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Diverse anion exchange of pliable $[X_2@Pd_3L_4]^{4+}$ double cages: A molecular ruler for recognition of polyatomic anions

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Table S1. Crystallographic data

	$[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$	$[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$	$[(NO_3)_2(H_2O)_2@Pd_3L_4](NO_3)_4\cdot 2C_6H_6\cdot Me_2SO$
Formula	$C_{62}H_{64}B_2F_8N_8O_8Pd$	$C_{110}H_{138}B_4F_{16}N_{20}O_{30}Pd_3$	$C_{106}H_{114}N_{18}O_{37}Pd_3S$
M_w	1329.23	2886.84	2565.39
Cryst.sys.	Monoclinic	Monoclinic	Monoclinic
Space group	*P2₁/c*	*C2/c*	*P2/n*
a (Å)	17.540(5)	41.454(3)	24.117(5)
b (Å)	14.333(3)	16.3397(12)	16.548(3)
c (Å)	12.987(3)	19.2485(13)	37.143(7)
α (°)	90	90	90
β (°)	108.92(3)	95.4160(10)	101.83(3)
γ (°)	90	90	90
V (Å^3)	3088.5(14)	12979.8(16)	14508(5)
Z	2	4	4
ρ (g cm^{-3})	1.429	1.477	1.174
μ (mm^{-1})	0.340	0.513	0.612
R_{int}	0.0339	0.0471	0.1078
GoF on F^2	1.088	1.063	1.012
R_1 [$I>2\sigma(I)$][a]	0.0677	0.0659	0.0944
wR_2 (all data)[b]	0.1965	0.2140	0.3063

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR_2 = (\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2])^{1/2}$

	$[(NO_3)_2@Pd_3L_4](PF_6)_4\cdot 6Me_2SO$	$[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4\cdot 3C_3H_7NO$	$[(PF_6)_2@Pd_3L_4](PF_6)_4\cdot 4C_3H_7NO$
Formula	$C_{96}H_{104}F_{24}N_{14}O_{24}P_4Pd_3S_2$	$C_{184}H_{188}F_{60}N_{26}O_{40}P_{10}Pd_6$	$C_{92}H_{92}F_{36}N_{12}O_{16}P_6Pd_3$
M_w	2801.13	5491.69	2810.79
Cryst.sys.	Triclinic	Triclinic	Monoclinic
Space group	*P-1*	*P-1*	*C2/m*
a (Å)	13.814(3)	14.451(3)	17.463(4)
b (Å)	16.319(3)	19.150(4)	42.738(9)
c (Å)	18.370(4)	23.820(5)	9.1170(18)
α (°)	68.07(3)	96.52(3)	90
β (°)	88.03(3)	106.07(3)	93.09(3)
γ (°)	71.71(3)	90.14(3)	90
V (Å^3)	3631.2(16)	6289(2)	6794(3)
Z	1	1	2
ρ (g cm^{-3})	1.281	1.450	1.374
μ (mm^{-1})	0.412	0.807	0.770
R_{int}	0.0214	0.0132	0.0550
GoF on F^2	1.215	1.011	2.123
R_1 [$I>2\sigma(I)$][a]	0.0538	0.0506	0.1115
wR_2 (all data)[b]	0.1730	0.1426	0.3340

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR_2 = (\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2])^{1/2}$

	$[(NO_3)_2@Pd_3L_4](ClO_4)_4\cdot 2C_6H_6\cdot 4Me_2SO$	$[(NO_3)(H_2O)(ClO_4)@Pd_3L_4](ClO_4)_4\cdot 3C_3H_7NO$	$[(ClO_4)_2@Pd_3L_4](ClO_4)_4\cdot 2Me_2SO$
Formula	$C_{112}H_{128}Cl_{14}N_{14}O_{42}Pd_3S_4$	$C_{95}H_{101}Cl_4N_{15}O_{40}Pd_3$	$C_{96}H_{104}Cl_{16}N_{12}O_{42}Pd_3S_2$
M_w	2931.52	2553.90	2693.93
Cryst.sys.	Triclinic	Triclinic	Monoclinic
Space group	*P-1*	*P-1*	*P2₁/n*
a (Å)	14.016(5)	14.393(3)	9.3150(19)
b (Å)	16.030(6)	19.113(4)	22.198(4)

c (Å)	18.468(7)	23.510(5)	28.653(6)
α (°)	66.969(2)	98.23(3)	90
β (°)	86.217(3)	106.16(3)	92.76(3)
γ (°)	70.922(3)	90.40(3)	90
V (Å^3)	3600(2)	6140(2)	5918(2)
Z	1	2	2
ρ (g cm^{-3})	1.352	1.381	1.512
μ (mm^{-1})	0.581	0.819	0.964
R_{int}	0.2015	0.0497	0.0817
GoF on F^2	0.972	1.106	2.067
R_1 [$I>2\sigma(I)$][a]	0.0746	0.1065	0.1057
wR_2 (all data)[b]	0.1824	0.3226	0.3159

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR_2 = (\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2])^{1/2}$

Table S2. Bond lengths (Å) and angles (°)

