

Supporting Information

Computational Insights into Fused Heterocyclic-Based 2D COFs for Photocatalytic Hydrogen Evolution

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Calculation Details of Gibbs Free Energy Changes and Reaction Energy for 2D COFs

The photocatalytic water-splitting hydrogen production reaction of CTF-x and CHF-x was simulated using the model proposed by Nørskov et al.¹ In aqueous solution, the HER process can be decomposed into two single-electron steps, each consuming one proton and one electron:



In the equation, * denotes a site on the surface, and (radical)* denotes the corresponding radical adsorbed on the surface. Using the Gibbs free energy formula: $G(T) = E_{\text{elec}} + H_{\text{corr}}(T) - TS(T)$, here, $G(T)$ represents the Gibbs free energy at temperature T , $H(T)$ is the enthalpy derived from the total energy, and $S(T)$ is the entropy. In the context of our DFT calculations, the term E refers to the electronic energy, while $H(T)$ incorporates the thermal corrections to enthalpy (translational, rotational, and vibrational contributions). For gaseous substances, this includes contributions from vibrational, rotational, and translational motions. For adsorbed substances, rotational and translational motions are hindered, thus only vibrational contributions are considered.² Therefore, the Gibbs free energy change ΔG resulting from the influence of the external potential U on the above steps can be obtained from the following equation:

$$\Delta G_1 = G(\text{H}^*) - G(*) - 1/2G(\text{H}_2) - eU_e$$

$$\Delta G_2 = G(*) + 1/2G(\text{H}_2) - G(\text{H}^*) - eU_e$$

Here, $G(\text{H}^+ + \text{e}^-)$ is replaced by $1/2G(\text{H}_2)$, considering that the reaction $\text{H}^+ + \text{e}^- = \text{H}_2$ is at equilibrium under standard conditions ($\text{pH} = 0$, $T = 298 \text{ K}$, 1 atm). Due to the presence of photoelectrons, the Gibbs free energy shifts with the applied reduction potential (eU_e). For photocatalytic reactions, U_e denotes the HER potential, representing the energy difference between the CBM and the hydrogen reduction potential (H^+/H_2).

The reaction energies (E_r) for CTF-TCT, CTF-DTBT, CTF-MTBT, CHF-TCT, CHF-DTBT, and CHF-MTBT in this paper can be calculated from the dechlorination reaction. As shown in Figures S3-S4. Taking Figure S3a as an example, the generation energy is defined as $E_r = E(\text{CTF-TCT}) + 6E(\text{HCl}) - 3E(4,4\text{-dimethyl-4H-cyclopenta}[2,1\text{-b}:3,4\text{-b}']\text{dithiophene}) - 2E(2,4,6\text{-trichloro-1,3,5-triazine})$. The reaction energies (E_r) for CTF-TCT2, CTF-DTBT2 and CHF-TCT2 can be calculated from the aldehyde-amine condensation reaction,³⁻⁵ as shown in Figures S5-S6. Taking Figure S5a as an example, the generation energy is defined as $E_r = E(\text{CTF-TCT2}) + 6E(\text{H}_2\text{O}) + 6E(\text{H}_2) - 3E(4,4\text{-dimethyl-4H-cyclopenta}[2,1\text{-b}:3,4\text{-b}']\text{dithiophene-2,6-dicarbaldehyde}) - 2E(\text{benzene-1,3,5-triamine})$.

Optimized 2D COFs Structure

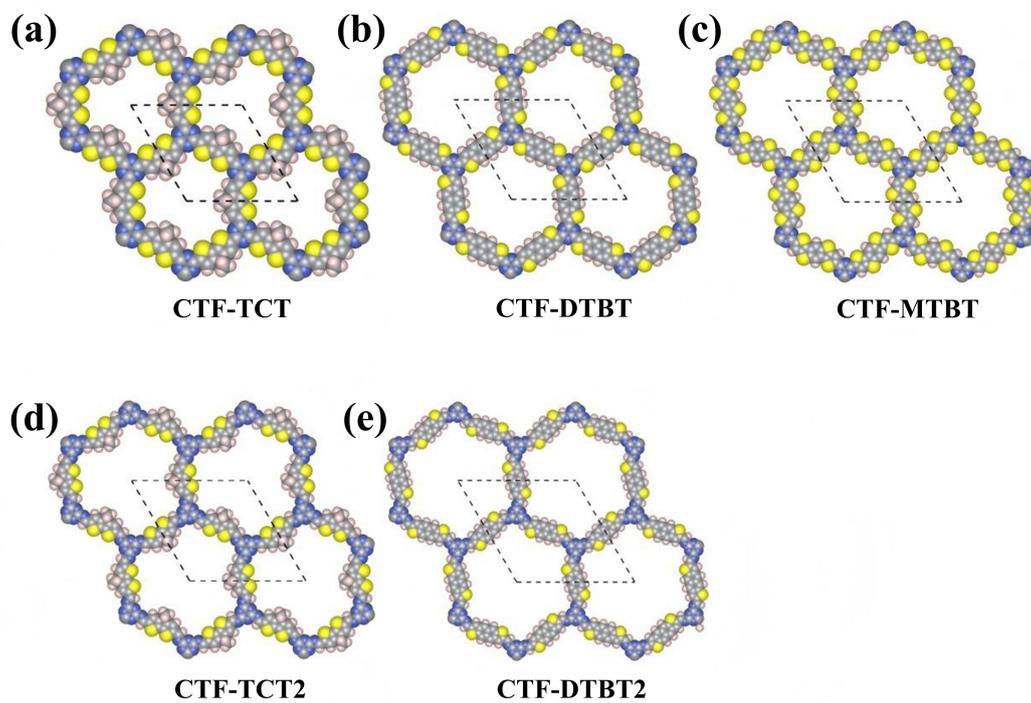


Figure S1. Optimized 2D CTFs

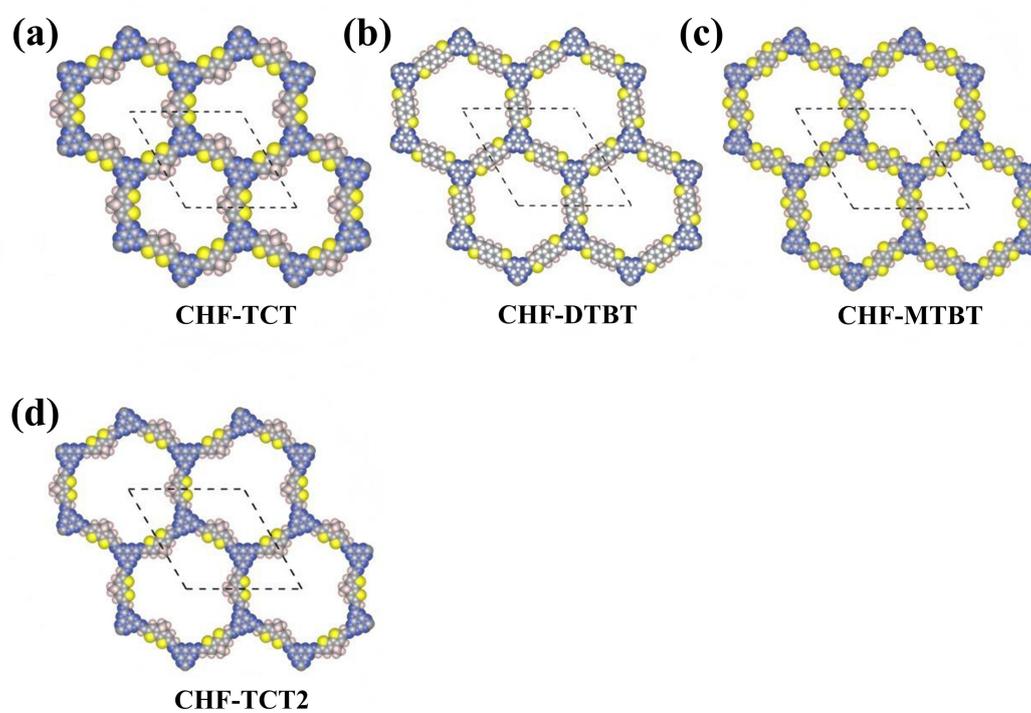


Figure S2. Optimized 2D CHFs

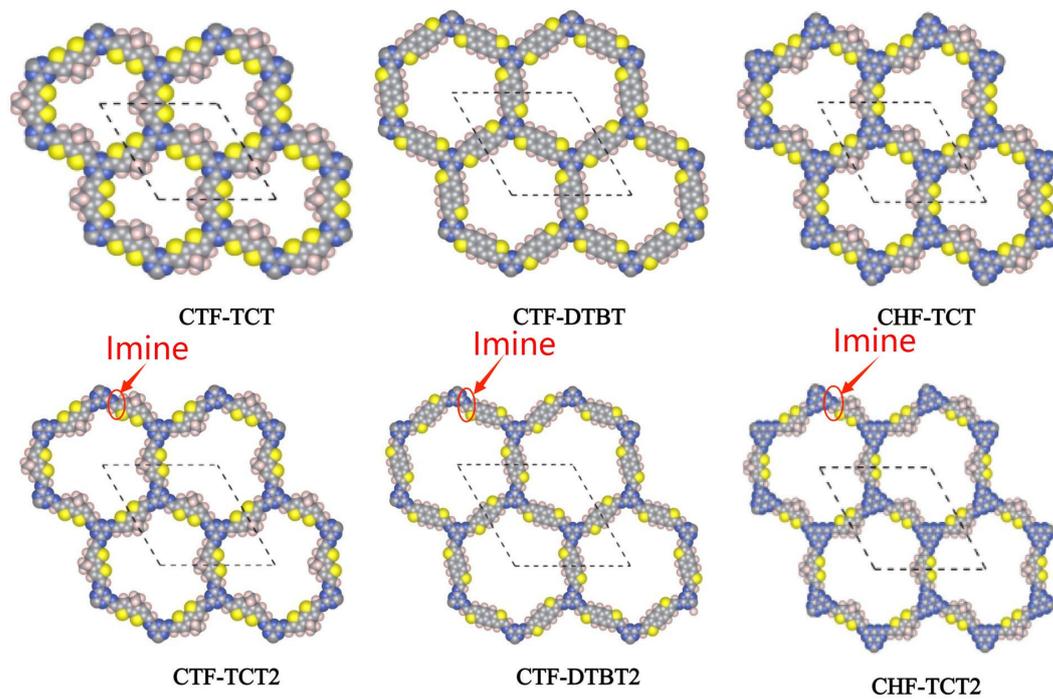
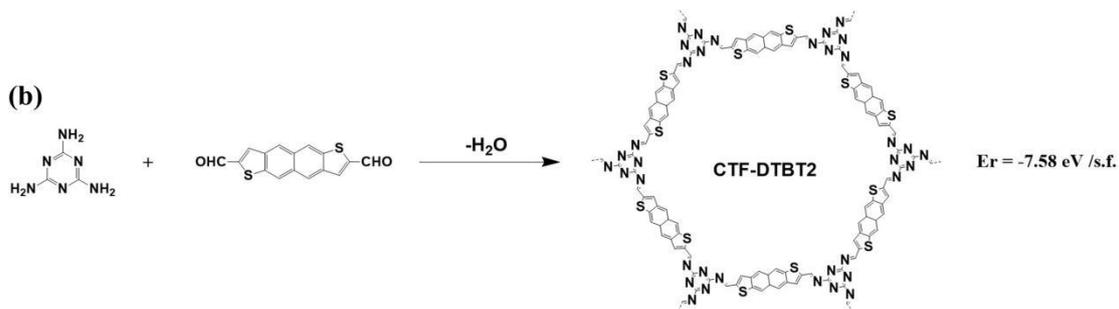
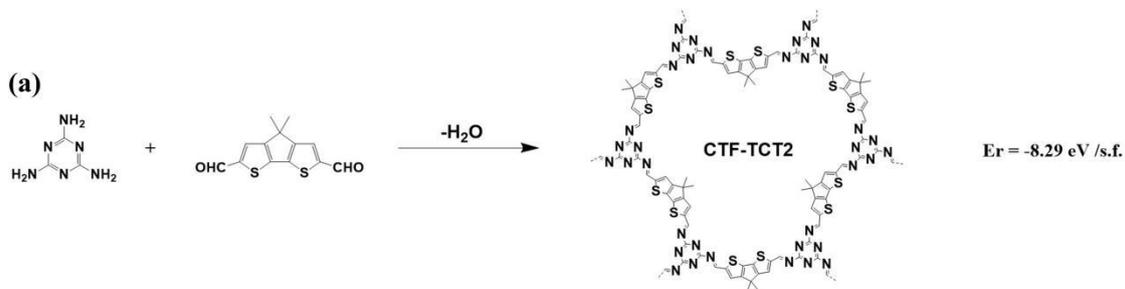
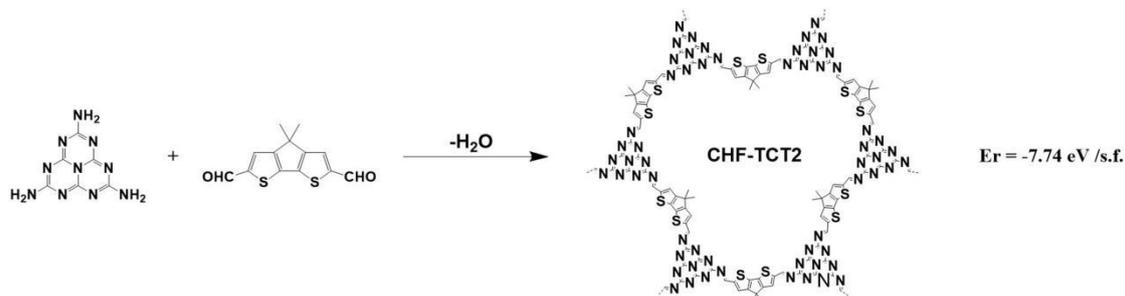


