Supplementary Material

Spin-Orbit Charge Transfer from Guanine and 9-Methylguanine Radical Cations to Nitric Oxide Radicals and The Induced Triplet-to-Singlet Intersystem Crossing

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Cartesian coordinates of the ^{1}CT complex calculated at ωB97XD/6-31+G(d,p)

N	-1.27497500	-1.81869000	-0.00038600
C	-0.02407500	-2.40523100	-0.03280500
H	0.08798400	-3.48075900	-0.04637700
N	0.95743300	-1.54408700	-0.05029500
C	0.32063300	-0.32388100	-0.02763800
C	0.84146300	0.96787000	-0.03352300
O	2.06918500	1.30345200	-0.06720200
N	-0.11765900	1.95812300	-0.01461000
H	0.22885800	2.91041500	-0.02140700
C	-1.48106700	1.71099800	0.00330200
N	-2.29709100	2.77802600	0.00772600
H	-1.97264700	3.73021500	-0.00505400
H	-3.29053600	2.60644000	0.01895700
N	-1.98912700	0.49743700	0.01836100
C	-1.06630400	-0.47538700	0.00067800
C	-2.56972800	-2.48823100	0.01154000
H	-2.40415900	-3.56475800	0.03684400
H	-3.13231700	-2.18548700	0.89555900
H	-3.13079800	-2.22609600	-0.88652400
O	3.99098500	-0.25229600	-0.24466100
N	3.15095100	-0.17310300	0.46400200

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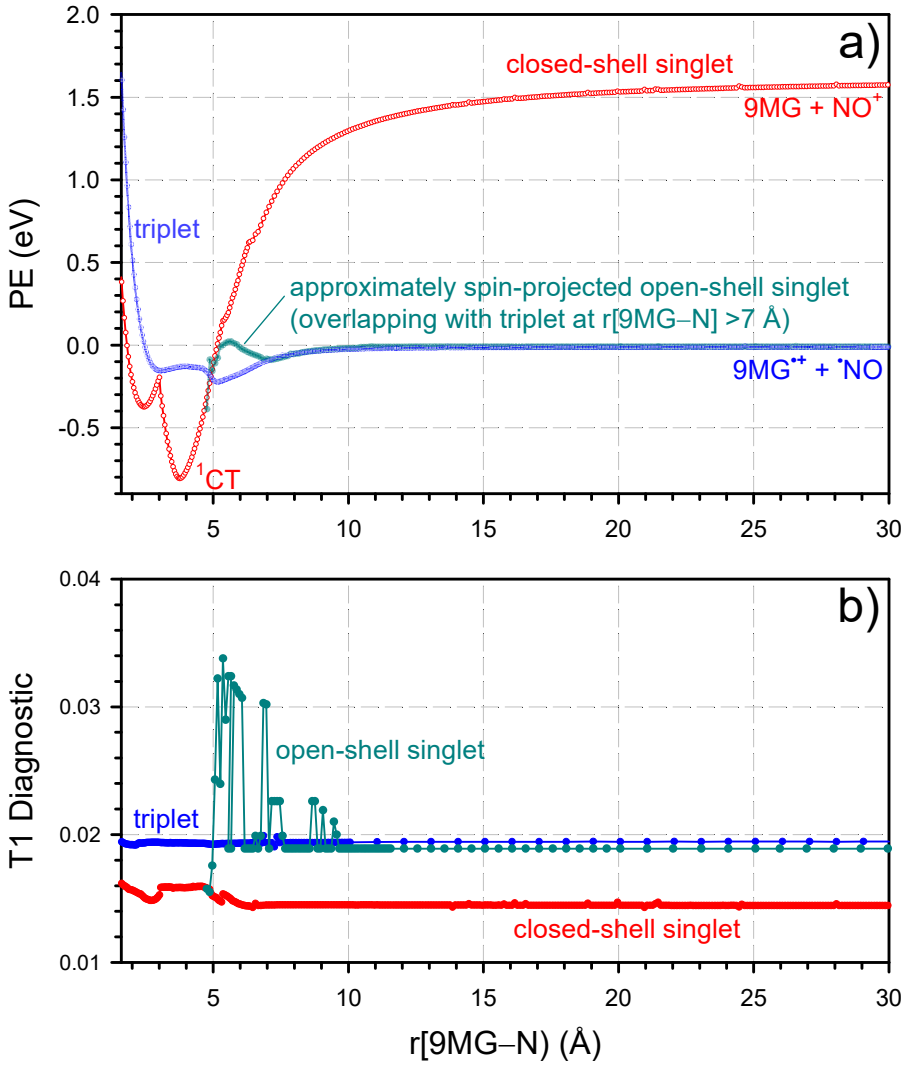

Figure S1 a) Potential energies (with respect to $9MG^{\bullet+}$ + •NO, no ZPE) and b) T1 diagnostic for closed-shell singlet, open-shell singlet, and triplet reaction structures along r[9MG–N] (the distance between the center-of-mass of 9MG and the N-terminal of •NO). Energies were calculated at ωB97XD/6-31+G(d,p) with approximate spin projection for the open-shell singlet. T1 diagnostics were done at DLPNO-CCSD(T)/aug-cc-pVTZ using the ωB97XD/6-31+G(d,p) optimized structures.