$[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$		$[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$		$[(NO_3)_2(H_2O)_2@Pd_3L_4](NO_3)_4\cdot 2C_6H_6\cdot Me_2SO$	
Pd(01)-N(00A)#1	2.020(2)	Pd(1)-N(12)	2.009(4)	Pd(1)-N(7)	2.003(7)
Pd(01)-N(00A)	2.020(2)	Pd(1)-N(10)	2.013(4)	Pd(1)-N(3)	2.016(10)
Pd(01)-N(1)	2.021(2)	Pd(1)-N(6)#1	2.036(3)	Pd(1)-N(5)	2.025(7)
Pd(01)-N(1)#1	2.021(2)	Pd(1)-N(6)	2.037(3)	Pd(1)-N(1)	2.027(10)
		Pd(2)-N(8)#1	2.018(4)	Pd(2)-N(2)	1.959(12)
N(00A)#1-Pd(01)-N(00A)	180.0	Pd(2)-N(11)	2.023(4)	Pd(2)-N(4)	2.003(12)
N(00A)#1-Pd(01)-N(1)	89.86(9)	Pd(2)-N(7)	2.027(4)	Pd(2)-N(6)#1	2.040(7)
N(00A)-Pd(01)-N(1)	90.14(9)	Pd(2)-N(9)#1	2.034(4)	Pd(2)-N(6)	2.040(7)
N(00A)#1-Pd(01)-N(1)#1	90.14(9)			Pd(3)-N(11)	2.014(8)
N(00A)-Pd(01)-N(1)#1	89.86(9)	N(12)-Pd(1)-N(10)	180.0	Pd(3)-N(13)	2.019(9)
N(1)-Pd(01)-N(1)#1	180.00(12)	N(12)-Pd(1)-N(6)#1	89.58(8)	Pd(3)-N(10)#2	2.029(7)
		N(10)-Pd(1)-N(6)#1	90.42(8)	Pd(3)-N(8)	2.043(7)
		N(12)-Pd(1)-N(6)	89.58(8)	Pd(4)-N(14)	2.017(11)
		N(10)-Pd(1)-N(6)	90.42(8)	Pd(4)-N(12)	2.023(10)
		N(6)#1-Pd(1)-N(6)	179.16(17)	Pd(4)-N(9)	2.036(6)
		N(8)#1-Pd(2)-N(11)	88.62(17)	Pd(4)-N(9)#2	2.036(6)
		N(8)#1-Pd(2)-N(7)	176.70(16)		
		N(11)-Pd(2)-N(7)	90.85(17)	N(7)-Pd(1)-N(3)	89.6(3)
		N(8)#1-Pd(2)-N(9)#1	90.40(16)	N(7)-Pd(1)-N(5)	175.5(3)
		N(11)-Pd(2)-N(9)#1	177.06(17)	N(3)-Pd(1)-N(5)	91.9(3)
		N(7)-Pd(2)-N(9)#1	90.40(16)	N(7)-Pd(1)-N(1)	88.7(3)
				N(3)-Pd(1)-N(1)	178.2(3)
				N(5)-Pd(1)-N(1)	89.7(3)
				N(2)-Pd(2)-N(4)	180.0
				N(2)-Pd(2)-N(6)#1	88.9(2)
				N(4)-Pd(2)-N(6)#1	91.1(2)
				N(2)-Pd(2)-N(6)	88.9(2)
				N(4)-Pd(2)-N(6)	91.1(2)
				N(6)#1-Pd(2)-N(6)	177.9(4)
				N(11)-Pd(3)-N(13)	177.5(3)
				N(11)-Pd(3)-N(10)#2	90.1(3)
				N(13)-Pd(3)-N(10)#2	88.6(3)
				N(11)-Pd(3)-N(8)	90.1(3)
				N(13)-Pd(3)-N(8)	91.0(3)

				N(10)#2-Pd(3)-N(8)	177.5(3)
				N(14)-Pd(4)-N(12)	180.0
				N(14)-Pd(4)-N(9)	89.93(19)
				N(12)-Pd(4)-N(9)	90.07(19)
				N(14)-Pd(4)-N(9)#2	89.93(19)
				N(12)-Pd(4)-N(9)#2	90.07(19)
				N(9)-Pd(4)-N(9)#2	179.9(4)

[#1] −x+1, −y, −z+1 [#1] −x+1, y, −z+3/2 [#1] −x+1/2,y,−z+1/2
[#2] −x+3/2,y,−z+1/2

$[(NO_3)_2@Pd_3L_4](PF_6)_4\cdot 6Me_2SO$		$[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4\cdot 3C_3H_7NO$		$[(PF_6)_2@Pd_3L_4](PF_6)_4\cdot 4C_3H_7NO$	
Pd(01)-N(2)	2.0214(18)	Pd(01)-N(8)	2.032(3)	Pd(1)-N(5)#1	1.978(11)
Pd(01)-N(2)#1	2.0214(18)	Pd(01)-N(5)	2.037(3)	Pd(1)-N(5)	1.978(11)
Pd(01)-N(5)	2.0356(19)	Pd(01)-N(11)	2.044(3)	Pd(1)-N(2)	2.053(9)
Pd(01)-N(5)#1	2.0356(19)	Pd(01)-N(2)	2.053(3)	Pd(1)-N(2)#1	2.053(9)
N(1)-Pd(02)#1	2.023(2)	N(1)-Pd(03)	2.025(3)	Pd(2)-N(4)#2	1.999(10)
Pd(02)-N(6)	2.019(2)	Pd(02)-N(3)	2.021(3)	Pd(2)-N(4)	1.999(10)
Pd(02)-N(3)	2.020(2)	Pd(02)-N(9)	2.021(3)	Pd(2)-N(1)#2	2.009(9)
Pd(02)-N(4)#1	2.029(2)	Pd(02)-N(12)	2.027(3)	Pd(2)-N(1)	2.009(9)
		Pd(02)-N(6)	2.031(4)		
N(2)-Pd(01)-N(2)#1	180.0	Pd(03)-N(4)	2.025(4)	N(5)#1-Pd(1)-N(5)	180.0
N(2)-Pd(01)-N(5)	94.36(8)	Pd(03)-N(10)	2.036(3)	N(5)#1-Pd(1)-N(2)	86.1(3)
N(2)#1-Pd(01)-N(5)	85.65(8)	Pd(03)-N(7)	2.040(3)	N(5)-Pd(1)-N(2)	93.9(3)
N(2)-Pd(01)-N(5)#1	85.65(8)			N(5)#1-Pd(1)-N(2)#1	93.9(3)
N(2)#1-Pd(01)-N(5)#1	94.35(8)	N(8)-Pd(01)-N(5)	90.97(12)	N(5)-Pd(1)-N(2)#1	86.1(3)
N(5)-Pd(01)-N(5)#1	180.0	N(8)-Pd(01)-N(11)	87.45(12)	N(2)-Pd(1)-N(2)#1	180.0
N(6)-Pd(02)-N(3)	90.04(9)	N(5)-Pd(01)-N(11)	177.24(11)	N(4) -Pd(2)-N(4)#2	178.9(4)
N(6)-Pd(02)-N(1)#1	90.13(9)	N(8)-Pd(01)-N(2)	176.99(12)	N(4)-Pd(2)-N(1)#2	90.5(4)
N(3)-Pd(02)-N(1)#1	178.56(7)	N(5)-Pd(01)-N(2)	87.32(11)	N(4)#2-Pd(2)-N(1)#2	89.5(4)
N(6)-Pd(02)-N(4)#1	177.98(7)	N(11)-Pd(01)-N(2)	94.16(12)	N(4)-Pd(2)-N(1)	89.5(4)
N(3)-Pd(02)-N(4)#1	89.41(9)	N(3)-Pd(02)-N(9)	178.17(14)	N(4)#2-Pd(2)-N(1)	90.5(4)
N(1)#1-Pd(02)-N(4)#1	90.37(9)	N(3)-Pd(02)-N(12)	89.19(13)	N(1)#2-Pd(2)-N(1)	179.8(4)
		N(9)-Pd(02)-N(12)	89.44(14)		
		N(3)-Pd(02)-N(6)	90.76(14)		
		N(9)-Pd(02)-N(6)	90.59(15)		
		N(12)-Pd(02)-N(6)	179.26(13)		
		N(1)-Pd(03)-N(4)	89.73(13)		

		N(1)-Pd(03)-N(10)	89.78(13)		
		N(4)-Pd(03)-N(10)	177.65(14)		
		N(1)-Pd(03)-N(7)	177.34(14)		
		N(4)-Pd(03)-N(7)	89.50(14)		
		N(10)-Pd(03)-N(7)	90.89(13)		