Figure S3. Labeling the location of the imine.

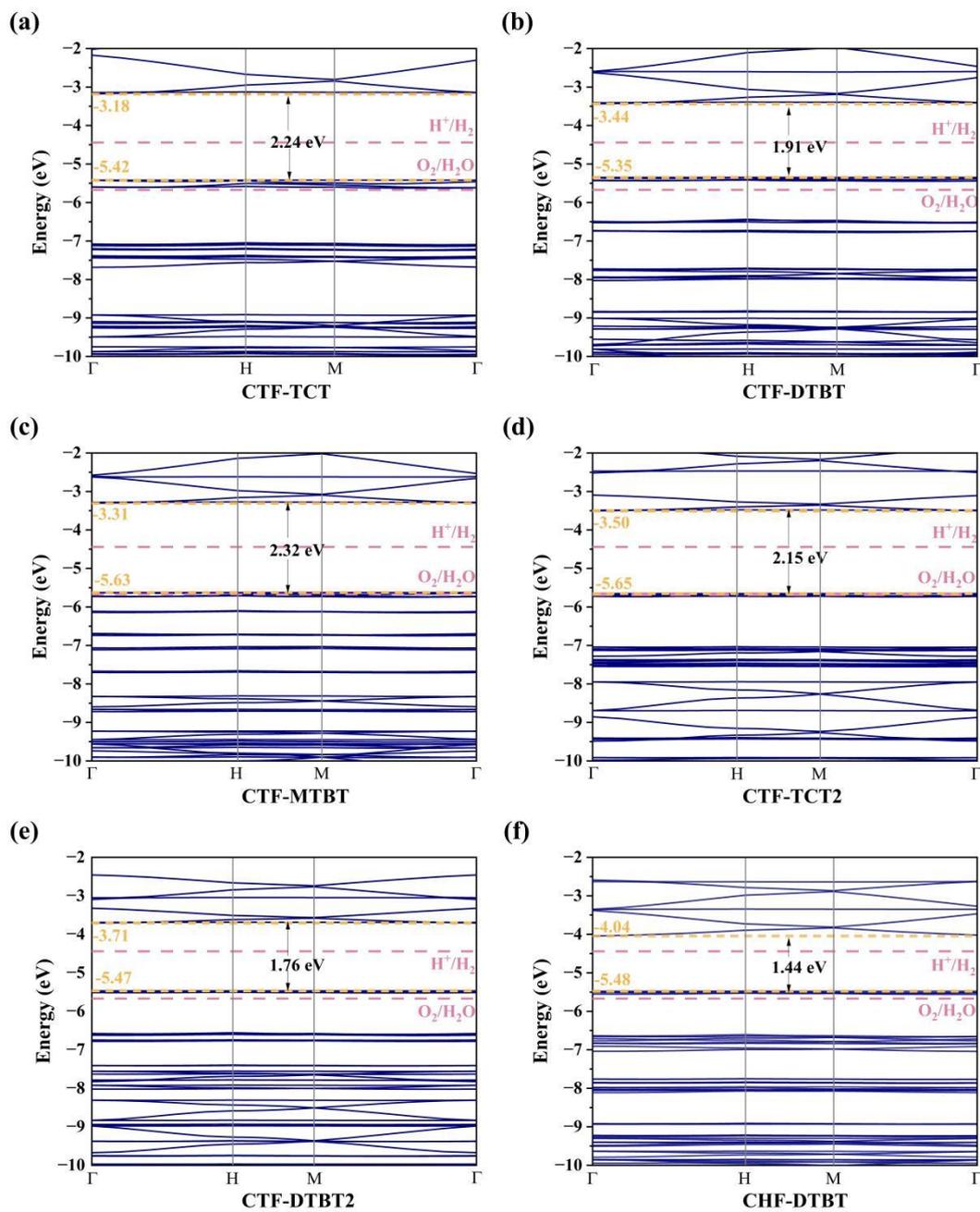


S6. Illustrates the experimentally feasible polymerization process of (a) CTF-TCT2, (b) CTF-DTBT2, respectively.



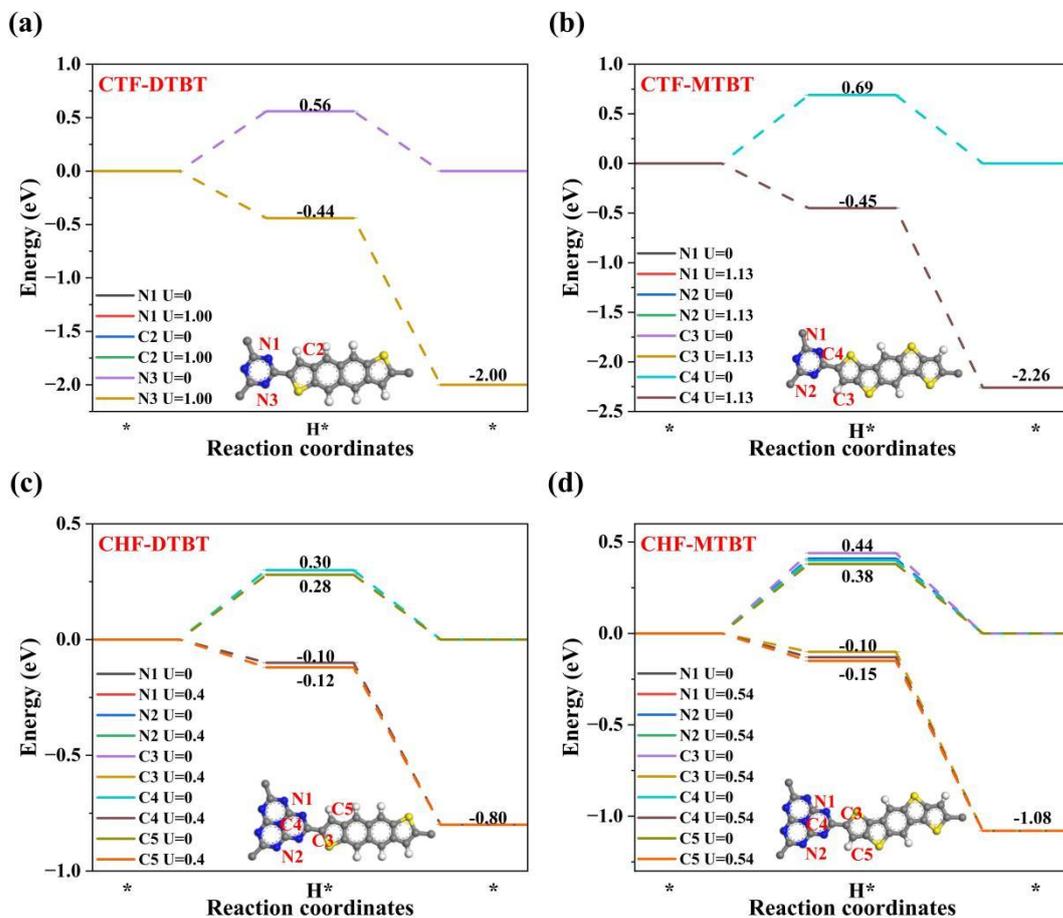
S7. Illustrates the experimentally feasible polymerization process of CHF-TCT2, respectively.

Detailed HSE06 band gap structures of 2D COFs



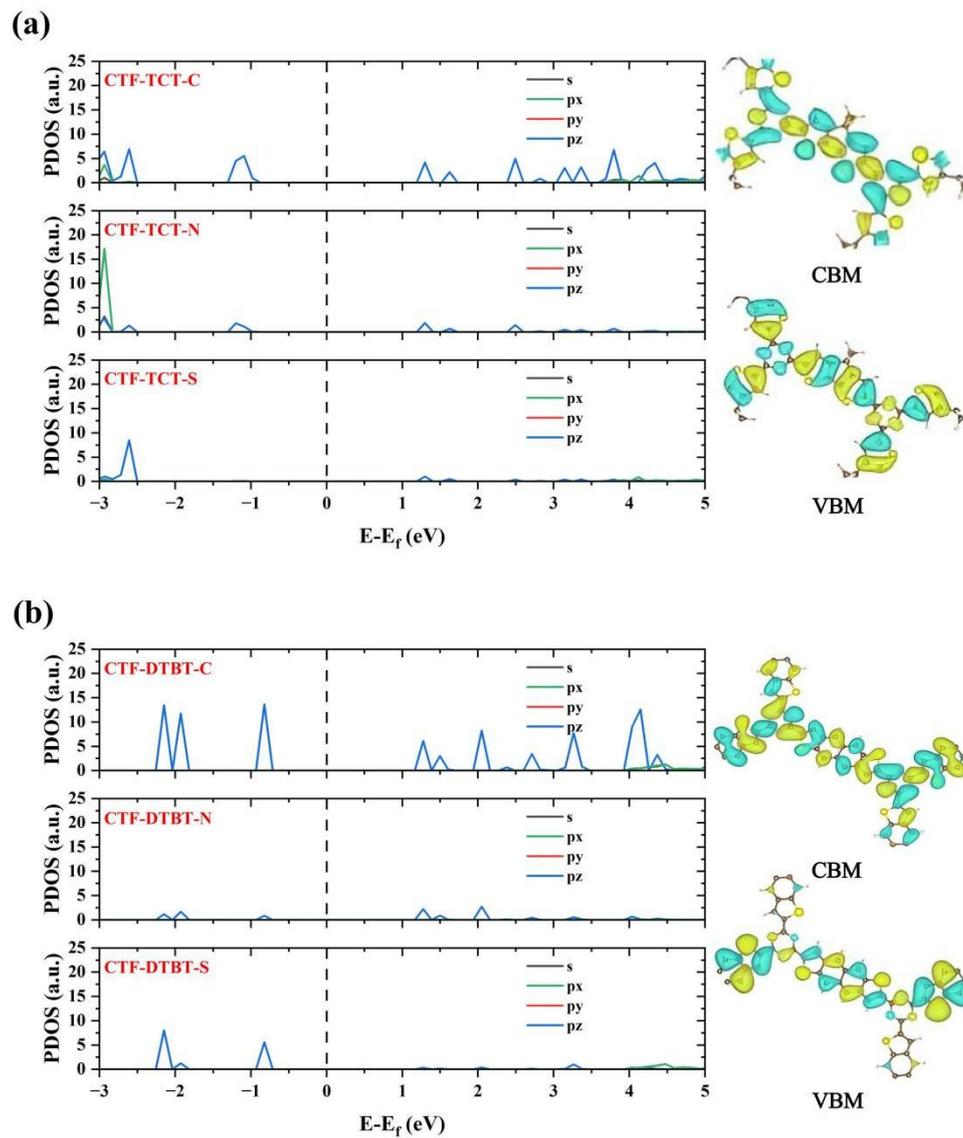
S8. Detailed analysis of the band structures of (a) CTF-TCT, (b) CTF-DTBT, (c) CTF-MTBT, (d) CTF-TCT2, (e) CTF-DTBT2, and (f) CHF-DTBT using the HSE06 function.⁶

