Supplementary Materials

Synthesis and Characterization of New Guanine Complexes of Pt(IV) and Pd(II) by X-Ray Diffraction and Hirshfeld Surface Analysis

Anton Novikov, Mikhail Volkov, Alexey Safonov, Mikhail Grigoriev and Evgeny Abkhalimov *

Frumkin Institute of Physical Chemistry and Electrochemistry, RAS
* Correspondence: abkhalimov@ipc.rssi.ru

Table S1. Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd1	N19	2.028(3)	N12	C12	1.313(6)
Pd1	N9	2.012(3)	N3	C4	1.373(5)
Pd1	Cl2	2.3260(11)	N3	C2	1.360(6)
Pd1	Cl1	2.3148(11)	N9	C4	1.340(5)
O2	C16	1.216(5)	N9	C8	1.362(5)
O1	C6	1.210(5)	N17	C18	1.334(6)
N19	C14	1.348(5)	N17	C15	1.375(5)
N19	C18	1.313(6)	N2	C2	1.309(6)
N13	C12	1.348(6)	N1	C6	1.408(6)
N13	C14	1.366(5)	N1	C2	1.343(6)
N11	C12	1.352(6)	C16	C15	1.426(6)
N11	C16	1.411(6)	C6	C5	1.429(6)
N7	C5	1.369(6)	C5	C4	1.378(6)
N7	C8	1.343(5)	C14	C15	1.373(6)

Table S2. Bond Angles for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N19	Pd1	Cl2	88.32(11)	O2	C16	C15	127.7(4)
N19	Pd1	Cl1	90.37(11)	N11	C16	C15	111.2(4)
N9	Pd1	N19	179.72(15)	O1	C6	N1	118.8(4)
N9	Pd1	Cl2	91.40(11)	O1	C6	C5	130.1(4)
N9	Pd1	Cl1	89.90(11)	N1	C6	C5	111.1(4)
Cl1	Pd1	Cl2	177.75(4)	N7	C5	C6	133.2(4)
C14	N19	Pd1	128.0(3)	N7	C5	C4	105.5(4)
C18	N19	Pd1	125.3(3)	C4	C5	C6	121.3(4)
C18	N19	C14	106.7(4)	N19	C14	N13	128.0(4)
C12	N13	C14	118.0(4)	N19	C14	C15	109.3(4)
C12	N11	C16	126.3(4)	N13	C14	C15	122.4(4)
C8	N7	C5	108.2(4)	N3	C4	C5	122.5(4)
C2	N3	C4	118.1(4)	N9	C4	N3	126.8(4)
C4	N9	Pd1	127.1(3)	N9	C4	C5	110.6(4)
C4	N9	C8	105.8(4)	N19	C18	N17	111.4(4)
C8	N9	Pd1	127.1(3)	N2	C2	N3	120.1(4)
C18	N17	C15	107.2(4)	N2	C2	N1	121.0(4)
C2	N1	C6	127.6(4)	N1	C2	N3	118.9(4)
N13	C12	N11	119.9(4)	N7	C8	N9	110.0(4)
N12	C12	N13	119.1(4)	N17	C15	C16	131.1(4)
N12	C12	N11	121.0(4)	C14	C15	N17	105.5(4)
O2	C16	N11	121.0(4)	C14	C15	C16	121.7(4)

Table S3. Hydrogen Bonds for **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N13	H13	Cl3	0.88	2.28	3.071(4)	150.2
N11	H11	O1[1]	0.88	1.83	2.688(5)	165.4
N7	H7	O2[2]	0.88	1.94	2.792(5)	163.0
N12	H12A	Cl3	0.88	2.43	3.206(4)	146.9
N12	H12B	O1[1]	0.88	2.60	3.257(5)	132.6
N12	H12B	O3[3]	0.88	2.15	2.830(5)	133.5
N3	H3	Cl3	0.88	2.26	3.051(4)	150.2
N17	H17	Cl4[4]	0.88	2.26	3.016(4)	143.4
N2	H2A	Cl4[5]	0.88	2.54	3.294(4)	143.8
N2	H2B	Cl3	0.88	2.38	3.158(4)	147.7
N1	H1	Cl4[5]	0.88	2.19	3.044(4)	162.3
O3	H3A	Cl4[6]	0.85	2.43	3.255(4)	163.3
O3	H3B	Cl2	0.85	2.47	3.308(4)	170.9

