Ultrafast Electron Transfer in Photosynthesis: Reduced Pheophytin and Quinone Interaction Mediated by Conical Intersections

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Supporting Information

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Table S1. Cartesian coordinates of the ground-state geometry for FBC, optimized at the B3PW91/6-31G* level, within the constraints of C_{2v} point group (data in Å).

C	0.000000	2.890366	1.206130
C	0.000000	-2.890366	1.206130
C	0.000000	1.099543	-2.824949
C	0.000000	-1.099543	-2.824949
C	0.000000	1.081124	2.929490
C	0.000000	-1.081124	2.929490
C	0.000000	0.766141	-4.309521
C	0.000000	-0.766141	-4.309521
C	0.000000	4.246434	0.755421
C	0.000000	-4.246434	0.755421
C	0.000000	4.236227	-0.616078
C	0.000000	-4.236227	-0.616078
C	0.000000	0.679592	4.323464
C	0.000000	-0.679592	4.323464
C	0.000000	2.419285	2.510553
C	0.000000	-2.419285	2.510553
C	0.000000	2.411276	-2.372596
C	0.000000	-2.411276	-2.372596
C	0.000000	2.871378	-1.049796
C	0.000000	-2.871378	-1.049796
N	0.000000	2.104663	0.076312
N	0.000000	-2.104663	0.076312
N	0.000000	0.000000	-2.043877
N	0.000000	0.000000	2.103204
H	0.000000	1.090988	0.101046
H	0.000000	-1.090988	0.101046
H	0.880339	1.190344	-4.806153
H	-0.880339	-1.190344	-4.806153
H	-0.880339	1.190344	-4.806153
H	0.880339	-1.190344	-4.806153
H	0.000000	5.108449	1.410210
H	0.000000	-5.108449	1.410210
H	0.000000	5.087776	-1.284202
H	0.000000	-5.087776	-1.284202
H	0.000000	3.177576	3.289192
H	0.000000	-3.177576	3.289192
H	0.000000	3.189424	-3.131395
H	0.000000	-3.189424	-3.131395
H	0.000000	1.352616	5.172927
H	0.000000	-1.352616	5.172927

Table S2. Cartesian coordinates of the ground-state geometry for FBC, optimized at the B3PW91/6-31G* level, within the constraints of C_s point group (data in Å).

C	-0.934236	2.989398	0.000000
C	2.914309	0.834129	0.000000
C	2.711353	-1.355532	0.000000
C	-2.817244	1.346879	0.000000
C	-3.016804	-0.806155	0.000000
C	0.780307	-2.955981	0.000000
C	-1.467764	-2.766783	0.000000
C	-1.144069	-4.158652	0.000000
C	0.222517	-4.275010	0.000000
C	4.361869	0.365073	0.000000
C	4.220458	-1.160529	0.000000
C	-0.360256	4.298073	0.000000
C	1.004440	4.161288	0.000000
C	-4.367593	-0.277687	0.000000
C	-4.242155	1.075678	0.000000
C	-2.276564	2.640733	0.000000
C	2.584999	2.182003	0.000000
C	-2.723138	-2.177343	0.000000
C	1.310315	2.762222	0.000000
C	2.139917	-2.619915	0.000000
N	0.118244	2.102755	0.000000
N	2.035074	-0.188612	0.000000
N	-0.270260	-2.088667	0.000000
N	-2.094242	0.194100	0.000000
H	0.000000	1.095693	0.000000
H	-0.201428	-1.077026	0.000000
H	-1.875583	-4.956585	0.000000
H	0.809241	-5.184557	0.000000
H	4.895421	0.741672	0.880545
H	4.895421	0.741672	-0.880545
H	-0.932661	5.216855	0.000000
H	1.748333	4.947516	0.000000
H	-5.275623	-0.869293	0.000000
H	-2.981878	3.467669	0.000000
H	3.412403	2.886771	0.000000
H	-3.568428	-2.860553	0.000000
H	4.675698	-1.628773	-0.880545
H	4.675698	-1.628773	0.880545
H	-5.025978	1.824092	0.000000
H	2.823689	-3.464746	0.000000

Table S3. Cartesian coordinates of the ground-state geometry for Q, optimized at the π-CASSCF level, using the ANO-S basis set with the contraction scheme C,O[3s2p1d]/H[2s] and within the constraints of D_{2h} point group (data in Å).

