Supplementary information for

Synthesis of a Hydroxy-Functionalized Poly(*m*-xylylene) via Visible-Light-Driven Reductive Coupling of Isophthalaldehyde using Perylene as a Photoredox Catalyst

Shusuke Okamoto[1], Seito Nose[2], and Atsushi Sudo[2]*

[1] School of Food and Nutritional Science, University of Shizuoka, Yada 52-1, Suruga-ku, Shizuoka, Shizuoka, 422-8526, Japan.

[2] Graduate School of Science and Engineering, Kindai University, Kowakae 3-4-1, Higashi Osaka, Osaka 577-8502, Japan.

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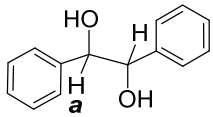
S1. NMR Data

^{1}H NMR

Conv. of **1** = >95 %
Yield of **2** = 72 %
dl : *meso* = 50 : 50



2

Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of crude **2**.

S2. IR Data

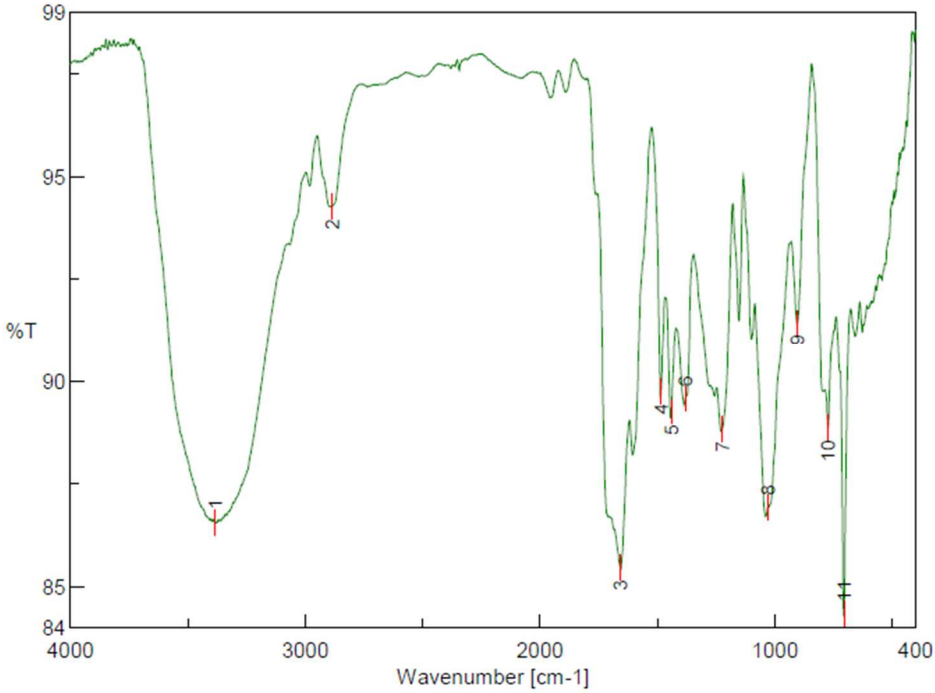


Figure S2. IR spectrum of **4** obtained using HE.

S3. SEC Data

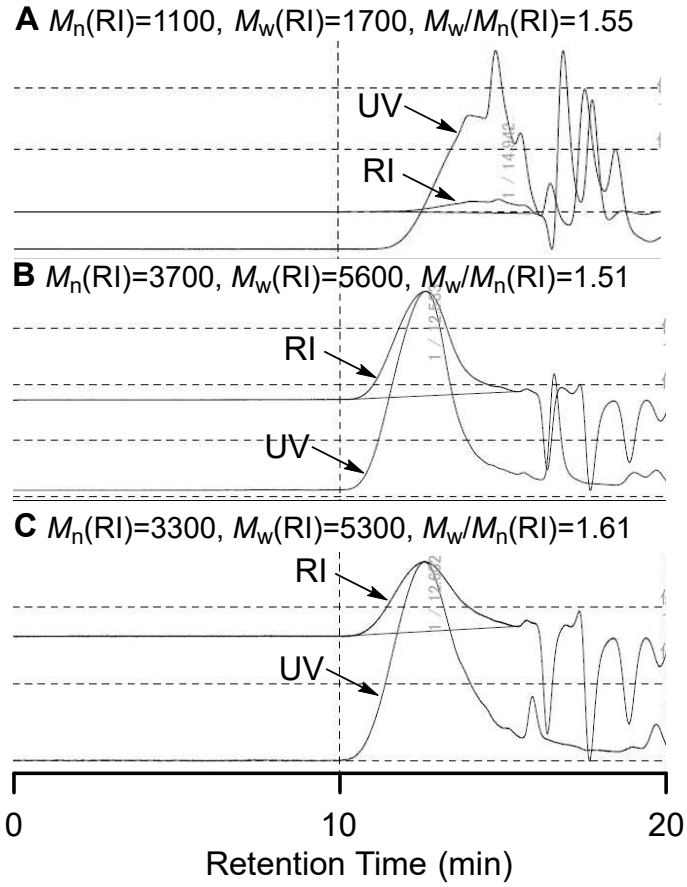


Figure S3. SEC traces of **4** obtained using (A) DIPEA, (B) HE, and (C) HE-TB.