Gibbs free energy change curve of the HER process under visible light irradiation and without visible light irradiation

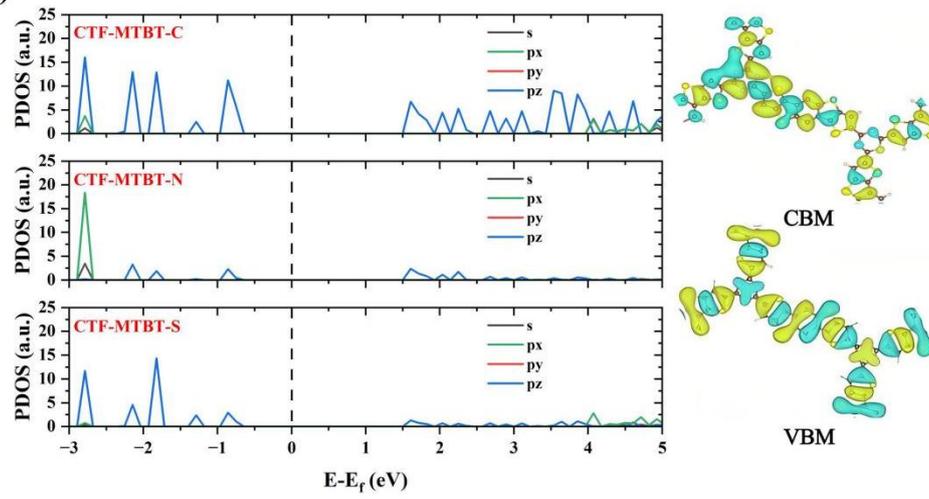


S9. (a) CTF-DTBT, (b) CTF-MTBT, (c) CHF-DTBT, (d) CHF-MTBT Gibbs free energy change for hydrogen adsorption at N and C sites with and without photobias potential U.

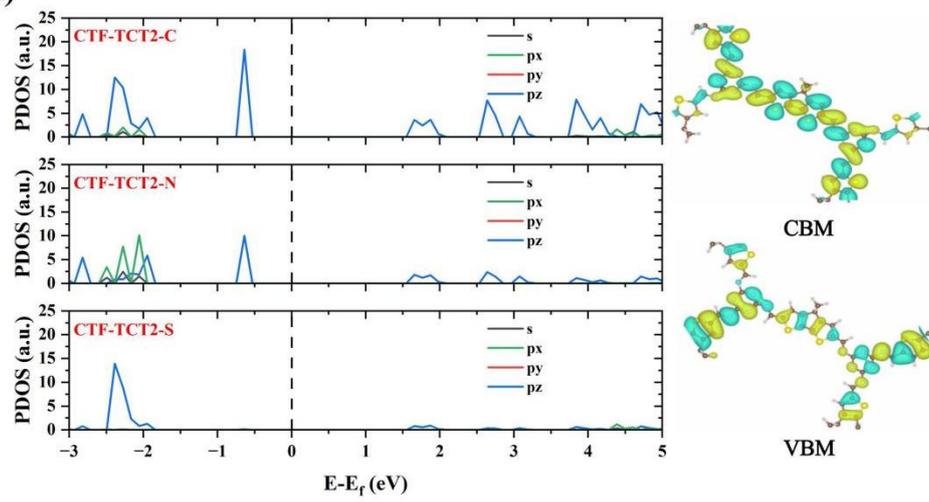
The projected density of states and charge distribution for the CBM and VBM of nine COF materials were calculated.

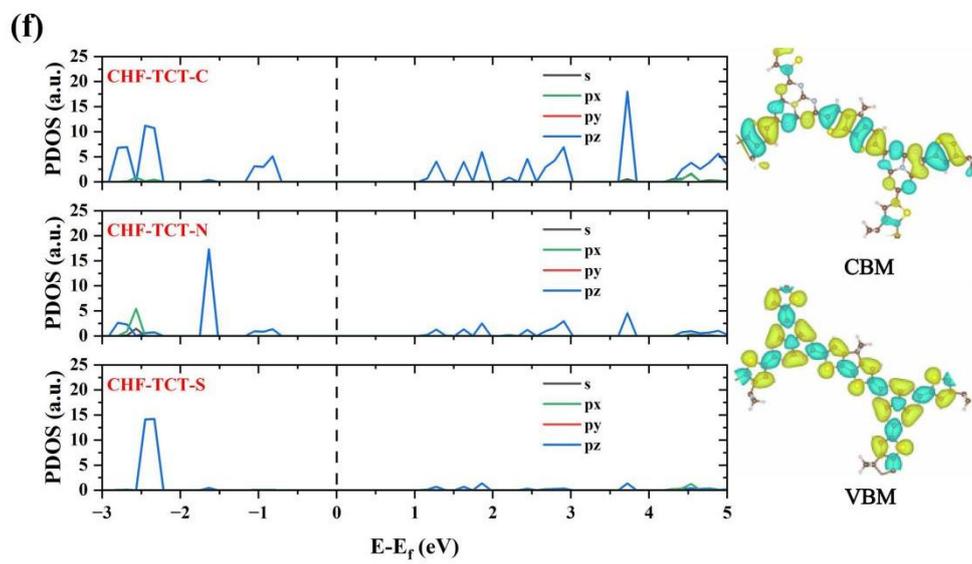
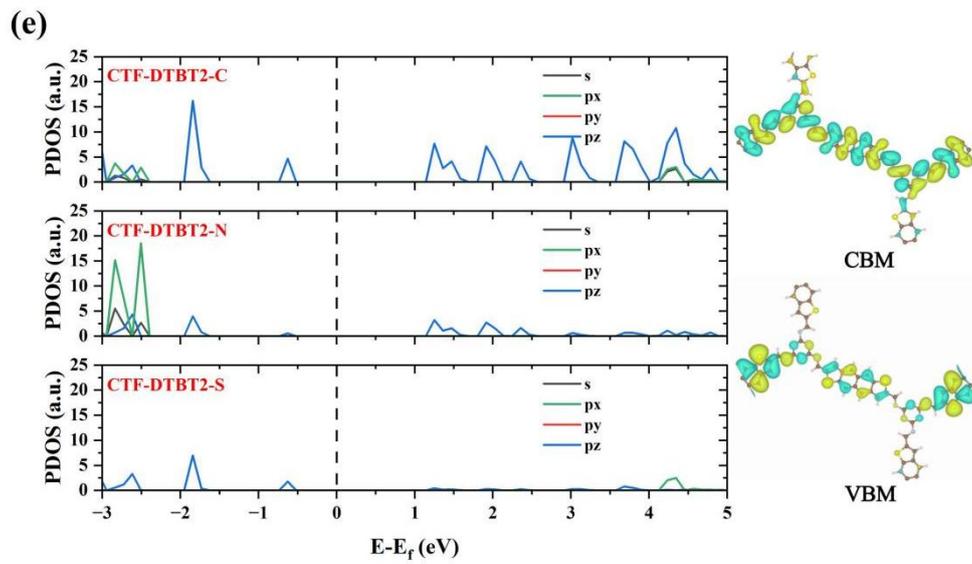


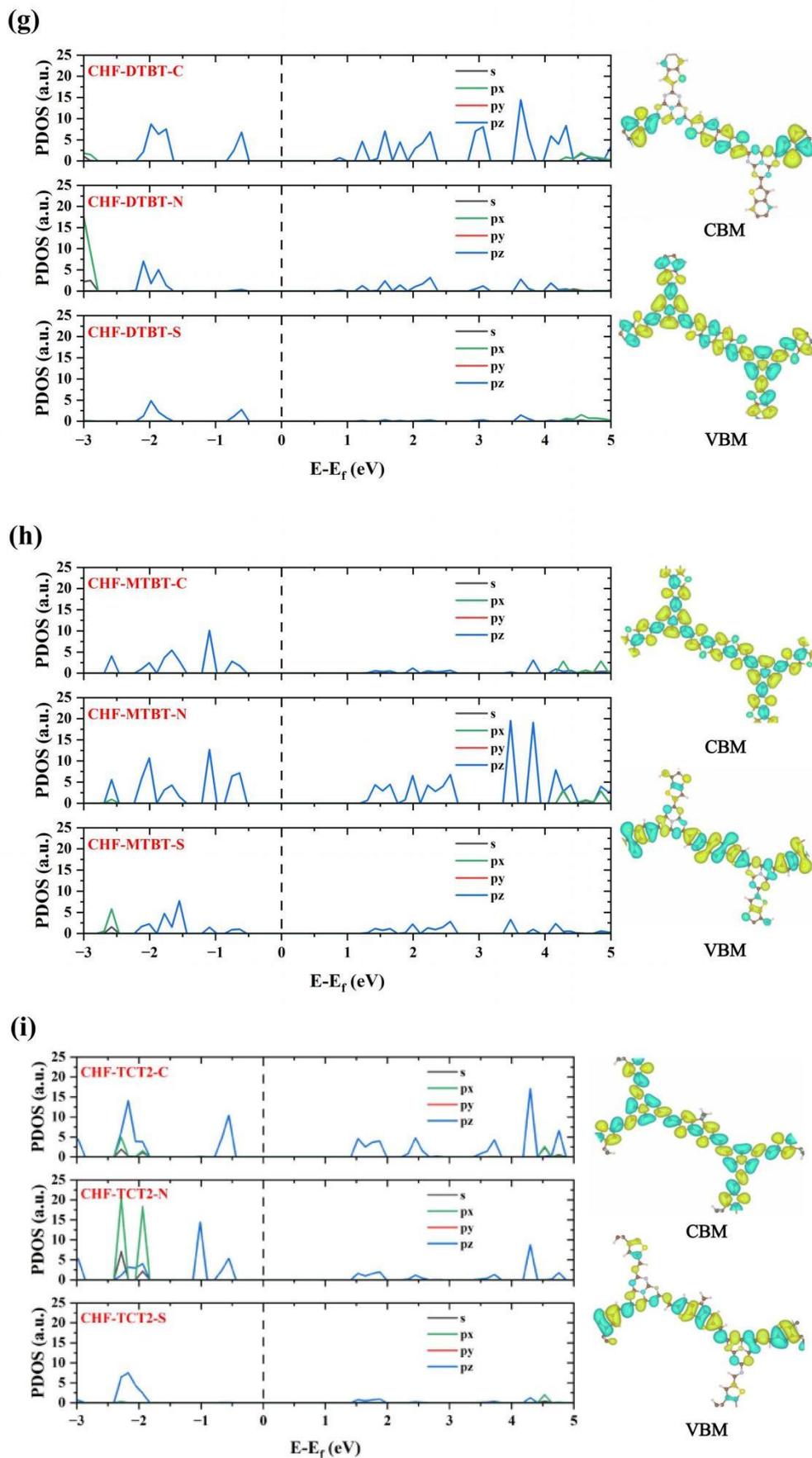
(c)