[1]1+X,-1+Y,+Z; [2]-1+X,1+Y,+Z; [3]2-X,1-Y,2-Z; [4]1-X,-Y,1-Z; [5]1-X,1-Y,2-Z; [6]+X,1+Y,+Z

Table S4. Torsion Angles for **1**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Pd1	N19	C14	N13	5.9(7)	C16	N11	C12	N12	177.9(5)
Pd1	N19	C14	C15	179.6(3)	C6	N1	C2	N3	2.6(7)
Pd1	N19	C18	N17	-179.7(3)	C6	N1	C2	N2	-178.2(5)
Pd1	N9	C4	N3	-1.9(7)	C6	C5	C4	N3	2.9(7)
Pd1	N9	C4	C5	179.5(3)	C6	C5	C4	N9	-178.4(4)
Pd1	N9	C8	N7	-179.1(3)	C5	N7	C8	N9	-0.4(5)
O2	C16	C15	N17	7.3(9)	C14	N19	C18	N17	0.8(5)
O2	C16	C15	C14	170.0(5)	C14	N13	C12	N11	2.9(7)
O1	C6	C5	N7	-1.4(9)	C14	N13	C12	N12	-176.4(4)
O1	C6	C5	C4	175.8(5)	C4	N3	C2	N2	175.3(4)
N19	C14	C15	N17	0.6(5)	C4	N3	C2	N1	-5.5(6)
N19	C14	C15	C16	-165.9(4)	C4	N9	C8	N7	0.0(5)
N13	C14	C15	N17	174.8(4)	C18	N19	C14	N13	-174.6(4)
N13	C14	C15	C16	8.2(7)	C18	N19	C14	C15	-0.9(5)
N11	C16	C15	N17	-168.6(5)	C18	N17	C15	C16	164.7(5)
N11	C16	C15	C14	-5.8(7)	C18	N17	C15	C14	-0.1(5)
N7	C5	C4	N3	-179.3(4)	C2	N3	C4	N9	-175.5(4)
N7	C5	C4	N9	-0.6(5)	C2	N3	C4	C5	3.0(7)
N1	C6	C5	N7	177.4(5)	C2	N1	C6	O1	-178.2(5)
N1	C6	C5	C4	-5.4(6)	C2	N1	C6	C5	2.9(7)
C12	N13	C14	N19	166.6(4)	C8	N7	C5	C6	178.1(5)
C12	N13	C14	C15	-6.3(7)	C8	N7	C5	C4	0.6(5)
C12	N11	C16	O2	-173.6(5)	C8	N9	C4	N3	179.0(4)
C12	N11	C16	C15	2.6(7)	C8	N9	C4	C5	0.3(5)
C16	N11	C12	N13	-1.3(7)	C15	N17	C18	N19	-0.4(5)

Table S5. Bond Lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pt1	Cl1	2.3027(8)	N2	C2	1.395(4)
Pt1	Cl2	2.3152(8)	N3	C1	1.341(3)
Pt1	Cl3	2.3084(7)	N3	C4	1.368(3)
Pt1	Cl4	2.3075(8)	N4	C3	1.382(4)
Pt1	Cl5	2.3216(7)	N4	C5	1.320(4)
Pt1	N5	2.038(2)	N5	C4	1.367(3)
O1	C2	1.210(4)	N5	C5	1.342(4)
N1	C1	1.303(4)	C2	C3	1.411(4)
N2	C1	1.338(4)	C3	C4	1.356(4)