S4. TG Data

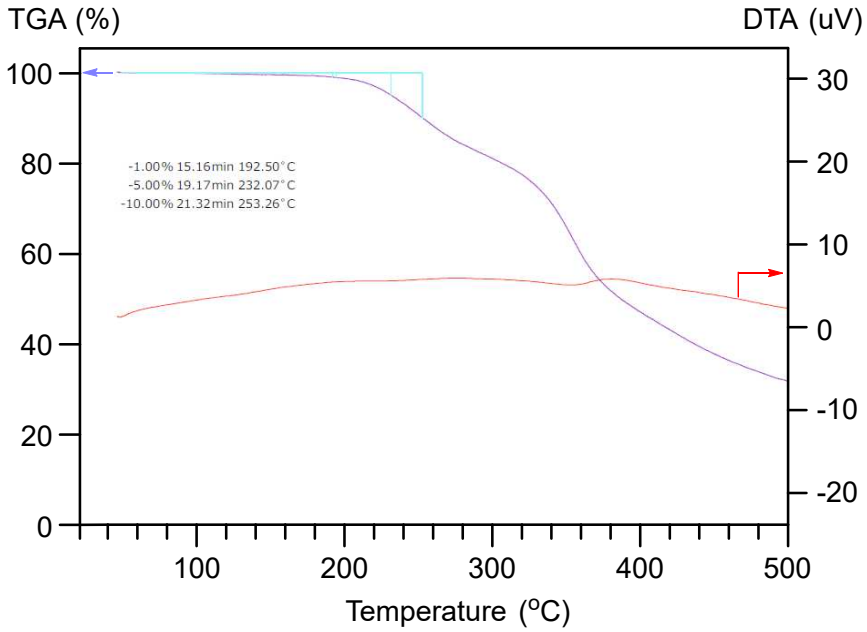


Figure S4. TG-thermogram of **4** obtained using HE.

S5. DSC Data

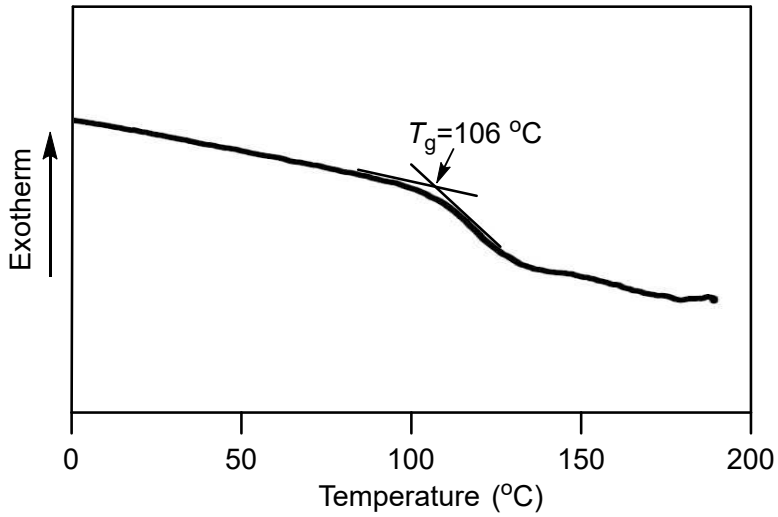


Figure S5. DSC-thermogram of **4** obtained using HE during the second heating cycle.

S6. Computational Data

All calculations were performed using the Gaussian 16 program suite [S1]. The geometries and electronic energies of **1**, HE, HE$^{\bullet+}$, the **1**–HE complex, the **1**–HE$^{\bullet+}$ complex, **3**, **Diol-1**, and **Diol-2** were calculated at the ωB97X-D/6-31+G(d,p) level of theory with the SMD solvation model for DMF. The nature of each optimized structure was confirmed by harmonic vibrational frequency calculations, and no imaginary frequencies were found.

Gas-phase calculations were subsequently performed using the checkpoint files of the DMF-optimized structures as initial geometries. The corresponding structures were reoptimized in the absence of a solvation model, followed by harmonic vibrational frequency calculations to confirm that each optimized structure corresponded to a local minimum.

The electronic energies of the optimized species are summarized in Table S1. Based on these values, the complexation energies of the **1**–HE and **1**–HE$^{\bullet+}$ complexes were estimated as the energy differences between the optimized complexes and their corresponding isolated components.

Harmonic vibration frequencies were computed at the same level of theory to verify the optimized geometries as minima with all real modes in the Hessian matrix. Color coding: O(red), N(blue), C(grey), H(white).

