

Na⁺ and Ca²⁺ Ion Selective Pyridylcarboxylate Rings of Pd(II) and Pt(II)

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Electronic Supplementary Information

Bond lengths/Å	1	2
Pt(1)-N(1)/ Pd(1)-N(1)	2.083 (6)	2.089 (4)
Pt(1)-O(1)/ Pd(1)-O(1)	2.083 (6)	2.083 (3)
Pd(2)-N(2)	2.087 (7)	-
Pd(2)-O(3)	2.086 (5)	-
Ca(1)-O(2)	2.337 (6)	-
Ca(1)-O(1W)	2.338 (7)	-
Ca(1)-O(8)	2.348 (7)	-
Ca(1)-O(2W)	2.349 (6)	-
Ca(1)-O(4)	2.355 (6)	-
Ca(1)-O(5)	2.360 (6)	-

Table 1: Selected bond lengths (Å) for [Pd₂Ca(OTf)₂(3-PyOAc)₂(H₂O)₂(dppf)₂](OTf)₂, **1** and [Pt₂(3-PyOAc)₂(dppf)₂](PF₆)₂, **2** (space group C2/c, symmetry operators: -x+1, y, -z+3/2).

Bond angles/°	1	2
N(1)-Pd(1)-O(1)/ N(1)#1-Pt(1)-O(1)	86.6 (2)	83.06 (14)
N(2)-Pd(2)-O(3)	86.8 (2)	-
N(1)-Pd(1)-P(1)/ N(1)#1-Pt(1)-P(1)	91.24 (19)	92.34 (11)
N(1)-Pd(1)-P(2)/ N(1)#1-Pt(1)-P(2)	169.0 (2)	167.99 (11)
O(1)-Pd(1)-P(1)/ O(1)-Pt(1)-P(1)	177.75 (16)	174.88 (10)
O(1)-Pd(1)-P(2)/ O(1)-Pt(1)-P(2)	84.65 (16)	84.94 (10)
P(1)-Pd(1)-P(2)/ P(1)-Pt(1)-P(2)	97.57 (8)	99.63 (4)
O(2)-Ca(1)-O(1W)	178.4 (3)	-
O(2)-Ca(1)-O(8)	93.6 (2)	-
O(1W)-Ca(1)-O(8)	87.2 (3)	-
O(2)-Ca(1)-O(2W)	91.3 (2)	-
O(1W)-Ca(1)-O(2W)	90.2 (3)	-
O(8)-Ca(1)-O(2W)	82.6 (2)	-
O(2)-Ca(1)-O(4)	90.6 (2)	-
O(1W)-Ca(1)-O(4)	87.9 (2)	-
O(8)-Ca(1)-O(4)	98.6 (2)	-
O(2W)-Ca(1)-O(4)	177.7 (2)	-
O(2)-Ca(1)-O(5)	95.4 (2)	-
O(1W)-Ca(1)-O(5)	84.1 (2)	-
O(8)-Ca(1)-O(5)	164.7 (2)	-
O(2W)-Ca(1)-O(5)	84.9 (2)	-

O(4)-Ca(1)-O(5) 93.6 (2) -

Table 2: Selected bond angles (deg) for [Pd₂Ca(OTf)₂(3-PyOAc)₂(H₂O)₂(dppf)₂](OTf)₂, **1** and [Pt₂(3-PyOAc)₂(dppf)₂](PF₆)₂, **2** (space group C2/c, symmetry operators: -x+1, y, -z+3/2).

Bond lengths (Å)		Bond angles (°)	
Pt(1)-N(1)	2.074 (2)	N(1)-Pt(1)-O(2)#1	84.04 (11)
Pt(1)-O(2)#1	2.084 (2)	N(1)-Pt(1)-P(2)	92.47 (8)
Pt(1)-P(1)	2.2631 (11)	N(1)-Pt(1)-P(1)	168.65 (8)
Pt(1)-P(2)	2.2452 (10)	O(2)#1-Pt(1)-P(2)	176.50 (8)
		O(2)#1-Pt(1)-P(1)	84.65 (7)
		P(2)-Pt(1)-P(1)	98.82 (4)

Table 3: Selected bond lengths (Å) and bond angles (deg) [Pt₂(3-PyOAc)₂(PPh₃)₄](PF₆)₂, **3**, with space group C2/c, symmetry operators: -x+1, y, -z+1/2.