(d)

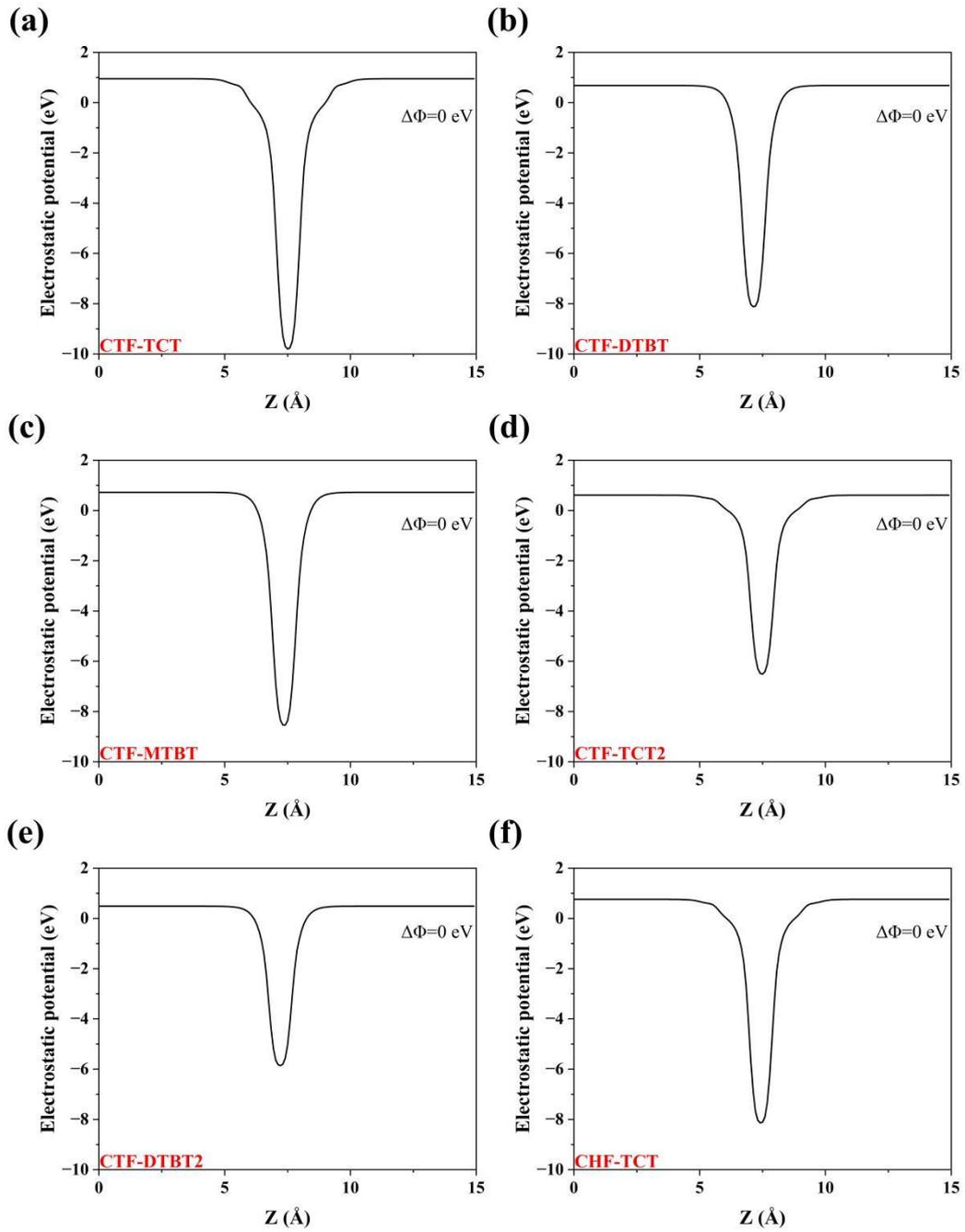


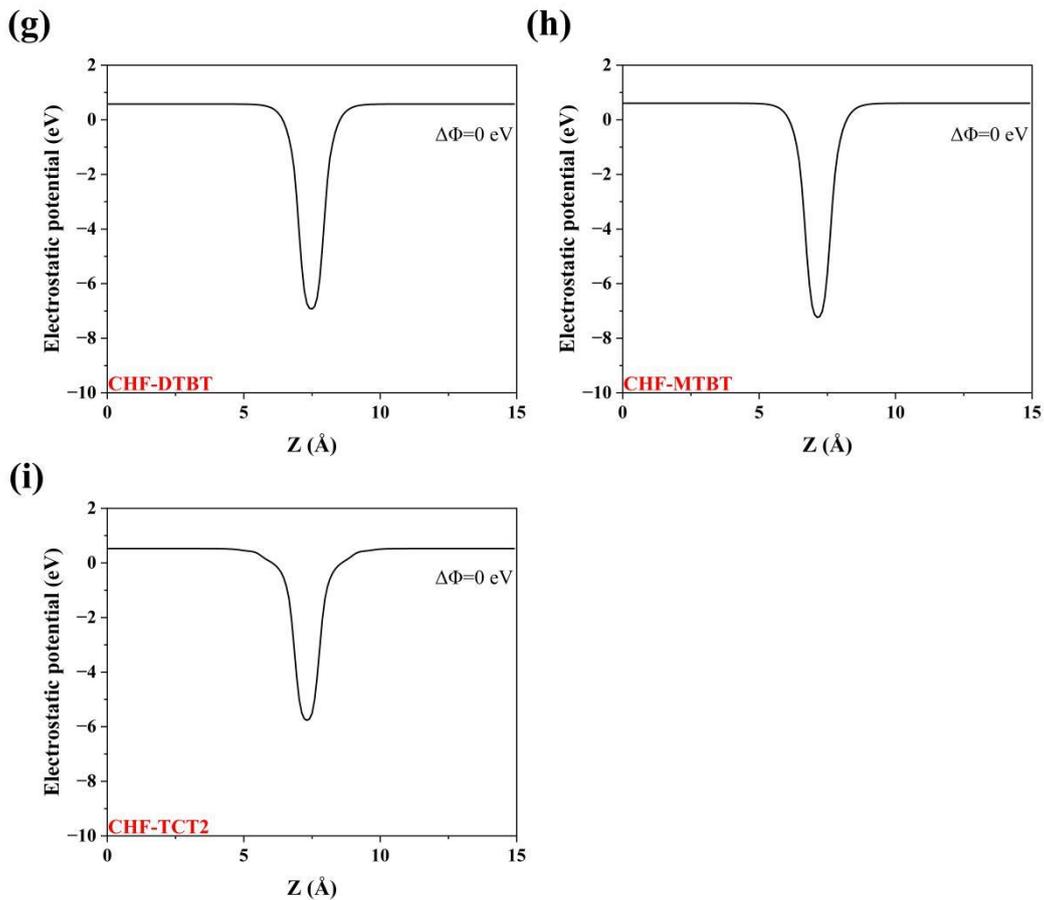




S10. Projected density of states and partial charge density for CBM and VBM on the atomic orbitals of (a) CTF-TCT, (b) CTF-DTBT, (c) CTF-MTBT, (d) CTF-TCT2, (e) CTF-DTBT2, (f) CHF-TCT, (g) CHF-DTBT, (h) CHF-MTBT, and (i) CHF-TCT2. The calculation method is HSE06. The Fermi level was set to zero.

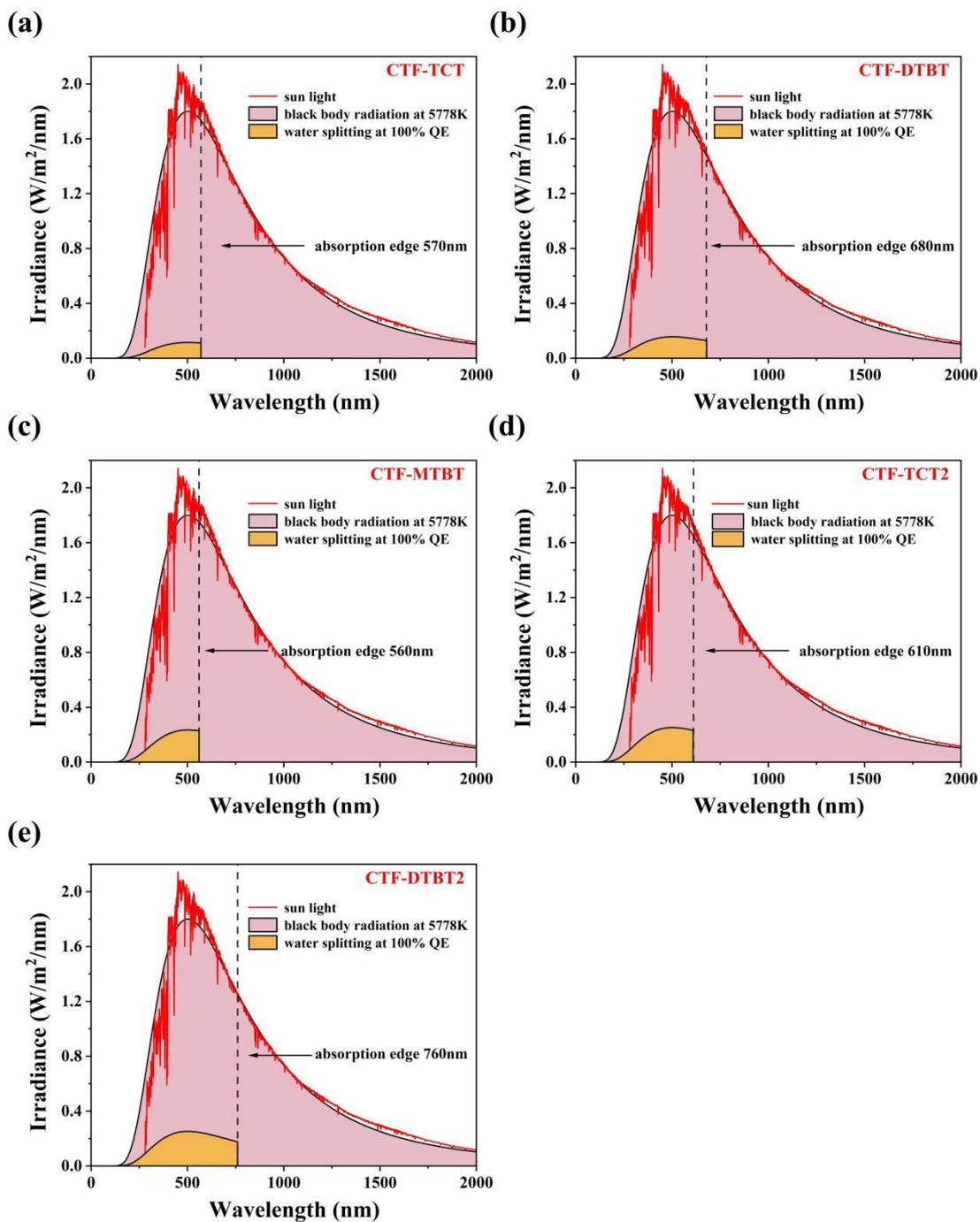
Plane-averaged Potential Curves of 2D COF Materials





S11. Plane-averaged potential curves of (a) CTF-TCT, (b) CTF-DTBT, (c) CTF-MTBT, (d) CTF-TCT2, (e) CTF-DTBT2, (f) CHF-TCT, (g) CHF-DTBT, (h) CHF-MTBT and (i) CHF-TCT2 monolayers along the perpendicular direction, plotted using the HSE06 method.

