SUPPORTING MATERIAL

Electron Transfer From Aromatic Amino Acids to Guanine and Adenine Radical Cations in π Stacked and T-Shaped Complexes

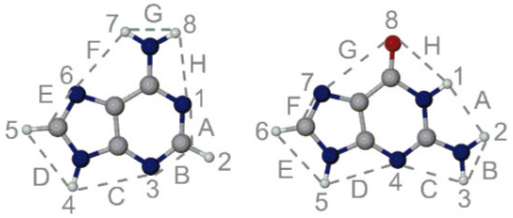
Cristina Butchosa,[a] Sílvia Simon,*[,a] and Alexander A. Voityuk *[,a,b]

[a]*Institut de Química Computational, Universitat de Girona, 17071 Girona, Spain*

[b]*Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain*

Table S1 Notation of dimer configurations

Current study	**Wetmore et al.** [1]
S1	stacked
S2	stacked′
E	edge
F1	face_A *for G* face_4 *for A*
F2	face_5 *for G-His G-Phe* face_E *for G-Trp G-Tyr* face_8 *for A*



Scheme. S1.

[1] L. R. Rutledge, H. F. Durst, S. D. Wetmore, J. Chem. Theory Comput., 2009, 5 (5), 1400-1410.

Table S2 Comparison of the ET driving force ΔE and electronic coupling *V* calculated with different DFT functionals and the Hartree-Fock method for S1 complex [G-Trp].

Functional	***ΔE (eV)***	***V* (eV)**
B3LYP	0.046	0.020
BHLHLYP	0.055	0.025
PBE0	0.054	0.020
M052X	0.046	0.025
M06	0.053	0.020
M06-2X	0.058	0.026
HF	0.175	0.032

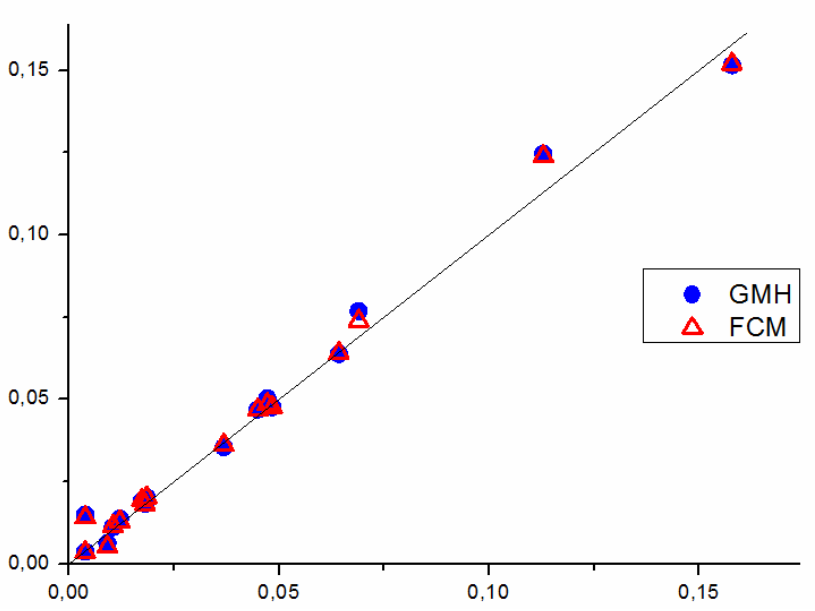


Fig. S2 Comparison of electronic couplings for A-X complexes calculated using the GMH and FCM schemes and the direct method (X-axis).

Table. S3 Computational results for complexes A-X. All energies in eV, electronic coupling *V* in meV, Charges in au

