Pairing Strength and Proton Characters of the N7, N9-dimethylated GC and AT Base Pairs: An Density Functional Theory Investigation

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Supporting Information

TABLE S1 Geometric Characteristics of All Species Derived From G-C /mG-C(bond lengths in Å, angle in degree)

	O6…H4a	N1-H1	N3…H1	N1-N3	O2…H2a	D1[a]	D2[a]
GC	1.789	(-)	1.934		1.920	0.04	0.00
$[mGC]^+$	1.941	1.048	1.868	2.915	1.767	0.00	0.00
$[mGC]^+_{PT}$	1.619	1.776	1.069	2.841	1.971	(-)	(-)
$[mGC]^+_{TS}$	1.660	1.382	1.273	2.654	1.789	-10.7	-6.6
mG(N1)C	(-)	1.885[b]	(-)		2.014[c]	0.03	0.03
mG(N2a)C	1.861	(-)	2.111		(-)	-54.9	-16.6
mG(N2b)C	1.817	(-)	2.050		2.260	0.0	0.0
mG(C8)C	1.798	(-)	1.927		1.920	0.00	0.00
mGC(N1)	2.000	(-)	1.689	2.781	1.454	9.7	10.6
mGC(N4a)	(-)	1.936	(-)	2.966	1.959	-32.2	-39.0
mGC(N4b)	2.090	1.961	(-)	2.995	1.899	0.0	0.0
mGC(C5)	1.871	1.914	(-)	2.953	1.881	0.0	0.0
mGC(C6)	1.851	1.899	(-)	2.937	1.874	-0.3	0.0

[a] The dihedral angles G(O6-C2)-C(C2-C4) and G(C6-N1)-C(N3-C4) are denoted by D1 and D2, respectively. [b] the length of N1…H4a; [c] the length of N3…H2a. A dash (-) denotes that the H-bond has been removed upon deprotonated structure formation.

TABLE S2. Geometric Characteristics of All Species Derived From AT /mAT (Bond Lengths in Å, Angle in Degree)

	O4…H6a	N1…H3N3	N6…HO4	N6…HN3	D1[a]	D2
AT	1.927	1.870	(-)	(-)	0.0	0.0
$[mAT]^+$	1.763	1.993	(-)	(-)	0.1	0.0
mA(C2)T	1.873	1.860	(-)	(-)	33.5	20.1
mA(N6a)T	(-)	1.904	(-)	(-)	-84.0	-67.6
mA(N6b)T	2.290	1.845	(-)	(-)	0.0	0.0
mA(C8)T	1.914	1.879	(-)	(-)	0.7	1.8
mAT(N1)	1.399	2.050	(-)	(-)	-0.1	0.0
mAT(N3)	(-)	(-)	(-)	1.840	34.7	11.4
mAT(C6)	(-)	1.883	1.712	(-)	0.0	0.0

[a] The dihedral angles A(C6-N1)-T(N3-C4) and A(N1-C2)-T(C2-N3) are denoted by D1 and D2, respectively. A dash (-) denotes that the H-bond has been removed upon deprotonated structure formation.

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