Table S6. Bond Angles for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	Pt1	Cl2	90.30(3)	C5	N4	C3	107.4(2)
Cl1	Pt1	Cl3	89.44(3)	C4	N5	Pt1	131.27(19)
Cl1	Pt1	Cl4	89.65(3)	C5	N5	Pt1	123.29(19)
Cl1	Pt1	Cl5	91.27(3)	C5	N5	C4	105.3(2)
Cl2	Pt1	Cl5	88.97(3)	N1	C1	N2	120.6(3)
Cl3	Pt1	Cl2	91.27(3)	N1	C1	N3	120.5(3)
Cl3	Pt1	Cl5	179.25(3)	N2	C1	N3	118.8(3)
Cl4	Pt1	Cl2	177.83(3)	O1	C2	N2	121.4(3)
Cl4	Pt1	Cl3	90.91(3)	O1	C2	C3	128.1(3)
Cl4	Pt1	Cl5	88.86(3)	N2	C2	C3	110.4(3)
N5	Pt1	Cl1	179.01(7)	N4	C3	C2	130.8(3)
N5	Pt1	Cl2	90.47(7)	C4	C3	N4	106.1(2)
N5	Pt1	Cl3	89.94(7)	C4	C3	C2	122.9(3)
N5	Pt1	Cl4	89.60(7)	N5	C4	N3	128.8(3)
N5	Pt1	Cl5	89.35(7)	C3	C4	N3	121.5(3)
C1	N2	C2	127.7(3)	C3	C4	N5	109.7(2)
C1	N3	C4	118.5(2)	N4	C5	N5	111.5(3)

Table S7. Hydrogen Bonds for **2**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1C	O2W	0.865(4)	2.154(4)	2.997(5)	164.8(2)
O1W	H1D	Cl3[1]	0.861(3)	2.7980(9)	3.335(3)	122.0(2)
O2W	H2B	Cl1[2]	0.829(18)	2.53(2)	3.345(3)	166(4)
O2W	H2C	O1W[3]	0.830(18)	1.974(19)	2.795(4)	170(5)
N1	H1A	Cl1[4]	0.86	2.53	3.288(3)	148.0
N1	H1B	O1[5]	0.86	1.98	2.746(3)	147.5
N2	H2A	Cl5[4]	0.86	2.46	3.221(3)	148.1
N3	H3A	Cl2	0.86	2.83	3.377(2)	122.6
N3	H3A	Cl3	0.86	2.65	3.159(3)	118.8
N3	H3A	O1[5]	0.86	2.25	2.942(3)	137.2
N4	H4A	O2W	0.86	1.89	2.734(4)	165.3

[1]1-X,1-Y,1-Z; [2]2-X,1-Y,1-Z; [3]2-X,1-Y,2-Z; [4]-1/2+X,1/2-Y,1/2+Z; [5]-1/2+X,1/2-Y,-1/2+Z

Table S8. Torsion Angles for **2**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Pt1	N5	C4	N3	2.2(4)	C2	N2	C1	N1	-177.5(3)
Pt1	N5	C4	C3	-176.4(2)	C2	N2	C1	N3	1.9(5)
Pt1	N5	C5	N4	176.67(19)	C2	C3	C4	N3	-1.4(5)
O1	C2	C3	N4	-4.6(6)	C2	C3	C4	N5	177.3(3)
O1	C2	C3	C4	179.4(3)	C3	N4	C5	N5	-0.2(3)
N2	C2	C3	N4	175.9(3)	C4	N3	C1	N1	176.2(3)
N2	C2	C3	C4	0.0(4)	C4	N3	C1	N2	-3.2(4)
N4	C3	C4	N3	-178.2(2)	C4	N5	C5	N4	0.5(3)
N4	C3	C4	N5	0.5(3)	C5	N4	C3	C2	-176.7(3)
C1	N2	C2	O1	-179.7(3)	C5	N4	C3	C4	-0.2(3)
C1	N2	C2	C3	-0.2(4)	C5	N5	C4	N3	178.0(3)
C1	N3	C4	N5	-175.4(3)	C5	N5	C4	C3	-0.6(3)
C1	N3	C4	C3	3.0(4)					