Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Predicting the Photoinduced Electron Transfer Thermodynamics in 1,3,5-Triarylpyrazolines Based on Multiple Linear Free Energy Relationships

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Supporting Information

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Table S1-1: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Benzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
H	0.000000	-2.473053	0.000000
C	0.000000	-1.391331	0.000000
C	0.000000	1.391331	0.000000
C	-1.205725	-0.695861	0.000000
C	1.205725	-0.695861	0.000000
C	1.205725	0.695861	0.000000
C	-1.205725	0.695861	0.000000
H	-2.142081	-1.237457	0.000000
H	2.142081	-1.237457	0.000000
H	2.142081	1.237457	0.000000
H	-2.142081	1.237457	0.000000
H	0.000000	2.473053	0.000000

Table S1-2: Cartesian Atomic Coordinates for the Geometry Optimized Structure of Fluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	0.000000	0.000000	1.829310
H	0.000000	0.000000	2.910127
C	1.204675	0.000000	1.132290
C	1.213587	0.000000	-0.259081
C	0.000000	0.000000	-0.924105
C	-1.213587	0.000000	-0.259081
C	-1.204675	0.000000	1.132290
H	-2.142543	0.000000	1.670292
H	-2.133709	0.000000	-0.824810
F	0.000000	0.000000	-2.278981
H	2.133709	0.000000	-0.824810
H	2.142543	0.000000	1.670292

Table S1-3: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2-Difluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	-0.694211	0.000000	0.532532
C	0.695220	0.000000	-1.861975
C	0.694211	0.000000	0.532532
C	-1.395699	0.000000	-0.659181
C	-0.695220	0.000000	-1.861975
C	1.395699	0.000000	-0.659181
H	-2.475745	0.000000	-0.629725
H	-1.240162	0.000000	-2.794924
H	2.475745	0.000000	-0.629725
H	1.240162	0.000000	-2.794924
F	-1.351059	0.000000	1.706266
F	1.351059	0.000000	1.706266

Table S1-4: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,3-Difluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	1.180585	0.000000	0.302609
C	-1.211601	0.000000	-1.081151
C	0.000000	0.000000	1.025917
C	1.211601	0.000000	-1.081151
C	0.000000	0.000000	-1.765201
C	-1.180585	0.000000	0.302609
H	0.000000	0.000000	2.104961
H	2.159230	0.000000	-1.598058
H	0.000000	0.000000	-2.845961
H	-2.159230	0.000000	-1.598058
F	2.347076	0.000000	0.984185
F	-2.347076	0.000000	0.984185

Table S1-5: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,4-Difluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	1.362760	0.000000	0.000000
C	-1.362760	0.000000	0.000000
C	0.695466	1.212592	0.000000
C	0.695466	-1.212592	0.000000
C	-0.695466	-1.212592	0.000000
C	-0.695466	1.212592	0.000000
H	1.257915	2.134358	0.000000
H	1.257915	-2.134358	0.000000
H	-1.257915	-2.134358	0.000000
H	-1.257915	2.134358	0.000000
F	2.716936	0.000000	0.000000
F	-2.716936	0.000000	0.000000

Table S1-6: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2,3-Trifluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	1.195569	0.000000	0.013059
C	-1.209769	0.000000	-1.370236
C	0.000000	0.000000	0.719129
C	1.209769	0.000000	-1.370236
C	0.000000	0.000000	-2.056270
C	-1.195569	0.000000	0.013059
H	2.158737	0.000000	-1.885226
F	2.345488	0.000000	0.706081
H	0.000000	0.000000	-3.136352
F	0.000000	0.000000	2.056260
H	-2.158737	0.000000	-1.885226
F	-2.345488	0.000000	0.706081

Table S1-7: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2,4-Trifluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	1.111940	0.560703	0.000000
C	-1.558011	-0.062445	0.000000
C	0.706716	-0.767589	0.000000
C	0.174462	1.576885	0.000000
C	-1.182788	1.268778	0.000000
C	-0.636908	-1.097445	0.000000
H	0.515762	2.601712	0.000000
F	2.425793	0.847885	0.000000
H	-1.934422	2.043382	0.000000
H	-0.952137	-2.129764	0.000000
F	1.632573	-1.738037	0.000000
F	-2.871885	-0.375253	0.000000

Table S1-8: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,3,5-Trifluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	0.000000	0.000000	1.361553
C	0.000000	0.000000	-1.405661
C	-1.218261	0.000000	0.703302
C	1.218261	0.000000	0.703302
C	1.179669	0.000000	-0.680623
C	-1.179669	0.000000	-0.680623
H	-2.151604	0.000000	1.243306
H	2.151604	0.000000	1.243306
H	0.000000	0.000000	-2.484160
F	0.000000	0.000000	2.709028
F	-2.346114	0.000000	-1.355066
F	2.346114	0.000000	-1.355066

Table S1-9: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2,3,4-Tetrafluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	0.695387	0.000000	1.726745
C	-0.694236	0.000000	-0.684469
C	-0.695387	0.000000	1.726745
C	1.377587	0.000000	0.524984
C	0.694236	0.000000	-0.684469
C	-1.377587	0.000000	0.524984
F	-2.720095	0.000000	0.502772
F	1.358521	0.000000	-1.841874
F	2.720095	0.000000	0.502772
H	1.257289	0.000000	2.648344
F	-1.358521	0.000000	-1.841874
H	-1.257289	0.000000	2.648344

Table S1-10: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2,3,5-Tetrafluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	0.000000	0.000000	1.089869
C	0.000000	0.000000	-1.663248
C	1.194122	0.000000	0.381511
C	-1.194122	0.000000	0.381511
C	-1.216213	0.000000	-1.002314
C	1.216213	0.000000	-1.002314
H	-2.151113	0.000000	-1.540130
H	2.151113	0.000000	-1.540130
F	-2.344372	0.000000	1.067706
F	0.000000	0.000000	2.426904
F	2.344372	0.000000	1.067706
F	0.000000	0.000000	-3.010075

Table S1-11: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2,4,5-Tetrafluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	0.000000	-1.397213	0.000000
C	0.000000	1.397213	0.000000
C	-1.191879	-0.693834	0.000000
C	1.191879	-0.693834	0.000000
C	1.191879	0.693834	0.000000
C	-1.191879	0.693834	0.000000
H	0.000000	2.476652	0.000000
H	0.000000	-2.476652	0.000000
F	-2.358881	-1.355647	0.000000
F	-2.358881	1.355647	0.000000
F	2.358881	1.355647	0.000000
F	2.358881	-1.355647	0.000000

Table S1-12: Cartesian Atomic Coordinates for the Geometry Optimized Structure of 1,2,3,4,5-Pentafluorobenzene (B3LYP/6-311+G(2d,2p)).

Atom	x/Å	y/Å	z/Å
C	0.000000	0.000000	1.669616
C	0.000000	0.000000	-1.113939
C	-1.190223	0.000000	0.964237
C	1.190223	0.000000	0.964237
C	1.205244	0.000000	-0.423129
C	-1.205244	0.000000	-0.423129
F	-2.357461	0.000000	1.621445
F	-2.357508	0.000000	-1.096785
F	2.357508	0.000000	-1.096785
F	2.357461	0.000000	1.621445
H	0.000000	0.000000	2.748674
F	0.000000	0.000000	-2.446657