Supporting Information: On the Role of the Special Pair in Photosystems as a Charge Transfer Rectifier

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S2-S5: SI Tables and Figures.

S4-S8: X-Ray atoms coord. (Å).

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SI Table S1. Excited states of the special pair calculated with SRSH-PCM scheme at various dielectric constants. Structures are obtained in corresponding constant.

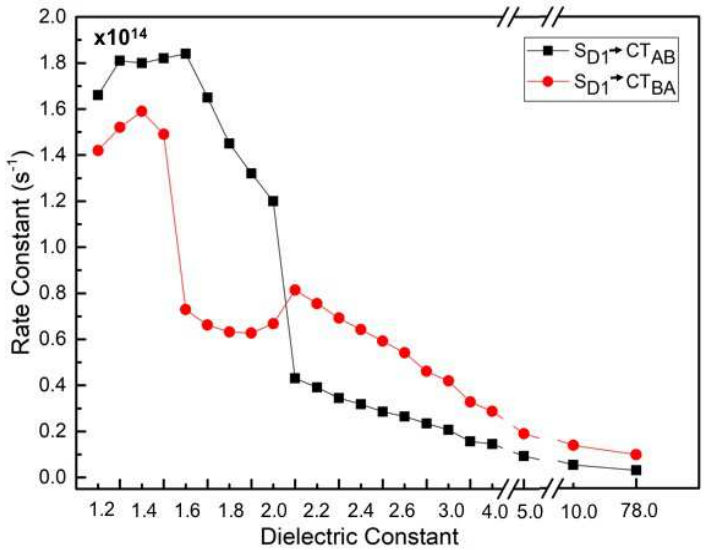
ϵ	state	main configuration	excitation energy(eV)	oscillator strength	net charge
GAS	S_1	H → L(0.80) H-1 → L+1(0.37)	1.8709	0.79	0.02
	S_2	H → L+1(0.67) H-1 → L(0.71)	1.9225	0.02	0.02
	CT_1	H-1 → L(-0.56) H → L(0.53) H → L+1(0.58)	2.3459	0.00	-0.46
	CT_2	H-1 → L(0.89) H → L(-0.22)	2.4091	0.00	0.65
1.2	S_1	H → L(0.92)	1.6690	0.89	-0.14
	S_2	H → L+1(0.92)	1.7273	0.05	0.01
	CT_1	H-1 → L(0.88) H-1 → L+1(0.27)	1.9992	0.10	-0.69
	CT_2	H-1 → L(-0.27) H-1 → L+1(0.94)	2.0858	0.08	0.78
1.3	S_1	H → L(0.94)	1.6603	0.81	-0.20
	S_2	H → L+1(0.95)	1.7193	0.07	0.02
	CT_1	H-1 → L(0.91) H-1 → L+1(0.27)	1.9606	0.13	-0.62
	CT_2	H-1 → L(-0.27) H-1 → L+1(0.91)	2.0395	0.10	0.75
1.4	S_1	H → L(0.96)	1.6496	0.72	-0.27
	S_2	H → L+1(0.97)	1.7101	0.11	0.09
	CT_1	H-1 → L(0.93) H-1 → L+1(0.27)	1.9327	0.15	-0.55
	CT_2	H-1 → L(-0.27) H-1 → L+1(0.94)	2.0025	0.13	0.72
1.5	S_1	H → L(0.98)	1.6384	0.64	-0.35
	S_2	H → L+1(0.98)	1.7001	0.14	0.14
	CT_1	H-1 → L(0.94) H-1 → L+1(0.27)	1.9086	0.18	-0.48
	CT_2	H-1 → L(-0.27) H-1 → L+1(0.94)	1.9714	0.16	0.67
1.6	S_1	H → L(0.98)	1.6261	0.56	-0.42
	S_2	H → L+1(0.98)	1.6904	0.16	0.20
	CT_1	H-1 → L(0.94) H-1 → L+1(0.27)	1.8911	0.20	-0.42
	CT_2	H-1 → L(-0.27) H-1 → L+1(0.94)	1.9458	0.20	0.62
1.7	S_1	H → L(0.98)	1.6128	0.49	-0.48
	S_2	H → L+1(0.98)	1.6840	0.18	0.27
	CT_1	H-1 → L(0.94) H-1 → L+1(0.28)	1.8769	0.22	-0.37
	CT_2	H-1 → L(-0.28)	1.9240	0.22	0.57
1.8	S_1	H → L(0.50) H → L+1(0.77) H-1 → L+1(0.32)	1.6035	0.47	-0.54
	S_2	H → L(0.83) H → L+1(-0.48)	1.6737	0.15	0.38
	CT_1	H → L+1(-0.40) H-1 → L+1(0.86) H → L+1(0.40)	1.8531	0.24	-0.35
	CT_2	H-1 → L(0.91) H-1 → L+1(-0.31)	1.8716	0.25	0.42
1.9	S_1	H → L(0.42) H → L+1(0.77) H-1 → L+1(0.36)	1.5986	0.42	-0.58
	S_2	H → L(0.85) H → L+1(-0.45)	1.6611	0.14	0.45
	CT_1	H → L+1(-0.43) H-1 → L+1(0.86)	1.8308	0.29	-0.31
	CT_2	H-1 → L(0.94) H-1 → L+1(-0.23)	1.8579	0.25	0.36
2.0	S_1	H → L(0.48) H → L+1(0.75) H-1 → L+1(0.39)	1.5911	0.39	-0.60
	S_2	H → L(0.86) H → L+1(-0.44)	1.6484	0.12	0.49
	CT_1	H → L+1(-0.46) H-1 → L+1(0.86)	1.8278	0.34	-0.28
	CT_2	H-1 → L(0.96)	1.8489	0.24	0.31
2.1	CT_1	H → L(0.90) H → L+1(0.37)	1.5772	0.30	-0.69
	CT_2	H → L(-0.38) H → L+1(0.84) H-1 → L(-0.33)	1.6267	0.15	0.55
	S_1	H-1 → L+1(0.97)	1.7789	0.62	0.13
	S_2	H → L+1(0.36) H-1 → L(0.92)	1.8071	0.02	-0.01
2.2	CT_1	H → L(0.88) H → L+1(0.38)	1.5708	0.27	-0.73
	CT_2	H → L(-0.39) H → L+1(0.82) H-1 → L(-0.35)	1.6185	0.15	0.61
	S_1	H-1 → L+1(0.95) H → L(0.23)	1.7948	0.64	0.13
	S_2	H → L+1(0.38) H-1 → L(0.91)	1.8069	0.03	-0.03
	CT_1	H → L(0.87) H → L+1(0.41)	1.5645	0.23	-0.78
	CT_2	H → L(-0.41) H → L+1(0.80) H-1 → L(-0.36)	1.6112	0.15	0.66
2.3	S_1	H-1 → L+1(0.94) H → L(0.26)	1.7915	0.67	0.12
	S_2	H → L+1(0.40) H-1 → L(0.90)	1.8069	0.03	-0.03
	CT_1	H → L(0.85) H → L+1(0.42)	1.5583	0.21	-0.79
	CT_2	H → L(-0.43) H → L+1(0.78) H-1 → L(-0.38)	1.6037	0.14	0.70
2.4	S_1	H-1 → L+1(0.93) H → L(0.28)	1.7891	0.68	0.11
	S_2	H → L+1(0.41) H-1 → L(0.89)	1.8070	0.04	-0.04
	CT_1	H → L(0.82) H → L+1(0.46)	1.5463	0.18	-0.84
	CT_2	H → L(-0.45) H → L+1(0.74) H-1 → L(-0.39)	1.5896	0.13	0.76
2.6	S_1	H-1 → L+1(0.91) H → L(0.33)	1.7849	0.71	0.09
	S_2	H → L+1(0.43) H-1 → L(0.87)	1.8073	0.05	-0.03
	CT_1	H → L(0.80) H → L+1(0.48)	1.5362	0.14	-0.86
	CT_2	H → L(-0.47) H → L+1(0.72) H-1 → L(-0.40) H-1 → L+1(0.31)	1.5776	0.12	0.81
2.8	S_1	H-1 → L+1(0.89) H → L(0.36)	1.7822	0.73	-0.08
	S_2	H → L+1(0.44) H-1 → L(0.86)	1.8073	0.05	0.03
	CT_1	H → L(0.78) H → L+1(0.50)	1.5247	0.12	-0.89
	CT_2	H → L(-0.48) H → L+1(0.69) H-1 → L(-0.41) H-1 → L+1(0.34)	1.5653	0.11	0.84
3.0	S_1	H → L(0.39) H-1 → L+1(0.88)	1.7798	0.75	0.06
	S_2	H-1 → L+1(0.85) H → L+1(0.46)	1.8073	0.05	-0.02
	CT_1	H → L(0.74) H → L+1(0.52) H-1 → L(0.36)	1.4873	0.06	-0.93
	CT_2	H-1 → L(-0.38) H → L+1(0.64) H → L(0.48)	1.5300	0.08	0.91
4.0...	S_1	H → L(0.46) H-1 → L+1(0.84)	1.7755	0.80	0.03
	S_2	H-1 → L(0.84) H → L+1(0.49)	1.8062	0.03	-0.01
	CT_1	H → L(0.61) H → L+1(0.61) H-1 → L(0.42)	1.4015	0.03	-0.94
	CT_2	H-1 → L(0.40) H → L+1(0.52) H → L(0.56)	1.4304	0.05	0.93
10.0...	S_1	H → L(0.53) H-1 → L+1(0.75)	1.7662	0.74	0.01
	S_2	H-1 → L(0.59) H → L+1(0.35)	1.7896	0.12	-0.01
	CT_1	H → L+1(0.69) H → L(0.48) H-1 → L(0.45)	1.3500	0.02	-0.91
	CT_2	H → L(0.64) H → L+1(0.40) H-1 → L+1(0.51) H-1 → L(0.42)	1.3697	0.05	0.90
78	S_1	H-1 → L+1(0.74) H → L(-0.56)	1.7637	0.74	0.09
	S_2	H-1 → L(0.74) H → L+1(-0.55)	1.7945	0.02	-0.07

