Supporting Information for:

A Conductive Metal-Organic Framework Photoanode

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Table of Contents:

Experimental Methods:

H_4TTFTB Synthesis:

H_4TTFTB (tetrathiafulvalene tetrabenzoic acid) was synthesized following the literature procedures without modification.[1,2]

TiO_2 and ZrO_2 Film Preparation:

FTO was purchased from Pilkington (NSG TEC). For THz measurements, quartz substrates purchased from GM associates. TiO_2 (Ti-Nanoxide T/SP) and ZrO_2 (Zr-Nanoxide ZT/SP) nanoparticle pastes were purchased from Solaronix and used as received. The films were deposited by doctor blading with Scotch tape as a spacer layer. One layer was applied followed by calcination in a programmable furnace. The furnace was heated to 370 ˚C by 180 ˚C /hour, held 10 minutes, then heated to 470 ˚C by 180 ˚C /hour, held 30 minutes, followed by ambient cooling to room temperature.

Zn_2TTFTB Film Growth:

Zn_2TTFTB was grown on FTO, TiO_2, or ZrO_2 substrates using the same procedure. Two pieces of cleaned substrate are placed back-to-back in a 20mL glass scintillation vial. Two solutions are then prepared separately, one containing the metal precursor and the other containing the ligand. In a typical synthesis, the metal solution is prepared by dissolving 37 mg (0.2 mmoles) of $Zn(NO_3)_2{\cdot}6H_2O$ into a mixture of 2.6 mL of DMF and 2.6 mL of ETOH. The ligand solution is then prepared by dissolving 21 mg of H_4TTFTB (0.03 mmoles) into a mixture of 2.6 mL of DMF and 1.5 mL of ETOH. The metal solution is then pipetted into the vial containing the substrates. Following the addition of the metal solution, the ligand solution is added slowly to the vial while gently swirling to mix. The vial is then tightly capped and suspended in an oil bath preheated to 40˚ C and is then ramped to 75˚ C. After cooling to room temperature, the film is removed from solution and rinsed with DMF followed by ETOH and is allowed to dry in air. For OPTP experiments, the metal oxides were deposited on Quartz rather than FTO prior to film growth.

X-ray Absorption Spectroscopy:

X-ray absorption spectroscopy was performed at the National Synchrotron Light Source II at Brookhaven National Laboratory at beamline 6-BM. Bulk powder samples were measured in transmission mode by preparing a thin layer in Kapton tape. Film samples were measured in fluorescence mode using a four-element Si-drift detector. Energy was calibrated against a Zn reference foil.

Data was analyzed using the Demeter suite of programs (version 0.9.25) which implements FEFF6. The input models for each unique Zn atom (Zn_1 and Zn_2) were prepared from the published crystal structure.[2] Fourier transforms to R-space were performed on the k-range of (2.35 - 8.50 $Å^{-1}$) for all data sets.

Standard Characterization:

UV-Visible spectroscopy was performed using a Shimadzu UV-2600 spectrometer in either transmission mode or in diffuse reflectance mode with an integrating sphere attachment. pXRD patterns were obtained using a Rigaku SmartLab X-ray diffractometer. Mercury (CCDC) was used to calculate the reference pXRD pattern using the published single crystal structure.[2]

Cyclic Voltammetry and Spectroelectrochemistry:

Cyclic voltammetry (CV) of H4TTFTB was performed in DMF electrolyte (0.1M $TBAPF_6$) using a glassy carbon working electrode, Pt wire counter electrode, and Ag/AgCl reference electrode (sat. NaCl) in an N_2 purged cell. CV of Zn_2TTFTB-FTO did not give clear features in a DMF electrolyte, and therefore a DCM electrolyte (0.1M $TBAPF_6$) was used for the reported CV.

Spectroelectrochemistry of H_4TTFTB was performed in a quartz spectroelectrochemistry cell cuvette (Basi, 1mm path length) with a Pt mesh working electrode in the beam path, a Pt wire counter electrode, and a Ag/AgCl reference electrode (sat. NaCl) in 0.1M $TBAPF_6$ electrolyte. Chronoamperometry was performed at each measured potential and given 60 seconds to equilibrate prior to measurement of the UV-Visible spectrum. Zn_2TTFTB-FTO was measured in a standard 1cm quartz cuvette using Pt wire counter electrode and Ag/AgCl reference electrode in 0.1M $TBAPF_6$ DMF electrolyte. Upon immersion into electrolyte, a gradual baseline shift is observed due to refractive index changes upon solvent intercalation into the MOF. As a result, the film was placed in electrolyte for 30 minutes prior to spectroelectrochemistry to allow equilibration. Starting from the no potential condition, oxidizing potentials were first applied with chronoamperometry. At each potential, approximately 20 minutes was allowed for equilibration after which a UV-Visible spectrum was collected.

Optical-pump THz-probe spectroscopy:

OPTP was performed using our time-resolved THz spectrometer described elsewhere .[3,4] The system is based on a Spectra-Physics Spitfire Ace amplifier (35 fs FWHM, 1 kHz repetition rate, 3.8 mJ pulse energy) that is first split into two beams. The first generates a frequency-doubled 400nm pulse in a β-barium borate (BBO) crystal that is sent to a delay line to control the pump delay (t_{pump}). The samples were excited from the front, meaning that the incident excitation pulse passes through the sensitizer and mesoporous TiO_2 followed by the quartz substrate. The second beam is split to generate a weak read-out pulse and the majority is used for THz generation in a two-color air plasma. The read-out pulse then gates the electro-optical sampling in a ZnTe (110) crystal. The OPTP experiments are performed at the peak of the THz pulse and are collected by chopping the excitation pulse and using a lock-in amplifier to directly measure the difference signal. The data is reported as % THz attenuation.

Nanosecond Transient Absorption Spectroscopy:

Transient absorption data was collected on an Edinburgh Instruments LP900 spectrometer. The excitation is based on the third harmonic of an Nd:YAG laser (Spectra-Physics, INDI-10, 355 nm, pulse

width 10 ns) that is sent through an optical parametric oscillator (OPO, Spectra-Physics) to generate a X mJ, 10 mm diameter, 430 nm pulse. The samples were excited from the front as in OPTP experiments. The probe is a pulsed 450 W Xe arc lamp with a 490 nm long pass filter after the sample to remove scattered pump light. The white probe light is passed through a monochromator and is detected by a photomultiplier tube.

Computational Methods

MOF Construction:

The Zn_2TTFTB MOF 3 and 1 layer systems and H_4TTFTB were cut from a crystal unit cell structure produced by Narayan et al.[2] Before truncating the structure, the crystal was optimized under periodic boundary conditions using the Perdew−Burke−Ernzerhof (PBE) exchange-correlation functional[5] with 5-5-5 k points, a 500 eV cutoff, and the PAW plane wave basis set. This periodic optimization was done to remove the concern of crystal structure resolution limitations. The coordination sphere of Zn in the truncated models was capped with either carboxylate or water groups as would occur in the crystal structure.

Energetics:

The truncated models were optimized with the density functional tight binding program DFTB+[6] using 3ob-3-1[7-10] parameters to improve energetics while maintaining computational tractability for all systems. A full example input is provided in the SI. Slight changes in angles (2-4°) of phenyl rings were seen upon optimization from crystal structure. Density of states were generated from these optimized structures in vacuum. Functionals and basis sets of the ligand system were benchmarked to match UV-Vis experimental spectra with a half width at half height of 0.4 eV with benchmarking data in the SI (Table S1). Use of functional Wb97xd[11] with basis set Def2TZV[12] was found to give the best reproduction while maintaining tractability. UV-Vis and oxidation potentials were calculated for each neutral and cationic ligand, 1 layer, and 3 layer system in DMF using the functional B3LYP[13,14] instead of Wb97xd to best reproduce the spectra.

Alignments of the H_4TTFTB ligand and TiO_2 fermi levels to experimental data were performed in both YAeHMOP and DynEMol programs detailed below. The aligned fermi levels were used for all subsequent DOS and interfacial electron transfer calculations. The experimental center of the band gap ("fermi level") for the ligand was determined from the average of $Ep_{1/2}$ for 50mV/s and 100 mV/s CV of H_4TTFTB and was found to be +0.118 V vs Ferrocene. Ferrocene vs Vacuum is -4.8eV[15] making the fermi level of the ligand -4.92eV vs Vacuum. The experimental fermi level of intrinsic, indirect bandgap TiO_2 was determined to be -6.34eV vs Vacuum by converting from the literature value +3.5eV vs SHE[16] and using the conversion factor of +4.44eV.[17] Shifts were determined by comparing the experimental value to the calculated value of the center of bandgap for the isolated ligand or fermi level for the isolated TiO_2 and determining the added value required to match experiment. The YAeHMOP shifts were +5.455eV for the ligand and +3.487eV for TiO_2. The DynEMol shifted were +4.783 for the ligand and +6.130 for TiO_2. These shifts were then used for the joint calculations.

To perform the shift in the YAeHMOP based IET code, one must add lines as follow to the .bind input file, where the first number is the adsorbate shift, the second the surface shift, the third and fourth are extended Huckel fitting parameters, and the fifth is the number of orbitals needed for the adsorbate.