Bond lengths (Å)		Bond angles (°)	
Pt(1)-O(4)	2.069(6)	O(4)-Pt(1)-N(1)	86.1(2)
Pt(1)-N(1)	2.070(7)	O(4)-Pt(1)-P(1)	173.28(18)
Pt(1)-P(1)	2.235(2)	N(1)-Pt(1)-P(1)	92.80(19)
Pt(1)-P(2)	2.262(2)	O(4)-Pt(1)-P(2)	82.50(17)
Pt(2)-O(1)	2.055(6)	N(1)-Pt(1)-P(2)	167.72(19)
Pt(2)-N(2)	2.063(6)	P(1)-Pt(1)-P(2)	99.08(8)
Pt(2)-P(4)	2.240(2)	O(1)-Pt(2)-N(2)	87.0(3)
Pt(2)-P(3)	2.267(2)	O(1)-Pt(2)-P(4)	174.48(18)
Na(1)-O(2)	2.274(6)	N(2)-Pt(2)-P(4)	91.4(2)
Na(1)-O(3)	2.285(7)	O(1)-Pt(2)-P(3)	83.10(17)
Na(1)-O(7)	2.293(13)	N(2)-Pt(2)-P(3)	170.1(2)
Na(1)-O(9)	2.441(11)	P(4)-Pt(2)-P(3)	98.48(8)
		O(2)-Na(1)-O(3)	102.8(3)
		O(2)-Na(1)-O(7)	115.5(4)
		O(3)-Na(1)-O(7)	119.8(4)
		O(2)-Na(1)-O(9)	86.0(3)
		O(3)-Na(1)-O(9)	121.3(3)
		O(7)-Na(1)-O(9)	106.5(4)

Table 4: Selected bond lengths (Å) and bond angles (°) for [Pt₂Na(3-PyPrO₂)₂(OTf)₂(dppf)₂](OTf), **4**

Bond lengths/Å	5	6
Pt(1)-O(1)/	2.104 (14)	2.098 (10)
Pd(1)-O(1)		
Pt(1)-N(1)/	2.049 (16)	2.157 (12)
Pd(1)-N(1)		
Pt(1)-P(1)/	2.269 (6)	2.334 (4)
Pd(1)-P(1)		
Pt(1)-P(2)/	2.256 (6)	2.314 (4)
Pd(1)-P(2)		
Pt(2)-O(3)/	2.075 (13)	-
Pd(2)-O(1)		
Pt(2)-N(2)/	2.086 (14)	-
Pd(2)-N(2)		
Pt(2)-P(4)/	2.277 (5)	-
Pd(2)-P(4)		
Pt(2)-P(3)/	2.242 (5)	-
Pd(2)-P(3)		
Na(1)-O(2)/	2.291 (15)	2.348 (14)
Ca(1)-O(2)		
Na(1)-O(4)/	2.251 (15)	2.345 (14)
Ca(1)-O(3)		
Na(1)-O(6)/	2.20 (2)	2.348 (14)
Ca(1)-O(2)#1		
Na(1)-O(9)/	2.438 (17)	2.345 (14)
Ca(1)-O(2)#1		

Table 5: Selected bond lengths (Å) for [Pt₂Na(3-PyPrO₂)₂(OTf)₂(PPh₃)₄](OTf), **5** and [Pd₂Ca(3-PyPrO₂)₂(OTf)₂(dppf)₂](OTf), **6** (space group Pccn, symmetry operators: -x+3/2, -y+1/2, z).