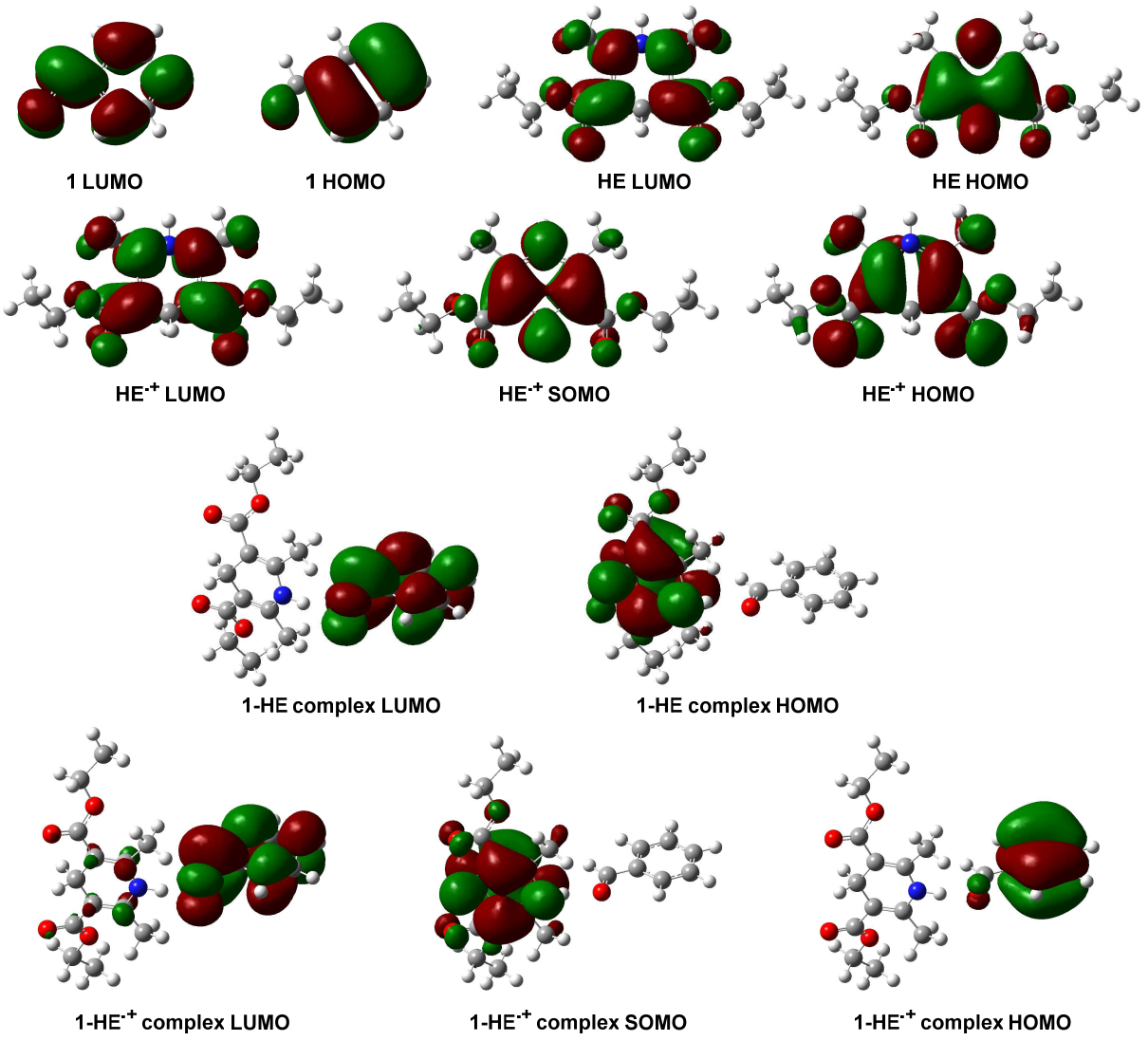


Figure S6. DFT (ωb97xd/6-31+G(d,p)/SMD(ε=DMF)) optimized geometry of **1**, HE, HE$^{\bullet+}$, **1**–HE complex, and **1**–HE$^{\bullet+}$ complex.

