952	6.0019	8.5956
C	7.6133	6.4514	9.1577
C	6.3919	5.9712	8.7232
C	6.3481	5.0138	7.7124
C	5.2614	4.4158	6.9476
C	3.3153	4.402	5.7431
C	2.1004	4.9353	5.1361
C	1.0653	5.7061	5.6279
C	0.0789	6.1334	4.7603
C	0.1177	5.8026	3.4086
C	1.1341	5.0265	2.8993
C	2.1336	4.5759	3.7482
C	3.3525	3.8168	3.5285
N	5.9156	2.9909	3.7602
N	5.8674	3.5708	6.0527
N	3.8808	3.6228	4.7771
N	7.9575	3.4372	4.9079
N	3.9601	4.7667	6.8612
N	4.0444	3.5931	2.3999
H	1.02798	5.96818	6.66464
H	-0.72831	6.72848	5.13338
H	-0.65327	6.15655	2.7565

H	1.15269	4.77371	1.85976
H	5.67679	3.81768	-0.33387
H	7.86545	3.92136	-1.3849
H	9.91742	3.61633	-0.07915
H	9.79673	3.4042	2.36851
H	9.69865	4.69079	7.17672
H	9.72889	6.39523	8.93972
H	7.64521	7.18099	9.93973
H	5.48509	6.33303	9.16101

subporphyrin

Electronic energy = −881.27251468 hartree, ZPE = 0.256842 hartree

Charge = 0 Multiplicity = 1

O	2.7407	1.976	2.0234
N	0.3871	1.2474	2.323
N	0.925	3.5626	2.1684
C	-1.1709	0.0765	1.243
H	-1.8059	-0.1954	0.5913
C	-0.7754	-0.6538	2.3289
H	-1.0892	-1.5208	2.561
C	0.3112	5.7176	2.11
H	0.2557	6.6439	2.3115
C	1.0161	4.728	2.8768
C	0.7748	0.0323	4.3528
C	-0.4639	1.3184	1.2579
C	-0.2664	5.0955	1.0403
H	-0.7955	5.5118	0.3702
N	1.459	2.3224	4.1231
C	1.302	1.2166	4.9139
C	0.0699	3.7002	1.1108
C	1.6587	3.0244	6.2405
H	1.7945	3.5811	6.9981
C	1.487	1.6729	6.2612
H	1.4896	1.1257	7.0366
C	-0.5777	2.5575	0.5804
C	0.1951	0.1128	3.0582
C	1.5988	3.4645	4.8755
C	1.4425	4.7157	4.2193
B	1.4655	2.2578	2.6297
C	3.4167	0.8078	2.4857
H	3.5531	0.8708	3.4538
H	4.2855	0.7349	2.0385
H	2.8766	0.0149	2.283
H	1.64491	5.63091	4.73536
H	0.81086	-0.89506	4.88534
H	-1.14702	2.62939	-0.32271

Pd-coordinated norcorrole

Electronic energy = −1038.71931640 hartree, ZPE = 0.240693 hartree

Charge = 0 Multiplicity = 1

C	5.3836	4.8244	7.6775
C	4.2436	4.2271	8.2877
H	4.017	3.3052	8.2854
C	3.5259	5.2586	8.8888
H	2.7255	5.1574	9.3904
C	4.1908	6.4868	8.6266
N	5.3509	6.1411	7.9691
C	3.7028	7.8415	8.6097
C	4.2209	8.9447	7.9058
C	3.5408	10.1223	7.4335
H	2.7382	10.4807	7.7928
C	4.25	10.6437	6.3737
H	4.0287	11.4152	5.8652
C	5.386	9.7935	6.1884
N	5.3918	8.8856	7.1759
C	6.3295	9.4717	5.0777
C	6.5391	9.8511	3.7275
H	6.2445	10.6535	3.3128
C	7.2558	8.8266	3.1275
H	7.5589	8.8126	2.227
C	7.4599	7.7965	4.0981
N	6.9525	8.2884	5.2698
C	7.7699	6.3927	3.9117
C	7.4761	5.3471	4.8156
C	7.3146	3.9432	4.6043
H	7.6469	3.4514	3.8619
C	6.5947	3.4233	5.6584
H	6.3324	2.5183	5.7714
C	6.3199	4.511	6.5499
N	6.9365	5.5888	6.0754
Pd	6.334	7.263	6.7628
H	2.83675	8.03374	9.20795
H	8.26818	6.12287	3.00406

sumanene

Electronic energy = −807.33073836 hartree, ZPE = 0.262572 hartree

Charge = 0 Multiplicity = 1

C	-1.2563	8.9751	1.931
C	-1.1913	10.3599	1.9333
C	-2.1541	11.1497	2.5495
C	-3.2765	10.4767	3.0409
C	1.1923	12.781	3.0432

C	0.0000	12.255	2.5487
C	-1.5001	12.5273	2.8345
H	-3.9104	10.9234	3.5585
H	1.2231	13.6182	3.5739
H	-1.664	12.8256	3.7434
H	-1.9053	13.2724	2.2722
C	1.1756	8.8353	1.931
C	-0.0562	8.1992	1.9333
C	-0.2588	6.9705	2.5495
C	0.8853	6.335	3.0409
C	-3.3447	9.0529	3.0432
C	-2.293	8.2833	2.5487
C	-1.7788	6.848	2.8345
H	0.8154	5.5626	3.5585
H	-4.0852	8.6609	3.5739
H	-1.9552	6.5569	3.7434
H	-2.2215	6.1246	2.2722
C	0.0807	11.0113	1.931
C	1.2475	10.2625	1.9333
C	2.4128	10.7015	2.5495
C	2.3912	12.01	3.0409
C	2.1524	6.9878	3.0432
C	2.293	8.2833	2.5487
C	3.279	9.4463	2.8345
H	3.0951	12.3357	3.5585
H	2.8621	6.5425	3.5739
H	3.6192	9.4391	3.7434
H	4.1268	9.4247	2.2722

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