Bond lengths/Å	5	6
O(1)-M(1)-N(1)	86.1 (6)	91.0 (4)
O(1)-M(1)-P(1)	85.4 (4)	80.0 (3)
N(1)-M(1)-P(1)	171.4 (4)	169.2 (4)
O(1)-M(1)-P(2)	176.8 (4)	176.5 (4)
N(1)-M(1)-P(2)	92.1 (4)	87.6 (3)
P(1)-M(1)-P(2)	96.4 (2)	101.10 (14)
O(3)-M(2)-N(2)	86.5 (5)	-
O(3)-M(2)-P(4)	86.6 (4)	-
N(2)-M(2)-P(4)	172.9 (4)	-
O(3)-M(2)-P(3)	175.7 (4)	-
N(2)-M(2)-P(3)	91.6 (4)	-
P(4)-M(2)-P(3)	95.25 (18)	-
O(2)-Na(1)-O(4)/ O(3)-Ca(1)-O(3)#1	113.2 (6)	107.7 (7)
O(4)-Na(1)-O(8)/ O(2)-Ca(1)-O(3)#1	134.4 (6)	127.2 (5)
O(2)-Na(1)-O(8)/ O(3)-Ca(1)-O(2)	108.0 (6)	101.5 (5)
O(4)-Na(1)-O(9)/ O(2)-Ca(1)-O(2)#1	92.9 (6)	94.1 (7)
O(2)-Na(1)-O(9)/ O(3)-Ca(1)-O(2)#1	111.3 (6)	127.2 (5)

O(6)-Na(1)-O(9)/ 133.1 (9) 101.5 (5)
 O(3)#1-Ca(1)-O(2)#1

Table 6: Selected bond angles (deg) for $[\text{Pt}_2\text{Na}(3\text{-PyPrO}_2)_2(\text{OTf})_2(\text{PPh}_3)_4](\text{OTf})$, **5** and $[\text{Pd}_2\text{Ca}(3\text{-PyPrO}_2)_2(\text{OTf})_2(\text{dppf})_2](\text{OTf})$, **6**, where M= Pt for **5** and M=Pd for **6** (space group Pccn, symmetry operators: $-x+3/2, -y+1/2, z$).

Bond lengths/ Å		Bond angles/ °	
Pd(1)-O(1)	2.037 (7)	O(1)-Pd(1)-N(2)	90.8 (3)
Pd(1)-N(2)	2.105 (8)	O(1)-Pd(1)-P(2)	177.4 (2)
Pd(2)-O(3)	2.076 (7)	N(2)-Pd(1)-P(2)	90.3 (2)
Pd(2)-N(1)	2.077 (9)	O(1)-Pd(1)-P(1)	79.7 (2)
Pd(1)-P(1)	2.291 (3)	N(2)-Pd(1)-P(1)	170.1 (2)
Pd(1)-P(2)	2.263 (3)	P(2)-Pd(1)-P(1)	99.05 (11)
Pd(2)-P(3)	2.278 (3)	N(1)-Pd(2)-O(3)	87.7 (3)
Pd(2)-P(4)	2.281 (3)	N(1)-Pd(2)-P(4)	166.5 (2)
C(1)-O(1)	1.312 (12)	O(3)-Pd(2)-P(4)	84.4 (2)
C(1)-O(2)	1.231 (13)	N(1)-Pd(2)-P(3)	89.5 (3)
C(9)-O(3)	1.306 (13)	O(3)-Pd(2)-P(3)	176.8 (2)
C(9)-O(4)	1.230 (13)	P(4)-Pd(2)-P(3)	98.72 (11)

Table 7: Selected bond lengths (Å) and bond angles (°) for $[\text{Pd}(4\text{-PyPrO}_2)(\text{dppf})_2](\text{OTf})_2$, **7**.

Bond lengths/ Å		Bond angles/ °	
Pt(1)-N(1)	2.072(10)	N(1)-Pt(1)-P(1)	91.9(3)
Pt(1)-P(1)	2.251(3)	N(1)-Pt(1)-P(2)	170.0(3)

Pt(1)-P(2)	2.269(3)	P(1)-Pt(1)-P(2)	97.77(11)
Pt(1)-Cl(1)	2.336(3)	N(1)-Pt(1)-Cl(1)	83.9(3)
O(1)-C(8)	1.20(2)	P(1)-Pt(1)-Cl(1)	173.31(13)
O(2)-C(8)	1.31(2)	P(2)-Pt(1)-Cl(1)	86.74(11)

Table 8: Selected bond angles (°) and bond angles (°) for [PtCl(4-PyPrO₂H)(dppf)](OTf), **8**.