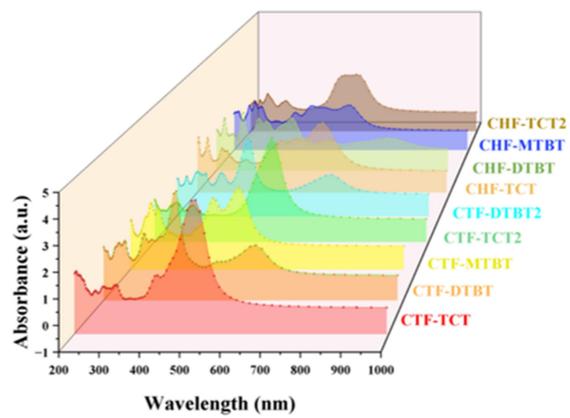
STH Efficiency of 2D COF Materials



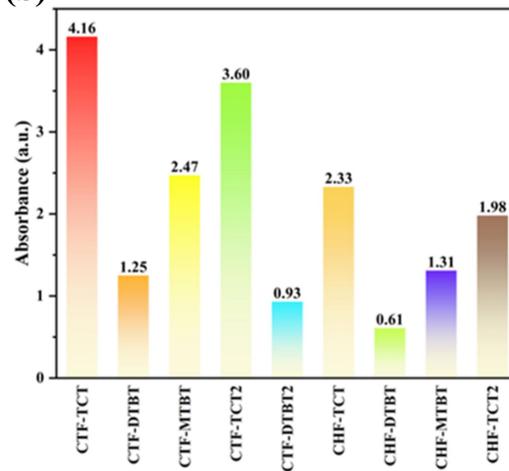
S12. Solar-to-hydrogen conversion efficiencies simulated for (a) CTF-TCT, (b) CTF-DTBT, (c) CTF-MTBT, (d) CTF-TCT2 and (e) CTF-DTBT2 under conditions of blackbody radiation at 5778 K and quantum efficiency (QE) of 100%.

Light Absorption Intensity of 2D COF Materials

(a)



(b)



S13. (a) 3D waterfall plot of absorption spectra for nine 2D COF materials; (b) visible light absorption intensity of nine 2D COF materials.

Table S1. Optimized lattice parameters using the PBE function, the VBM and CBM positions relative to the vacuum energy levels calculated by the HSE06 function, and the values of the electronic band gap for the 2D CTF ($c = 15 \text{ \AA}$, $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$).

CTFs	a=b/ \AA	VBM (V)	CBM (V)	Band gap (eV)
CTF-TCT	20.15	-5.42	-3.18	2.24
CTF-DTBT	25.73	-5.35	-3.44	1.91
CTF-MTBT	27.31	-5.63	-3.01	2.32
CTF-TCT2	27.62	-5.65	-3.50	2.15
CTF-DTBT2	32.98	-5.47	-3.71	1.76

Table S2. Optimized lattice parameters using the PBE function, the VBM and CBM positions relative to the vacuum energy levels calculated by the HSE06 function, and the values of the electronic band gap for the 2D CHF ($c = 15 \text{ \AA}$, $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$).

CHFs	a=b/ \AA	VBM (V)	CBM (V)	Band gap (eV)
CHF-TCT	24.81	-5.69	-3.87	1.82
CHF-DTBT	30.43	-5.48	-4.04	1.44
CHF-MTBT	32.00	-5.73	-3.90	1.83
CHF-TCT2	32.25	-5.94	-3.98	1.96

Table S3. STH efficiency η_{STH} of nine types of 2D COF materials.

COFs	η_{STH} (%)
CTF-TCT	15.74%
CTF-DTBT	24.24%
CTF-MTBT	14.98%
CTF-TCT2	18.82%
CTF-DTBT2	30.26%
CHF-TCT	25.01%
CHF-DTBT	40.50%
CHF-MTBT	23.47%
CHF-TCT2	22.70%

Table S4. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CTF-TCT

CTF-TCT	N1	N2	C3	C4
$\Delta G_{\text{HER}}(1)$	0.57	0.56	2.00	2.20
$\Delta G_{\text{HER}}(2)$	-0.57	-0.56	-2.00	-2.20

Table S5. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CTF-DTBT.

CTF-DTBT	N1	N2	C3	C4
$\Delta G_{\text{HER}}(1)$	0.56	0.56	0.56	1.50
$\Delta G_{\text{HER}}(2)$	-0.56	-0.56	-0.56	-1.50

Table S6. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CTF-MTBT .

CTF-MTBT	N1	N2	C3	C4
$\Delta G_{\text{HER}}(1)$	0.69	0.69	0.69	0.69
$\Delta G_{\text{HER}}(2)$	-0.69	-0.69	-0.69	-0.69

Table S7. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER and processes at the thermodynamic vantage point of CTF-TCT2 .

CTF-TCT2	N1	N2	C3	C4
$\Delta G_{\text{HER}}(1)$	-0.07	-0.19	2.12	1.82
$\Delta G_{\text{HER}}(2)$	0.07	0.19	-2.12	-1.82

Table S8. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CTF-DTBT2.

CTF-DTBT2	N1	N2	N3	C4
$\Delta G_{\text{HER}}(1)$	-0.04	-0.04	-0.18	-0.22
$\Delta G_{\text{HER}}(2)$	0.04	0.04	0.18	0.22

Table S9. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CHF-TCT.

CHF-TCT	N1	N2	C3	C4	C5
$\Delta G_{\text{HER}}(1)$	0.31	0.32	0.33	0.32	0.29
$\Delta G_{\text{HER}}(2)$	-0.31	-0.32	-0.33	-0.32	-0.29

Table S10. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CHF-DTBT.

CHF-DTBT	N1	N2	C3	C4	C5
$\Delta G_{\text{HER}}(1)$	0.30	0.30	0.30	0.30	0.28
$\Delta G_{\text{HER}}(2)$	-0.30	-0.30	-0.30	-0.30	-0.28

Table S11. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CHF-MTBT.

CHF-MTBT	N1	N2	C3	C4	C5
$\Delta G_{\text{HER}}(1)$	0.44	0.41	0.44	0.40	0.38
$\Delta G_{\text{HER}}(2)$	-0.44	-0.41	-0.44	-0.40	-0.38

Table S12. Calculated Gibbs free energy changes (ΔG , eV) for the 2e HER processes at the thermodynamic vantage point of CHF-TCT2.

CHF-TCT2	N1	N2	N3	C4	C5
$\Delta G_{\text{HER}}(1)$	-0.27	-0.01	-0.34	1.73	-0.32
$\Delta G_{\text{HER}}(2)$	0.27	0.01	0.34	-1.73	0.32

Table S13. The model structure of CTF-TCT was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CTF-TCT P-62M (189) Hexagonal

$a = b = 20.14750 \text{ \AA}$; $c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	0.39325	0.82981	0.50119
S2	0.49111	0.89498	0.50083
C3	0.46646	0.96397	0.50100
C4	0.39090	0.94045	0.50132
C5	0.34618	0.86241	0.50140
C6	0.37579	1.00290	0.50146
C7	0.33323	1.00299	0.58651
C8	0.36293	0.74656	0.50130
N9	0.28613	0.69726	0.50125
C10	0.25810	0.62040	0.50141
N11	0.30740	0.59291	0.50162
C12	0.38426	0.64174	0.50166
N13	0.41175	0.71853	0.50150
C14	0.17484	0.56748	0.50133
S15	0.10967	0.60016	0.50098
C16	0.04068	0.50653	0.50116
C17	0.06420	0.45449	0.50147
C18	0.14224	0.48781	0.50158
C19	0.43719	0.61141	0.50174
S20	0.40450	0.51355	0.50176
C21	0.49813	0.53819	0.50156
C22	0.55018	0.61376	0.50151
C23	0.51686	0.65848	0.50163
C24	0.62773	0.62887	0.50129
C25	0.61262	0.55132	0.50122
C26	0.53706	0.49928	0.50140
S27	0.51242	0.40564	0.50144
C28	0.61027	0.43833	0.50124
C29	0.65734	0.51800	0.50117
C30	0.67072	0.67171	0.58606
C31	0.67041	0.67170	0.41637
C32	0.64059	0.38540	0.50112
N33	0.59177	0.30854	0.50105
C34	0.61925	0.25923	0.50090
N35	0.69611	0.28726	0.50084
C36	0.74542	0.36406	0.50093
N37	0.71738	0.41288	0.50107

C38	1.00176	0.37693	0.50162
C39	0.93931	0.39204	0.50133
C40	0.96284	0.46761	0.50107
S41	0.89384	0.49224	0.50075
C42	0.82867	0.39438	0.50094
C43	0.86127	0.34731	0.50125
C44	1.00182	0.33391	0.41700
C45	0.45334	0.06534	0.50115
C46	0.50538	0.04181	0.50090
S47	0.59901	0.11081	0.50062
C48	0.56632	0.17598	0.50087
C49	0.48666	0.14338	0.50114
C50	0.33270	0.00282	0.41682
C51	1.00168	1.33429	1.58667
H52	0.28415	0.83133	0.50161
H53	0.27517	0.95129	0.58848
H54	0.32675	1.05462	0.58825
H55	0.36503	1.00312	0.64722
H56	0.17333	0.45687	0.50182
H57	0.54780	0.72051	0.50161
H58	0.71937	0.54894	0.50108
H59	0.67693	0.72968	0.58796
H60	0.72888	0.67836	0.58742
H61	0.63939	0.64003	0.64696
H62	0.63863	0.64025	0.35555
H63	0.72843	0.67796	0.41436
H64	0.67701	0.72986	0.41487
H65	0.83018	0.28528	0.50144
H66	1.00192	0.36537	0.35598
H67	0.95014	0.27584	0.41537
H68	1.05344	0.32741	0.41553
H69	0.45571	0.17446	0.50136
H70	0.27458	-0.04876	0.41539
H71	0.36404	0.00267	0.35582
H72	0.32637	0.05452	0.41515
H73	1.00148	1.36592	1.64738
H74	1.05340	1.32799	1.58868
H75	0.95011	1.27615	1.58838

Table S14. The model structure of CTF-DTBT was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CTF-DTBT P6/M (175) Hexagonal

$a = b = 25.73050 \text{ \AA}; c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ; \gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-0.46555	-0.57126	0.47661
C2	-0.41493	-0.51510	0.47661
C3	-0.41948	-0.46337	0.47661
C4	-0.47674	-0.46911	0.47661
C5	-0.52914	-0.52748	0.47661
C6	-0.52307	-0.57875	0.47661
C7	-0.58640	-0.53323	0.47661
C8	-0.59096	-0.48150	0.47661
C9	-0.54034	-0.42533	0.47661
C10	-0.48281	-0.41784	0.47661
C11	-0.55396	-0.38038	0.47661
C12	-0.61548	-0.40386	0.47661
S13	-0.65696	-0.48102	0.47661
C14	-0.45193	-0.61621	0.47661
C15	-0.39039	-0.59274	0.47661
S16	-0.34892	-0.51558	0.47661
C17	-0.63491	-0.27087	0.47661
N18	-0.69560	-0.29711	0.47661
C19	-0.73035	-0.35773	0.47661
N20	-0.70412	-0.39220	0.47661
C21	-0.64349	-0.36632	0.47661
N22	-0.60903	-0.30562	0.47661
C23	-0.89254	-0.46089	0.47661
C24	-0.89808	-0.41026	0.47661
C25	-0.95436	-0.41481	0.47661
C26	-0.99992	-0.52448	0.47661
C27	-0.94258	-0.51841	0.47661
C28	-0.83397	-0.44727	0.47661
C29	-0.79591	-0.38574	0.47661
S30	-0.83159	-0.34426	0.47661
C31	-0.53216	-0.00132	0.47661
C32	-0.46804	-0.04686	0.47661
C33	-0.51976	-0.10314	0.47661
C34	-0.57593	-0.10870	0.47661
C35	-0.58343	-0.05866	0.47661
C36	-0.62087	-0.16728	0.47661
C37	-0.59738	-0.20532	0.47661