EFalignment2

5.455 3.487 1.75 1.75 226

To perform the shift in the DynEmol code add the following lines to the tuning.f file.

!--

! define %DPF (Dipole Fragment)

! define %V_shift (FMO offset shift)

!--

where(univ% atom% residue == "LA1") univ% atom% V_shift =+4.783d0

where(univ% atom% residue == "CCC") univ% atom% V_shift =+6.130d0

Interfacial Electron Transfer:

Interfacial electron transfer was conducted for three different orientations of the ligand on TiO_2 following the procedure outlined in Rego, et al[18] which utilizes the YAeHMOP package.[19] Orientations each had two carboxylate groups embedded into the TiO_2 surface and were oriented flat, long, or tall with respect to the surface (Figure 6, main text). Dynamics were calculated for every 0.1 fs for a total of 100 fs. 1 k point was used with an absorbing potential in the bottom layer of the TiO_2. Survival probabilities, density of states, and electron and hole density visualizations were produced. The visualizations can be seen in Figure 6 and Figure 7 in the main text, and Figure S13 and Figure S20.

Interlayer Electron /Hole dynamics:

To investigate the inter-layer charger transfer dynamics in the Zn_2TTFTB MOF, a six-layer stack of ligands (one unit cell from the crystal structure) was used after replacing the Zn nodes with capping hydrogen atoms on the carboxylates. This model was submitted to four 250 fs NVT molecular dynamics trajectories at 298.15 K using the GNF2-XTB level of theory. In these simulations, a harmonic potential of 0.3 Hartrees was applied to the benzoic acid oxygen atoms to mimic the rigid framework to which they would otherwise be coordinated. The time step for the MD trajectories was 0.1 fs. Subsequently, electron and hole wavepackets were propagated on the correlated configurations of the MD trajectories according to a previously reported time-slice methodology. This sequential QM/QM' approach incorporates the influence of nuclear dynamics on the electorn/hole prorogation, which we found to be an important consideration.

The wavepackets were initialed on each of the six ligands, and the results were averaged for across the four MD trajectories. The quantum dynamics simulations were performed with the Dynamics of Electronics in Molecules (DynEMol) suite of programs,[18] which was also used to optimize the parameters of the Extended Hückel (EH) Hamiltonian used for the simulations. The EH parameters were optimized to reasonably reproduce the topologies and HOMO-LUMO gap of the frontier orbitals as obtained at the DFT (B3LYP/def2TZVP) level of theory (SI figure).

Interlayer Electron /Hole Coupling Constants:

Electronic coupling constants were calculated for every adjacent pair of layers in the six-layer stack model used for the quantum dynamics simulations. The coupling calculations were performed on structures taken from a separate, 250 ps NVT molecular dynamics simulation using the GNF2-XTB method . In this case, the sampled configurations were separated in time by 1.0 ps. The transfer integral approach implemented in the Amsterdam Density Functional program (version 2017.107) was used to compute the electron couplings at the B3LYP/TZ2P level of theory.

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Supplementary Figures:

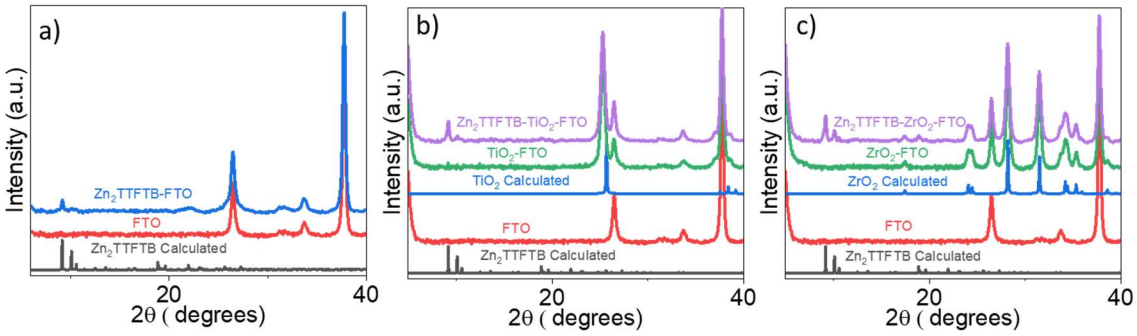


Figure S1. pXRD patterns comparing the calculated Zn_2TTFTB film samples to the patterns for the substrate(s) for Zn_2TTFTB-FTO (a), Zn_2TTFTB-TiO_2 (b), and Zn_2TTFTB-ZrO_2 (c).

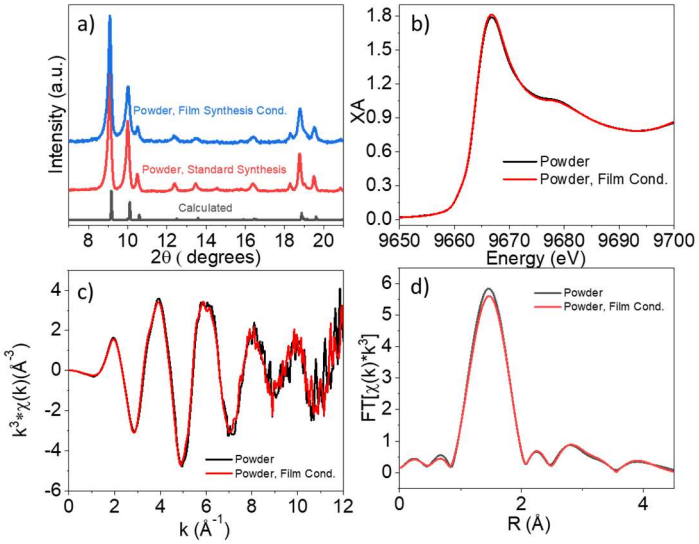


Figure S2. (a) pXRD patterns comparing the polycrystalline powder sample obtained from the standard published synthesis to the powder synthesized under the film synthesis condition. (b) Zn K-edge XANES spectra comparing the two synthesis conditions. (c) K-space and (d) R-space comparisons of the two synthesis methods.

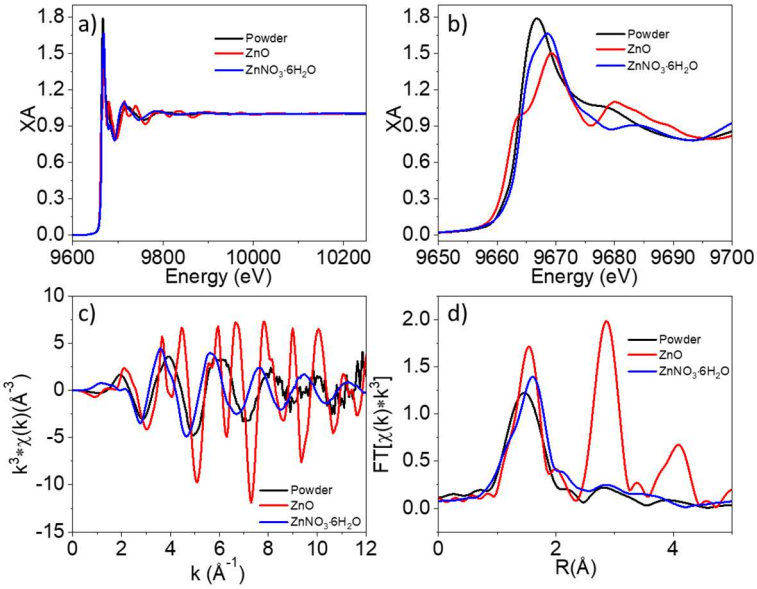


Figure S3. (a) EXAFS spectra of Zn_2TTFTB powder compared to reference samples and (b) enlarged XANES region. (c) K-space and (d) R-space EXAFS spectra. ZnO is a material with tetrahedral Zn coordination with O and significant second shell Zn-Zn scattering. $ZnNO_3$•$6H_2O$ has octahedral coordination of Zn with H_2O ligands and crystallizes along with NO_3 ions and does not give significant Zn-Zn second shell interactions. While the XANES region differs between Zn_2TTFTB powder and $ZnNO_3$•$6H_2O$ in the white line region, the structure and oxidation state of Zn in Zn_2TTFTB appears to be consistent with Zn^{2+} in octahedral or pseudo-octahedral coordination environment. Quantitative EXAFS fitting (main text) confirms the structure of Zn^{2+} in Zn_2TTFTB.

