Mononuclear 1,3-Dideazaadenine–Ag(I)–Thyminate Base Pairs

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Supporting Information

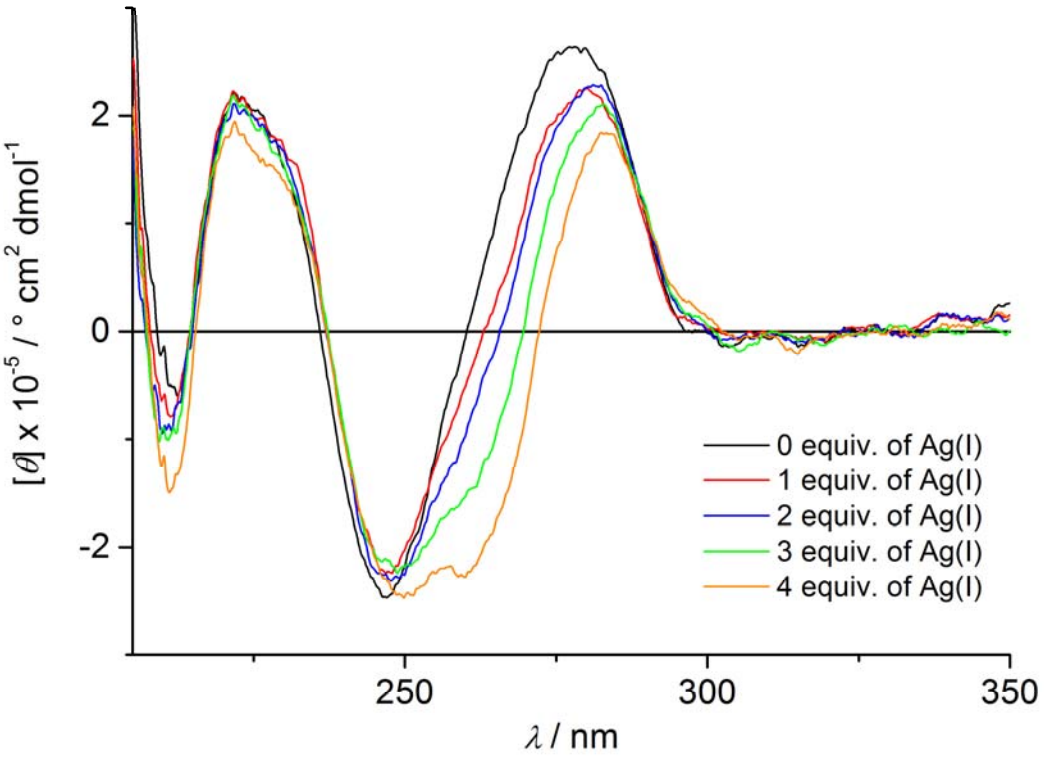

Figure S1. CD spectra of the oligonucleotide duplex comprising one central D:T mispair at pH 6.8 in the presence of various amounts of $AgNO_3$ (1 μM duplex, 150 mM $NaClO_4$, 5 mM MOPS pH 6.8).

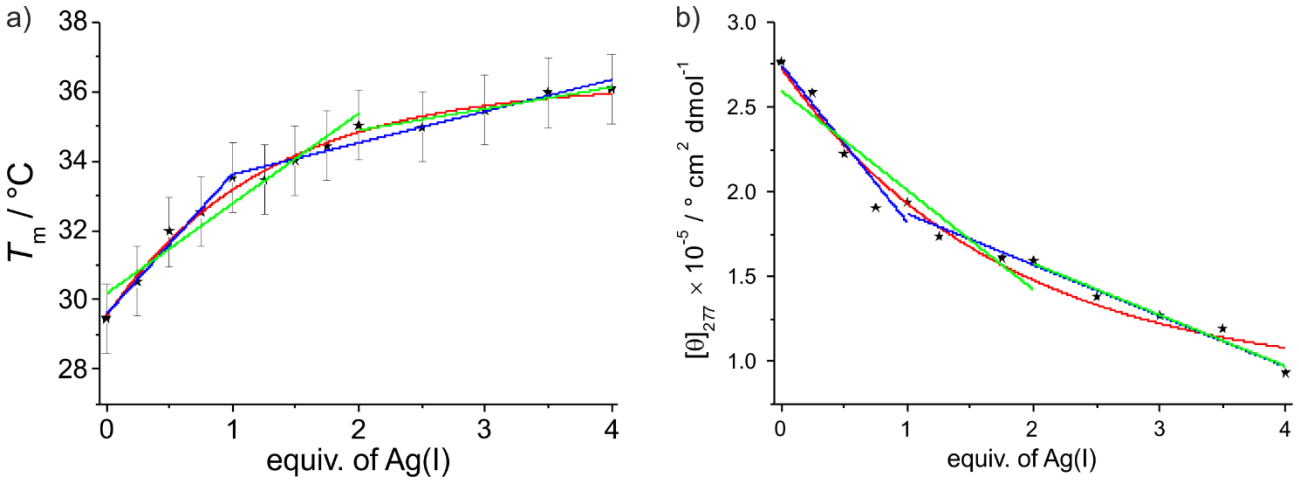

Figure S2. Experimental data a) from the inset of Figure 1 and b) from Figure 3b, including an asymptotic curve fit (y = a – b c^x, red) and two combinations of two linear fits (y = a + b x, blue for 1:1 stoichiometry, green for 2:1 stoichiometry).

a) asymptotic curve fit: a = 36.2(2), b = 6.7(2), c = 0.46(3), R^2 = 0.987

two linear fits: x = 0 → 1, a = 29.6(2), b = 4.0(3), R^2 = 0.978

x = 1 → 4, a = 32.7(2), b = 0.91(9), R^2 = 0.926

The lines intersect at x = 1.0(3), confirming an assumed 1:1 stoichiometry.

two linear fits: x = 0 → 2, a = 30.2(3), b = 2.6(3), R^2 = 0.925

x = 2 → 4, a = 33.6(4), b = 0.6(1), R^2 = 0.878

The lines intersect at x = 1.7(5), being ambiguous regarding an assumed 2:1 stoichiometry.

For these experimental data, the linear fits assuming a 1:1 stoichiometry are significantly better than those for a 2:1 stoichiometry. Nonetheless, the asymptotic fit is better than any of the two linear fits, in particular with respect to the data points at x > 1. Hence, the stoichiometry between metal-mediated base pair and included metal ions cannot be deduced unambiguously.

b) asymptotic curve fit: a = 0.9(2), b = –1.8(1), c = 0.56(7), R^2 = 0.966

two linear fits: x = 0 → 1, a = 2.75(9), b = –0.9(2), R^2 = 0.900

x = 1 → 4, a = 2.17(5), b = –0.30(2), R^2 = 0.970

Both lines intersect at x = 1.0(3), confirming an assumed 1:1 stoichiometry.

two linear fits: x = 0 → 2, a = 2.6(1), b = –0.59(9), R^2 = 0.857

x = 2 → 4, a = 2.2(1), b = –0.30(3), R^2 = 0.952

Both lines intersect at x = 1.4(1), contradicting an assumed 2:1 stoichiometry.

For these experimental data, the linear fits assuming a 1:1 stoichiometry are significantly better than those for a 2:1 stoichiometry. The asymptotic fit is of similar quality as the 1:1 linear fit, but the latter is better for data points at x > 1. Hence, these data tend to point towards a 1:1 stoichiometry.