SI Table S2. Excited states energies at ϵ=2.0 for the dimers of Figure 5(B) and 5(C) where the distinctly oriented PFGs are removed. Figure 5(B) dimer exhibits same orientation as in Figure 5(A). In Figure 5(C), the monomers are shifted towards each other to obtain a stacked dimer geometry.

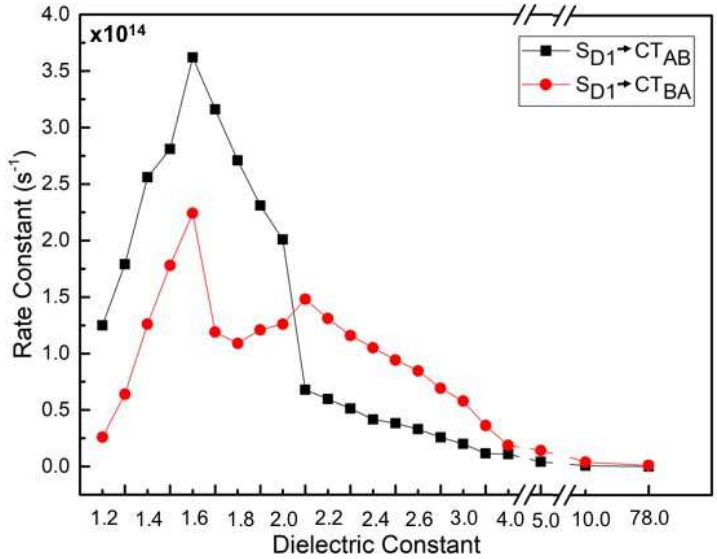
	state	excitation energy(eV)	oscillator strength	net charge (e)
5(b)	S_1	1.9371	0.91	0.00
	S_2	2.0131	0.00	0.00
	CT_1	2.2277	0.00	0.61
	CT_2	2.2597	0.05	-0.62
5(c)	CT_1	2.0530	0.02	-0.80
	CT_2	2.0675	0.02	0.76
	S_1	2.1392	0.00	0.05
	S_2	2.2905	0.53	0.02

SI Table S3. Diabatic states-based energy parameters and rates. Excited state (S_{D1}), Electronic coupling ($V_{\rm el}$), CT state energy, and CT-optimized energies (CT*), driving force (ΔE), reorganization energy ($E_r^{\rm tot}$), activation energy (E_A), Marcus CT rate ($k_{\rm M}$) and Fermi golden rule CT rate ($k_{\rm FGR}$). For the CT states, CT_{AB} and CT_{BA} are provided at the first and second row, respectively, for each dielectric value.

