

Supporting Information for

Observation of Proton-Coupled Electron Transfer by Transient Absorption Spectroscopy in a Hydrogen-Bonded, Porphyrin Donor-Acceptor Assembly

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Supporting Material

Structure of 1:3 from energy optimized geometry calculation	S1
xyz-coordinates for energy optimized geometry calculation of 1:3	S2-S3

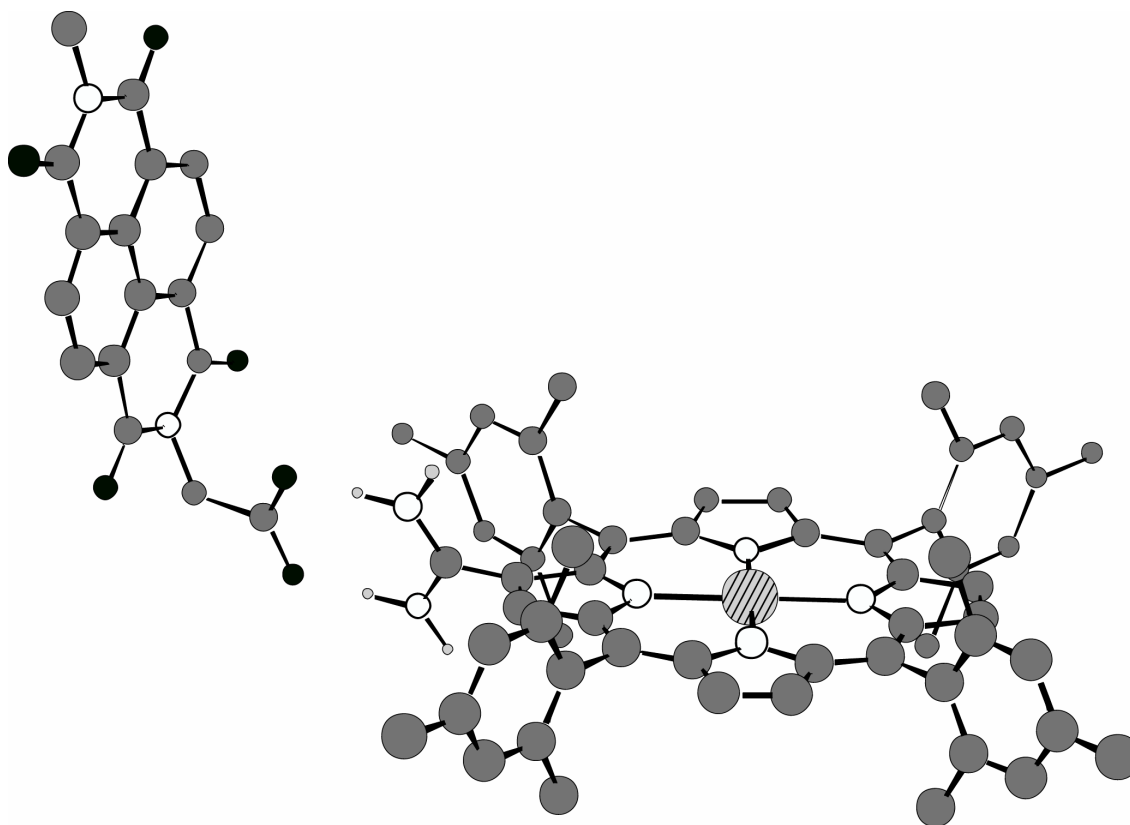


Figure S1. Optimized geometry for 1:3 complex (where the aryl substituent of the diimide has been replaced by a methyl group) determined using density functional theory: C (dark grey), N (white), O (black), H (light gray) Zn (striped grey). All hydrogen atoms except those of the amidinium moiety have been hidden for clarity. Details of the method and basis set are discussed in the Experimental.

Table S1. xyz-Coordinates for energy optimized geometry calculation of **1:3**.