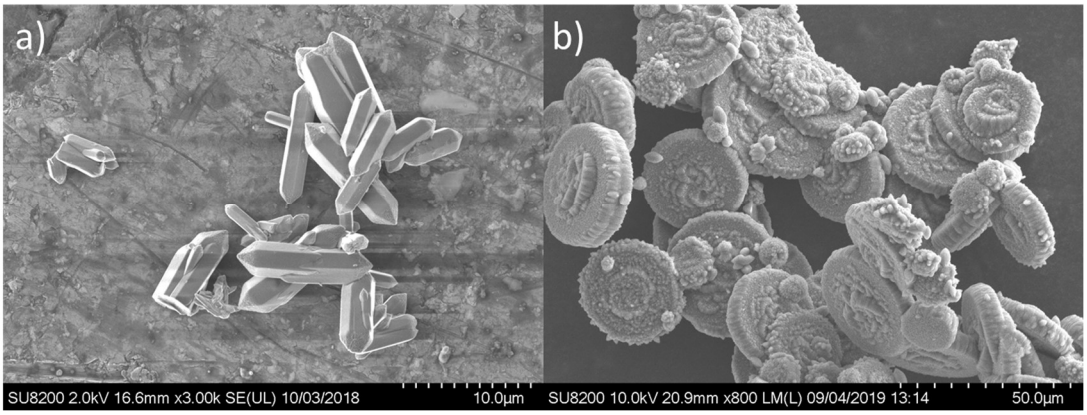


Figure S4. SEM images of (a) Zn_2TTFTB powder synthesized under the standard synthesis conditions containing added H_2O and (b) Zn_2TTFTB powder synthesized under the film conditions without added H_2O and also with a larger Zn:TTFTB ratio than the standard synthesis.

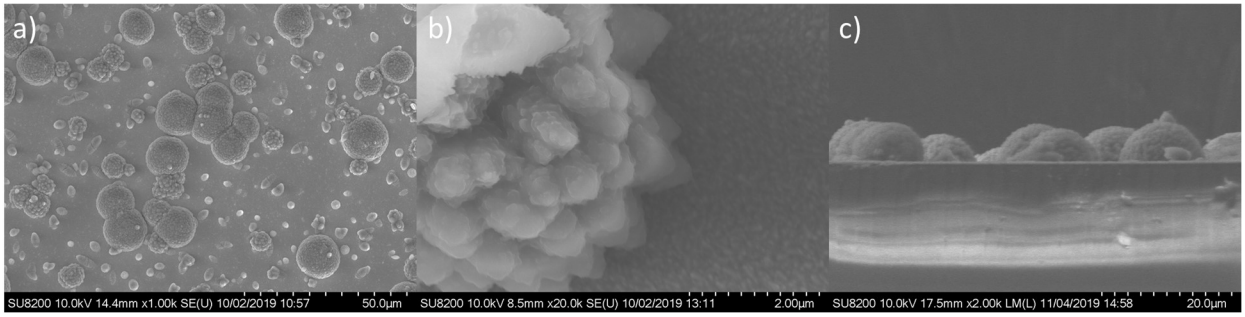


Figure S5. SEM results for Zn_2TTFTB-FTO. Top-view images (a,b) and cross-section image (c) show the formation of a monolayer of hemispherical flower-like MOF structures.

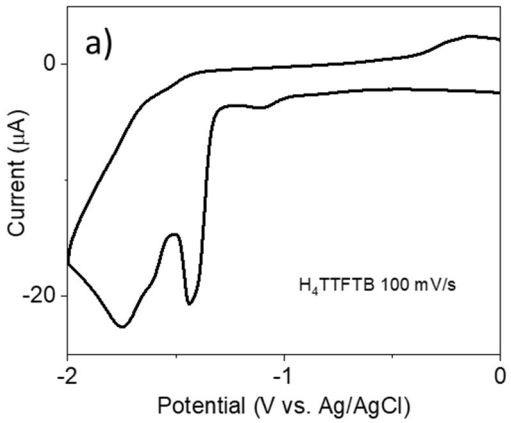


Figure S6. CV data collected on the reduction side for H_4TTTB in N_2 purged 0.1M $TBAPF_6$ at 100 mV/s. The working electrode is glassy carbon.

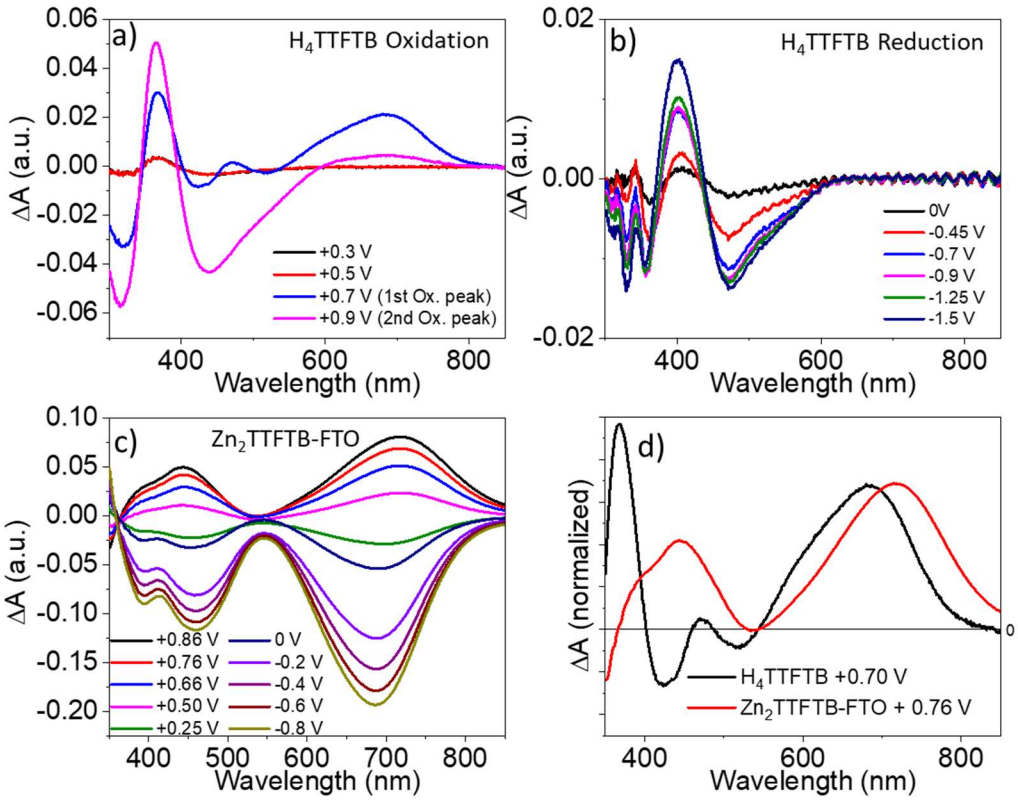


Figure S7. ΔA spectra for the spectroelectrochemical oxidation (a) and reduction (b) of H_4TTFB generated by subtracting the "no potential" spectrum from the spectrum of each applied potential. (c) ΔA spectrum of Zn2TTFTB generated similarly as (a) and (b). (d) Comparison of the ΔA spectra for the ligand (H_4TTFTB) compared to the MOF (Zn_2TTFTB-FTO). Overall, the ΔA spectra are similar with shifting of the red-most feature and difference in the splitting of the feature at 420 nm.

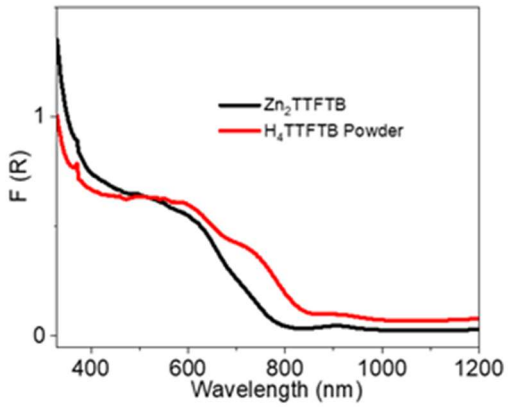


Figure S8. Diffuse reflectance UV-Visible-NIR spectra for Zn_2TTFTB powder and H_4TTFTB powder. Both display absorption in the region between 600-nm corresponding to TTF cation radical absorption.

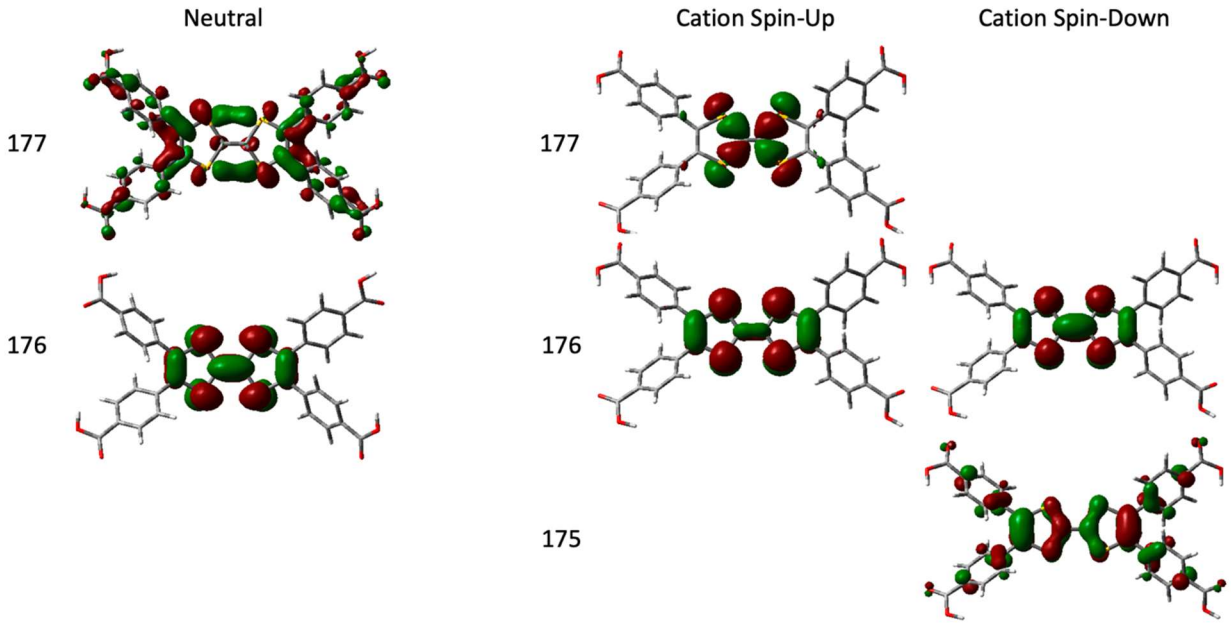


Figure S9. Natural Transition Orbitals for H_4TTFTB neutral and cationic structures. Optimized with B3LYP/6-31(g) in n,n-DiMethylFormamide using SMD and gd3bj empirical dispersion. The neutral NTOs show that upon excitation from the HOMO (176) to the LUMO (177), the electron density becomes delocalized from the center.