#1 −x+1, −y+1, −z+1

#1 −x, −y, −z+1
#2 −x, y, −z+1

$[(NO_3)_2@Pd_3L_4](ClO_4)_4\cdot 2C_6H_6\cdot 4Me_2SO$		$[(NO_3)(H_2O)(ClO_4)@Pd_3L_4](ClO_4)_4\cdot 3C_3H_7NO$		$[(ClO_4)_2@Pd_3L_4](ClO_4)_4\cdot 2Me_2SO$	
N(1)-Pd(02)#1	2.025(7)	N(1)-Pd(03)	2.002(10)	Pd(1)-N(2)	2.014(8)
Pd(01)-N(5)#1	2.039(6)	Pd(01)-N(11)	2.030(7)	Pd(1)-N(2)#1	2.014(8)
Pd(01)-N(5)	2.039(6)	Pd(01)-N(5)	2.042(7)	Pd(1)-N(5)#1	2.028(8)
Pd(01)-N(2)	2.048(7)	Pd(01)-N(2)	2.048(7)	Pd(1)-N(5)	2.028(8)
Pd(01)-N(2)#1	2.048(7)	Pd(01)-N(8)	2.058(6)	N(1)-Pd(2)#1	2.050(7)
Pd(02)-N(4)	2.014(7)	Pd(02)-N(12)	2.029(8)	Pd(2)-N(3)	2.032(7)
Pd(02)-N(3)	2.019(6)	Pd(02)-N(6)	2.019(7)	Pd(2)-N(6)	2.026(8)
Pd(02)-N(6)#1	2.042(7)	Pd(02)-N(9)	2.027(7)	Pd(2)-N(4)#1	2.056(8)
		Pd(02)-N(3)	2.041(8)		
N(5)#1-Pd(01)-N(5)	180.0	Pd(03)-N(10)	1.961(6)	N(2)#1-Pd(1)-N(2)	180.0
N(5)#1-Pd(01)-N(2)	85.4(2)	Pd(03)-N(7)	2.011(8)	N(2)#1-Pd(1)-N(5)#1	89.0(3)
N(5)-Pd(01)-N(2)	94.6(2)	Pd(03)-N(4)	2.020(8)	N(2)-Pd(1)-N(5)#1	91.0(3)
N(5)#1-Pd(01)-N(2)#1	94.6(2)			N(2)#1-Pd(1)-N(5)	91.0(3)
N(5)-Pd(01)-N(2)#1	85.4(2)	N(11)-Pd(01)-N(5)	175.8(2)	N(2)-Pd(1)-N(5)	89.0(3)
N(2)-Pd(01)-N(2)#1	180.0	N(11)-Pd(01)-N(2)	91.3(3)	N(5)#1-Pd(1)-N(5)	180.0
N(4)-Pd(02)-N(3)	90.1(3)	N(5)-Pd(01)-N(2)	86.9(3)	N(3)-Pd(2)-N(6)	90.3(3)
N(4)-Pd(02)-N(1)#1	90.2(4)	N(11)-Pd(01)-N(8)	86.6(3)	N(3)-Pd(2)-N(1)#1	178.8(3)
N(3)-Pd(02)-N(1)#1	178.2(3)	N(5)-Pd(01)-N(8)	95.1(3)	N(6)-Pd(2)-N(1)#1	88.8(3)
N(4)-Pd(02)-N(6)#1	177.0(3)	N(2)-Pd(01)-N(8)	176.2(3)	N(3)-Pd(2)-N(4)#1	89.9(3)
N(3)-Pd(02)-N(6)#1	88.9(3)	N(12)-Pd(02)-N(6)	177.7(3)	N(6)-Pd(2)-N(4)#1	178.2(3)
N(1)#1-Pd(02)-N(6)#1	90.7(3)	N(12)-Pd(02)-N(9)	89.1(3)	N(1)#1-Pd(2)-N(4)#1	91.0(3)
		N(6)-Pd(02)-N(9)	90.6(3)		
		N(6)-Pd(02)-N(12)	177.9(3)		
		N(9)-Pd(02)-N(12)	89.4(3)		
		N(6)-Pd(02)-N(3)	89.4(3)		
		N(9)-Pd(02)-N(3)	177.4(3)		
		N(12)-Pd(02)-N(3)	90.5(3)		
		N(10)-Pd(03)-N(1)	92.1(4)		

N(10)-Pd(03)-N(7)	90.2(3)
N(1)-Pd(03)-N(7)	177.3(4)
N(10)-Pd(03)-N(4)	179.0(3)
N(1)-Pd(03)-N(4)	88.9(4)
N(7)-Pd(03)-N(4)	88.8(3)

[#1] –x+1, –y+1, –z+1

[#1] –x, –y+1, –z+1

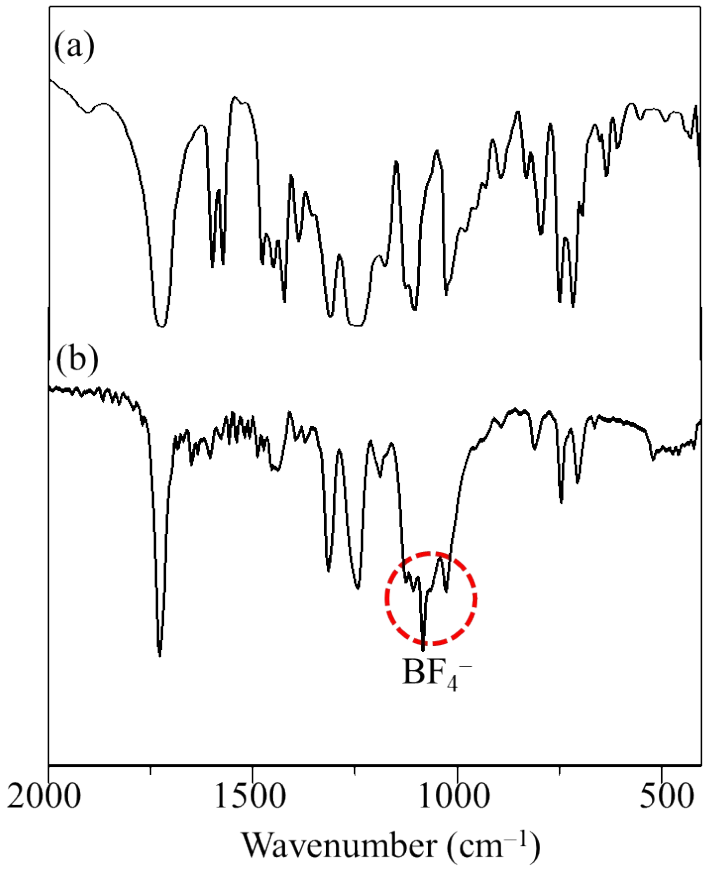

Fig. S1 IR spectra of Ligand (a) and $[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$ (b).