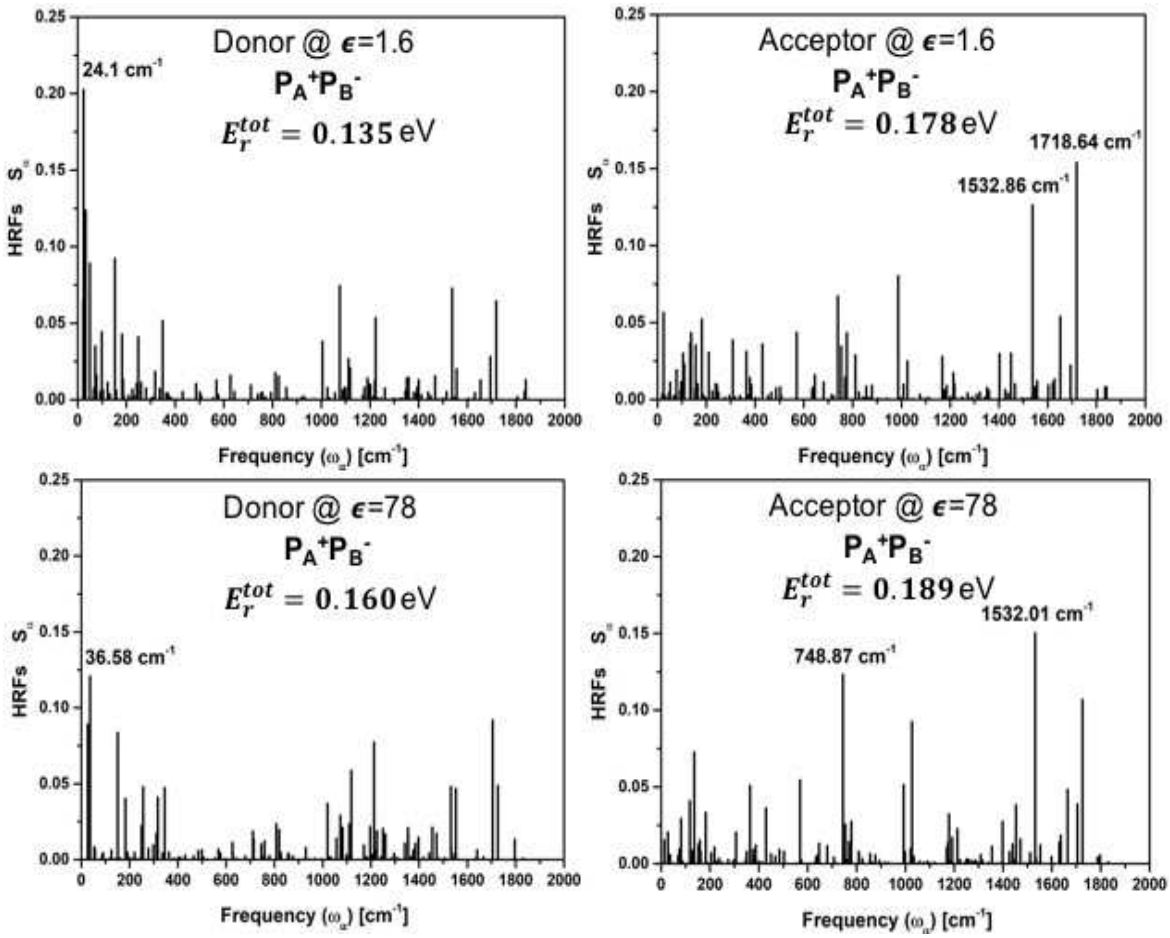
ϵ	S_{D1} [eV]	CT [eV]	CT* [eV]	$V_{\rm el}$ [eV]	$\lvert\Delta E\rvert$ [eV]	$E_r^{\rm tot}$ [eV]	$E_{\rm a}$ [eV]	$k_{\rm M}$ [s^{-1}]	$k_{\rm FGR}$ [s^{-1}]
1.2	1.7493	1.9136	1.6126	0.099	0.136	0.301	0.023	$1.25\text{x}10^{14}$	$1.66\text{x}10^{14}$
		2.0274	1.7264	0.102	0.022		0.064	$2.60\text{x}10^{13}$	$1.42\text{x}10^{14}$
1.3	1.7506	1.8626	1.5536	0.097	0.188	0.309	0.012	$1.79\text{x}10^{14}$	$1.81\text{x}10^{14}$
		1.9739	1.6649	0.107	0.077		0.044	$6.40\text{x}10^{13}$	$1.52\text{x}10^{14}$
1.4	1.7515	1.8185	1.5085	0.099	0.243	0.310	0.0036	$2.56\text{x}10^{14}$	$1.80\text{x}10^{14}$
		1.9289	1.6189	0.105	0.134		0.0250	$1.26\text{x}10^{14}$	$1.59\text{x}10^{14}$
1.5	1.7531	1.7819	1.4709	0.098	0.282	0.311	0.0007	$2.81\text{x}10^{14}$	$1.82\text{x}10^{14}$
		1.8892	1.5782	0.102	0.175		0.0147	$1.78\text{x}10^{14}$	$1.49\text{x}10^{14}$
1.6	1.7323	1.7257	1.4127	0.110	0.320	0.313	0.0001	$3.62\text{x}10^{14}$	$1.84\text{x}10^{14}$
		1.8215	1.5085	0.060	0.224		0.0063	$2.24\text{x}10^{14}$	$7.29\text{x}10^{13}$
1.7	1.7370	1.7042	1.3912	0.104	0.341	0.313	0.0006	$3.16\text{x}10^{14}$	$1.65\text{x}10^{14}$
		1.7899	1.4769	0.063	0.260		0.0022	$1.19\text{x}10^{14}$	$6.62\text{x}10^{13}$
1.8	1.7325	1.6902	1.3752	0.098	0.357	0.315	0.0014	$2.71\text{x}10^{14}$	$1.45\text{x}10^{14}$
		1.7624	1.4474	0.064	0.285		0.0007	$1.09\text{x}10^{14}$	$6.32\text{x}10^{13}$
1.9	1.7454	1.6750	1.3600	0.095	0.385	0.315	0.0039	$2.31\text{x}10^{14}$	$1.32\text{x}10^{14}$
		1.7375	1.4225	0.064	0.323		0.00001	$1.22\text{x}10^{14}$	$6.27\text{x}10^{13}$
2.0	1.7474	1.6614	1.3454	0.092	0.402	0.316	0.0059	$2.01\text{x}10^{14}$	$1.20\text{x}10^{14}$
		1.7160	1.4000	0.066	0.347		0.0183	$1.26\text{x}10^{14}$	$6.68\text{x}10^{13}$
2.1	1.7326	1.6193	1.3023	0.058	0.430	0.317	0.0101	$6.78\text{x}10^{13}$	$4.31\text{x}10^{13}$
		1.6773	1.3603	0.074	0.373		0.0025	$1.48\text{x}10^{14}$	$8.14\text{x}10^{13}$
2.2	1.7356	1.6086	1.2896	0.058	0.449	0.319	0.0132	$5.98\text{x}10^{13}$	$3.91\text{x}10^{13}$
		1.6637	1.3447	0.072	0.391		0.0041	$1.31\text{x}10^{14}$	$7.55\text{x}10^{13}$
2.3	1.7386	1.5986	1.2786	0.056	0.460	0.320	0.0153	$5.13\text{x}10^{13}$	$3.45\text{x}10^{13}$
		1.6523	1.3323	0.070	0.406		0.0058	$1.16\text{x}10^{14}$	$6.92\text{x}10^{13}$
2.4	1.7403	1.5897	1.2687	0.055	0.472	0.321	0.0196	$4.18\text{x}10^{13}$	$3.18\text{x}10^{13}$
		1.6414	1.3204	0.069	0.420		0.0076	$1.05\text{x}10^{14}$	$6.42\text{x}10^{13}$
2.5	1.7422	1.5819	1.2619	0.053	0.480	0.320	0.0200	$3.84\text{x}10^{13}$	$2.85\text{x}10^{13}$
		1.6312	1.3112	0.068	0.431		0.0002	$9.43\text{x}10^{13}$	$5.92\text{x}10^{13}$
2.6	1.7438	1.5733	1.2523	0.052	0.492	0.321	0.0227	$3.31\text{x}10^{13}$	$2.65\text{x}10^{13}$
		1.6222	1.3012	0.067	0.443		0.0116	$8.47\text{x}10^{13}$	$5.41\text{x}10^{13}$
2.8	1.7465	1.5600	1.2350	0.050	0.512	0.325	0.0269	$2.59\text{x}10^{13}$	$2.34\text{x}10^{13}$
		1.6062	1.2812	0.065	0.465		0.0151	$6.93\text{x}10^{13}$	$4.61\text{x}10^{13}$
3.0	1.7480	1.5462	1.2202	0.048	0.528	0.326	0.0312	$2.01\text{x}10^{13}$	$2.07\text{x}10^{13}$
		1.5911	1.2651	0.064	0.483		0.0003	$5.78\text{x}10^{13}$	$4.19\text{x}10^{13}$
3.5	1.7527	1.5207	1.1937	0.044	0.559	0.327	0.0411	$1.15\text{x}10^{13}$	$1.57\text{x}10^{13}$
		1.5654	1.2384	0.059	0.514		0.0015	$3.62\text{x}10^{13}$	$3.28\text{x}10^{13}$
4.0	1.7560	1.5022	1.1702	0.042	0.586	0.332	0.0486	$1.09\text{x}10^{13}$	$1.45\text{x}10^{13}$
		1.5477	1.2157	0.058	0.540		0.0067	$1.86\text{x}10^{13}$	$2.87\text{x}10^{13}$
5.0	1.7600	1.4757	1.1437	0.039	0.616	0.332	0.0607	$4.22\text{x}10^{12}$	$9.26\text{x}10^{12}$
		1.5226	1.1906	0.050	0.569		0.0423	$1.42\text{x}10^{13}$	$1.90\text{x}10^{13}$
10.0	1.7573	1.4115	1.0685	0.033	0.689	0.343	0.0872	$1.07\text{x}10^{12}$	$5.12\text{x}10^{12}$
		1.4409	1.0979	0.050	0.659		0.0223	$4.28\text{x}10^{12}$	$1.36\text{x}10^{13}$
78.0	1.7534	1.3584	1.0094	0.027	0.744	0.349	0.1118	$2.74\text{x}10^{11}$	$2.77\text{x}10^{12}$
		1.3773	1.0283	0.048	0.725		0.1013	$1.30\text{x}10^{12}$	$9.63\text{x}10^{12}$