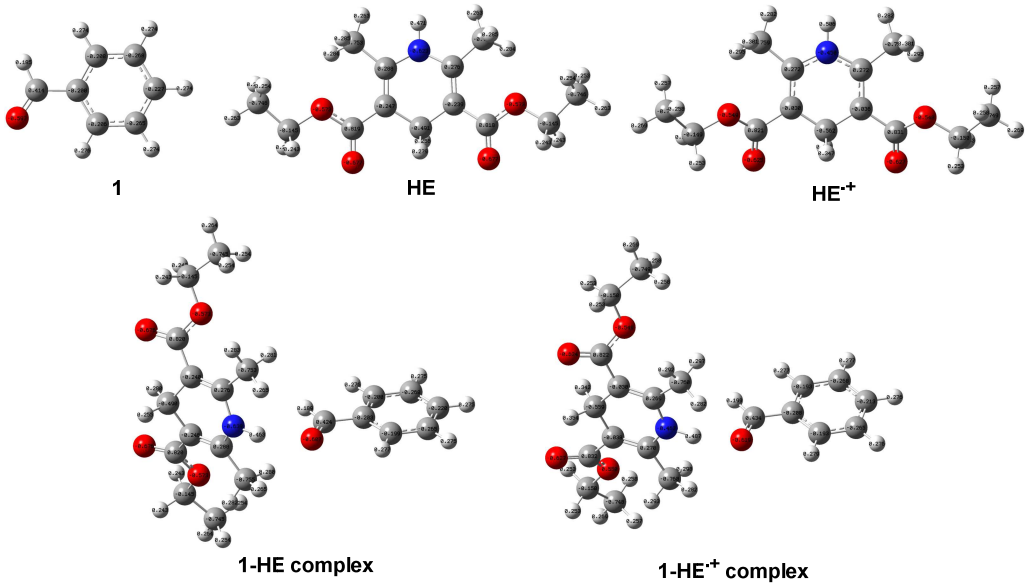


Figure S7. NPA of **1**, HE, HE$^{\bullet+}$, **1**–HE complex, and **1**–HE$^{\bullet+}$ complex in DMF

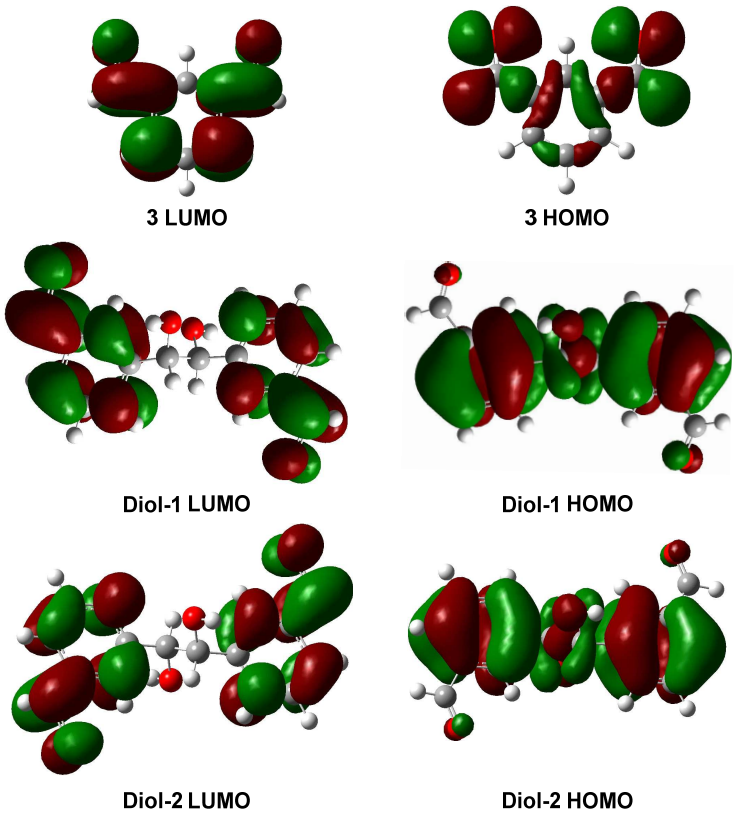


Figure S8. DFT (ωb97xd/6-31+G(d,p)/SMD(ε=DMF)) optimized geometry of **3**, **Diol-1**, and **Diol-2**.

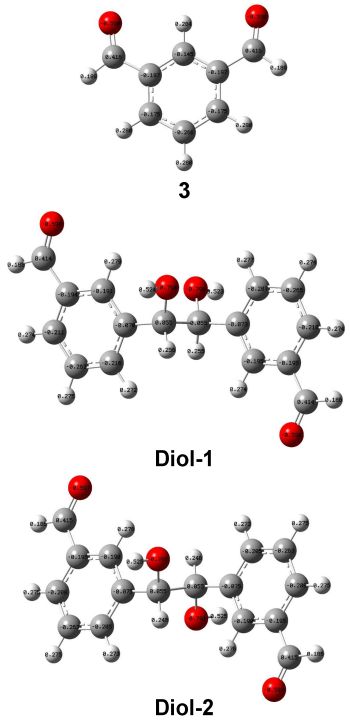


Figure S9. NPA of **3**, **Diol-1**, and **Diol-2**.

XYZ Coordinate

1 in DMF

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(rωB97XD) = -345.4860 Hartree. Lowest harmonic frequency (cm^{-1}) = 113.41.

LUMO：-0.00167×27.2114 = -0.0454 (ev). HOMO：-0.33977×27.2114 = -9.25 (ev)

0 1

O	2.85078813	-0.39400087	-0.00001061
C	1.98741553	0.46613409	0.00000464
H	2.26647707	1.53695881	0.00002775
C	0.53380595	0.19977784	0.00000432
C	-0.34773274	1.28584503	0.00000103
C	0.03443038	-1.10932050	0.00000494
C	-1.72338546	1.06798202	-0.00000404
H	0.04708505	2.29894059	0.00000254
C	-1.33831229	-1.32442347	0.00000199
H	0.72636667	-1.94612712	0.00000843
C	-2.21626482	-0.23633454	-0.00000333
H	-2.40800317	1.91032246	-0.00000823
H	-1.72953047	-2.33706072	0.00000373
H	-3.28843950	-0.40898982	-0.00000652

1 in gas

E(rωB97XD) = -345.4728 Hartree. Lowest harmonic frequency (cm^{-1}) = 113.41.