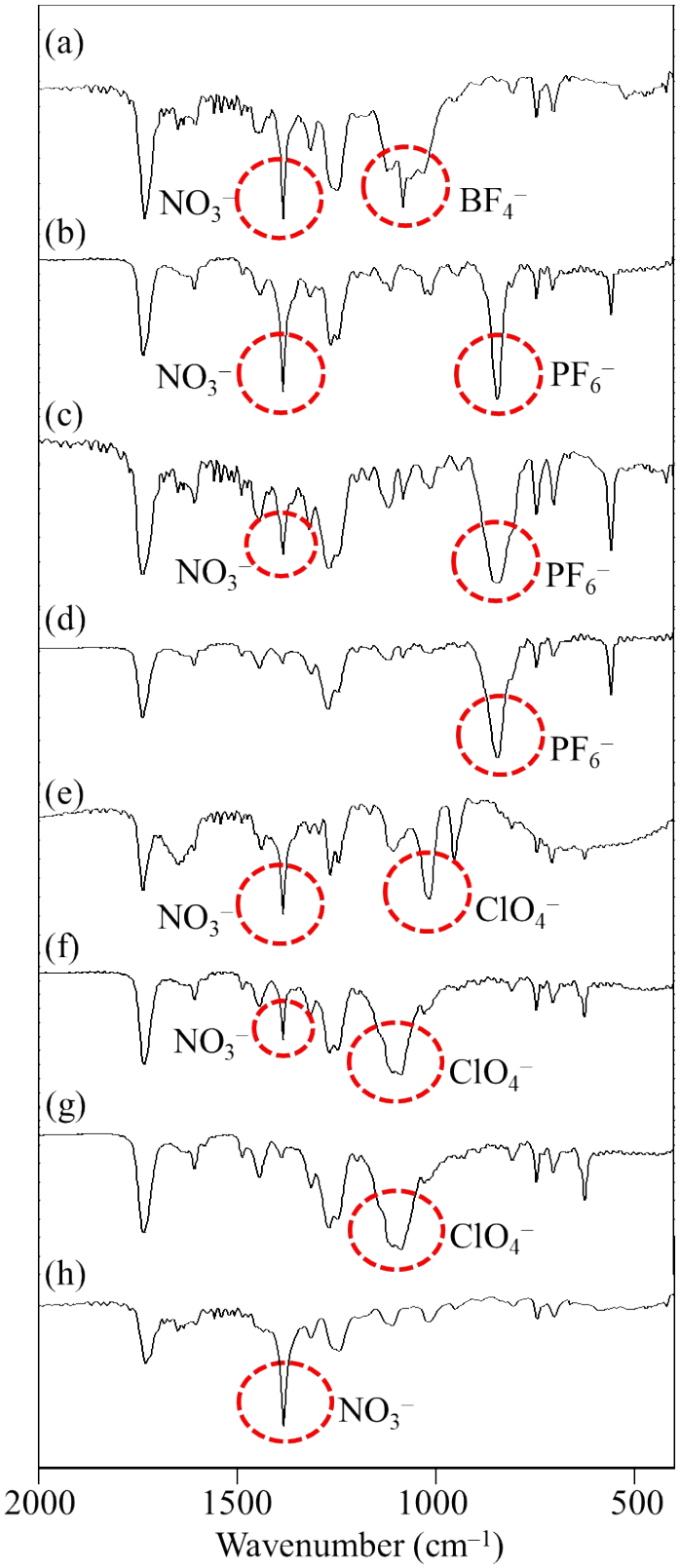

Fig. S2 IR spectra of $[(NO_3)_2(H_2O)_2Pd_3L_4](BF_4)_4 \cdot 6C_3H_7NO$ (a), $[(NO_3)_2@Pd_3L_4](PF_6)_4 \cdot 6Me_2SO$ (b), $[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4 \cdot 3C_3H_7NO$ (c), $[(PF_6)_2@Pd_3L_4](PF_6)_4 \cdot 4C_3H_7NO$ (d), $[(NO_3)_2@Pd_3L_4](ClO_4)_4 \cdot 2C_6H_6 \cdot 4Me_2SO$ (e), $[(NO_3)(H_2O)(ClO_4)@Pd_3L_4](ClO_4)_4 \cdot 3C_3H_7NO$ (f), $[(ClO_4)_2@Pd_3L_4](ClO_4)_4 \cdot 2Me_2SO$ (g), and $[(NO_3)_2(H_2O)_2@Pd_3L_4](NO_3)_4 \cdot 2C_6H_6 \cdot Me_2SO$ (h).