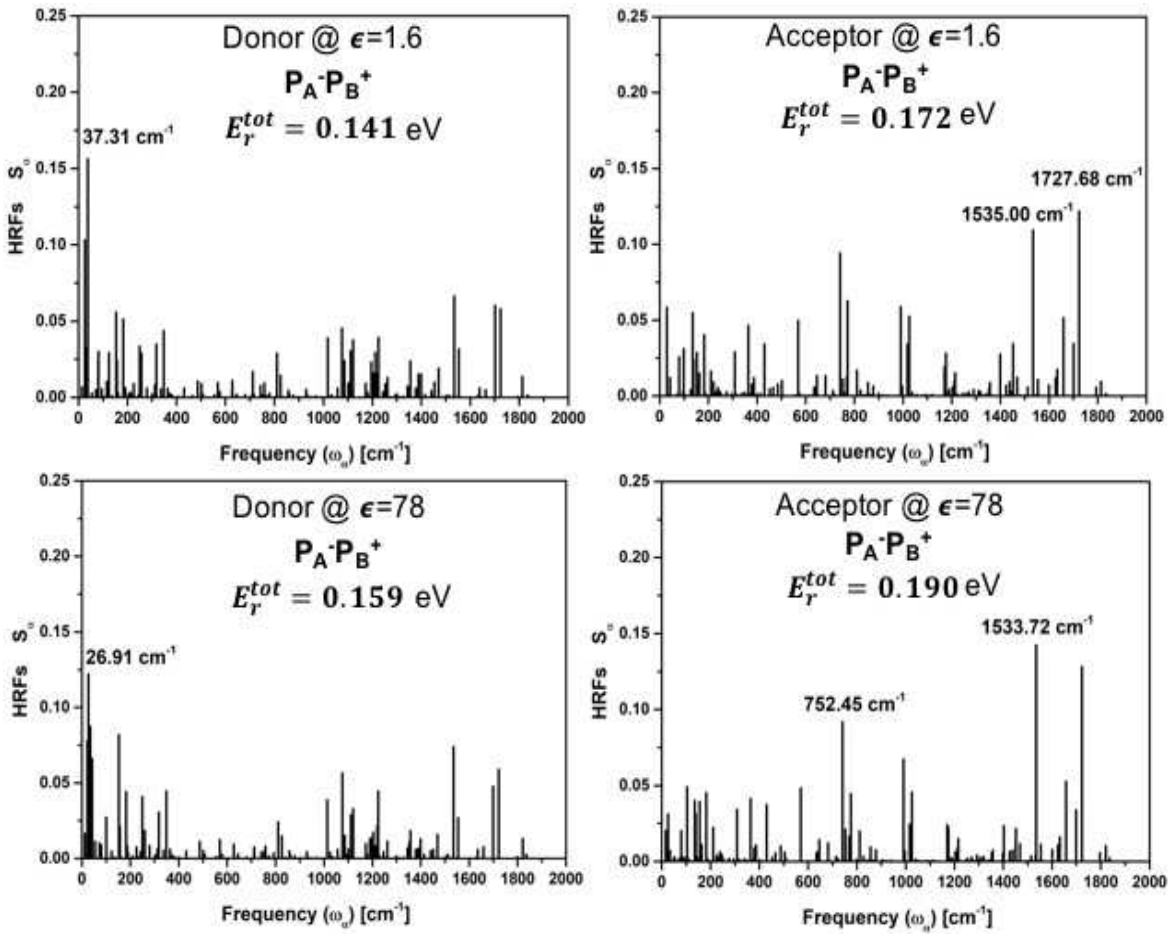
SI Figure S1. FGR CT rates for the full range of dielectric constants up to 78. Black and red curves correspond to CT_{AB} and CT_{BA} processes, respectively.



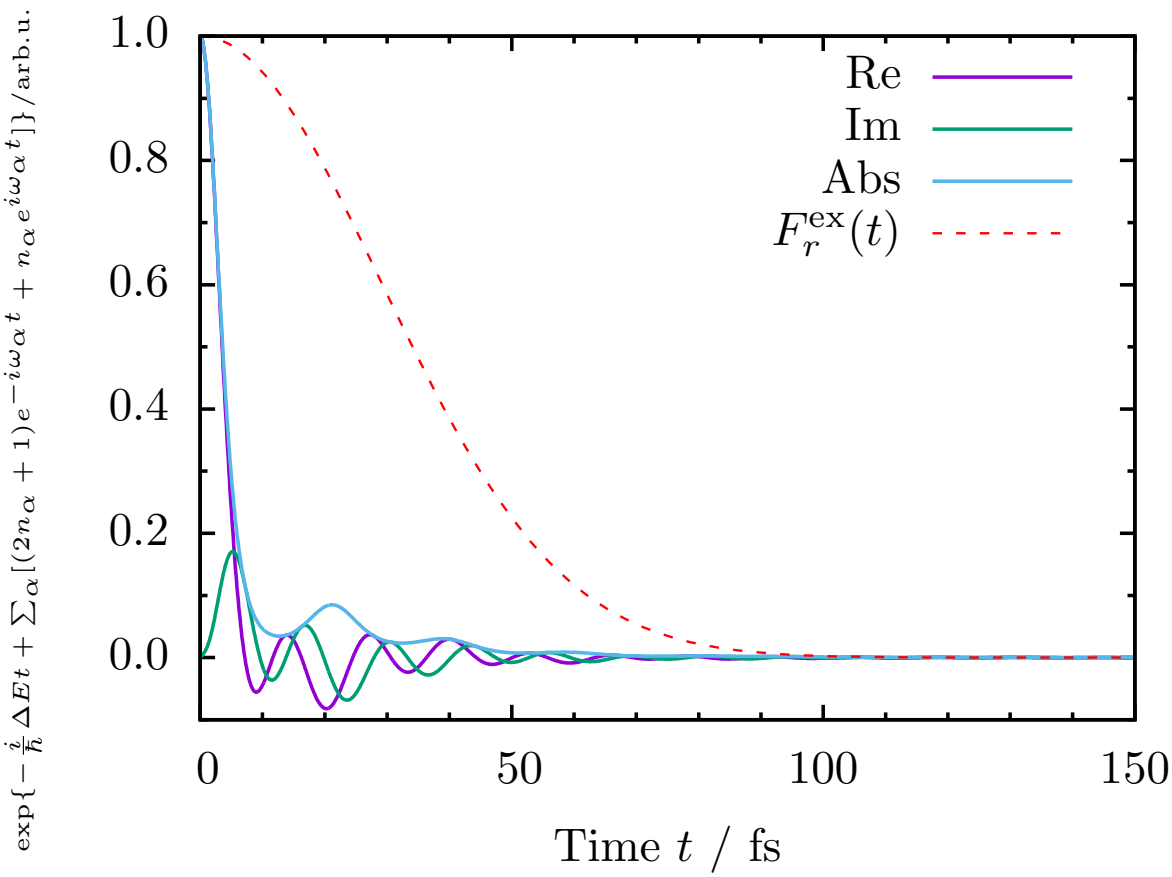
SI Figure S2. Marcus CT rates for the full range of dielectric constants up to 78. Black and red curves correspond to CT_{AB} and CT_{BA} processes, respectively



SI Figure S3. HRF distributions due to electron transfer ($P_A^+ P_B^-$) in the special pair for dielectric constants 1.6 (upper panel) and 78 (lower panel) due to acceptor and donor monomer contributions.



SI Figure S4. HRF distributions due to electron transfer ($P_A^- \; P_B^+$) in the special pair for dielectric constants 1.6 (upper panel) and 78 (lower panel) due to acceptor and donor monomer contributions.



SI Figure S5. The time-dependent integrand of the FGR-expression (solid lines), without the $F_r^{\mathrm{ex}}(t)$ window function, decays at $\epsilon = 1.6$ (highest rate) on a sub-100 fs timescale. The semi-classical contribution of an external reorganization energy E^{ex} of 0.01 eV leads to a window function $F_r^{\mathrm{ex}}(t)$ (red dashed line) with only negligible effect on the FGR rate.

SI Table S4. The atomic coordinates of the X-Ray structure of special pair (Å).

