SUPPLEMENTARY INFORMATION

ic-2008-01004a

Table SI. Summary of bond distances and angles for the crystal and calculated structures of metal complexes of 1-MeCyt.

	exp	**DFT/mPW1PW91**	**DFT/mPW1PW91**
	1	***exo* 1**	***endo* 1**
Pd-N1	2.0494 (16)	2.082	2.077
Pd-N2	2.0001 (14)	2.030	2.036
Pd-N3	2.0429 (15)	2.060	2.060
Pd-N3C	2.0462 (13)	2.067	2.065
N2-Pd-N3	84.16 (6)	84.01	84.13
N2-Pd-N3C	178.40 (6)	176.70	175.03
N3-Pd-N3C	94.31 (6)	95.25	94.64
N2-Pd-N1	84.17 (6)	83.88	84.25
N3-Pd-N1	167.10 (6)	167.67	165.65
N3C-Pd-N1	97.40 (6)	96.97	96.21
N1-Pd-N3C-C2C	72.37	61.56	-107.7
O2C…H2N1	2.955	2.224	2.198[a]
	2	***exo* 2**	***endo* 2**
Pt-N1	2.039 (5)	2.077	2.075
Pt-N2	2.018 (5)	2.036	2.040
Pt-N3	2.056 (5)	2.057	2.058
Pt-N3C	2.045 (5)	2.066	2.064
N2-Pt-N3	83.4 (2)	84.26	84.31
N2-Pt-N3C	179.6 (2)	177.3	176.3
N3- Pt-N3C	97.0 (2)	95.0	94.6
N2-Pt-N1	84.4 (2)	84.0	84.4
N3-Pt-N1	167.7 (2)	168.2	166.3
N3c-Pt-N1	95.2 (2)	96.8	96.2
N1-Pt-N3C-C2C	65.12	57.91	-114.5
O2C…H2N1	2.547	2.168	2.134[a]

a. O2C…H1N1

Table SII. Summary of bond distances and angles for the crystal and calculated structures of metal complexes incorporating Guanine nucleobases.

	exp	**DFT/mPW1PW91**	**DFT/mPW1PW91**
	[Pd(dien)(Guanosine)]$^{2+,a}$	**3**	**4**
Pd,Pt-N4	2.029 (16)	2.051	2.051
Pd,Pt-N5	1.988 (14)	2.034	2.037
Pd,Pt-N6	2.019 (15)	2.086	2.079
Pd,Pt-N7	2.013 (13)	2.048	2.044
N4-Pd,Pt-N5	84.16 (6)	84.08	84.33
N5-Pd,Pt-N6	83.68 (6)	84.10	84.24
N4-Pd,Pt-N7	98.55 (6)	94.40	94.22
N4-Pd,Pt-N6	167.11 (6)	165.95	166.58
N5-Pd,Pt-N7	177.25 (6)	176.40	177.23
N7-Pd,Pt-N6	93.58 (6)	96.96	96.90
N6-Pd,Pt-N7-C8	-115.95	-57.24	-54.60

a: from Ref. 49