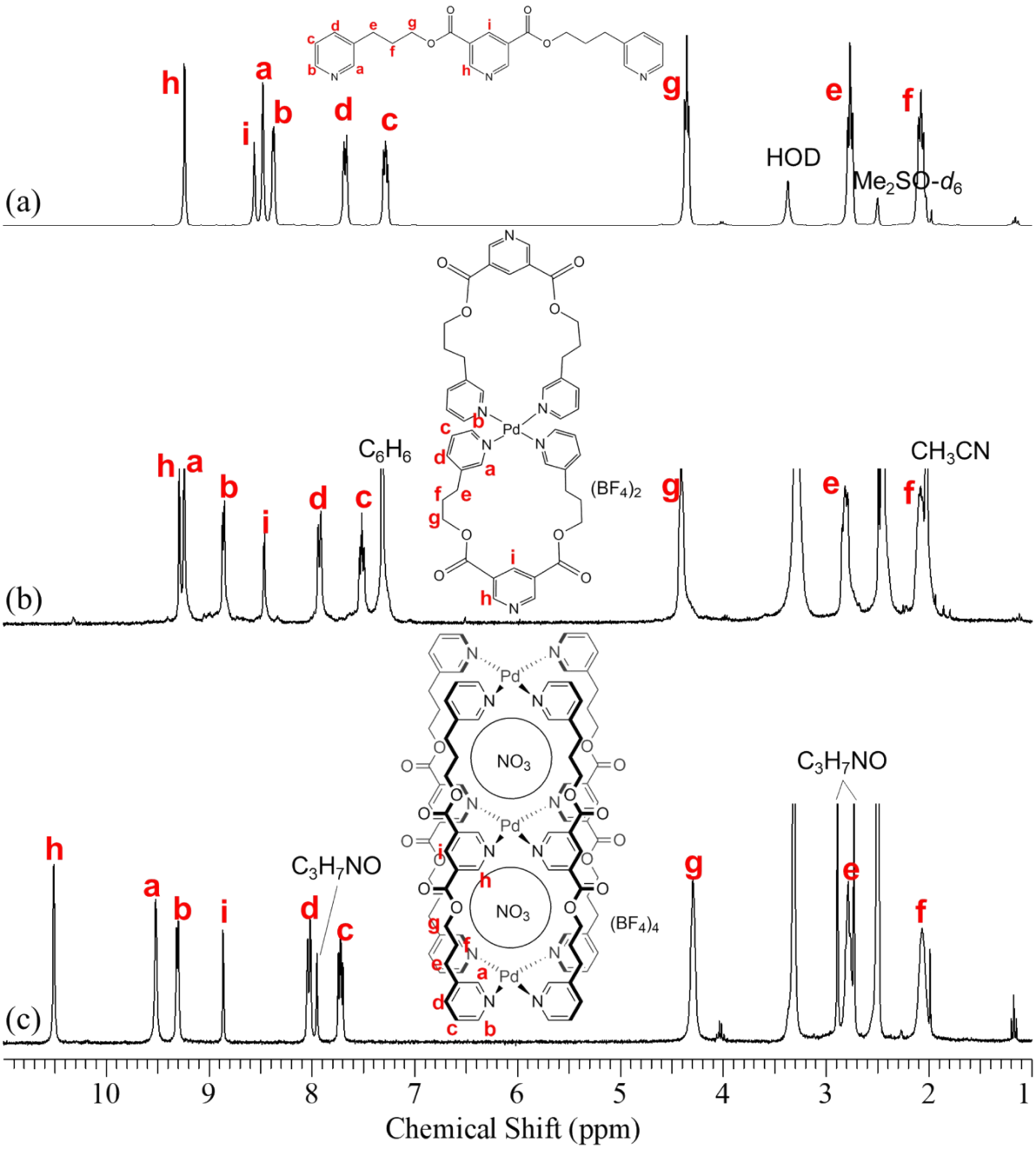

Fig. S3 ^{1}H NMR spectra of Ligand (a), $[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$ (b), and $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$ (c).

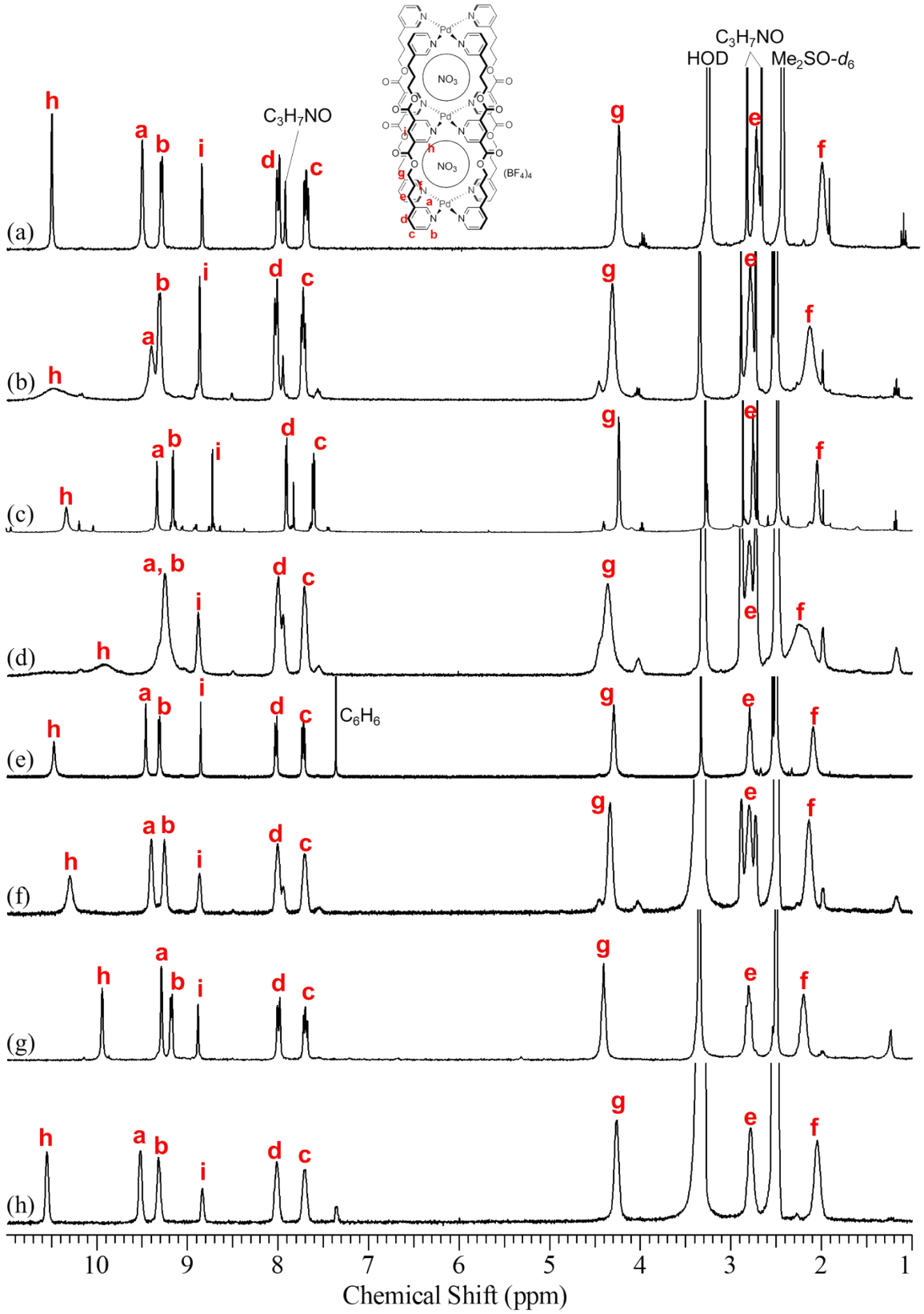

Fig. S4 ^{1}H NMR spectra of $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4{\cdot}6C_3H_7NO$ (a), $[(NO_3)_2@Pd_3L_4](PF_6)_4{\cdot}6Me_2SO$ (b), $[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4{\cdot}3C_3H_7NO$ (c), $[(PF_6)_2@Pd_3L_4](PF_6)_4{\cdot}4C_3H_7NO$ (d), $[(NO_3)_2@Pd_3L_4](ClO_4)_4{\cdot}2C_6H_6{\cdot}4Me_2SO$ (e), $[(NO_3)(H_2O)(ClO_4)@Pd_3L_4](ClO_4)_4{\cdot}3C_3H_7NO$ (f), $[(ClO_4)_2@Pd_3L_4](ClO_4)_4{\cdot}2Me_2SO$ (g), and $[(NO_3)_2(H_2O)_2@Pd_3L_4](NO_3)_4{\cdot}2C_6H_6{\cdot}Me_2SO$ (h).