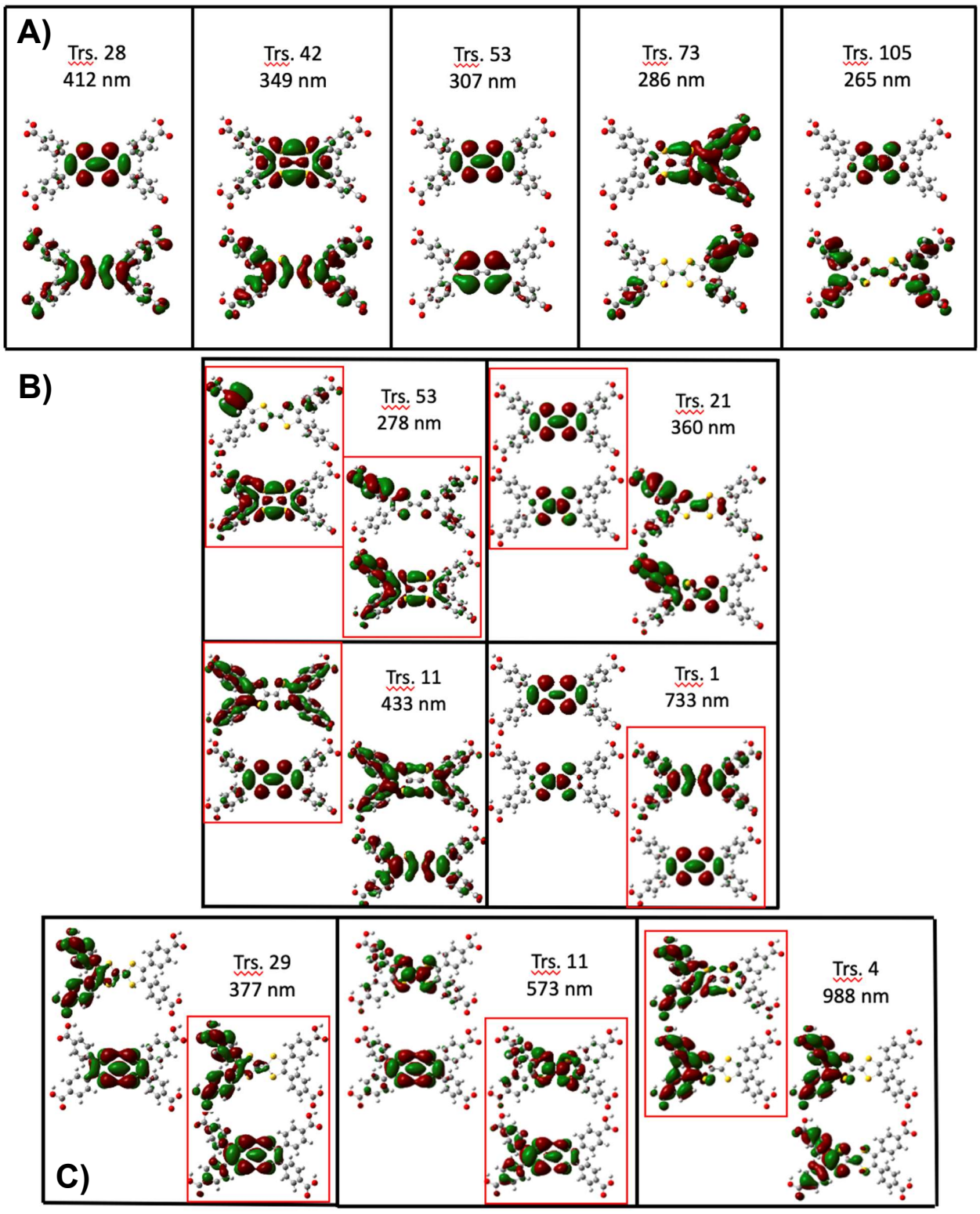


Figure S10. NTO's for various transitions in the absorption spectra of the anionic (A), cationic (B), and dicationic (C) of the H_4TTFTB ligand. Red boxed transitions note the more favorable transition when multiple are possible.

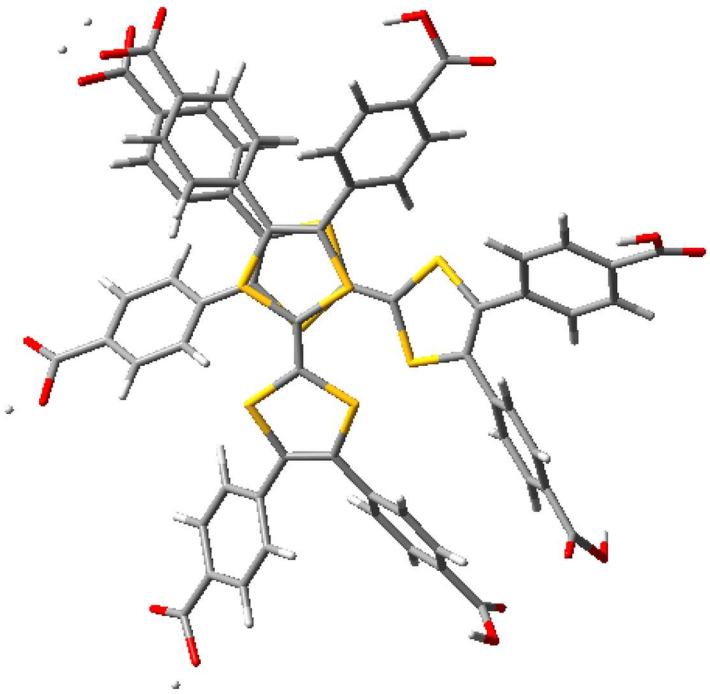


Figure S11. Two H_4TTFTB Ligands Optimized. Optimization performed with wb97xd/def2tzv in n,n-dimethylformamide using the pcm solvation model.

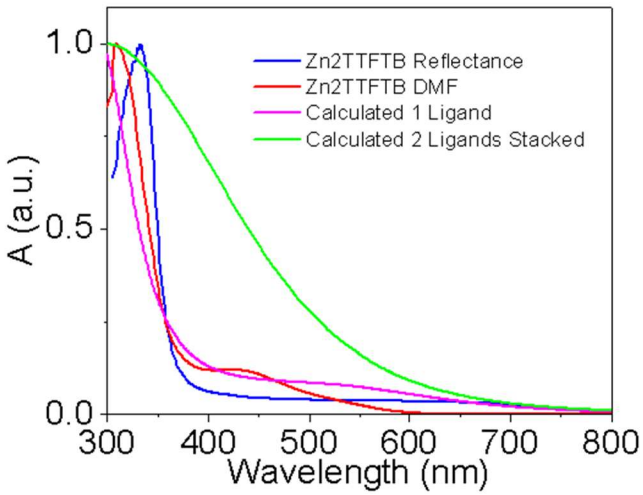


Figure S12. Comparison of 2 ligand stacked model to experimental and theoretically calculated single ligand UV-Visible spectra. The 2 ligand shows absorption broadening between the 400-600 nm region but does not show a prominent feature in the 600 – 800nm region seen in the MOF and cation structures.