Zn	0.00000	0.00000	0.00000	C	1.10934	2.86334	0.00883
N	2.06380	0.00000	0.00000	C	0.68045	4.24451	0.03462
C	2.88480	1.11195	0.00000	N	-2.08620	0.00000	0.00000
C	4.27084	0.68846	-0.00358	C	-2.91765	1.10840	0.04723
C	2.45618	2.45018	0.00438	C	-4.30453	0.64446	-0.00069
C	3.51724	3.52130	0.00284	C	-5.60678	1.36229	0.00545
C	4.01807	4.01843	-1.22075	N	-6.07576	1.92364	-1.10090
C	5.00149	5.01894	-1.19748	N	-6.35072	1.33099	1.10036
C	5.50322	5.53748	0.00285	C	-2.88142	-1.12839	-0.07139
C	6.58795	6.59526	0.00110	C	-4.26372	-0.74213	-0.06089
C	3.50490	3.49764	-2.54970	C	-2.46043	-2.46337	0.03204
C	4.01059	4.02963	1.23077	C	-3.52680	-3.52899	0.04488
C	4.99363	5.02945	1.20505	C	-4.04833	-4.01679	-1.17636
C	3.49398	3.51219	2.56015	C	-5.05739	-4.99029	-1.14302
C	2.88736	-1.10567	-0.00714	C	-5.56251	-5.49350	0.06298
C	2.46423	-2.44847	-0.01422	C	-6.63258	-6.56550	0.07245
C	3.53300	-3.50830	-0.04076	C	-3.54339	-3.49918	-2.50925
C	4.02154	-3.98603	-1.27699	C	-4.01997	-4.02215	1.27399
C	5.03030	-4.95968	-1.28188	C	-5.03041	-4.99547	1.25902
C	5.57177	-5.47055	-0.09527	C	-3.47959	-3.51804	2.59858
C	6.67767	-6.50543	-0.12573	N	-0.00180	-2.05778	0.00862
C	3.46758	-3.45869	-2.60649	C	1.12071	-2.87018	-0.00347
C	4.06073	-4.01664	1.17325	C	0.68352	-4.28758	0.00064
C	5.06941	-4.98868	1.12079	C	-1.12026	-2.87367	0.02316
C	3.54910	-3.52755	2.51422	C	-0.67736	-4.29012	0.01812
C	4.27370	-0.67823	-0.00867	N	-10.82566	3.98957	1.55005
N	-0.00285	2.03767	-0.01031	C	-10.29228	4.89280	2.48703
C	-1.11739	2.85798	-0.00222	C	-10.62375	4.64690	3.92081
C	-0.68544	4.24343	0.03101	C	-11.36842	3.49920	4.29208
C	-2.46889	2.46167	-0.02524	C	-11.82027	2.57337	3.31887
C	-3.47091	3.58860	-0.01806	C	-11.55717	2.82327	1.87083
C	-3.96216	4.08873	1.21211	C	-8.98560	3.23623	0.04964
C	-4.85145	5.16907	1.20399	C	-10.47201	5.30983	6.25186
C	-5.26104	5.78235	0.01105	C	-12.78985	2.73280	9.78678
C	-6.25417	6.92409	0.03408	O	-11.19126	4.78745	8.95201
C	-3.49186	3.50758	2.56156	O	-13.44412	0.92945	7.81984
C	-3.84885	4.20913	-1.22902	C	-10.29885	4.07205	0.17481
C	-4.73997	5.29094	-1.19152	H	5.12722	1.35776	0.00001
C	-3.29462	3.74912	-2.56537	H	6.52905	7.22886	0.89873

H	6.51047	7.24477	0.88379	H	-5.11741	-1.41315	-0.11116
H	7.58715	6.12721	-0.01396	H	-7.28988	-6.48036	-0.80582
H	5.38182	5.40437	-2.14716	H	-7.25686	-6.49805	0.97587
H	4.00684	4.00574	-3.38590	H	-6.17622	-7.57004	0.05370
H	2.41959	3.65968	-2.64993	H	-5.46338	-5.35963	-2.08845
H	3.68014	2.41449	-2.64992	H	-4.07103	-3.98843	-3.34072
H	5.36923	5.42229	2.15357	H	-2.46388	-3.68576	-2.62771
H	3.65973	2.42722	2.65785	H	-3.69434	-2.41142	-2.59959
H	2.41018	3.68353	2.66232	H	-5.41364	-5.37079	2.21146
H	4.00195	4.01473	3.39593	H	-3.58150	-2.42458	2.68510
H	6.61008	-7.13445	-1.02608	H	-2.40763	-3.75021	2.70642
H	6.63321	-7.16245	0.75588	H	-4.01728	-3.98081	3.43873
H	7.66751	-6.01791	-0.13094	H	1.35680	-5.14180	-0.00861
H	5.40088	-5.32960	-2.24130	H	-1.34761	-5.14674	0.02627
H	3.96003	-3.95838	-3.45307	H	-9.57998	6.38991	4.58314
H	3.63137	-2.37318	-2.70032	H	-12.83836	0.73111	2.93590
H	2.38255	-3.63337	-2.68223	H	-10.13481	6.00315	7.02097
H	5.47083	-5.38168	2.05860	H	-13.38518	0.36344	5.36936
H	2.46711	-3.70778	2.61912	H	-12.90861	3.73141	10.22203
H	3.70752	-2.44337	2.63102	H	-12.02380	2.18030	10.35218
H	4.06507	-4.04144	3.33798	H	-13.72810	2.16996	9.79999
H	5.13344	-1.34320	-0.00984	H	-11.05128	3.67448	-0.51616
H	-1.34747	5.10453	0.04799	H	-10.08703	5.12164	-0.05580
H	-6.38994	7.35534	-0.96859				
H	-5.91699	7.72635	0.71049				
H	-7.23478	6.57578	0.39455				
H	-5.24200	5.54042	2.15490				
H	-3.48963	2.40769	2.55855				
H	-4.14231	3.85891	3.37543				
H	-2.45970	3.83202	2.77861				
H	-5.04570	5.75491	-2.13298				
H	-3.94408	4.07847	-3.39037				
H	-3.18364	2.65548	-2.61768				
H	-2.28967	4.17193	-2.74018				
H	1.34584	5.10364	0.05163				
H	-7.00767	2.46618	-1.11278				
H	-5.48931	1.91270	-1.93073				
H	-7.31438	1.84149	1.12452				
H	-5.94921	0.92002	1.93963				