Complex	X	E(A)	E(A)-E0(A)	E(X)	E(X)-E0(X)	ΔE	V(meV)	Q(A)	Q(X)	K(sec-1)
∞	HIS	5.876	0.000	6.092	0.000	0.216	--	--	--	--
S1	HIS	5.841	-0.035	5.976	-0.116	0.135	157,800	0.627	0.373	1.51E+09
S2	HIS	5.836	-0.040	5.934	-0.158	0.098	44,950	0.713	0.287	2.74E+08
E	HIS	6.293	0.417	5.819	-0.273	-0.474	10,470	0.001	0.999	1.25E+11
F1	HIS	5.696	-0.180	6.520	0.428	0.824	8,796	1.000	0.000	1.15E-02
F2	HIS	5.789	-0.087	6.262	0.170	0.473	68,950	0.977	0.023	5.45E+04
∞	PHE	5.876	0.000	6.701	0.000	0.825	--	--	--	--
S1	PHE	5.739	-0.137	6.550	-0.151	0.811	3,891	0.995	0.005	3.55E-03
E	PHE	5.982	0.106	6.512	-0.189	0.530	17,400	0.998	0.002	6.56E+02
F1	PHE	5.666	-0.210	7.236	0.535	1.570	18,290	1.000	0.000	7.02E-16
F2	PHE	5.708	-0.168	6.895	0.194	1.187	70,160	0.996	0.004	5.14E-07
∞	TRP	5.876	0.000	5.384	0.000	-0.492	--	--	--	--
S1	TRP	5.657	-0.219	5.357	-0.027	-0.300	112,900	0.113	0.887	1.82E+12
S2	TRP	5.720	-0.156	5.336	-0.048	-0.384	9,181	0.012	0.988	3.53E+10
E	TRP	6.221	0.345	5.179	-0.205	-1.042	18,500	0.001	0.999	5.65E+12
F1	TRP	5.630	-0.246	5.761	0.377	0.131	3,891	0.999	0.001	1.00E+06
F2	TRP	5.733	-0.143	5.515	0.131	-0.218	36,860	0.028	0.972	5.96E+10
∞	TYR	5.876	0.000	5.971	0.000	0.095	--	--	--	--
S1	TYR	5.721	-0.155	5.851	-0.120	0.130	64,260	0.818	0.182	2.80E+08
S2	TYR	5.734	-0.142	5.855	-0.116	0.121	48,360	0.839	0.161	1.93E+08
E	TYR	6.214	0.338	5.755	-0.216	-0.459	18,110	0.002	0.998	3.20E+11
F1	TYR	5.698	-0.179	6.412	0.441	0.714	12,150	1.000	0.000	9.62E-01
F2	TYR	5.747	-0.129	6.139	0.168	0.392	47,210	0.984	0.016	2.44E+05

Table. S4 Computational results for complexes G-X. All energies in eV, electronic coupling *V* in meV, Charges in au

Complex	X	E(G)	E(G)-E0(G)	E(X)	E(X)-E0(X)	ΔE	V (meV)	Q(G)	Q(X)	K (sec-1)
∞	HIS	5.514	0.000	6.092	0.000	0.578	--	--	--	--
S1	HIS	5.493	-0.021	6.108	0.016	0.615	40.930	0.994	0.006	2.70E+02
S2	HIS	5.390	-0.124	5.950	5.726	0.560	41.420	0.993	0.007	1.51E+03
E	HIS	5.910	0.401	5.805	5.581	-0.105	5.849	0.005	0.995	2.38E+08
F1	HIS	5.324	-0.185	6.643	0.550	1.319	1.004	1.000	0.000	3.21E-13
F2	HIS	5.346	-0.165	6.613	0.520	1.267	9.943	1.000	0.000	3.22E-10
∞	PHE	5.514	0.000	6.701	0.000	1.187	--	--	--	--
S1	PHE	5.370	-0.144	6.548	-0.153	1.178	21.660	0.996	0.004	7.18E-08
E	PHE	5.611	0.102	6.451	-0.250	0.840	6.057	0.999	0.001	3.07E-03
F1	PHE	5.276	-0.233	7.409	0.708	2.133	0.211	0.999	0.001	2.55E-33
F2	PHE	5.315	-0.196	7.250	0.549	1.935	38.270	1.000	0.000	9.98E-24
∞	TRP	5.514	0.000	5.384	0.000	-0.130	--	--	--	--
S1	TRP	5.312	-0.202	5.343	-0.041	0.031	20.080	0.832	0.168	2.19E+08
S2	TRP	5.304	-0.210	5.330	-0.054	0.026	3.588	0.813	0.187	7.73E+06
E	TRP	5.851	0.342	5.118	-0.266	-0.733	16.430	0.001	0.999	2.27E+12
F1	TRP	5.238	-0.273	5.896	0.512	0.658	16.470	0.998	0.002	1.11E+01
F2	TRP	5.202	-0.307	5.841	0.457	0.639	17.480	0.998	0.002	2.30E+01
∞	TYR	5.514	0.000	5.971	0.000	0.457	--	--	--	--
S1	TYR	5.397	-0.117	5.959	-0.012	0.562	16.840	0.994	0.006	2.35E+02
S2	TYR	5.373	-0.141	5.870	-0.101	0.497	51.260	0.977	0.023	1.51E+04
E	TYR	5.821	0.312	5.616	-0.355	-0.205	16.550	0.007	0.993	9.84E+09
F1	TYR	5.307	-0.204	6.590	0.619	1.283	28.580	0.999	0.001	1.31E-09
F2	TYR	5.281	-0.230	6.500	0.529	1.219	5.242	1.000	0.000	7.28E-10