Supporting Information

For

Charge Photoinjection in Intercalated and Covalently Bound $[Re(CO)_3(dppz)(py)]^+$-DNA Constructs Monitored by Time Resolved Visible and Infrared Spectroscopy

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Strand sequences and MALDI data.

Strand	Sequence	Mass (calc.)	Mass (MALDI)
ATa	5′-TTT ATA TTA TTA AAT AAA TTT TAT ATA TTT-3′	9172	9165
ATb	3′-AAA TAT AAT AAT TTA TTT AAA ATA TAT AAA-5′	9226	9222
GCa	5′-CCC GCG CCG CCG GGC GGG CCC CGC GCG CCC-3′	9094	9094
GCb	3′-GGG CGC GGC GGC CCG CCC GGG GCG CGC GGG-5′	9334	9333
Re-25(G)a	5′-Re′-AGC GTT GGT GAC TGA CTG ACT GAC T-3′	8583	8582
Re-25(G)b	3′-TCG CAA CCA CTG ACT GAC TGA CTG A-5′	7611	7614
Re-25(I)a	5′-Re′-AIC ITT GGT GAC TGA CTG ACT GAC T-3′	8553	8550
Re-25(I)b	3′-TCI CAA CCA CTG ACT GAC TGA CTG A-5′	7596	7597

FIGURE S1

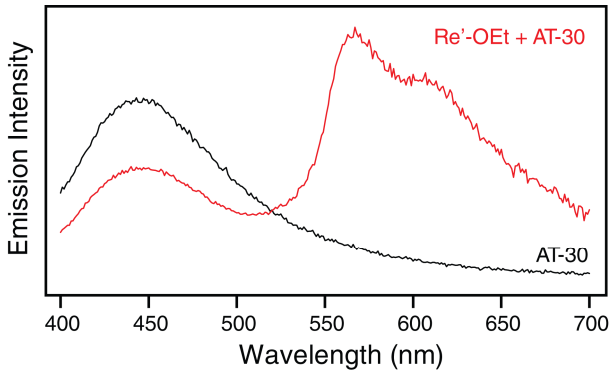

Figure S1. Steady-state emission spectra of 20 μM Re′-OEt in the presence of 0.5 mM (base pairs) AT-30 (red), and of 0.5 mM (base pairs) AT-30 (black) alone following excitation at 355 nm. Samples were prepared in D_2O buffer (10 mM NaP_i, 50 mM NaCl; pD 7.0).