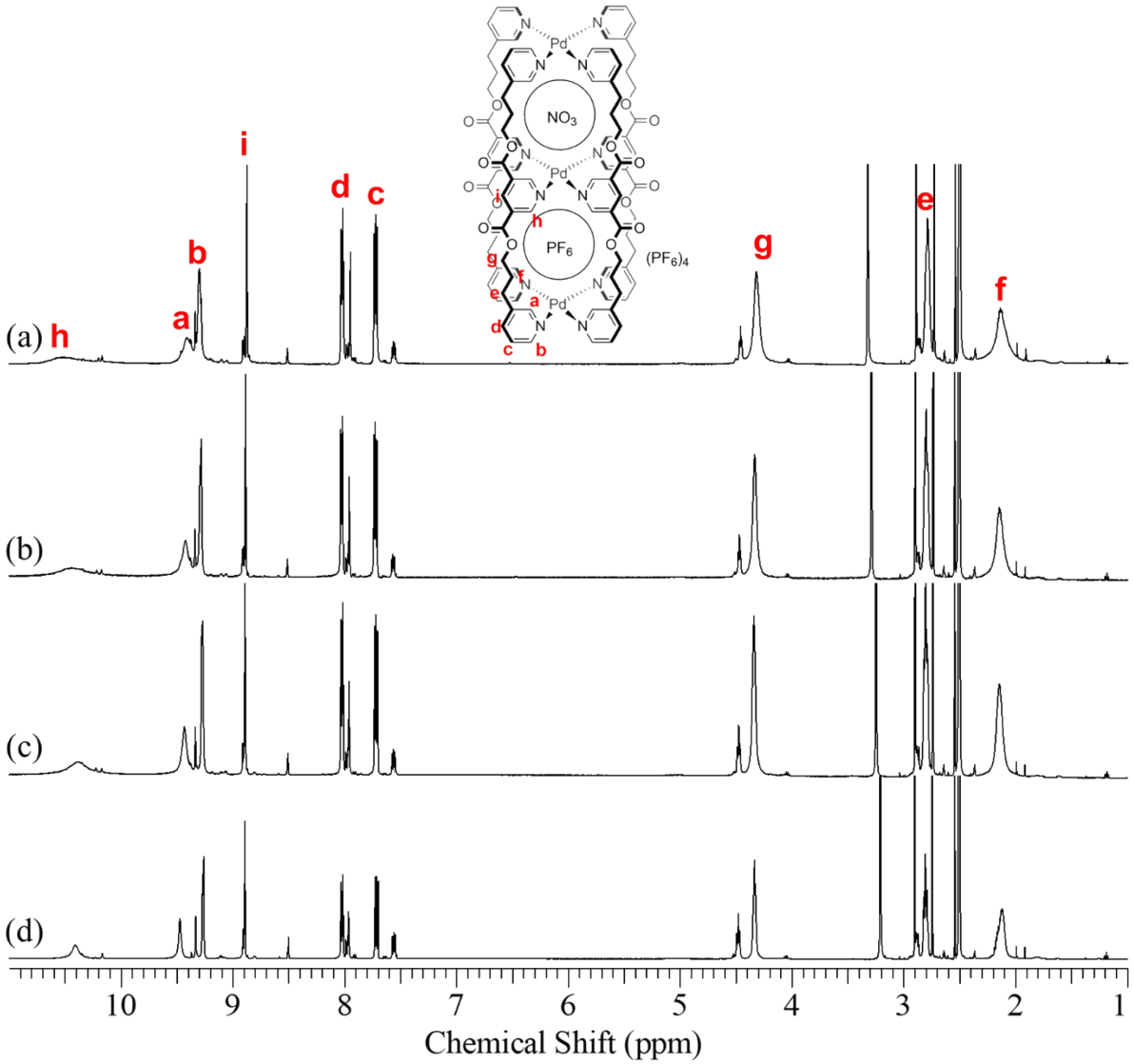

Fig. S5 ^{1}H NMR spectra of

$[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4 \cdot 3C_3H_7NO$ at 25 ℃ (a),
$[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4 \cdot 3C_3H_7NO$ at 35 ℃ (b),
$[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4 \cdot 3C_3H_7NO$ at 45 ℃ (c), and
$[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4 \cdot 3C_3H_7NO$ at 55 ℃ (d).

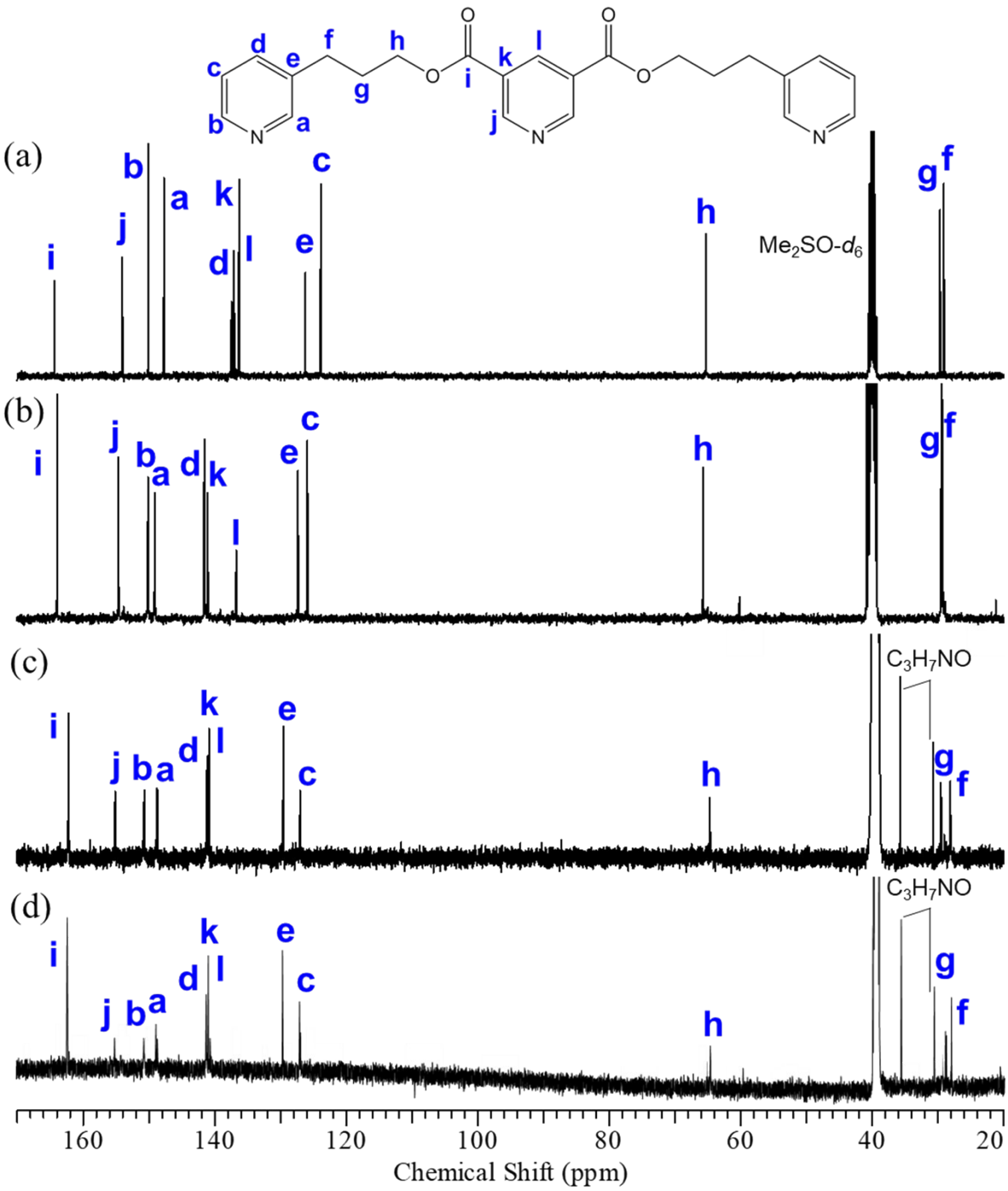

Fig. S6 ^{13}C NMR spectra of Ligand (a), $[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$ (b), $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$ (c), and $[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4\cdot 3C_3H_7NO$ (d).