Mg	-4.285600000000000	4.1406700000000001	-3.9274900000000001
C	-0.978600000000000	3.5786699999999998	-4.8334900000000003
C	-5.054600000000000	0.9996699999999999	-5.1644899999999998
C	-7.349600000000000	4.2586700000000004	-2.3654899999999999
C	-3.107600000000000	6.6666699999999999	-1.7944899999999999
N	-3.183600000000000	2.5906699999999998	-4.9374900000000004
C	-1.851600000000000	2.6466699999999999	-5.3034900000000000
C	-1.561600000000000	1.5626700000000000	-6.3024899999999997
C	-2.767600000000000	0.6706700000000000	-6.2544899999999997
C	-3.754600000000000	1.4086700000000001	-5.3894900000000003
C	-0.325600000000000	0.7356700000000000	-6.0104899999999999
C	-0.159600000000000	-0.4323300000000000	-6.9514899999999997
C	0.831400000000000	-1.4203300000000001	-6.4334899999999999
O	0.607400000000000	-2.6133299999999999	-6.5784900000000004
O	1.969400000000000	-1.0423300000000000	-5.7294900000000002
N	-5.933600000000000	2.9086699999999999	-3.8534899999999999
C	-6.043600000000000	1.6746700000000001	-4.4654900000000000
C	-7.386600000000000	1.1766700000000001	-4.2814899999999998
C	-8.054600000000001	2.0616699999999999	-3.4804900000000001
C	-7.113600000000000	3.1486700000000001	-3.1774900000000001
C	-9.365600000000001	1.9616700000000000	-2.8414899999999998
O	-10.094600000000000	0.9626700000000000	-2.8494899999999999
C	-10.018599999999999	3.2616700000000001	-2.4964900000000001
N	-5.118600000000000	5.3536700000000002	-2.4554900000000002
C	-6.460600000000000	5.2806699999999998	-2.0494900000000000
C	-6.789600000000000	6.5676699999999997	-1.3304900000000000
C	-5.463600000000000	6.9576700000000002	-0.7454900000000000
C	-4.467600000000000	6.3646700000000003	-1.7254900000000000
N	-2.504600000000000	4.9356700000000000	-3.3694899999999999
C	-2.168600000000000	5.9976700000000003	-2.5664899999999999
C	-0.739600000000000	6.2876700000000003	-2.6424900000000000
C	-0.252600000000000	5.4276700000000000	-3.5684900000000002
C	-1.324600000000000	4.5446700000000000	-3.9414899999999999
C	0.890400000000000	5.0406700000000004	-4.3484900000000000
O	2.064400000000000	5.4646699999999999	-4.3504899999999997
C	0.419400000000000	3.9516700000000000	-5.3264899999999997
C	0.239400000000000	4.5876700000000001	-6.6664899999999996
O	0.837400000000000	4.0656699999999999	-7.6194899999999999
O	-0.576600000000000	5.6456700000000000	-6.8344899999999997
C	-0.759600000000000	6.2616699999999996	-8.0714900000000007
C	2.627400000000000	-2.0983299999999998	-4.9834899999999998
H	-5.320610000000000	0.0856000000000000	-5.5629000000000000
H	-8.292370000000000	4.3294800000000002	-1.9517400000000000
H	-2.770530000000000	7.4561700000000002	-1.2216800000000001
H	-1.367810000000000	2.0106299999999999	-7.2546900000000001
H	-3.165030000000000	0.5202900000000000	-7.2365000000000004
H	-2.537780000000000	-0.3004400000000000	-5.8684500000000002
H	0.534370000000000	1.3666300000000000	-6.0956799999999998
H	-0.433770000000000	0.3374600000000000	-5.0232599999999996
H	-1.105020000000000	-0.9190300000000000	-7.0705900000000002
H	0.199290000000000	-0.0586700000000000	-7.8876999999999997
H	-7.773340000000000	0.3080800000000000	-4.6827300000000003
H	-9.290039999999999	4.0448800000000000	-2.5230199999999998
H	-10.440049999999999	3.1997000000000000	-1.5149400000000000
H	-10.793020000000000	3.4708000000000001	-3.2046100000000002
H	-7.518820000000000	6.4074499999999999	-0.5640300000000000
H	-7.213320000000000	7.3165800000000001	-1.9664900000000001
H	-5.364580000000000	8.0218299999999996	-0.6937400000000000
H	-5.326750000000000	6.6084100000000001	0.2566000000000000
H	-0.213910000000000	6.9954900000000002	-2.1061399999999999
H	1.096340000000000	3.1250200000000001	-5.3838499999999998
H	-1.446890000000000	7.0750299999999999	-7.9667000000000003
H	-1.151360000000000	5.5513100000000000	-8.7691999999999997
H	0.178990000000000	6.6315299999999997	-8.4280899999999992
H	3.485210000000000	-1.7001900000000001	-4.4829299999999996
H	2.934010000000000	-2.8722099999999999	-5.6558000000000002
H	1.948310000000000	-2.5014400000000001	-4.2615299999999996
Mg	-9.747600000000000	-0.1673300000000000	0.0385100000000000
C	-12.562600000000000	-2.0153300000000001	-0.9554900000000000
C	-7.827600000000000	-2.1383299999999998	-2.0474899999999998
C	-7.185600000000000	2.1506699999999999	0.1625100000000000
C	-11.905600000000000	2.1856700000000000	1.4395100000000001
N	-10.110600000000000	-1.9173300000000000	-1.1684900000000000
C	-11.355600000000001	-2.5283300000000000	-1.3974899999999999
C	-11.160600000000001	-3.6923300000000001	-2.3084899999999999
C	-9.669600000000001	-3.9023300000000001	-2.2834900000000000
C	-9.119600000000000	-2.5673300000000001	-1.8704900000000000
C	-11.621600000000001	-3.3353299999999999	-3.7214900000000002
C	-11.654600000000000	-4.4413299999999998	-4.7204899999999999
C	-12.848599999999999	-5.3313300000000003	-4.5364899999999997
O	-13.459600000000000	-5.3023300000000004	-3.4584899999999998
O	-13.298600000000000	-6.2343299999999999	-5.5794899999999998
N	-7.833600000000000	-0.0643300000000000	-0.7264900000000000
C	-7.240600000000000	-0.9973300000000000	-1.5244899999999999
C	-5.873600000000000	-0.6153300000000000	-1.7184900000000001
C	-5.743600000000000	0.7106700000000000	-1.3704900000000000
C	-6.956600000000000	0.9866700000000000	-0.5914900000000000
C	-4.713600000000000	1.5856699999999999	-0.8254899999999999
O	-4.000600000000000	1.3196699999999999	0.0875100000000000
C	-3.914600000000000	1.8966700000000001	-2.0634899999999998
N	-9.534599999999999	1.7696700000000001	0.9025100000000000
C	-8.350600000000000	2.5286700000000000	0.8515100000000000
C	-8.526600000000000	3.7686700000000002	1.7095100000000001
C	-10.029600000000000	3.9256700000000002	1.7955099999999999
C	-10.565600000000000	2.5416699999999999	1.4665100000000000
N	-11.725600000000000	0.0366700000000000	0.3275100000000000
C	-12.467599999999999	1.0276700000000001	0.9105100000000000
C	-13.889600000000000	0.6796700000000000	0.8805100000000000
C	-13.980600000000001	-0.4313300000000000	0.1125100000000000
C	-12.645600000000000	-0.8553300000000000	-0.1824900000000000
C	-14.873600000000000	-1.3423300000000000	-0.5654900000000000
O	-16.102599999999999	-1.4343300000000001	-0.5334900000000000
C	-14.014600000000000	-2.3323299999999998	-1.3804900000000000
C	-14.390599999999999	-3.7433299999999998	-0.9714900000000000
O	-13.642600000000000	-4.3553300000000004	-0.1924900000000000
O	-15.585599999999999	-4.2893299999999996	-1.3904900000000000
C	-16.049600000000002	-5.4153300000000000	-0.8634900000000000
C	-14.679600000000001	-6.6613300000000004	-5.5124899999999997
H	-7.224940000000000	-2.7333699999999999	-2.6372000000000000
H	-6.396250000000000	2.8132299999999999	0.2171600000000000
H	-12.563879999999999	2.8591099999999998	1.8616200000000001
H	-11.713609999999999	-4.5597899999999996	-2.0142300000000000
H	-9.404170000000001	-4.6584899999999996	-1.5745000000000000
H	-9.284979999999999	-4.2315800000000001	-3.2261299999999999
H	-12.612019999999999	-2.9372500000000001	-3.6473300000000002
H	-10.887210000000000	-2.6495199999999999	-4.0892400000000002
H	-11.687410000000000	-4.0183700000000000	-5.7027999999999999
H	-10.775630000000000	-5.0359400000000001	-4.5835600000000003
H	-5.116800000000000	-1.2281599999999999	-2.0601200000000000
H	-4.580020000000000	2.1320299999999999	-2.8676800000000000
H	-3.321760000000000	1.0462199999999999	-2.3283700000000001
H	-3.274300000000000	2.7327599999999999	-1.8740600000000001
H	-8.078469999999999	4.6222200000000004	1.2452399999999999
H	-8.060150000000000	3.6825199999999998	2.6686299999999998
H	-10.324830000000000	4.2233499999999999	2.7799499999999999
H	-10.402670000000001	4.6789500000000004	1.1334599999999999
H	-14.662660000000001	1.1783399999999999	1.3482000000000001
H	-14.147640000000001	-2.2494700000000001	-2.4389500000000002
H	-16.982730000000000	-5.6662200000000000	-1.3230700000000000
H	-16.194120000000002	-5.2837399999999999	0.1885100000000000
H	-15.346090000000000	-6.2039499999999999	-1.0309699999999999
H	-14.889419999999999	-7.3196099999999999	-6.3295199999999996
H	-15.320449999999999	-5.8063700000000003	-5.5696500000000002
H	-14.850080000000000	-7.1737299999999999	-4.5887599999999997