FIGURE S2

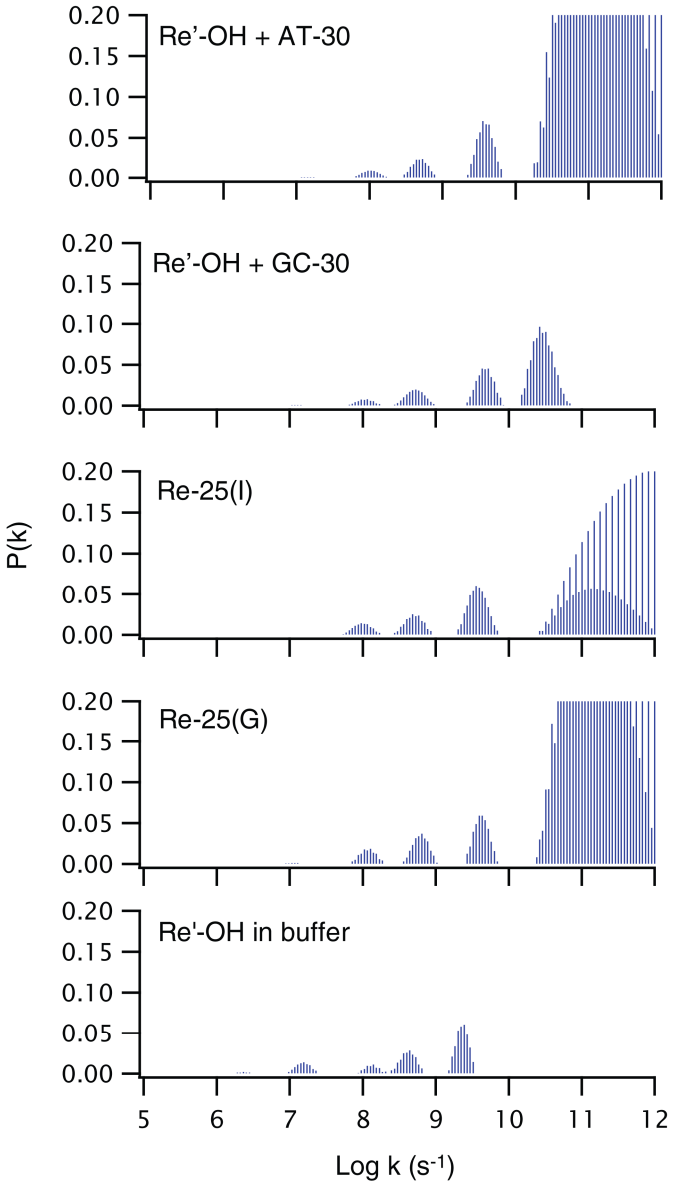

Figure S2. Lifetime distributions from maximum entropy analysis of emission from (64 μM) Re′-OH in the presence of 1.6 mM (base pairs) DNA and of 64 μM Re-25(I) or Re-25(G) measured on the picosecond timescale (λ_{ex} = 355 nm, 1 ps pulse width). Samples were prepared in D_2O buffer (10 mM NaP_i, 50 mM NaCl; pD 7.0) and were irradiated at 355 nm. Probability P is plotted as a function of rate k. Large distributions at k = 10^{11}-10^{12} s^{-1} are caused by convolution of the measurement signal with instrumental noise. The emission decay from Re′-OH in buffer is expected to be monoexponential; the complex distribution of rates observed here may be due to the formation of aggregates (solubility is quite low) or it may simply be an effect of the low emission intensity observed for this sample.

FIGURE S3

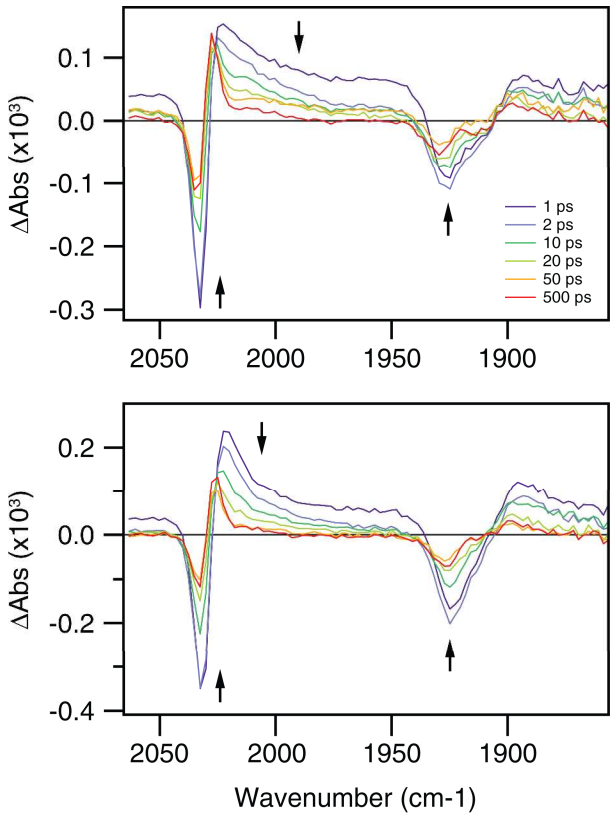

Figure S3. Picosecond-timescale TRIR difference spectra of 100 μM Re-25(I) (top) and Re-25(G) (bottom) measured at the indicated delay times after 355 nm, 50 fs excitation. Each probe data point is separated by ca. 2.1 cm^{-1}. Arrows indicate changes in the spectra with time. Delay times displayed are a subset of the data collected.

FIGURE S4

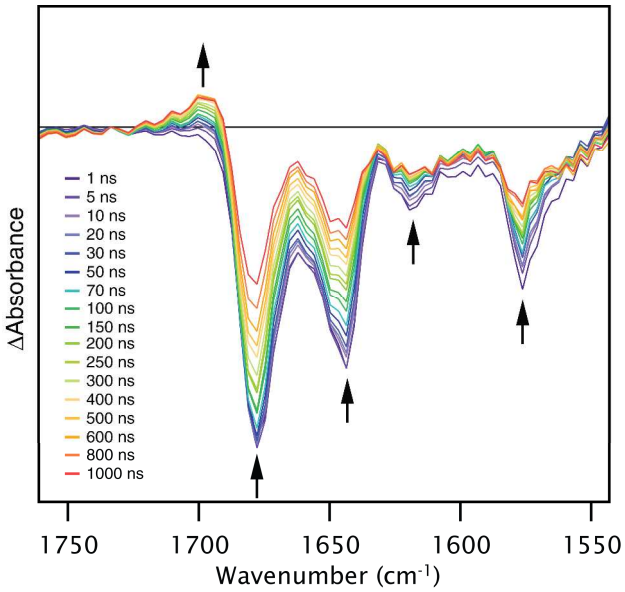

Figure S4. Nanosecond-timescale TRIR difference spectra showing changes in the IR absorbance of 4.8 mM (base pairs) GC-30 in the presence of 0.5 mM Re′-OH following excitation at 355 nm. Arrows indicate changes in the spectra with time. The increase in absorbance at ~1700 cm^{-1} is clearly displayed.