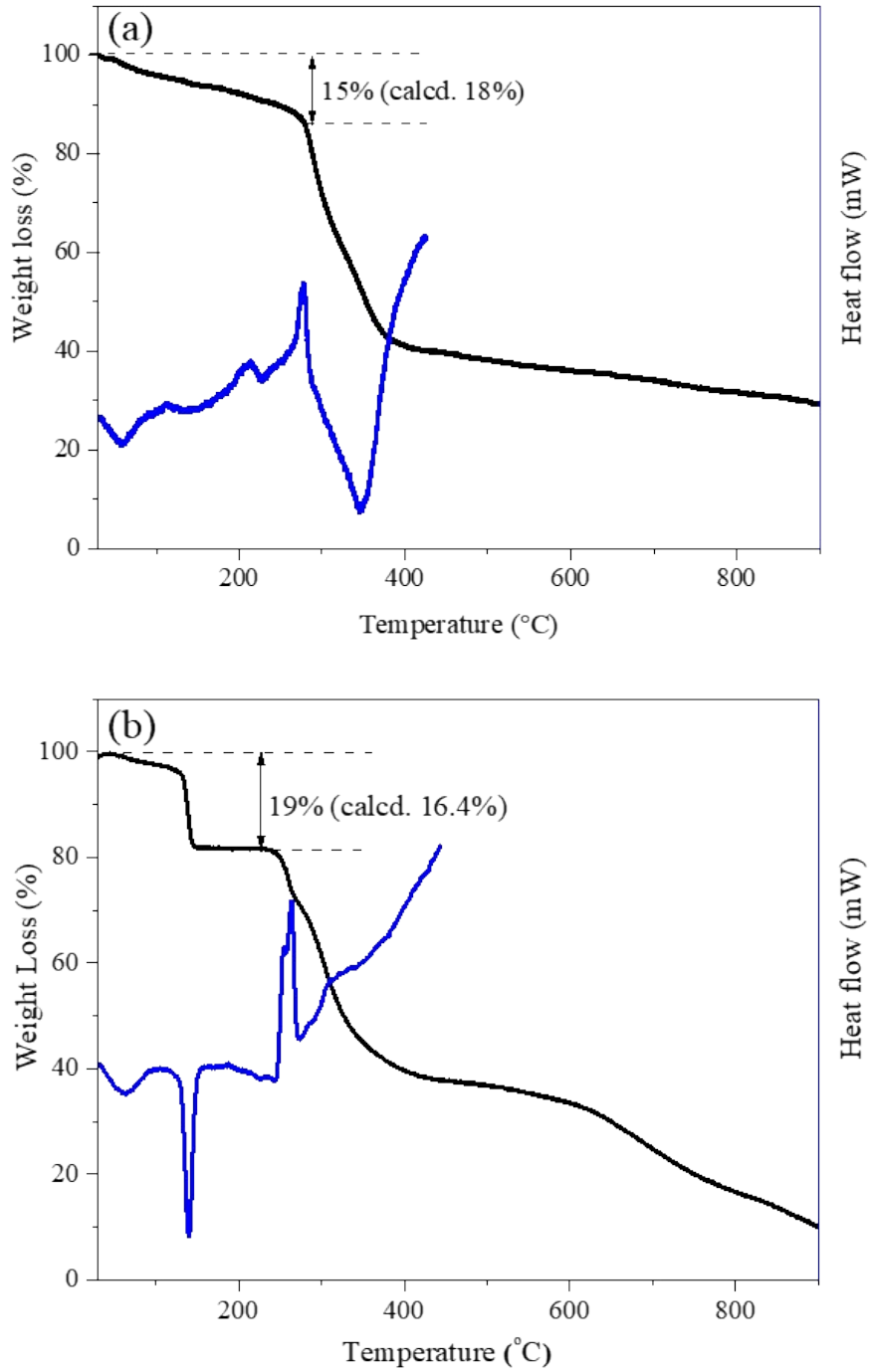

Fig. S7 TGA and DSC overlay of $[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$ (a) and $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$ (b).