SI Table S5. The atomic coordinates of the X-Ray structure of BChl monomer (P_A) molecule (Å).

Mg	-9.747600000000000	-0.1673300000000000	0.0385100000000000
C	-12.562600000000000	-2.0153300000000001	-0.9554900000000000
C	-7.827600000000000	-2.1383299999999998	-2.0474899999999998
C	-7.185600000000000	2.1506699999999999	0.1625100000000000
C	-11.905600000000000	2.1856700000000000	1.4395100000000001
N	-10.110600000000000	-1.9173300000000000	-1.1684900000000000
C	-11.355600000000001	-2.5283300000000000	-1.3974899999999999
C	-11.160600000000001	-3.6923300000000001	-2.3084899999999999
C	-9.669600000000001	-3.9023300000000001	-2.2834900000000000
C	-9.119600000000000	-2.5673300000000001	-1.8704900000000000
C	-11.621600000000001	-3.3353299999999999	-3.7214900000000002
C	-11.654600000000000	-4.4413299999999998	-4.7204899999999999
C	-12.848599999999999	-5.3313300000000003	-4.5364899999999997
O	-13.459600000000000	-5.3023300000000004	-3.4584899999999998
O	-13.298600000000000	-6.2343299999999999	-5.5794899999999998
N	-7.833600000000000	-0.0643300000000000	-0.7264900000000000
C	-7.240600000000000	-0.9973300000000000	-1.5244899999999999
C	-5.873600000000000	-0.6153300000000000	-1.7184900000000001
C	-5.743600000000000	0.7106700000000000	-1.3704900000000000
C	-6.956600000000000	0.9866700000000000	-0.5914900000000000
C	-4.713600000000000	1.5856699999999999	-0.8254899999999999
O	-4.000600000000000	1.3196699999999999	0.0875100000000000
C	-3.914600000000000	1.8966700000000001	-2.0634899999999998
N	-9.534599999999999	1.7696700000000001	0.9025100000000000
C	-8.350600000000000	2.5286700000000000	0.8515100000000000
C	-8.526600000000000	3.7686700000000002	1.7095100000000001
C	-10.029600000000000	3.9256700000000002	1.7955099999999999
C	-10.565600000000000	2.5416699999999999	1.4665100000000000
N	-11.725600000000000	0.0366700000000000	0.3275100000000000
C	-12.467599999999999	1.0276700000000001	0.9105100000000000
C	-13.889600000000000	0.6796700000000000	0.8805100000000000
C	-13.980600000000001	-0.4313300000000000	0.1125100000000000
C	-12.645600000000000	-0.8553300000000000	-0.1824900000000000
C	-14.873600000000000	-1.3423300000000000	-0.5654900000000000
O	-16.102599999999999	-1.4343300000000001	-0.5334900000000000
C	-14.014600000000000	-2.3323299999999998	-1.3804900000000000
C	-14.390599999999999	-3.7433299999999998	-0.9714900000000000
O	-13.642600000000000	-4.3553300000000004	-0.1924900000000000
O	-15.585599999999999	-4.2893299999999996	-1.3904900000000000
C	-16.049600000000002	-5.4153300000000000	-0.8634900000000000
C	-14.679600000000001	-6.6613300000000004	-5.5124899999999997
H	-7.224940000000000	-2.7333699999999999	-2.6372000000000000
H	-6.396250000000000	2.8132299999999999	0.2171600000000000
H	-12.563879999999999	2.8591099999999998	1.8616200000000001
H	-11.713609999999999	-4.5597899999999996	-2.0142300000000000
H	-9.404170000000001	-4.6584899999999996	-1.5745000000000000
H	-9.284979999999999	-4.2315800000000001	-3.2261299999999999
H	-12.612019999999999	-2.9372500000000001	-3.6473300000000002
H	-10.887210000000000	-2.6495199999999999	-4.0892400000000002
H	-11.687410000000000	-4.0183700000000000	-5.7027999999999999
H	-10.775630000000000	-5.0359400000000001	-4.5835600000000003
H	-5.116800000000000	-1.2281599999999999	-2.0601200000000000
H	-4.580020000000000	2.1320299999999999	-2.8676800000000000
H	-3.321760000000000	1.0462199999999999	-2.3283700000000001
H	-3.274300000000000	2.7327599999999999	-1.8740600000000001
H	-8.078469999999999	4.6222200000000004	1.2452399999999999
H	-8.060150000000000	3.6825199999999998	2.6686299999999998
H	-10.324830000000000	4.2233499999999999	2.7799499999999999
H	-10.402670000000001	4.6789500000000004	1.1334599999999999
H	-14.662660000000001	1.1783399999999999	1.3482000000000001
H	-14.147640000000001	-2.2494700000000001	-2.4389500000000002
H	-16.982730000000000	-5.6662200000000000	-1.3230700000000000
H	-16.194120000000002	-5.2837399999999999	0.1885100000000000
H	-15.346090000000000	-6.2039499999999999	-1.0309699999999999
H	-14.889419999999999	-7.3196099999999999	-6.3295199999999996
H	-15.320449999999999	-5.8063700000000003	-5.5696500000000002
H	-14.850080000000000	-7.1737299999999999	-4.5887599999999997

SI Table S6. The atomic coordinates of the X-Ray structure of BChl monomer (P_B) molecule (Å).