S38	-0.52022	-0.16962	0.47661
C39	-0.11327	-0.53567	0.47661
C40	-0.10772	-0.58628	0.47661
C41	-0.05144	-0.58173	0.47661
C42	-0.00588	-0.47207	0.47661
C43	-0.06322	-0.47814	0.47661
C44	-0.17185	-0.54929	0.47661
C45	-0.20992	-0.61083	0.47661
S46	-0.17422	-0.65229	0.47661
C47	-0.36237	-0.63029	0.47661
N48	-0.39683	-0.69099	0.47661
C49	-0.37095	-0.72574	0.47661
N50	-0.31025	-0.69950	0.47661
C51	-0.27550	-0.63886	0.47661
N52	-0.30174	-0.60440	0.47661
C53	-0.47379	-0.99535	0.47661
C54	-0.53790	-0.94980	0.47661
C55	-0.48616	-0.89351	0.47661
C56	-0.43000	-0.88796	0.47661
C57	-0.42251	-0.93801	0.47661
C58	-0.38504	-0.82939	0.47661
C59	-0.40850	-0.79132	0.47661
S60	-0.48567	-0.82701	0.47661
H61	-0.37925	-0.41958	0.47661
H62	-0.56216	-0.62340	0.47661
H63	-0.62664	-0.57701	0.47661
H64	-0.44373	-0.37319	0.47661
H65	-0.52093	-0.33297	0.47661
H66	-0.48495	-0.66362	0.47661
H67	-0.95791	-0.37457	0.47661
H68	-0.93701	-0.55749	0.47661
H69	-0.81958	-0.48030	0.47661
H70	-0.42426	-0.04332	0.47661
H71	-0.62809	-0.06425	0.47661
H72	-0.66829	-0.18168	0.47661
H73	-0.04788	-0.62197	0.47661
H74	-0.06878	-0.43905	0.47661
H75	-0.18623	-0.51626	0.47661
H76	-0.58168	-0.95335	0.47661
H77	-0.37786	-0.93244	0.47661
H78	-0.33762	-0.81501	0.47661

Table S15. The model structure of CTF-MTBT was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CTF-MTBT P6/M (175) Hexagonal

$a = b = 27.31270 \text{ \AA}; c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ; \gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-0.93522	-0.47538	0.49075
C2	-0.96172	-0.44291	0.49075
C3	-0.96588	-0.53460	0.49075
C4	-0.87796	-0.44103	0.49075
C5	-0.86267	-0.38589	0.49075
S6	-0.91634	-0.37079	0.49075
C7	-0.80547	-0.35094	0.49075
C8	-0.77887	-0.38314	0.49075
S9	-0.82429	-0.45557	0.49075
C10	-0.55354	-0.02923	0.49075
C11	-0.52498	-0.05990	0.49075
C12	-0.46601	-0.03339	0.49075
S13	-0.43927	-0.07877	0.49075
C14	-0.50804	-0.13246	0.49075
C15	-0.54789	-0.11716	0.49075
S16	-0.61611	-0.17086	0.49075
C17	-0.58908	-0.21628	0.49075
C18	-0.53028	-0.18966	0.49075
C19	-0.43307	-0.97437	0.49075
C20	-0.46163	-0.94370	0.49075
C21	-0.52061	-0.97021	0.49075
S22	-0.54735	-0.92483	0.49075
C23	-0.47857	-0.87114	0.49075
C24	-0.43872	-0.88644	0.49075
S25	-0.37051	-0.83274	0.49075
C26	-0.39753	-0.78733	0.49075
C27	-0.45633	-0.81395	0.49075
C28	-0.62582	-0.27803	0.49075
N29	-0.68286	-0.30114	0.49075
C30	-0.71713	-0.35814	0.49075
N31	-0.69403	-0.39207	0.49075
C32	-0.63703	-0.36934	0.49075
N33	-0.60310	-0.31230	0.49075
C34	-0.51975	-0.47015	0.49075
C35	-0.55220	-0.52912	0.49075
C36	-0.52609	-0.56204	0.49075
C37	-0.46686	-0.53345	0.49075
C38	-0.43442	-0.47448	0.49075

C39	-0.46053	-0.44156	0.49075
S40	-0.36229	-0.44772	0.49075
C41	-0.37736	-0.51649	0.49075
C42	-0.43250	-0.55635	0.49075
C43	-0.55411	-0.44725	0.49075
C44	-0.60925	-0.48711	0.49075
S45	-0.62432	-0.55588	0.49075
S46	-0.44702	-0.62456	0.49075
C47	-0.37458	-0.59752	0.49075
C48	-0.34240	-0.53871	0.49075
C49	-0.64422	-0.46489	0.49075
C50	-0.61203	-0.40608	0.49075
S51	-0.53959	-0.37904	0.49075
C52	-0.34959	-0.63426	0.49075
N53	-0.38352	-0.69130	0.49075
C54	-0.36079	-0.72557	0.49075
N55	-0.30376	-0.70246	0.49075
C56	-0.26949	-0.64546	0.49075
N57	-0.29259	-0.61153	0.49075
C58	-0.05140	-0.52822	0.49075
C59	-0.02489	-0.56069	0.49075
C60	-0.02074	-0.46900	0.49075
C61	-0.10865	-0.56257	0.49075
C62	-0.12395	-0.61771	0.49075
S63	-0.07027	-0.63281	0.49075
C64	-0.18114	-0.65266	0.49075
C65	-0.20774	-0.62046	0.49075
S66	-0.16233	-0.54803	0.49075
H67	-0.94489	-0.55934	0.49075
H68	-0.78439	-0.30522	0.49075
H69	-0.59927	-0.05021	0.49075
H70	-0.50565	-0.21074	0.49075
H71	-0.38735	-0.95339	0.49075
H72	-0.48096	-0.79286	0.49075
H73	-0.55079	-0.60776	0.49075
H74	-0.43582	-0.39584	0.49075
H75	-0.29668	-0.51406	0.49075
H76	-0.68994	-0.48954	0.49075
H77	-0.04172	-0.44426	0.49075
H78	-0.20223	-0.69838	0.49075

Table S16. The model structure of CTF-TCT2 was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CTF-TCT2 P-6 (174) Hexagonal

$a = b = 27.61920 \text{ \AA}$; $c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	0.44448	0.58321	0.49802
S2	0.43166	0.51498	0.49833
C3	0.50208	0.54350	0.49733
C4	0.53304	0.59983	0.49684
C5	0.50089	0.62466	0.49723
C6	0.59205	0.61997	0.49608
C7	0.59042	0.56723	0.49630
C8	0.53783	0.52319	0.49699
S9	0.53076	0.45864	0.49736
C10	0.60341	0.49303	0.49655
C11	0.62999	0.55128	0.49602
C12	0.61963	0.65334	0.41080
C13	0.62052	0.65397	0.58046
C14	0.42003	0.88905	0.49789
S15	0.48827	0.94448	0.49836
C16	0.45974	0.98637	0.49756
C17	0.40341	0.96099	0.49700
C18	0.37859	0.90402	0.49718
C19	0.38327	-0.00015	0.49637
C20	0.43600	0.05098	0.49667
C21	0.48005	0.04244	0.49737
S22	0.54460	0.09993	0.49783
C23	0.51019	0.13818	0.49701
C24	0.45194	0.10649	0.49642
C25	0.34926	-0.00577	0.58076
C26	0.95216	0.41280	0.50259
C27	0.96074	0.46539	0.50115
S28	0.90328	0.47249	0.49981
C29	0.86499	0.39984	0.50116
C30	0.89664	0.37326	0.50257
C31	0.11413	0.55866	0.50008
S32	0.05873	0.57151	0.49914
C33	0.01682	0.50111	0.50074
C34	0.04216	0.47012	0.50189
C35	0.09914	0.50225	0.50155
C36	0.00325	0.41112	0.50322
C37	0.00873	0.38223	0.41930
C38	0.34151	0.73208	0.49839

N39	0.28663	0.69231	0.49880
C40	0.27112	0.63719	0.49910
N41	0.31088	0.62208	0.49894
C42	0.36599	0.66169	0.49847
N43	0.38111	0.71656	0.49821
N44	0.35676	0.78982	0.49812
C45	0.40798	0.83095	0.49820
N46	0.40849	0.64646	0.49818
C47	0.39842	0.59525	0.49850
N48	0.21339	0.59468	0.49964
C49	0.17223	0.60473	0.49943
C50	0.63492	0.37578	0.49723
N51	0.60302	0.31924	0.49718
C52	0.62741	0.28698	0.49773
N53	0.68395	0.31162	0.49842
C54	0.71621	0.36827	0.49851
N55	0.69157	0.40016	0.49789
N56	0.60823	0.40880	0.49685
C57	0.63471	0.46303	0.49665
N58	0.77592	0.39499	0.49928
C59	0.80369	0.36853	0.50057
N60	0.59439	0.22726	0.49765
C61	0.54016	0.19948	0.49698
C62	1.00901	1.38391	1.58898
C63	0.34990	0.99412	1.41113
H64	0.51695	0.66933	0.49698
H65	0.67474	0.57953	0.49555
H66	0.59895	0.62811	0.35029
H67	0.66456	0.66562	0.40892
H68	0.61658	0.69194	0.40867
H69	0.61793	0.69285	0.58198
H70	0.66538	0.66584	0.58163
H71	0.60015	0.62935	0.64168
H72	0.33391	0.87540	0.49683
H73	0.42368	0.12297	0.49589
H74	0.31048	-0.04730	0.58241
H75	0.33720	0.02705	0.58189
H76	0.37388	-0.00142	0.64194
H77	0.88012	0.32852	0.50339
H78	0.12774	0.48617	0.50236
H79	0.00448	0.40227	0.35777
H80	-0.02421	0.33740	0.41862
H81	0.05018	0.38479	0.41794
H82	0.44274	0.82317	0.49858
H83	0.35588	0.56048	0.49905
H84	0.17998	0.64726	0.49869
H85	0.68001	0.48680	0.49664
H86	0.78218	0.32323	0.50120
H87	0.51636	0.22099	0.49643
H88	1.00633	1.40605	1.64909
H89	1.04991	1.38527	1.59005

H90	0.97518	1.33947	1.59280
H91	0.31117	0.95255	1.40907
H92	0.37502	0.99847	1.35057
H93	0.33778	1.02690	1.40916

Table S17. The model structure of CTF-DTBT2 was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CTF-DTBT2 P6/M (175) Hexagonal