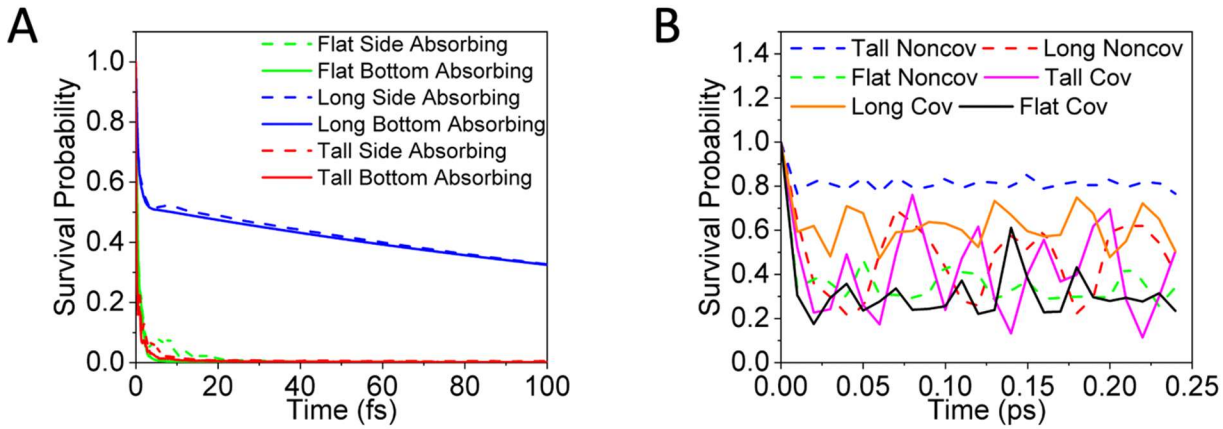


Figure S13. Survival probabilities calculated using utilizing Yaehmop according to Luis Rego's prescription and default extended Huckel parameters (A) and Dynemol using tuned parameters to match DFT results following the Dynemolmanual prescription (B). (A,B) show survival probability for the electron in H_4TTFTB on TiO_2 in the long, tall, and flat orientations. (A) shows results utilizing an absorbing boundary on either the side or bottom of the TiO_2 and shows little difference between the two with the long side showing the most difference with a longer lifetime. In (A) the H_4TTFTB is bound covalently on TiO_2. (B) shows covalent and noncovalently bound H_4TTFTB with no absorbing boundary in either case.

The lack of an absorbing boundary shows a great deal of recombination after an initial loss of probability on the ligand. (A) suggests that when an appropriate absorbing boundary is present, as would be found in an extended TiO_2 slab in experiment, the survival probability decreases rapidly to 0 within the instrument response time of the experiment. Differing the location of the absorbing potential showed some initial recombination probability in the side absorbing cases, but generally followed the finding that electrons injected within the instrument response time. The lengthened long orientation probability is seen to be due to only the electrons from the phenyl ring in contact with the surface injecting initially followed by a slow drain from the farther phenyl. This can be seen in the electronic SI movies of injection.

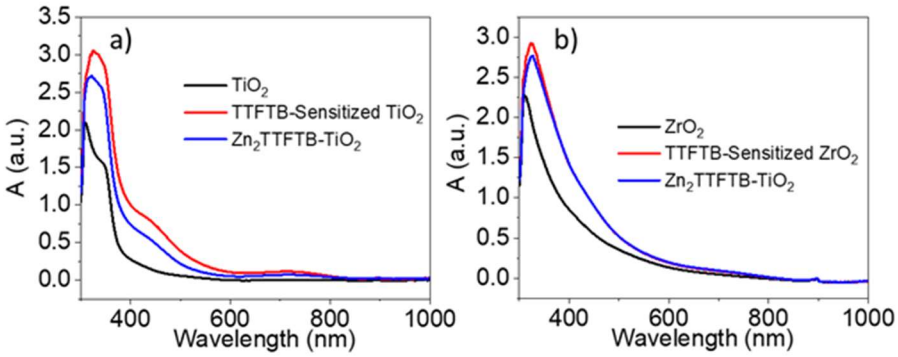


Figure S14. Transmission mode UV-Visible spectra for TiO_2 samples (a), ZrO_2 samples (b). The cation radical band is observed clearly in the TTFTB-Sensitized TiO2 sample (a). Additionally, it is observed in the diffuse reflectance spectrum of H4TTFTB powder (c). Evidently, oxidation occurs when the ligands are aggregated in either the solid powder, on a sensitized film, or in the MOF structure.

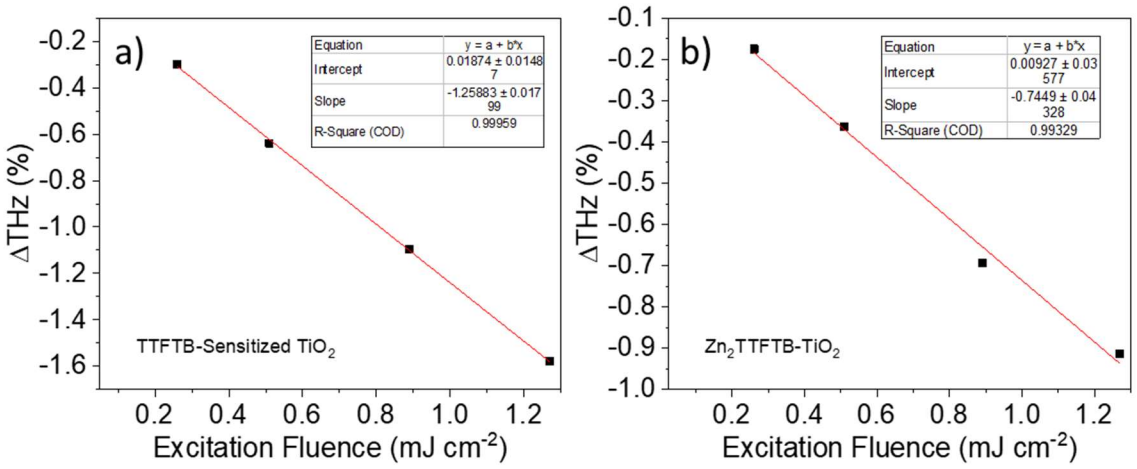


Figure S15. Linear dependence of the THz attenuation amplitude on the 400 nm pump fluence.

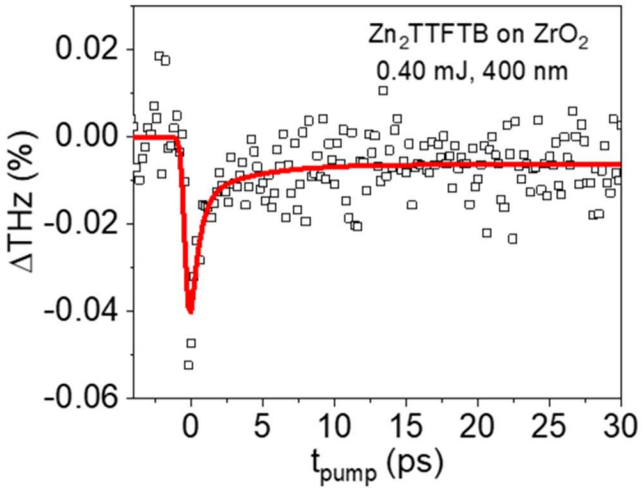


Figure S16. Control experiment for Zn_2TTFTB on ZrO_2 under 400nm excitation. The intrinsic photoconductivity of the MOF is over an order of magnitude weaker than the observed injection signal and is therefore disregarded in modelling.

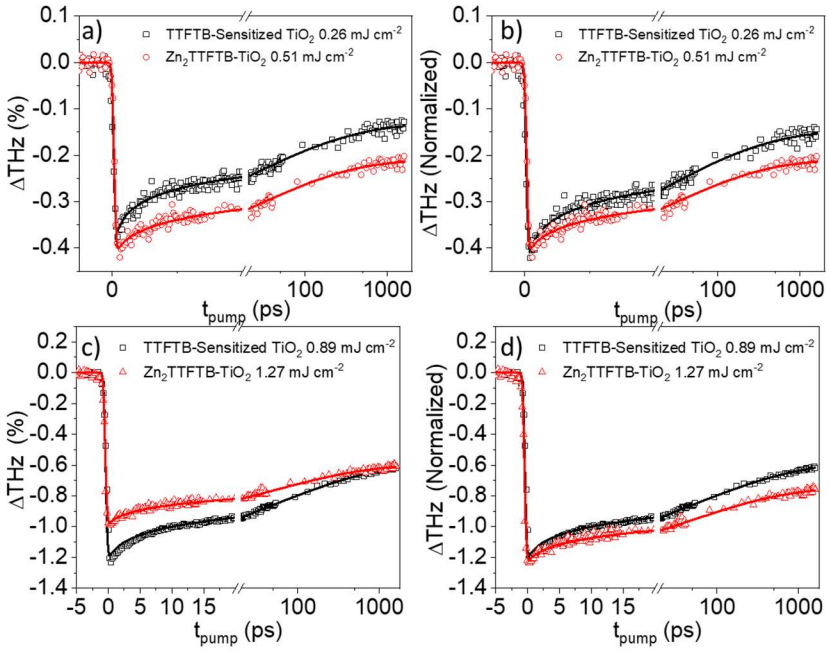
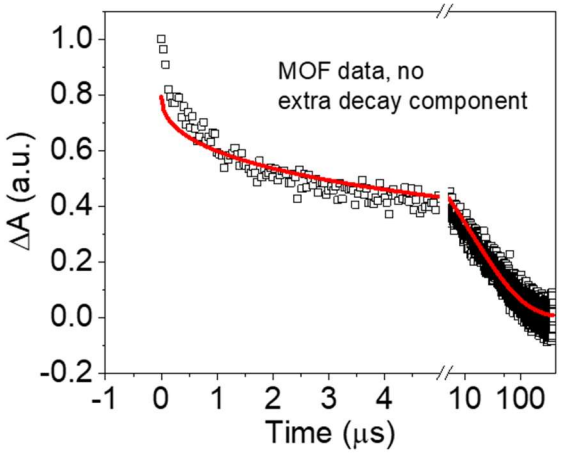


Figure S17. OPTP comparisons of TTFTB-Sensitized TiO_2 to Zn_2TTFTB-TiO_2 at similar ΔTHz attenuation magnitudes. Unnormalized (a) and normalized (b) comparisons at 0.26 mJ cm^{-2} and 0.51 mJ $cm^{-2,}$ respectively. Unnormalized (c) and normalized (d) comparisons at 0.89 mJ cm^{-2} and 1.27 mJ cm^{-2}, respectively.