Mg	-4.285600000000000	4.1406700000000001	-3.9274900000000001
C	-0.978600000000000	3.5786699999999998	-4.8334900000000003
C	-5.054600000000000	0.9996699999999999	-5.1644899999999998
C	-7.349600000000000	4.2586700000000004	-2.3654899999999999
C	-3.107600000000000	6.6666699999999999	-1.7944899999999999
N	-3.183600000000000	2.5906699999999998	-4.9374900000000004
C	-1.851600000000000	2.6466699999999999	-5.3034900000000000
C	-1.561600000000000	1.5626700000000000	-6.3024899999999997
C	-2.767600000000000	0.6706700000000000	-6.2544899999999997
C	-3.754600000000000	1.4086700000000001	-5.3894900000000003
C	-0.325600000000000	0.7356700000000000	-6.0104899999999999
C	-0.159600000000000	-0.4323300000000000	-6.9514899999999997
C	0.831400000000000	-1.4203300000000001	-6.4334899999999999
O	0.607400000000000	-2.6133299999999999	-6.5784900000000004
O	1.969400000000000	-1.0423300000000000	-5.7294900000000002
N	-5.933600000000000	2.9086699999999999	-3.8534899999999999
C	-6.043600000000000	1.6746700000000001	-4.4654900000000000
C	-7.386600000000000	1.1766700000000001	-4.2814899999999998
C	-8.054600000000001	2.0616699999999999	-3.4804900000000001
C	-7.113600000000000	3.1486700000000001	-3.1774900000000001
C	-9.365600000000001	1.9616700000000000	-2.8414899999999998
O	-10.094600000000000	0.9626700000000000	-2.8494899999999999
C	-10.018599999999999	3.2616700000000001	-2.4964900000000001
N	-5.118600000000000	5.3536700000000002	-2.4554900000000002
C	-6.460600000000000	5.2806699999999998	-2.0494900000000000
C	-6.789600000000000	6.5676699999999997	-1.3304900000000000
C	-5.463600000000000	6.9576700000000002	-0.7454900000000000
C	-4.467600000000000	6.3646700000000003	-1.7254900000000000
N	-2.504600000000000	4.9356700000000000	-3.3694899999999999
C	-2.168600000000000	5.9976700000000003	-2.5664899999999999
C	-0.739600000000000	6.2876700000000003	-2.6424900000000000
C	-0.252600000000000	5.4276700000000000	-3.5684900000000002
C	-1.324600000000000	4.5446700000000000	-3.9414899999999999
C	0.890400000000000	5.0406700000000004	-4.3484900000000000
O	2.064400000000000	5.4646699999999999	-4.3504899999999997
C	0.419400000000000	3.9516700000000000	-5.3264899999999997
C	0.239400000000000	4.5876700000000001	-6.6664899999999996
O	0.837400000000000	4.0656699999999999	-7.6194899999999999
O	-0.576600000000000	5.6456700000000000	-6.8344899999999997
C	-0.759600000000000	6.2616699999999996	-8.0714900000000007
C	2.627400000000000	-2.0983299999999998	-4.9834899999999998
H	-5.320610000000000	0.0856000000000000	-5.5629000000000000
H	-8.292370000000000	4.3294800000000002	-1.9517400000000000
H	-2.770530000000000	7.4561700000000002	-1.2216800000000001
H	-1.367810000000000	2.0106299999999999	-7.2546900000000001
H	-3.165030000000000	0.5202900000000000	-7.2365000000000004
H	-2.537780000000000	-0.3004400000000000	-5.8684500000000002
H	0.534370000000000	1.3666300000000000	-6.0956799999999998
H	-0.433770000000000	0.3374600000000000	-5.0232599999999996
H	-1.105020000000000	-0.9190300000000000	-7.0705900000000002
H	0.199290000000000	-0.0586700000000000	-7.8876999999999997
H	-7.773340000000000	0.3080800000000000	-4.6827300000000003
H	-9.290039999999999	4.0448800000000000	-2.5230199999999998
H	-10.440049999999999	3.1997000000000000	-1.5149400000000000
H	-10.793020000000000	3.4708000000000001	-3.2046100000000002
H	-7.518820000000000	6.4074499999999999	-0.5640300000000000
H	-7.213320000000000	7.3165800000000001	-1.9664900000000001
H	-5.364580000000000	8.0218299999999996	-0.6937400000000000
H	-5.326750000000000	6.6084100000000001	0.2566000000000000
H	-0.213910000000000	6.9954900000000002	-2.1061399999999999
H	1.096340000000000	3.1250200000000001	-5.3838499999999998
H	-1.446890000000000	7.0750299999999999	-7.9667000000000003
H	-1.151360000000000	5.5513100000000000	-8.7691999999999997
H	0.178990000000000	6.6315299999999997	-8.4280899999999992
H	3.485210000000000	-1.7001900000000001	-4.4829299999999996
H	2.934010000000000	-2.8722099999999999	-5.6558000000000002
H	1.948310000000000	-2.5014400000000001	-4.2615299999999996

SI Table S7. The atomic coordinates of structure demonstrated in Figure 5(b) (Å).

Mg	5.065200000000000	-6.520420000000000	-8.902910000000000
C	5.207590000000000	-9.885529999999999	-8.058790000000000
C	1.678220000000000	-6.634730000000000	-8.341070000000000
C	4.727610000000000	-3.437980000000000	-10.323510000000001
C	8.259480000000000	-6.752640000000000	-10.315910000000001
N	3.655650000000000	-8.057570000000000	-8.228149999999999
C	3.969790000000000	-9.364260000000000	-7.851000000000000
C	2.736710000000000	-10.090890000000000	-7.342350000000000
C	1.652870000000000	-9.002380000000000	-7.409060000000000
C	2.363270000000000	-7.830260000000000	-8.040310000000000
N	3.464380000000000	-5.311080000000000	-9.395210000000001
C	2.194580000000000	-5.496010000000000	-8.928319999999999
C	1.448270000000000	-4.260220000000000	-9.062720000000001
C	2.287410000000000	-3.339120000000000	-9.600790000000000
C	3.575430000000000	-4.019360000000000	-9.827240000000000
N	6.303330000000000	-5.289270000000000	-10.180040000000000
C	5.985720000000000	-4.053410000000000	-10.522259999999999
C	7.137660000000000	-3.311510000000000	-11.170500000000001
C	8.253460000000000	-4.366310000000000	-11.206000000000000
C	7.619770000000000	-5.571890000000000	-10.530510000000000
N	6.456600000000000	-7.973750000000000	-9.169359999999999
C	7.735760000000000	-7.935260000000000	-9.693310000000000
C	8.380929999999999	-9.174189999999999	-9.527490000000000
C	7.443670000000000	-9.996990000000000	-8.873880000000000
C	6.298930000000000	-9.209840000000000	-8.685510000000001
C	7.200330000000000	-11.313420000000001	-8.334050000000000
O	7.916750000000000	-12.297689999999999	-8.280989999999999
C	5.724690000000000	-11.283550000000000	-7.750960000000000
H	0.635330000000000	-6.595750000000000	-8.041639999999999
H	4.681170000000000	-2.397710000000000	-10.620260000000000
H	9.286470000000000	-6.813630000000000	-10.668410000000000
H	2.509160000000000	-10.878629999999999	-8.068220000000000
H	1.290630000000000	-8.710640000000000	-6.414520000000000
H	7.400190000000000	-2.431770000000000	-10.572469999999999
H	8.558270000000000	-4.610160000000000	-12.228540000000001
H	5.820460000000000	-11.468700000000000	-6.675270000000000
H	0.776730000000000	-9.300739999999999	-7.992220000000000
H	0.418000000000000	-4.118930000000000	-8.760220000000000
H	6.848550000000000	-2.950410000000000	-12.162580000000000
H	9.150570000000000	-4.040340000000000	-10.671370000000000
H	9.381539999999999	-9.419790000000001	-9.859299999999999
H	2.830980000000000	-10.527100000000001	-6.369860000000000
H	5.052390000000000	-12.008620000000001	-8.159829999999999
H	2.066470000000000	-2.353160000000000	-9.810790000000001
Mg	0.983660000000000	-1.193780000000000	-6.986180000000000
C	-2.405500000000000	-0.988070000000000	-6.407670000000000
C	0.906500000000000	-4.374470000000000	-5.661050000000000
C	4.372940000000000	-1.329980000000000	-7.141720000000000
C	1.147400000000000	2.280720000000000	-7.336490000000000
N	-0.564970000000000	-2.514400000000000	-6.194710000000000
C	-1.931370000000000	-2.235950000000000	-6.168350000000000
C	-2.728040000000000	-3.487950000000000	-5.851660000000000
C	-1.629420000000000	-4.428180000000000	-5.320050000000000
C	-0.351080000000000	-3.741410000000000	-5.744560000000000
N	2.407700000000000	-2.551080000000000	-6.359230000000000
C	2.136500000000000	-3.838220000000000	-5.992580000000000
C	3.345360000000000	-4.632380000000000	-6.105680000000000
C	4.326810000000000	-3.812380000000000	-6.558640000000000
C	3.730180000000000	-2.470730000000000	-6.697730000000000
N	2.547090000000000	0.281440000000000	-7.147970000000000
C	3.822640000000000	-0.031890000000000	-7.283470000000000
C	4.686140000000000	1.165810000000000	-7.625600000000000
C	3.675690000000000	2.324450000000000	-7.655770000000000
C	2.348550000000000	1.643200000000000	-7.363540000000000
N	-0.301390000000000	0.365050000000000	-6.816280000000000
C	-0.148710000000000	1.711350000000000	-7.090360000000000
C	-1.397690000000000	2.360350000000000	-7.106520000000000
C	-2.347500000000000	1.354050000000000	-6.840090000000000
C	-1.615040000000000	0.170410000000000	-6.675300000000000
C	-3.752460000000000	1.049100000000000	-6.682010000000000
O	-4.739480000000000	1.765510000000000	-6.728420000000000
C	-3.849050000000000	-0.500690000000000	-6.418270000000000
H	0.901960000000000	-5.413540000000000	-5.347240000000000
H	5.426050000000000	-1.406050000000000	-7.384520000000000
H	1.163410000000000	3.349740000000000	-7.536570000000000
H	-3.484450000000000	-3.288930000000000	-5.085880000000000
H	-1.683100000000000	-5.444560000000000	-5.721860000000000
H	5.186070000000000	1.010620000000000	-8.587750000000000
H	3.901330000000000	3.084550000000000	-6.902020000000000
H	-4.435730000000000	-0.950740000000000	-7.225010000000000
H	3.420640000000000	-5.690480000000000	-5.887360000000000
H	-1.559170000000000	3.415730000000000	-7.286120000000000
H	-1.650730000000000	-4.508370000000000	-4.227130000000000
H	5.468910000000000	1.299430000000000	-6.872470000000000
H	3.652470000000000	2.823080000000000	-8.628869999999999
H	-3.272640000000000	-3.882780000000000	-6.683780000000000
H	-4.332740000000000	-0.759440000000000	-5.499580000000000
H	5.302680000000000	-4.076510000000000	-6.765900000000000