$a = b = 32.98430 \text{ \AA}$; $c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-0.54604	-0.08672	0.48054
C2	-0.49964	-0.07512	0.48054
C3	-0.46393	-0.02842	0.48054
C4	-0.47582	0.00702	0.48054
C5	-0.55918	-0.05255	0.48054
C6	-0.57575	-0.13409	0.48054
C7	-0.55079	-0.15762	0.48054
S8	-0.49099	-0.12201	0.48054
C9	-0.64266	-0.28486	0.48053
N10	-0.69012	-0.30851	0.48053
C11	-0.71421	-0.35609	0.48053
N12	-0.69055	-0.37989	0.48053
C13	-0.64298	-0.35641	0.48053
N14	-0.61918	-0.30895	0.48053
N15	-0.61745	-0.38095	0.48053
N16	-0.76428	-0.38162	0.48053
N17	-0.61812	-0.23479	0.48054
C18	-0.63671	-0.42621	0.48053
C19	-0.79028	-0.36236	0.48053
C20	-0.57286	-0.20880	0.48054
C21	-1.00611	-0.48117	0.48054
C22	-0.97067	-0.43385	0.48054
C23	-0.92397	-0.42286	0.48054
C24	-0.91237	-0.45766	0.48054
C25	-0.94655	-0.50497	0.48054
C26	-0.86500	-0.43999	0.48053
C27	-0.84146	-0.39149	0.48053
S28	-0.87708	-0.36731	0.48053
C29	-0.54145	-0.45304	0.48053
C30	-0.57624	-0.49944	0.48053
C31	-0.56527	-0.53516	0.48053
C32	-0.51794	-0.52328	0.48053
C33	-0.48196	-0.47510	0.48054
C34	-0.49415	-0.43992	0.48053
C35	-0.43463	-0.46321	0.48054
C36	-0.42364	-0.49891	0.48054
C37	-0.45844	-0.54532	0.48054
C38	-0.50576	-0.55846	0.48054

C39	-0.44076	-0.57500	0.48054
C40	-0.39228	-0.55002	0.48054
S41	-0.36808	-0.49023	0.48054
C42	-0.55911	-0.42333	0.48053
C43	-0.60760	-0.44827	0.48053
S44	-0.63179	-0.50809	0.48053
C45	-0.08765	-0.54068	0.48054
C46	-0.07604	-0.57547	0.48054
C47	-0.02935	-0.56448	0.48054
C48	0.00609	-0.51715	0.48054
C49	-0.05348	-0.49337	0.48054
C50	-0.13502	-0.55836	0.48054
C51	-0.15853	-0.60685	0.48054
S52	-0.12291	-0.63103	0.48054
C53	-0.35693	-0.64186	0.48054
N54	-0.38073	-0.68931	0.48054
C55	-0.35726	-0.71342	0.48054
N56	-0.30981	-0.68978	0.48054
C57	-0.28572	-0.64220	0.48054
N58	-0.30936	-0.61839	0.48054
N59	-0.23567	-0.61670	0.48054
N60	-0.38181	-0.76346	0.48054
N61	-0.38244	-0.61732	0.48054
C62	-0.20969	-0.63598	0.48054
C63	-0.42706	-0.78943	0.48054
C64	-0.36315	-0.57206	0.48054
C65	-0.52400	-1.00519	0.48054
C66	-0.53589	-0.96976	0.48054
C67	-0.50020	-0.92307	0.48054
C68	-0.45379	-0.91145	0.48054
C69	-0.44065	-0.94562	0.48054
C70	-0.42410	-0.86409	0.48054
C71	-0.44910	-0.84059	0.48054
S72	-0.50889	-0.87621	0.48054
H73	-0.42766	-0.01990	0.48054
H74	-0.59589	-0.06259	0.48054
H75	-0.61357	-0.15071	0.48054
H76	-0.67445	-0.44841	0.48053
H77	-0.77475	-0.32463	0.48053
H78	-0.55066	-0.22435	0.48054
H79	-0.97919	-0.40610	0.48054
H80	-0.93651	-0.53164	0.48054
H81	-0.84837	-0.46119	0.48053
H82	-0.59302	-0.57143	0.48053
H83	-0.46748	-0.40321	0.48053
H84	-0.40688	-0.42694	0.48054
H85	-0.53244	-0.59517	0.48054
H86	-0.46194	-0.61283	0.48054
H87	-0.53789	-0.38550	0.48053
H88	-0.02083	-0.59223	0.48054
H89	-0.06353	-0.46669	0.48054

H90	-0.15166	-0.53717	0.48054
H91	-0.22524	-0.67372	0.48054
H92	-0.44927	-0.77389	0.48054
H93	-0.32541	-0.54987	0.48054
H94	-0.57216	-0.97828	0.48054
H95	-0.40393	-0.93557	0.48054
H96	-0.38628	-0.84745	0.48054

Table S18. The model structure of CHF-TCT was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CHF-TCT P-62M (189) Hexagonal

$a = b = 24.80850 \text{ \AA}; c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ; \gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-0.69249	-0.28056	0.49539
N2	-0.65249	-0.30322	0.49559
C3	-0.58985	-0.26322	0.49552
N4	-0.56748	-0.20093	0.49530
C5	-0.60728	-0.17820	0.49511
N6	-0.66979	-0.21822	0.49515
N7	-0.75477	-0.32047	0.49535
C8	-0.77751	-0.38301	0.49549
N9	-0.73750	-0.40551	0.49571
C10	-0.67515	-0.36586	0.49576
N11	-0.55020	-0.28591	0.49560
C12	-0.57270	-0.34843	0.49573
N13	-0.63524	-0.38823	0.49582
C14	-0.58263	-0.11054	0.49481
S15	-0.50316	-0.05758	0.49486
C16	-0.52314	-0.00152	0.49462
C17	-0.58451	-0.02063	0.49446
C18	-0.62083	-0.08402	0.49457
C19	-0.63141	0.03022	0.40961
C20	-0.52970	-0.37311	0.49559
S21	-0.55625	-0.45259	0.49537
C22	-0.48021	-0.43264	0.49518
C23	-0.43794	-0.37128	0.49527
C24	-0.46499	-0.33493	0.49553
C25	-0.37496	-0.35903	0.49512
C26	-0.38722	-0.42202	0.49498
C27	-0.44859	-0.46427	0.49503
S28	-0.46855	-0.54031	0.49508
C29	-0.38906	-0.51378	0.49510
C30	-0.35088	-0.44906	0.49504
C31	-0.34008	-0.32432	0.57994
C32	-0.34023	-0.32419	0.41029
C33	-0.27916	-0.57394	0.49545
N34	-0.31916	-0.63658	0.49558
C35	-0.29652	-0.67658	0.49568
N36	-0.23417	-0.65389	0.49564
C37	-0.19414	-0.59137	0.49549
N38	-0.21688	-0.55158	0.49540

N39	-0.30185	-0.53428	0.49529
C40	-0.36437	-0.55676	0.49526
N41	-0.40417	-0.61930	0.49537
C42	-0.38182	-0.65922	0.49552
N43	-0.33646	-0.73886	0.49567
C44	-0.39900	-0.76160	0.49556
N45	-0.42148	-0.72156	0.49550
C46	0.01420	-0.58076	0.49509
C47	-0.03653	-0.56851	0.49509
C48	-0.01743	-0.50715	0.49510
S49	-0.07351	-0.48719	0.49536
C50	-0.12646	-0.56669	0.49536
C51	-0.09992	-0.60486	0.49523
C52	0.01421	-0.61552	0.57995
C53	-0.59678	-0.96991	0.49453
C54	-0.53379	-0.91918	0.49479
C55	-0.49153	-0.93828	0.49480
S56	-0.41548	-0.88223	0.49520
C57	-0.44200	-0.82927	0.49535
C58	-0.50672	-0.85579	0.49513
C59	-0.63169	-0.97004	0.57926
C60	-0.84518	-0.42601	0.49532
S61	-0.89812	-0.39947	0.49524
C62	-0.95419	-0.47551	0.49508
C63	-0.93509	-0.51778	0.49508
C64	-0.87170	-0.49072	0.49526
C65	1.01420	1.38444	1.41027
H66	-0.67121	-0.10925	0.49458
H67	-0.67841	-0.01197	0.40739
H68	-0.60542	0.03077	0.34884
H69	-0.63710	0.07192	0.40831
H70	-0.43984	-0.28456	0.49572
H71	-0.30051	-0.42390	0.49509
H72	-0.33467	-0.27707	0.58166
H73	-0.29298	-0.31927	0.58151
H74	-0.36570	-0.34990	0.64083
H75	-0.36620	-0.34950	0.34943
H76	-0.29328	-0.31950	0.40805
H77	-0.33446	-0.27678	0.40914
H78	-0.12512	-0.65523	0.49522

Table S19. The model structure of CHF-DTBT was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CHF-DTBT P6/M(175) Hexagonal

$a = b = 30.42850 \text{ \AA}$; $c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-0.47009	-0.03568	0.49834
C2	-0.51344	-0.08358	0.49834
C3	-0.56121	-0.08894	0.49834
C4	-0.56822	-0.04703	0.49834
C5	-0.59876	-0.13868	0.49834
C6	-0.57832	-0.17035	0.49834
S7	-0.51303	-0.13941	0.49834
C8	-0.61554	-0.30601	0.49834
N9	-0.66712	-0.32870	0.49834
C10	-0.69600	-0.38028	0.49834
N11	-0.67334	-0.40891	0.49834
C12	-0.62189	-0.38632	0.49834
N13	-0.59311	-0.33484	0.49834
N14	-0.58692	-0.25473	0.49834
C15	-0.60951	-0.22588	0.49834
N16	-0.66100	-0.24858	0.49834
C17	-0.68981	-0.29982	0.49834
N18	-0.74725	-0.40271	0.49834
C19	-0.76995	-0.37393	0.49834
N20	-0.74109	-0.32248	0.49834
C21	-0.99757	-0.51734	0.49834
C22	-1.00333	-0.47344	0.49834
C23	-0.96017	-0.42473	0.49834
C24	-0.91227	-0.42018	0.49834
C25	-0.90689	-0.46257	0.49834
C26	-0.94879	-0.51150	0.49834
C27	-0.85715	-0.45039	0.49834
C28	-0.82548	-0.39826	0.49834
S29	-0.85644	-0.36394	0.49834
C30	-0.53325	-0.43462	0.49834
C31	-0.57566	-0.48239	0.49834
C32	-0.57111	-0.52575	0.49834
C33	-0.52241	-0.52021	0.49834
C34	-0.47851	-0.47057	0.49834
C35	-0.48433	-0.42762	0.49834
C36	-0.42980	-0.46503	0.49834
C37	-0.42525	-0.50839	0.49834
C38	-0.46766	-0.55616	0.49834

C39	-0.51658	-0.56316	0.49834
C40	-0.45548	-0.59371	0.49834
C41	-0.40335	-0.57326	0.49834
S42	-0.36901	-0.50797	0.49834
C43	-0.54542	-0.39706	0.49834
C44	-0.59755	-0.41751	0.49834
S45	-0.63189	-0.48280	0.49834
C46	-0.30490	-0.61049	0.49834
N47	-0.33379	-0.66206	0.49834
C48	-0.31109	-0.69095	0.49834
N49	-0.25981	-0.66829	0.49834
C50	-0.23095	-0.61684	0.49834
N51	-0.25365	-0.58806	0.49834
N52	-0.32756	-0.58187	0.49834
C53	-0.37901	-0.60446	0.49834
N54	-0.40779	-0.65594	0.49834
C55	-0.38536	-0.68476	0.49834
N56	-0.33992	-0.74220	0.49834
C57	-0.39140	-0.76490	0.49834
N58	-0.41399	-0.73604	0.49834
C59	-0.09401	-0.52821	0.49834
C60	-0.08864	-0.57061	0.49834
C61	-0.04074	-0.56605	0.49834
C62	-0.05212	-0.47929	0.49834
C63	-0.14375	-0.54039	0.49834
C64	-0.17542	-0.59251	0.49834
S65	-0.14447	-0.62684	0.49834
C66	-0.43969	-0.90183	0.49834
C67	-0.48746	-0.90719	0.49834
C68	-0.53082	-0.95509	0.49834
C69	-0.52527	-0.99825	0.49834
C70	-0.47563	-0.99252	0.49834
C71	-0.43268	-0.94374	0.49834
C72	-0.40213	-0.85210	0.49834
C73	-0.42259	-0.82043	0.49834
S74	-0.48788	-0.85138	0.49834
H75	-0.43283	-0.03214	0.49834
H76	-0.60619	-0.05228	0.49834
H77	-0.63896	-0.15133	0.49834
H78	-0.96371	-0.39101	0.49834
H79	-0.94354	-0.54422	0.49834
H80	-0.84450	-0.47794	0.49834
H81	-0.60483	-0.56300	0.49834
H82	-0.45160	-0.38965	0.49834
H83	-0.39607	-0.42777	0.49834
H84	-0.54930	-0.60113	0.49834
H85	-0.48302	-0.63391	0.49834
H86	-0.51786	-0.35686	0.49834
H87	-0.03719	-0.59977	0.49834
H88	-0.05736	-0.44656	0.49834
H89	-0.15640	-0.51285	0.49834