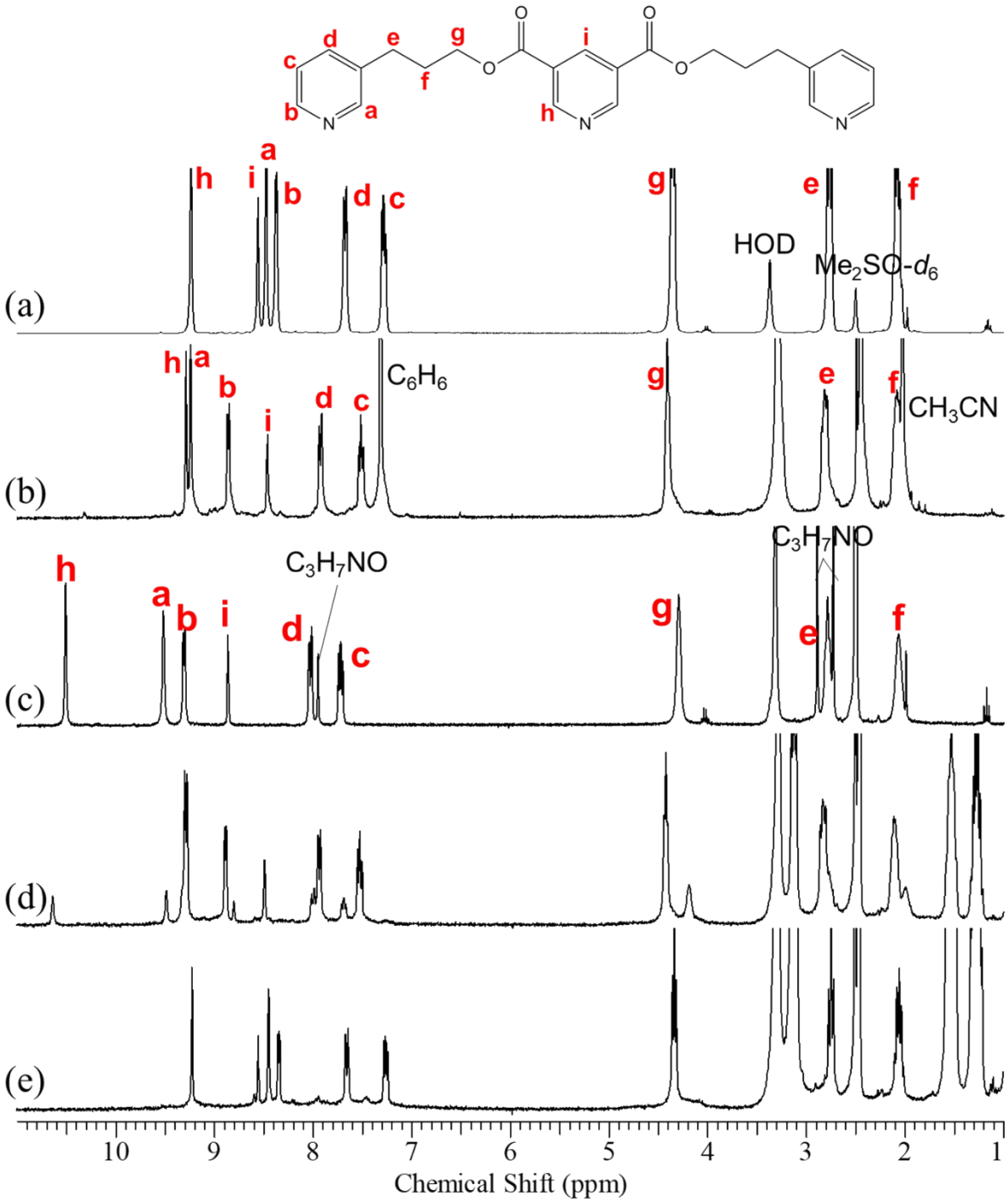

Fig. S8 ^{1}H NMR of Ligand (a), $[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$ (b), $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$ (c), $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$+TBAF (2 eq) (d), and $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$+TBAF (10 eq) (e).

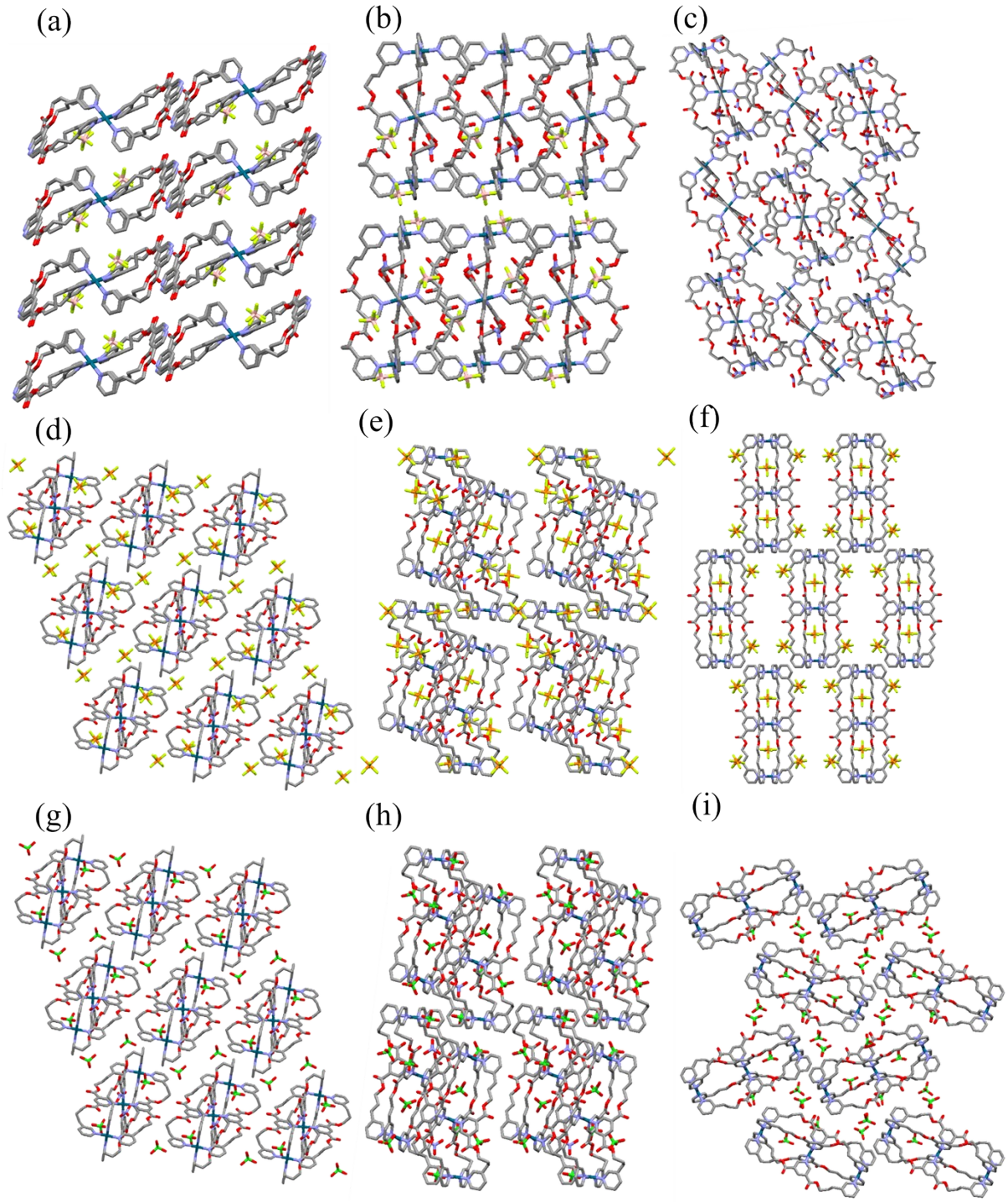

Fig. S9 Crystal structures of $[PdL_2]\cdot(BF_4)_2\cdot 2C_6H_6\cdot 2CH_3CN$ (a), $[(NO_3)_2(H_2O)_2@Pd_3L_4](BF_4)_4\cdot 6C_3H_7NO$ (b), $[(NO_3)_2(H_2O)_2@Pd_3L_4](NO_3)_4\cdot 2C_6H_6\cdot Me_2SO$ (c), $[(NO_3)_2@Pd_3L_4](PF_6)_4\cdot 6Me_2SO$ (d), $[(NO_3)(H_2O)(PF_6)@Pd_3L_4](PF_6)_4\cdot 3C_3H_7NO$ (e), $[(PF_6)_2@Pd_3L_4](PF_6)_4\cdot 4C_3H_7NO$ (f), $[(NO_3)_2@Pd_3L_4](ClO_4)_4\cdot 2C_6H_6\cdot 4Me_2SO$ (g), $[(NO_3)(H_2O)(ClO_4)@Pd_3L_4](ClO_4)_4\cdot 3C_3H_7NO$ (h), and $[(ClO_4)_2@Pd_3L_4](ClO_4)_4\cdot 2Me_2SO$ (i). (solvate molecules were omitted for clarity.)