SI Table S8. The atomic coordinates of structure demonstrated in Figure 5(c) (Å).

Mg	4.681670112386202	-6.263147802153376	-8.642919665162513
C	4.730720566929421	-9.684315730269967	-7.837267430732884
C	1.251702788122455	-6.434709870454210	-8.486620030547767
C	4.428080055271212	-3.387776310741616	-10.460169815820498
C	8.006358115153320	-6.581795012681004	-9.826468070487380
N	3.221421571753294	-7.837626330432863	-8.139795415629605
C	3.487744295029743	-9.162113216216895	-7.788211724839771
C	2.210705781752119	-9.904597811779963	-7.466517057531822
C	1.152365913162021	-8.794785596314640	-7.519049935897088
C	1.917549684413736	-7.615615074657518	-8.089181944373992
N	3.096724945793976	-5.227426042980416	-9.548443850374188
C	1.798945554848192	-5.350623361010955	-9.142275744842891
C	1.062687787153023	-4.131055970351833	-9.480294685425386
C	1.946496822083173	-3.284415334698339	-10.041026690351835
C	3.243817759497623	-3.964686618105522	-10.050338233804862
N	6.033170760741695	-5.143445329793540	-9.913311685445334
C	5.716714413113182	-3.967182304280490	-10.430570585823396
C	6.920765454393149	-3.241189688010459	-10.993877540740447
C	8.002376785177292	-4.326392597322386	-10.993494841065337
C	7.371001579457968	-5.437856829743915	-10.173244782024653
N	6.132175253227115	-7.711845052522822	-8.665099808409238
C	7.439450915177679	-7.725545262548480	-9.171190307945331
C	8.009327378966429	-8.995402326739764	-9.037706479676253
C	7.008955913897452	-9.811924238374949	-8.471835070400260
C	5.897331226537328	-8.996290419665449	-8.286877906566597
C	6.662184774836515	-11.163634287212243	-8.040336224799427
O	7.349238645793972	-12.167751410911430	-7.992112398654382
C	5.168489858528879	-11.117345302949561	-7.610279306371367
H	0.188241783884702	-6.390725212441435	-8.271494080497009
H	4.370865678414465	-2.379535512020332	-10.859134152636011
H	9.045026630017778	-6.676946883844566	-10.133417248193405
H	2.019509099711206	-10.680848725245415	-8.215948257610922
H	0.772332206885941	-8.529711972313292	-6.524694656808907
H	7.170589952964700	-2.409541432876201	-10.322679328334781
H	8.207112332618482	-4.682944807048016	-12.009367728563934
H	5.094843685161185	-11.442762293723376	-6.566258423598884
H	0.286097711282160	-9.045525440411762	-8.137528800647029
H	0.009376344650441	-3.975047230976777	-9.285536727689802
H	6.720296968408930	-2.816767859044978	-11.981264036725435
H	8.952903298656379	-3.988489997637410	-10.572503759483466
H	9.004099056407393	-9.276690369522784	-9.356779863665558
H	2.260163784517465	-10.400701887585464	-6.492917867256669
H	4.594362468306144	-11.832026860594315	-8.212049097382748
H	1.777486084130031	-2.281118550798253	-10.410820084441989
Mg	6.602557400992416	-6.887881603952142	-6.446523257236870
C	3.297973847750372	-6.459162631615193	-5.292917824277263
C	6.683373192465033	-9.802441350011572	-4.635419174807075
C	10.013198088796907	-6.844357371644583	-6.488864222793953
C	6.653732661643051	-3.463247751945231	-7.312256882933360
N	5.138697700825863	-7.998603847064761	-5.212485159186647
C	3.817886760002219	-7.648536625589023	-4.923767116659348
C	3.134891819617389	-8.728701585662893	-4.114670062188452
C	4.200706599306234	-9.831415673135851	-4.052948164429667
C	5.418008967989281	-9.172515758903932	-4.670794737706442
N	8.097628302334325	-8.005451750890444	-5.501480527141549
C	7.896625395856415	-9.263188720270023	-5.008995912837230
C	9.176100794363839	-9.974910866963178	-4.957047263241190
C	10.106539660699218	-9.143869290219847	-5.463998472083304
C	9.415929752157167	-7.909226265327106	-5.843849735533272
N	8.096310667469661	-5.386658003936782	-6.879397773137692
C	9.390493693452374	-5.658005279823011	-6.936927234858023
C	10.184287703258166	-4.541320437957602	-7.584750424489431
C	9.169369846259858	-3.395160963168493	-7.647737691271595
C	7.859534757959295	-4.078393904255023	-7.298389716381434
N	5.275852696144304	-5.329701291580429	-6.452913100579930
C	5.397358940549040	-3.997821438273901	-6.871066468402473
C	4.191892009963001	-3.310157613670424	-6.693390549858547
C	3.302150224254378	-4.233070558290241	-6.107202803318210
C	4.010638593585860	-5.422336123581426	-5.966785394798322
C	1.957361926543933	-4.434195681420544	-5.573018493120300
O	1.008781312708722	-3.671496983636784	-5.540294027613346
C	1.921766935486729	-5.887158713053486	-5.017615242884024
H	6.701347244244525	-10.810224585949445	-4.231877861598499
H	11.082374267518993	-6.917899354892501	-6.665284105312816
H	6.633245071798373	-2.430601909393331	-7.651847407410062
H	2.873726873102780	-8.355512240347053	-3.117934255954284
H	3.924651686731669	-10.710939679010618	-4.647509963596705
H	10.504145144412609	-4.873384139043625	-8.580699854849998
H	9.399793309056838	-2.621875088282586	-6.906942557501343
H	1.115923977308537	-6.434713276838148	-5.520389182727316
H	9.299103440365045	-10.983883878848520	-4.585560268003750
H	4.020374069818506	-2.271463974131486	-6.942612962985045
H	4.408008607858338	-10.183226743305575	-3.038312696026619
H	11.087822891459020	-4.300028684239243	-7.017884347235350
H	9.132207402787055	-2.910039945331830	-8.626285876424587
H	2.202845100081345	-9.061198700262814	-4.581197197652243
H	1.672636390897452	-5.861540342898767	-3.949736381909533
H	11.166932470908383	-9.320999202371636	-5.593296299762109