H90	-0.56807	-0.95863	0.49834
H91	-0.39471	-0.93851	0.49834
H92	-0.36192	-0.83946	0.49834

Table S20. The model structure of CHF-MTBT was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CHF-MTBT P6/M (175) Hexagonal

$a = b = 32.00200 \text{ \AA}$; $c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-0.47073	-0.95406	-0.52323
C2	-0.52111	-0.97744	-0.52323
C3	-0.54851	-1.02787	-0.52323
S4	-0.54489	-0.93952	-0.52323
C5	-0.48652	-0.89301	-0.52323
C6	-0.45194	-0.90528	-0.52323
S7	-0.39405	-0.85877	-0.52323
C8	-0.41808	-0.82082	-0.52323
C9	-0.46830	-0.84430	-0.52323
C10	-0.52036	-0.47736	-0.52323
C11	-0.54735	-0.52773	-0.52323
C12	-0.52433	-0.55513	-0.52323
C13	-0.47377	-0.53001	-0.52323
C14	-0.44677	-0.47964	-0.52323
C15	-0.46980	-0.45224	-0.52323
S16	-0.38507	-0.45586	-0.52323
C17	-0.39693	-0.51422	-0.52323
C18	-0.44378	-0.54881	-0.52323
C19	-0.55034	-0.45856	-0.52323
C20	-0.59720	-0.49315	-0.52323
S21	-0.60906	-0.55151	-0.52323
S22	-0.45516	-0.60669	-0.52323
C23	-0.39318	-0.58267	-0.52323
C24	-0.36644	-0.53244	-0.52323
C25	-0.62769	-0.47493	-0.52323
C26	-0.60094	-0.42470	-0.52323
S27	-0.53897	-0.40068	-0.52323
C28	-0.61478	-0.31665	-0.52323
N29	-0.66373	-0.33702	-0.52323
C30	-0.69231	-0.38596	-0.52323
N31	-0.67194	-0.41429	-0.52323
C32	-0.62310	-0.39404	-0.52323
N33	-0.59466	-0.34519	-0.52323
N34	-0.58646	-0.26796	-0.52323
C35	-0.60671	-0.23937	-0.52323
N36	-0.65556	-0.25978	-0.52323
C37	-0.68409	-0.30844	-0.52323
N38	-0.74097	-0.40609	-0.52323

C39	-0.76138	-0.37765	-0.52323
N40	-0.73279	-0.32880	-0.52323
C41	-0.30182	-0.62141	-0.52323
N42	-0.33040	-0.67035	-0.52323
C43	-0.31003	-0.69893	-0.52323
N44	-0.26134	-0.67857	-0.52323
C45	-0.23275	-0.62972	-0.52323
N46	-0.25316	-0.60128	-0.52323
N47	-0.32218	-0.59308	-0.52323
C48	-0.37103	-0.61333	-0.52323
N49	-0.39947	-0.66218	-0.52323
C50	-0.37934	-0.69072	-0.52323
N51	-0.33856	-0.74759	-0.52323
C52	-0.38741	-0.76800	-0.52323
N53	-0.40767	-0.73941	-0.52323
C54	-0.52339	-0.05331	-0.52323
C55	-0.47302	-0.02993	-0.52323
C56	-0.44561	0.02050	-0.52323
S57	-0.44923	-0.06785	-0.52323
C58	-0.50760	-0.11436	-0.52323
C59	-0.54219	-0.10209	-0.52323
S60	-0.60007	-0.14860	-0.52323
C61	-0.57605	-0.18655	-0.52323
C62	-0.52582	-0.16307	-0.52323
C63	-0.94744	-0.48039	-0.52323
C64	-0.97082	-0.45340	-0.52323
C65	-1.02125	-0.47642	-0.52323
C66	-0.89866	-0.45041	-0.52323
C67	-0.88639	-0.40355	-0.52323
S68	-0.93290	-0.39169	-0.52323
C69	-0.83768	-0.37306	-0.52323
C70	-0.81420	-0.39981	-0.52323
S71	-0.85215	-0.46178	-0.52323
C72	-0.04669	-0.52698	-0.52323
C73	-0.02331	-0.55397	-0.52323
C74	0.02712	-0.53095	-0.52323
C75	-0.09547	-0.55696	-0.52323
C76	-0.10774	-0.60382	-0.52323
S77	-0.06123	-0.61568	-0.52323
C78	-0.15645	-0.63431	-0.52323
C79	-0.17993	-0.60756	-0.52323
S80	-0.14198	-0.54559	-0.52323
H81	-0.58756	-1.04637	-0.52323
H82	-0.48990	-0.82691	-0.52323
H83	-0.54488	-0.59418	-0.52323
H84	-0.44925	-0.41319	-0.52323
H85	-0.32746	-0.51085	-0.52323
H86	-0.66667	-0.49652	-0.52323
H87	-0.40657	0.03900	-0.52323
H88	-0.50423	-0.18046	-0.52323
H89	-1.03974	-0.45587	-0.52323

H90	-0.82029	-0.33408	-0.52323
H91	0.04562	-0.55150	-0.52323
H92	-0.17384	-0.67329	-0.52323

Table S21. The model structure of CHF-TCT2 was generated in Materials Studio. The unit cell, space group, lattice parameters, and atomic positions are below.

CHF-TCT2 P3 (143) Hexagonal

$a = b = 32.24700 \text{ \AA}$; $c = 15 \text{ \AA}$

$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$

Atom Name	x(Å)	y(Å)	z(Å)
C1	-1.31466	-0.61619	0.49018
N2	-1.33931	-0.66502	0.49042
C3	-1.31514	-0.68967	0.49069
N4	-1.26659	-0.66552	0.49071
C5	-1.24199	-0.61681	0.49048
N6	-1.26610	-0.59226	0.49021
N7	-1.33881	-0.59180	0.48980
C8	-1.38752	-0.61591	0.48967
N9	-1.41207	-0.66457	0.48993
C10	-1.38814	-0.68919	0.49031
N11	-1.33976	-0.73823	0.49080
C12	-1.38842	-0.76234	0.49065
N13	-1.41254	-0.73775	0.49042
N14	-1.18954	-0.59051	0.49029
N15	-1.41457	-0.81479	0.49050
N16	-1.41381	-0.58977	0.48907
C17	-1.16604	-0.61347	0.49014
C18	-1.46103	-0.83831	0.49020
C19	-1.39086	-0.54330	0.48843
C20	-1.53129	-0.41678	0.48478
S21	-1.54849	-0.47704	0.48594
C22	-1.48923	-0.45855	0.48577
C23	-1.45866	-0.41087	0.48487
C24	-1.48175	-0.38505	0.48428
C25	-1.40936	-0.39880	0.48493
C26	-1.41611	-0.44629	0.48605
C27	-1.46274	-0.48063	0.48650
S28	-1.47511	-0.53823	0.48780
C29	-1.41330	-0.51458	0.48767
C30	-1.38610	-0.46478	0.48669
C31	-1.38332	-0.37075	0.56927
C32	-1.38358	-0.37179	0.39958
C33	-1.62664	-0.29463	0.48492
N34	-1.67267	-0.33175	0.48491
C35	-1.68158	-0.37778	0.48466
N36	-1.64458	-0.38649	0.48443
C37	-1.59865	-0.34946	0.48442
N38	-1.58979	-0.30359	0.48467

N39	-1.61793	-0.24892	0.48528
C40	-1.65496	-0.24001	0.48560
N41	-1.70083	-0.27703	0.48555
C42	-1.70979	-0.32284	0.48521
N43	-1.72739	-0.41463	0.48475
C44	-1.76440	-0.40578	0.48505
N45	-1.75550	-0.35985	0.48529
N46	-1.55860	-0.35875	0.48435
N47	-1.81375	-0.44585	0.48530
N48	-1.64567	-0.19066	0.48612
C49	-1.56686	-0.40250	0.48462
C50	-1.84922	-0.43759	0.48597
C51	-1.60193	-0.15517	0.48653
C52	-1.89908	-0.47316	0.48652
S53	-1.94212	-0.45594	0.48713
C54	-1.98290	-0.51519	0.48779
C55	-1.96582	-0.54579	0.48754
C56	-1.91689	-0.52271	0.48681
C57	-1.58765	-0.10531	0.48713
S58	-1.52739	-0.06226	0.48795
C59	-1.54585	-0.02147	0.48827
C60	-1.59354	-0.03857	0.48781
C61	-1.61938	-0.08750	0.48710
C62	-1.00307	-0.59508	0.48820
C63	-1.04379	-0.58830	0.48885
C64	-1.03147	-0.54166	0.48860
S65	-1.07669	-0.52926	0.48912
C66	-1.11488	-0.59105	0.48970
C67	-1.09230	-0.61828	0.48948
C68	-1.00105	-0.62078	0.57304
C69	-1.60558	-1.00132	0.48813
C70	-1.55809	-0.96059	0.48885
C71	-1.52375	-0.97289	0.48889
S72	-1.46614	-0.92766	0.48953
C73	-1.48976	-0.88948	0.48979
C74	-1.53957	-0.91207	0.48940
C75	-1.63340	-1.00328	0.57279
C76	0.99812	1.37878	1.40335
C77	0.36716	0.99738	1.40308
H78	-1.46381	-0.34639	0.48365
H79	-1.34740	-0.44397	0.48645
H80	-1.38137	-0.33536	0.57013
H81	-1.34625	-0.36469	0.57116
H82	-1.40237	-0.39066	0.63048
H83	-1.40246	-0.39272	0.33914
H84	-1.34631	-0.36520	0.39847
H85	-1.38220	-0.33671	0.39643
H86	-1.89619	-0.54066	0.48660
H87	-1.65803	-0.10819	0.48655
H88	-1.11023	-0.65699	0.48969
H89	-1.00152	-0.60129	0.63388

H90	-0.96780	-0.62309	0.57387
H91	-1.03227	-0.65772	0.57569
H92	-1.56036	-0.89416	0.48950
H93	-1.66880	-1.03672	0.57392
H94	-1.63945	-0.97226	0.57483
H95	-1.61330	-1.00235	0.63378
H96	0.99633	1.39756	1.34251
H97	0.96725	1.34159	1.40248
H98	1.03169	1.37708	1.40078
H99	0.33185	0.96386	1.40063
H100	0.38774	0.99898	1.34237
H101	0.36095	1.02830	1.40176
H102	0.42923	0.83758	0.48642
H103	0.39472	0.56635	0.48473
H104	0.15803	0.60082	0.48615
H105	0.64996	0.47735	0.48846
H106	0.81379	0.34571	0.49037
H107	0.51831	0.18185	0.49025

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