Sample	$A_{stretch}$	$\tau_{stretch}$ (μs)	β
Zn_2TTFTB-TiO_2	0.79	14.4	0.48

Figure S18. Fitting of Zn_2TTFTB-TiO2 ns-TA data with a single stretched exponential.

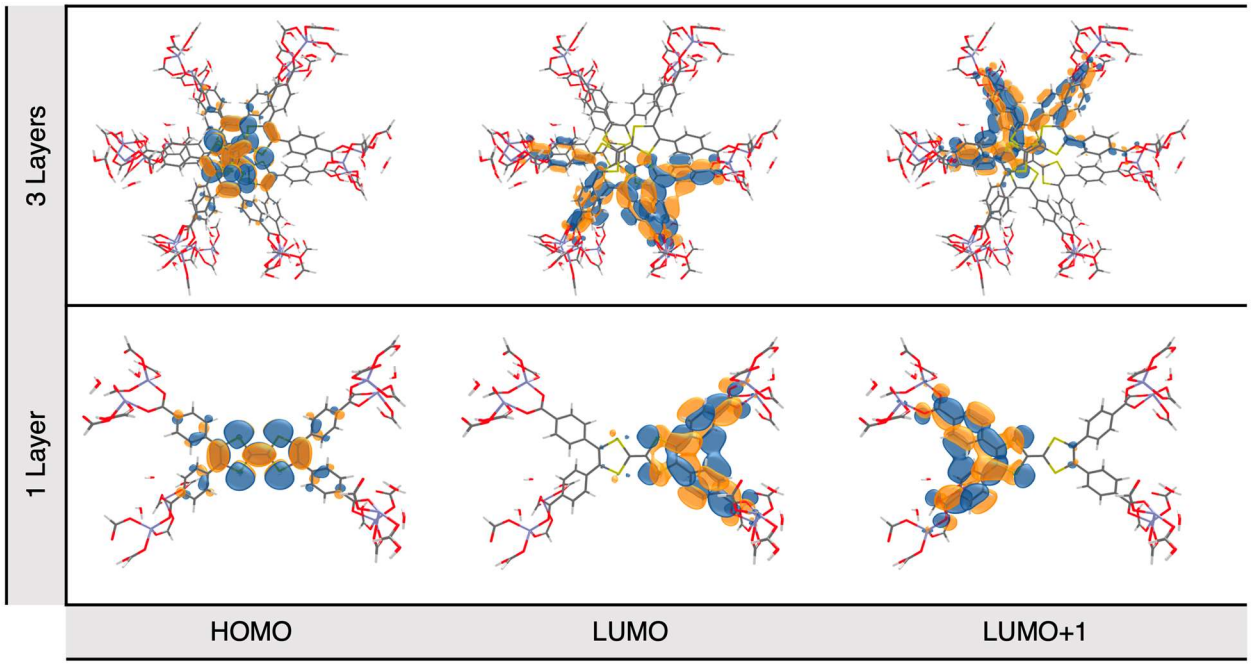


Figure S19. Molecular orbitals on 1 and 3 Layer MOF.

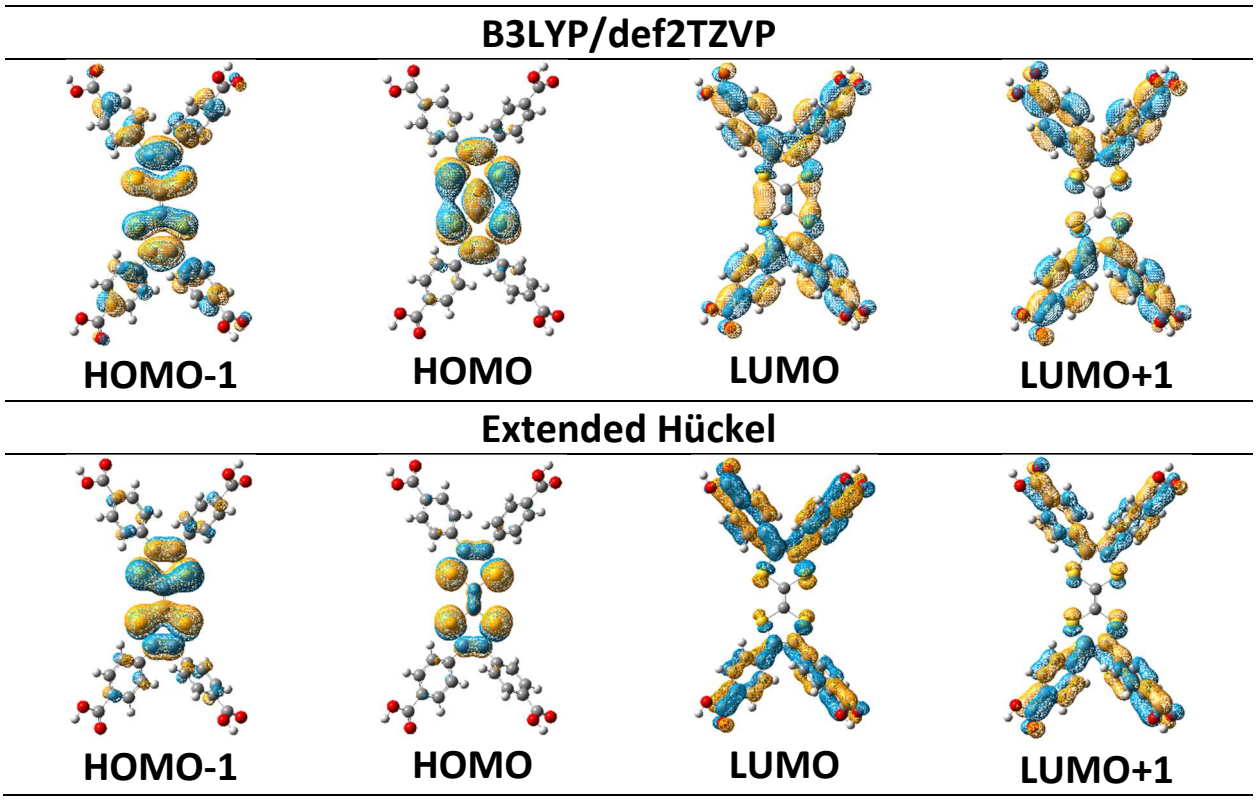


Figure S20. Comparison of the molecular orbital topologies at the DFT (B3LYP/def2TZVP) and Extended Hückel (EH) levels for the H_4TTFTB ligand. The parameters of the EH Hamiltonian were optimized to closely reproduce the symmetries and HOMO-LUMO gap of the DFT orbitals. The HOMO-LUMO gap at the DFT and EH levels are 2.56 and 3.15 eV, respectively.