HE in DMF

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(rωB97XD) = -862.3082 Hartree. Lowest harmonic frequency (cm^{-1}) = 15.69.

LUMO：-0.01722×27.2114 = -0.469 (ev). HOMO：-0.27308×27.2114 = -7.43 (ev).

0 1

C	-1.22291939	1.28759140	-0.27896262
C	1.22292112	1.28758610	-0.27894118
C	1.25566511	-0.07071932	-0.33141962
C	-1.25566805	-0.07071311	-0.33143823
C	-0.00000122	-0.85328568	-0.65611362
H	-0.00000752	-1.79014340	-0.09364610
H	0.00000626	-1.15368950	-1.71590158
N	0.00000387	1.92281036	-0.39732621
C	2.37297327	2.23713233	-0.09363187
H	2.70574563	2.23796659	0.94813204
H	3.22620824	1.95759516	-0.71075354
H	2.06807670	3.25360443	-0.35564250
C	-2.37296890	2.23714496	-0.09367705
H	-3.22622414	1.95756877	-0.71075179
H	-2.70570328	2.23804889	0.94809938
H	-2.06808270	3.25360063	-0.35576468
C	-2.46497052	-0.88521433	-0.17641492
C	2.46495963	-0.88522606	-0.17637171
O	-2.49108278	-2.08560450	-0.41766705
O	2.49105384	-2.08563117	-0.41755316
O	3.54561210	-0.22548568	0.26885639
O	-3.54560360	-0.22548869	0.26888100
C	-4.76518208	-0.97786127	0.40092387
H	-4.60980707	-1.78130210	1.12705060
H	-5.01172975	-1.42965511	-0.56431223
C	4.76517934	-0.97786882	0.40093686
H	5.01170229	-1.42974429	-0.56426720
H	4.60980349	-1.78124912	1.12713061
C	5.84077330	-0.01828560	0.85634384
H	5.58307525	0.43333336	1.81917528
H	6.78345108	-0.56162387	0.97316461
H	5.99265971	0.77940728	0.12286715
C	-5.84075166	-0.01829631	0.85642688
H	-6.78343616	-0.56162865	0.97322089
H	-5.58302884	0.43324047	1.81929023
H	-5.99263844	0.77945806	0.12301722
H	0.00000556	2.93131432	-0.33492618

HE in gas

E(rωB97XD) = -862.2815 Hartree. Lowest harmonic frequency (cm^{-1}) = 12.02.

$HE^{\bullet+}$ in DMF

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(uωB97XD) = -862.1181 Hartree. Lowest harmonic frequency (cm^{-1}) = 15.95.

LUMO：-0.01402×27.2114 = -0.382 (ev). SOMO：-0.32540×27.2114 = -8.85 (ev).

HOMO ：-0.38035×27.2114 = -10.35 (ev).

1 2

C	-1.22703726	1.31517700	-0.25998966
C	1.22703718	1.31517454	-0.25996844
C	1.25241730	-0.05900022	-0.24545170
C	-1.25242071	-0.05899635	-0.24546997
C	-0.00000326	-0.84858185	-0.27692761
H	-0.00001127	-1.57570262	0.55357601
H	0.00000055	-1.50264556	-1.16669733
N	0.00000053	1.91608579	-0.27353178
C	2.40015991	2.24368267	-0.28085388
H	2.79725132	2.36766596	0.73044476
H	3.19682011	1.85064838	-0.91139245
H	2.10372883	3.22326360	-0.66239472
C	-2.40015807	2.24368645	-0.28089943
H	-3.19682759	1.85062967	-0.91141153
H	-2.79723472	2.36771520	0.73039982
H	-2.10372666	3.22324979	-0.66248549
C	-2.50729963	-0.86654650	-0.26321928
C	2.50729017	-0.86655967	-0.26318520
O	-2.55183577	-1.96842167	-0.77474482
O	2.55180622	-1.96846162	-0.77465575
O	3.52021141	-0.27802347	0.35388125
O	-3.52020043	-0.27803134	0.35390069
C	-4.78773896	-0.98387335	0.36675235
H	-4.64134885	-1.94171703	0.87253219
H	-5.08523396	-1.17260235	-0.66802806
C	4.78773905	-0.98388373	0.36675083
H	5.08521335	-1.17267701	-0.66802374
H	4.64134298	-1.94169620	0.87258814
C	5.78236123	-0.10844123	1.08930952
H	5.46628054	0.08005890	2.11935805
H	6.74973704	-0.61864006	1.11459129
H	5.91137549	0.84865631	0.57564146
C	-5.78233493	-0.10845685	1.08937841
H	-6.74972011	-0.61863893	1.11464157
H	-5.46623699	0.07997428	2.11943426
H	-5.91133792	0.84867444	0.57577036
H	0.00000085	2.93440213	-0.29822864

$HE^{\bullet+}$ in gas

E(uωB97XD) = -862.0217 Hartree. Lowest harmonic frequency (cm^{-1}) = 10.76.

