Electronic Supplementary Information (ESI)

Intermolecular interactions in dictating the self-assembly of halogen derivatives of bis-(*N*-substituted oxamato)palladate(II) complexes

Francisco Ramón Fortea-Pérez, [†] Nadia Marico, [‡] Giovanni De Munno, [‡] Donatella Armentano, [‡,*] Miguel Julve, [†] Salah-Eddine Stiriba[†,‖,*]

[†] *Instituto de Ciencia Molecular (ICMol), Universitat de València, C/ Catedrático José Beltrán 2, 46980 Paterna, València, Spain*

[‡]*Dipartimento di Chimica e Tecnologie Chimiche (CTC), Università della Calabria, 87036 Rende, Cosenza, Italy.*

‖ *Equipe de Chimie Moléculaire, Matériaux et Modélisation- C3M, Faculté Polydisciplinaire de Safi, Université Cadi Ayyad, Safi, Morocco.*

Table S1. Crystal Data and Data Collection Parameters for **1-3**

	1	**2**	**3**
Formula	$C_{48}H_{80}N_4O_6F_2Pd$	$C_{48}H_{88}N_4O_{10}Cl_2Pd$	$C_{48}H_{88}N_4O_{10}Br_2Pd$
*M*r	953.56	1058.52	1147.44
Crystal	Monoclinic	Triclinic	Monoclinic
Space	$P2_{1/c}$	*P*-1	$P2_{/c}$
a /Å	9.6448(7)	12.5224(9)	14.827(4)
b /Å	16.3141(12)	15.6996(11)	14.635(4)
c /Å	16.9067(13)	17.1433(13)	15.017(4)
α / º	90	65.551(3)	90
β / º	92.808(3)	69.815(4)	114.983(9)
γ / º	90	82.697(4)	90
V / Å^3	2657.0(3)	2830.8(4)	2953.8(13)
Z	2	2	2
D_c / g cm $^{-3}$	1.192	1.242	1.290
T / K	293(2)	293(2)	293
μ / mm^{-1}	0.402	0.475	1.718
F(000)	1016	11128	1200
Reflections collected	34933	54404	27339
Independent reflections	5622 [*R*(int) = 0.0507]	11951 [*R*(int) = 0.0600]	5573 [*R*(int) = 0.0615]
Data/restraints/ parameters	5622/190 /281	11951/0/597	5573/242/309
Goodness-of-fit on F^2	1.094	1.000	1.045
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0294, wR_2 = 0.0855	R_1 = 0.0583, wR_2 = 0.1630	R_1 = 0.0433, wR_2 = 0.1189
R indices (all data)	R_1 = 0.0422, wR_2 = 0.1008	R_1 = 0.0840, wR_2 = 0.1878	R_1 = 0.0554, wR_2 = 0.1276
Largest diff. peak and hole / e Å^{-3}	0.390 and -0.570	0.947 and -0.438	0.867 and -0.927

Table S2. Selected bond lengths (Å) and angles (deg) for **1***

Pd(1)-O(1)	Pd(1)-N(1)
O(1)-Pd(1)-O(1a)	O(1a)-Pd(1)-N(1)
O(1)-Pd(1)-N(1)	

*Symmetry transformations used to generate equivalent atoms:
(a) = -*x*+1, -*y*+1, -*z*.

Table S3. Selected bond lengths (Å) and angles (deg) for **2***

Pd(1)-O(1)	O(4)-Pd(2)
Pd(1)-N(1)	N(2)-Pd(2)
O(1a)-Pd(1)-O(1)	O(4b)-Pd(2)-N(2)
O(1)-Pd(1)-N(1a)	O(4)-Pd(2)-N(2)
O(1)-Pd(1)-N(1)	O(4)-Pd(2)-N(2b)
N(1a)-Pd(1)-N(1)	N(2)-Pd(2)-N(2b)
O(4b)-Pd(2)-O(4)	

*Symmetry transformations used to generate equivalent atoms:
(a) = -*x*+2, -*y*, -*z*+1. (b) = -*x*+2, -*y*, -*z*+2.

Table S4. Selected bond lengths (Å) and angles (deg) for **3***

Pd(1)-O(1)	Pd(1)-N(1)
O(1a)-Pd(1)-O(1)	O(1)-Pd(1)-N(1)
O(1a)-Pd(1)-N(1)	N(1)-Pd(1)-N(1a)

*Symmetry transformations used to generate equivalent atoms:
(a) = -*x*+1, *y*, -*z*+1/2.

Table S5. Hydrogen bonds lengths (Å) for **2***

O(1W)···O(3)	2.853(4)	O(2W)···O(2)	2.915(4)
O(1W)···O(3c)	2.900(4)	O(2W)···O(3W)	2.782(4)
O(1W)···O(2W)	2.660(4)	O(3W)···O(3Wd)	2.817(4)

*Symmetry transformations used to generate equivalent atoms:
(c) = 1-*x*, -*y*, 1-*z*; (d) = 1-*x*, 1-*y*, 1-*z*.

Table S6. Hydrogen bonds lengths (Å) for **3***

O(1W)···O(2)	2.840(4)	O(1W)···O(2W)	2.859(4)
O(1W)···O(1Wb)	2.893(4)	O(2W)···O(3)	2.817(4)
O(2W)···O(2Wb)	2.840(4)		

*Symmetry transformations used to generate equivalent atoms:
(b) = -*x*, *y*, -*z*+1/2.