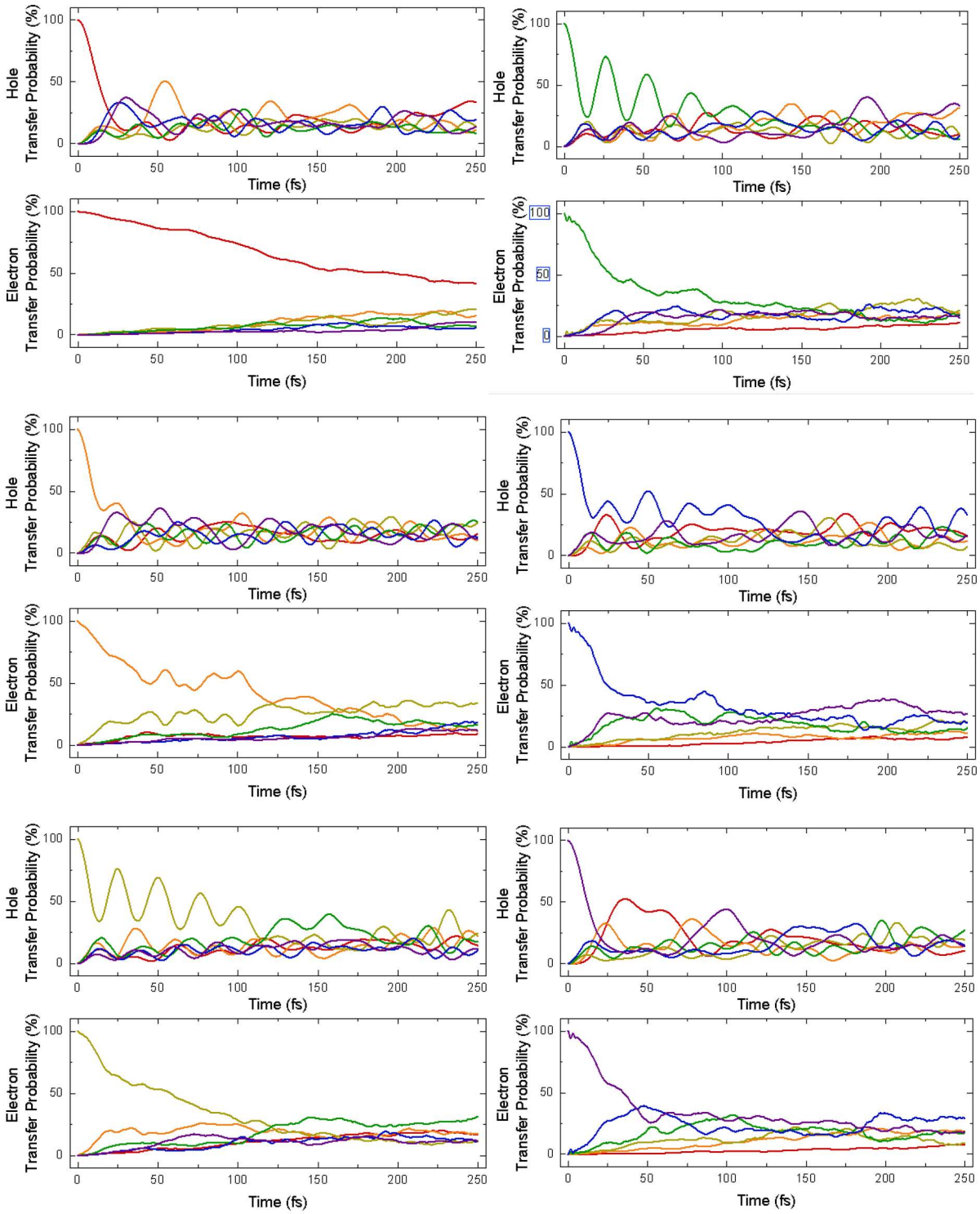


Figure S21. Inter-layer charge dynamics simulations with the hole and electron wavepackets initiated in the HOMO or LUMO, respectively, of each H_4TTFTB layer of a six-layer columnar stack. The left-hand column of the figure depicts the post-photoexcitation charge dynamics for wavepackets initialed on layers 1, 2 and 3, whereas the right-hand column shows the dynamics after initialization on layers 4, 5 and 6. Layers 1-6 are respectively indicated with red, orange, yellow, green, blue, and purple curves.

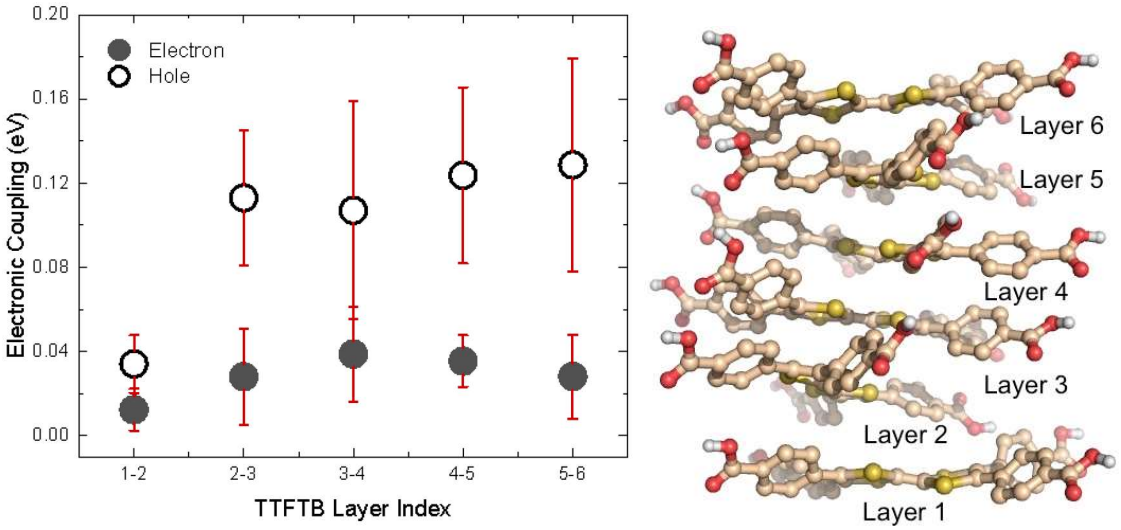


Figure S22. Inter-layer coupling constants averaged over ten 1-ps separated frames for a six-layer H_4TTFTB stack from a molecular dynamics trajectory at the GNF2-XTB level of theory. The LUMO-LUMO and HOMO-HOMO couplings for electron and hole transfer, respectively, were computed at the B3LYP/TZ2P level in the ADF program suite on the geometries from the GNF2-XTB trajectory.

Table S1. Benchmarking data for selection of basis set and functional for calculations of energies and UV-Visible spectra which were also compared to experiment. Triple zeta would be preferential for energetics, while double zeta would be appropriate for frequency and geometry. Dispersion corrected functionals like B3 with dispersion and Wb97xd would be preferred due to the electron transfer interest of the studies. Abbreviations Pseudo = [H,C](6-31g);[O,S](6-31g(d)) , Def = Def2TZV , CAM = CAMB3LYP, Wb = Wb97xd, B3 = B3LYP, B3/Disp = B3LYP with gdb3j dispersion.

Cation H_4TTFTB			
Basis Set	**Functional**	**E (Hartree)**	**G (Hartree)**
Pseudo	CAM	-3500.7313	-3500.3363
Pseudo	Wb	-3501.018	-3500.6229
Pseudo	B3	-3501.6969	-3501.3102
Pseudo	B3/Disp	-3501.887	-3501.4986
Def	CAM	-3499.3413	-3498.9504
Def	Wb	-3499.7839	-3499.3943
Def	B3	-3500.2896	-3499.9063
Anion H_4TTFTB			
Basis Set	**Functional**	**E (Hartree)**	**G (Hartree)**
Pseudo	CAM	-3500.9988	-3500.6082
Pseudo	Wb	-3501.286	-3500.8951
Pseudo	B3	-3501.9671	-3501.5853
Pseudo	B3/Disp	-3502.1574	-3501.7741
Def	CAM	-3499.6153	-3499.2286
Def	Wb	-3499.8823	-3499.4954
Def	B3	-3500.5663	-3500.1875
Neutral H_4TTFTB			
Basis Set	**Functional**	**E (Hartree)**	**G (Hartree)**
Pseudo	CAM	-3500.907	-3500.5132
Pseudo	Wb	-3501.1949	-3500.802
Pseudo	B3	-3501.8678	-3501.4829
Pseudo	B3/Disp	-3502.0579	-3501.6724
Def	CAM	-3499.5173	-3499.1287
Def	Wb	-3499.7839	-3499.3943
Def	B3	-3500.4615	-3500.0813

Calculation Optimized Coordinates:

All of these optimizations were performed with the following route card.

#p opt/freq wb97xd scrf=(solvent=n,n-dimethylformamide) def2TZV int=ultrafine

Frequency calculations could not be performed on the 3Layer structures. Initial optimization was performed with DFTB+.

2Ligand_Stacked

C	2.95339100	-1.85559300	1.44113200
C	2.16450800	-2.95848600	1.48677600
C	7.14347700	-1.75316100	0.32430300
C	6.21002200	-2.45260500	-0.46647400
C	4.86008700	-2.49442800	-0.10380100
C	4.40775900	-1.82801200	1.05790200
C	5.34216000	-1.10354700	1.83031700
C	6.69509000	-1.07200700	1.47303200
C	8.61325000	-1.70910400	-0.14629000
C	7.13513200	1.79707500	-0.33754700
C	3.45888100	-7.04040000	0.81001100
C	6.69067400	1.11513100	-1.48734500
C	2.25431200	-6.57122800	0.25035500
C	5.33781800	1.14070900	-1.84543600
C	1.83655000	-5.25467400	0.46989600
C	4.39958000	1.85983100	-1.07269000
C	2.61712800	-4.37255000	1.25187500
C	4.84797500	2.52688500	0.09013100
C	3.81911400	-4.85413700	1.82065800
C	6.19789200	2.49103800	0.45355800
C	4.23751100	-6.17065300	1.59964300