1-HE complex in DMF

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(rωB97XD) = -1207.8016 Hartree. Lowest harmonic frequency (cm^{-1}) = 8.33.

LUMO：-0.00849×27.2114 = -0.231 eV. HOMO：-0.27390×27.2114 = -7.453 eV.

0 1

C	0.93447089	-1.22408994	-0.99787453
C	0.97073760	1.21326573	-0.99362994
C	2.19268144	1.22492381	-0.39717548
C	2.15511717	-1.27425489	-0.40095057
C	3.02933147	-0.03755807	-0.38574679
H	3.66395810	-0.04838258	0.50273718
H	3.72321460	-0.04676305	-1.24173248
N	0.46389332	0.00269659	-1.43437170
C	0.04580984	2.36922962	-1.24908375
H	-0.60257020	2.53775552	-0.38271211
H	0.59190004	3.29040353	-1.44053133
H	-0.59152128	2.15050656	-2.10986011
C	-0.02421433	-2.35067919	-1.25937088
H	0.49356733	-3.28933088	-1.44380368
H	-0.68660668	-2.49566678	-0.39927076
H	-0.64537309	-2.11332338	-2.12701108
C	2.76555094	-2.48030954	0.16801360
C	2.83914954	2.41039270	0.17496301
O	3.95410357	-2.55261257	0.45309743
O	4.02845197	2.44473229	0.46414621
O	2.02474795	3.45596994	0.38919257
O	1.91878427	-3.49925212	0.38493777
C	2.48118095	-4.72048487	0.89869417
H	2.93764486	-4.51893463	1.87224063
H	3.26375983	-5.06681896	0.21729140
C	2.62440056	4.65836141	0.90526667
H	3.42295164	4.97705650	0.22897223
H	3.06710469	4.44298632	1.88222788
C	1.53374203	5.70006867	1.00707413
H	0.73659940	5.37055238	1.68037341
H	1.95699947	6.62780963	1.40415988
H	1.09958878	5.91305256	0.02549642
C	1.35673804	-5.72467880	1.00961397
H	1.75128228	-6.66584773	1.40464082
H	0.57618597	-5.36766529	1.68833631
H	0.90845471	-5.92373189	0.03146611
H	-0.48092154	0.01741788	-1.81542975
O	-2.48129720	0.04245315	-1.76455081
C	-2.74426091	0.04263769	-0.57015833
H	-1.92912608	0.03823756	0.17797033

C	-4.10699285	0.04826577	-0.01665952
C	-4.26520396	0.04780184	1.37359358
C	-5.23076424	0.05346638	-0.85427552
C	-5.54240608	0.05256074	1.92793239
H	-3.38701771	0.04370381	2.01440172
C	-6.50335031	0.05814244	-0.29823612
H	-5.09572760	0.05368164	-1.93147896
C	-6.65814519	0.05768960	1.09153728
H	-5.66854278	0.05221655	3.00586098
H	-7.37769734	0.06205662	-0.94143928
H	-7.65512100	0.06131992	1.52194670

1-HE complex in gas

E(rωB97XD) = -1207.7660 Hartree. Lowest harmonic frequency (cm^{-1}) = 5.05.

1-$HE^{\bullet+}$ complex in DMF

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(uωB97XD) = -1207.6132 Hartree. Lowest harmonic frequency (cm^{-1}) = 6.33.

LUMO：-0.01688×27.2114 = -0.459 (ev). SOMO：-0.32310×27.2114 = -8.792 (ev).

HOMO：-0.34587×27.2114 = -9.412 (ev).

1 2

C	-0.96873534	1.21308771	-0.76608941
C	-0.79686051	-1.22788580	-0.79260238
C	-2.07678184	-1.35185420	-0.30900839
C	-2.25406416	1.14592414	-0.28442748
C	-2.92643288	-0.15938559	-0.07924774
H	-3.36148842	-0.19999557	0.93324662
H	-3.81853147	-0.21511285	-0.72925022
N	-0.32297207	0.03452926	-1.00657409
C	0.15842619	-2.33009746	-1.13129595
H	0.77110107	-2.57522742	-0.25803252
H	-0.36951118	-3.23017557	-1.44040896
H	0.81994446	-2.01811587	-1.94233716
C	-0.17338621	2.44329248	-1.07604642
H	-0.81755920	3.26440794	-1.38435473
H	0.38445686	2.76004978	-0.18918182
H	0.53868537	2.23847306	-1.87796560
C	-3.09384700	2.34154617	0.01750727
C	-2.73366550	-2.66262229	-0.03002851
O	-4.30300284	2.32514194	-0.10680504
O	-3.92688676	-2.83168003	-0.18764058
O	-1.89575126	-3.57626777	0.43751552
O	-2.39395016	3.37405297	0.46378383
C	-3.12522592	4.59048798	0.76415075
H	-3.84204568	4.37195747	1.56000066