C	0.000000	0.000000	1.444813
C	0.000000	0.000000	-1.444813
C	0.000000	1.270034	0.673993
C	0.000000	-1.270034	0.673993
C	0.000000	1.270034	-0.673993
C	0.000000	-1.270034	-0.673993
O	0.000000	0.000000	2.653992
O	0.000000	0.000000	-2.653992
H	0.000000	2.184291	1.251504
H	0.000000	-2.184291	1.251504
H	0.000000	2.184291	-1.251504
H	0.000000	-2.184291	-1.251504

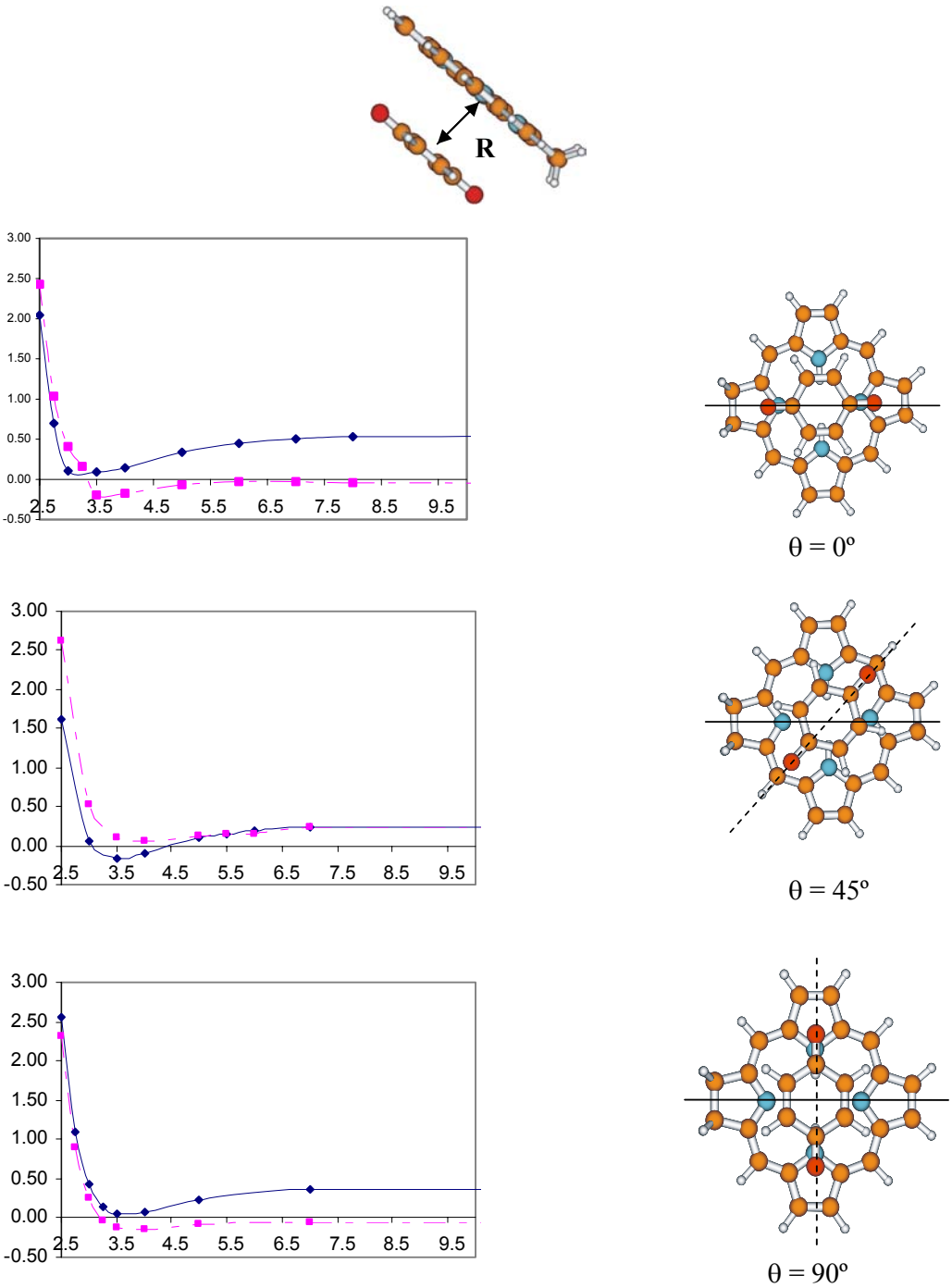

Figure S1. Potential energy curves (PECs) for $[FBC/Q]^-$ along the intermolecular distance R for the orientations defined by angle Θ. The results have been obtained at the CASSCF/ANO-S C,N,O [3s2p1d]/H[2s] level. Energies referred to the subsystems at infinity separation.