H	-3.67373622	4.89168410	-0.13198570
C	-2.44080246	-4.89037854	0.72225354
H	-2.90785947	-5.27314463	-0.18875671
H	-3.20777761	-4.78314046	1.49374973
C	-1.29698430	-5.76245909	1.17960083
H	-0.83352895	-5.36199135	2.08583983
H	-1.68146542	-6.76193574	1.40326117
H	-0.53481387	-5.85359405	0.40025541
C	-2.11506051	5.63073698	1.18331484
H	-2.64149756	6.56040822	1.41874819
H	-1.56607541	5.31167950	2.07401064
H	-1.40172549	5.83361734	0.37926502
H	0.65709498	0.10698668	-1.34407402
O	2.42365332	0.21041029	-1.43034918
C	2.87607717	0.16770276	-0.28937496
H	2.18870184	0.09680058	0.57292879
C	4.30369095	0.20423546	0.03600182
C	4.68345532	0.13791859	1.38211407
C	5.27677289	0.30159340	-0.96934148
C	6.03188133	0.16842292	1.72492865
H	3.92134821	0.06200900	2.15347590
C	6.62063912	0.33248882	-0.62266506
H	4.97150082	0.35252572	-2.00975800
C	6.99656505	0.26582303	0.72271393
H	6.33040016	0.11671978	2.76692842
H	7.37957454	0.40854175	-1.39479463
H	8.04914564	0.29014400	0.98842432

1-HE$^{\bullet+}$ complex in gas

E(uωB97XD) = -1207.5265 Hartree. Lowest harmonic frequency (cm^{-1}) = 8.78.

3

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_2

E(rωB97XD) = -458.7816 Hartree. Lowest harmonic frequency (cm^{-1}) = 100.25.

LUMO：-0.00788×27.2114 = -0.214 eV. HOMO：-0.34677×27.2114 = -9.436 eV

0 1

C	1.20578303	0.12812004	-0.00000247
C	1.20221466	1.52908292	-0.00000934
C	-0.00000354	-0.57350137	0.00000527
C	0.00000000	2.23056309	-0.00000618
H	2.14758326	2.06599756	-0.00001659
C	-1.20579031	0.12812398	0.00000873
H	-0.00001283	-1.65941065	0.00000761
C	-1.20222095	1.52908246	0.00000587
H	0.00000193	3.31538604	-0.00001253

H	-2.14758772	2.06599892	0.00001339
C	-2.50406252	-0.58454851	0.00001544
H	-3.39735789	0.06758031	0.00006228
O	-2.62242763	-1.79609265	-0.00002674
C	2.50406288	-0.58454329	-0.00000271
H	3.39734984	0.06759684	-0.00001379
O	2.62244311	-1.79608548	0.00001073

Diol-1

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(rωB97XD) = -918.7958 Hartree. Lowest harmonic frequency (cm^{-1}) = 17.25.

LUMO：-0.00162×27.2114 = -0.044 eV. HOMO：-0.32528×27.2114 = -8.851 eV

0 1

C	0.35088500	0.09223700	0.60786900
H	-0.18188500	0.88510400	1.15079900
C	-0.43698800	-0.12574200	-0.69555200
C	1.76152700	0.58089400	0.32582900
C	1.97637900	1.93843600	0.05592400
C	2.84469800	-0.29005300	0.31098500
C	3.25048300	2.42015300	-0.23257900
H	1.13356500	2.62559100	0.07498400
C	4.12964900	0.18871500	0.02766600
H	2.69831800	-1.34519400	0.51714300
C	4.33290500	1.54420700	-0.24627100
H	3.39837500	3.47569100	-0.43777400
H	5.33405500	1.90793400	-0.46343800
C	-1.88369500	-0.49044400	-0.41241800
C	-2.28886700	-1.82562000	-0.30098100
C	-2.82438300	0.51856600	-0.23396300
C	-3.61334000	-2.14732800	-0.01380000
H	-1.55622000	-2.61347300	-0.44142900
C	-4.15554300	0.20229900	0.06135200
H	-2.53313600	1.56225700	-0.32437500
C	-4.55060900	-1.13403100	0.17081400
H	-3.91208500	-3.18764100	0.06863000
H	-5.58691800	-1.37431900	0.39506400
O	0.32659600	-1.11145800	1.35029300
H	0.68795300	-0.93455800	2.22639600
C	5.29427600	-0.72102600	0.01068000
H	6.26107000	-0.23874700	-0.23018500
C	-5.16573700	1.26301600	0.25223900
H	-6.18626300	0.90214800	0.48186800
O	5.24408200	-1.91718600	0.23851600
O	-4.93926200	2.45809100	0.17343100
O	0.23403600	-1.10897400	-1.46166500
H	-0.18485700	-1.15352800	-2.32880500

H	-0.42543400	0.83928600	-1.22024900

Diol-2

#p opt=tight freq wb97xd/6-31+g(d,p), scrf=(smd,solvent=n,n-dimethylformamide), pop=npa int=ultrafine, C_1.

E(rωB97XD) = -918.7958 Hartree. Lowest harmonic frequency (cm^{-1}) = 15.76 cm^{-1}.

LUMO：-0.00161×27.2114 = -0.044 eV. HOMO：-0.32508×27.2114 = -8.846 eV

0 1

C	-0.33954000	0.24739400	-0.64395100
H	0.20519800	1.13607400	-0.99198000
C	0.33954000	-0.24739400	0.64395100
H	-0.20519800	-1.13607400	0.99198000
C	-1.78848000	0.62473500	-0.40733400
C	-2.18617300	1.96544500	-0.42700000
C	-2.74241500	-0.36020900	-0.16371200
C	-3.51396000	2.32309600	-0.19878000
H	-1.44629000	2.73730000	-0.62183600
C	-4.07653800	-0.00895400	0.06430000
H	-2.45842400	-1.40876700	-0.15134900
C	-4.46278600	1.33564800	0.04779000
H	-3.80531200	3.36844600	-0.21775500
H	-5.50220500	1.60100200	0.22443600
C	1.78848000	-0.62473500	0.40733400
C	2.18617300	-1.96544500	0.42700000
C	2.74241500	0.36020900	0.16371200
C	3.51396000	-2.32309600	0.19878000
H	1.44629000	-2.73730000	0.62183600
C	4.07653800	0.00895400	-0.06430000
H	2.45842400	1.40876700	0.15134900
C	4.46278600	-1.33564800	-0.04779000
H	3.80531200	-3.36844600	0.21775500
H	5.50220500	-1.60100200	-0.22443600
O	-0.21548600	-0.81057000	-1.58303000
H	-0.61903400	-0.52681700	-2.41153600
O	0.21548600	0.81057000	1.58303000
H	0.61903400	0.52681700	2.41153600
C	-5.10070000	-1.04203500	0.32594700
H	-6.12294600	-0.65533800	0.49923600
C	5.10070000	1.04203500	-0.32594700
H	6.12294600	0.65533800	-0.49923600
O	-4.88273900	-2.24057100	0.35829000
O	4.88273900	2.24057100	-0.35829000

Calculation of intermolecular interaction

The complexation energy (E_{comp}) was estimated from the energy difference between the optimized complex and the corresponding isolated components using DFT calculations, according to the following equation:

$$E_{\mathrm{comp}}(A\text{–}B) = E_{A\text{–}B} - (E_A + E_B)$$

where E_A and E_B are the electronic energies of the optimized isolated components A and B, respectively, and $E_{A\text{–}B}$ is the electronic energy of the optimized A–B complex.

Table S1. Electronic energies of the optimized species calculated in DMF and in the gas phase

Substrate	Energy (Hartree)
1 in DMF	-345.4860
HE in DMF	-862.3082
$HE^{\bullet+}$ in DMF	-862.1181
1-HE in DMF	-1207.8016
1-$HE^{\bullet+}$ in DMF	-1207.6132
1 in Gas	-345.4728
HE in Gas	-862.2815
$HE^{\bullet+}$ in Gas	-862.0217
1-HE in Gas	-1207.7660
1-$HE^{\bullet+}$ in Gas	-1207.5265

DMF

Complexation energy between **1** and HE

$E_{\mathbf{comp}}$ (**1**-HE) = $E_{\mathbf{1}\text{-HE}} - (E_{\mathbf{1}} + E_{\mathrm{HE}})$

= -1207.8016 - (-345.4860 + -862.3082) = -0.0074 Hartree

= -0.0074 × 627.5095 = -4.64 (kcal/mol)

Complexation energy between **1** and $HE^{\bullet+}$

$E_{\mathbf{comp}}$ (**1**-$HE^{\bullet+}$) = $E_{\mathbf{1}\text{-HE}^{\bullet+}} - (E_{\mathbf{1}} + E_{\mathrm{HE}^{\bullet+}})$

= -1207.6132 - (-345.4860 + -862.1181) = -0.0091 Hartree

= -0.0091 × 627.5095 = -5.71 (kcal/mol)

Gas

Complexation energy between **1** and HE

$E_{\mathbf{comp}}$ (**1**-HE) = $E_{\mathbf{1}\text{-HE}} - (E_{\mathbf{1}} + E_{\mathbf{HE}})$

= -1207.7660 - (-345.4728 + -862.2815) = -0.0117 Hartree

= -0.0117 × 627.5095 = -7.34 (kcal/mol)

Complexation energy between **1** and $HE^{\bullet+}$

$E_{\mathbf{comp}}$ (**1**-$HE^{\bullet+}$) = $E_{\mathbf{1}\text{-HE}^{\bullet+}} - (E_{\mathbf{1}} + E_{\mathrm{HE}^{\bullet+}})$

= -1207.5265 - (-345.4728 + -862.0217) = -0.0320 Hartree

= -0.0320 × 627.5095 = -20.08 (kcal/mol)

S7. Reference

S1. Gaussian 16 (Revision C. 021, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A. *et al Gaussian, Inc., Wallingford CT* **2019**.