C	8.60487300	1.75960800	0.13386800
C	3.87815000	-8.48746000	0.54367300
H	7.39185700	0.53300400	-2.09867300
H	1.64922600	-7.25143100	-0.36194600
H	5.00446700	0.59789500	-2.73771600
H	0.90051000	-4.90017300	0.02400600
H	4.42533300	-4.18735100	2.44379700
H	6.53825300	3.00022300	1.36365300
H	5.17117500	-6.53322500	2.04530100
H	6.55332900	-2.96133800	-1.37571300
H	4.14255700	-3.04164900	-0.72564700
H	5.00571500	-0.56119400	2.72170500
H	7.39313300	-0.48583200	2.08406600
O	9.60414000	-1.63168300	0.85934200
O	8.96411900	-1.73480600	-1.34422700
O	8.95480200	1.78549400	1.33208000
O	5.10911700	-8.79327900	1.16376900
O	9.59670300	1.68834100	-0.87122800
O	3.24267700	-9.32623900	-0.13172800
S	2.20637600	0.30770400	-1.83458000
S	0.44657700	-2.72656100	1.90397000
C	-3.30424700	-6.04413700	-1.13161200
C	-3.91264600	-5.26865100	-2.13887500
C	-1.94127600	-4.12745300	-0.50312800
C	-2.55125600	-3.34456800	-1.50926600
C	-3.53957700	-3.93399200	-2.32926200
C	-2.31451500	-5.46267500	-0.31462300

C	-3.74186200	-7.50025700	-0.96124000
H	-4.67944600	-5.72801400	-2.77494300
H	-1.17925800	-3.67449100	0.14614100
H	-1.83951400	-6.06126500	0.47159200
O	-4.61204300	-8.09230800	-1.63635700
O	-3.03259400	-8.13617200	0.08098700
C	-0.53701600	-0.13727500	1.91382400
C	0.54656600	-0.94134200	1.89368800
C	2.15196900	2.98092200	-1.50301200
C	2.94543100	1.88132900	-1.45743300
C	3.43526700	7.06688000	-0.80078000
C	4.20766500	6.20295300	-1.60339500
C	3.79876400	4.88535100	-1.83173200
C	2.59979400	4.39564200	-1.26376400
C	1.81636800	5.27386500	-0.48175500
C	2.22860000	6.59134600	-0.25011600
C	3.93388900	8.51535700	-0.60321000
H	4.12751900	3.06968600	0.71245500
H	5.13581900	6.57834700	-2.05189500
H	4.40811500	4.22556300	-2.45943400
H	0.87617300	4.91893100	-0.04493100
H	1.58820800	7.24879800	0.35157000
O	3.57841000	9.15610100	0.60633100
O	4.62792400	9.13418500	-1.43617300
S	2.20727500	-0.28433000	1.81528600
C	-0.53718400	0.14951500	-1.93832100
C	0.54298500	0.95814200	-1.91548700

C	-2.12998900	-1.91338600	-1.70291300
C	-2.96117900	0.84435000	1.76703300
C	-2.95730500	-0.84326600	-1.79988200
C	-2.13797400	1.91796600	1.67288100
C	-7.28354700	0.96542100	1.47762500
C	-6.48961700	1.69418500	0.56995200
C	-5.26240100	0.14131900	2.55421300
C	-4.45992600	0.88363900	1.65827200
C	-5.09499900	1.65157300	0.65513900
C	-6.65819700	0.18323800	2.46775500
C	-8.80491000	1.03509700	1.34247300
C	-7.28005100	-0.98799500	-1.52601600
C	-3.34397000	6.04291900	1.09530600
C	-6.48695000	-1.70533100	-0.60834500
C	-3.94269700	5.26435300	2.10659600
C	-5.09192200	-1.65315300	-0.69177200
C	-3.55524400	3.93272200	2.29741800
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C	-2.56586200	3.34669400	1.47753700
C	-5.25864900	-0.15839200	-2.60308700
C	-1.95859600	4.13437800	0.47375900
C	-6.65369000	-0.21142500	-2.51976200
C	-2.34166800	5.46687500	0.28951600
C	-8.80782600	-1.01532800	-1.47185000
C	-3.70920600	7.52422300	0.85561700
H	-6.98084200	2.28716100	-0.21126800
H	-4.78464600	-0.46768800	3.33045200

H	-4.01298100	-3.33868100	-3.11822000
H	-4.48610300	2.20957800	-0.06428000
H	-7.27108400	-0.39239800	3.17105600
H	-6.96910400	-2.29774200	0.17776900
H	-4.70036000	5.69765500	2.77171900
H	-4.48196500	-2.20303500	0.03304700
H	-4.01978600	3.33863700	3.09270500
H	-4.78191100	0.44734600	-3.38245800
H	-1.19201700	3.68810100	-0.17510800
H	-7.27513500	0.35053800	-3.22789700
H	-1.86657800	6.07516700	-0.49028700
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O	-9.45076000	0.26248400	2.33207700
O	-9.58469900	-0.45276600	-2.27391500
O	-2.90806200	8.38115800	0.42879800
O	-9.27505400	-1.76893300	-0.37239100
O	-5.04141100	7.90759600	1.13609500
S	-0.38043800	-1.62752800	-1.83773200
S	-2.21129100	-0.75243000	2.01481600
S	-2.21370800	0.75718800	-2.04431000
S	-0.38773800	1.64057900	1.81386600
S	0.43595200	2.74318600	-1.92465700
H	3.09626900	8.43879700	1.14167200
H	-5.50875400	7.03869300	1.38176000
H	-10.43545200	0.40365700	2.10634000
H	-10.28714400	-1.69129400	-0.47313300
H	-3.42856100	-9.07617300	0.06907900

H	5.24735400	-9.76854200	0.89875900
H	9.07893700	1.75721200	-1.74359000
H	9.08613500	-1.70171000	1.73146900

H_4TTFTB

C	6.64969100	-3.33177800	0.40160100
C	5.55244300	-3.67353400	-0.40828800
C	4.46393200	-2.81511900	-0.53783500
C	4.43860800	-1.57238300	0.12379500
C	5.53197500	-1.23596400	0.94780600
C	6.61228700	-2.09962700	1.08028900
C	7.86009200	-4.21229100	0.60875800
H	5.53270600	-4.62451800	-0.94274400
H	3.62708600	-3.10493800	-1.17033800
H	7.45072000	-1.83888600	1.72297200
O	8.75132000	-3.91342500	1.38951100
O	7.92356000	-5.36393400	-0.11633800
S	1.66338600	-1.49065500	-0.00309200
C	-6.64223600	-3.32274100	-0.40483000
C	-6.61171400	-2.09217000	-1.08466400
C	-4.46069300	-2.81568800	0.53523500
C	-4.43586400	-1.57295200	-0.12786900
C	-5.52822400	-1.23187700	-0.95201900
C	-5.54927800	-3.67272400	0.40610600
C	-7.81982000	-4.22203800	-0.57122000
H	-7.45033600	-1.82696200	-1.72504900
H	-3.62283600	-3.10202500	1.16847400
H	-5.55569700	-4.62456000	0.93286600

O	-8.79167600	-3.96949800	-1.27862200
O	-7.76164100	-5.38976300	0.13105700
C	3.26226100	0.68524000	-0.00870000
C	3.26226000	-0.68524400	0.00857800
C	6.64971000	3.33177900	-0.40153000
C	6.61233600	2.09963800	-1.08023800
C	5.53201700	1.23597400	-0.94781900
C	4.43861700	1.57237900	-0.12384600
C	4.46391800	2.81509700	0.53781800
C	5.55243500	3.67351600	0.40832900
C	7.86013200	4.21228200	-0.60861600
H	5.52190100	-0.29821100	1.49898500
H	7.45080000	1.83890600	-1.72288500
H	5.52196500	0.29823000	-1.49901300
H	3.62705200	3.10489800	1.17030200
H	5.53268300	4.62447900	0.94282200
O	7.92343300	5.36406900	0.11626500
O	8.75155000	3.91325400	-1.38909100
C	-0.67763600	0.00000400	-0.00007000
C	0.68004700	0.00000200	-0.00009400
C	-3.25977800	-0.68504900	-0.01134000
C	-3.25977700	0.68505600	0.01127200
C	-6.64222200	3.32274400	0.40489400
C	-6.61166700	2.09217700	1.08473400
C	-5.52818200	1.23188500	0.95204600
C	-4.43586000	1.57295900	0.12784500
C	-4.46072000	2.81569100	-0.53526500

C	-5.54930100	3.67272400	-0.40609300
C	-7.81979900	4.22204300	0.57133400
H	-5.51529200	-0.29300100	-1.50112600
H	-7.45026100	1.82697100	1.72515800
H	-5.51522500	0.29301100	1.50115400
H	-3.62289100	3.10202500	-1.16854300
H	-5.55574600	4.62455700	-0.93285900
O	-7.76167300	5.38974200	-0.13099000
O	-8.79162300	3.96950300	1.27877900
S	-1.65956200	-1.49000600	-0.00196700
S	-1.65956200	1.49001300	0.00186800
S	1.66339100	1.49065700	0.00286900
H	7.15959900	5.46654100	0.70096900
H	7.15988000	-5.46626700	-0.70126800
H	-8.57223100	-5.89556100	-0.04700000
H	-8.57226200	5.89553400	0.04709100

H_4TTFTB Cation

C	6.64969100	-3.33177800	0.40160100
C	5.55244300	-3.67353400	-0.40828800
C	4.46393200	-2.81511900	-0.53783500
C	4.43860800	-1.57238300	0.12379500
C	5.53197500	-1.23596400	0.94780600
C	6.61228700	-2.09962700	1.08028900
C	7.86009200	-4.21229100	0.60875800
H	5.53270600	-4.62451800	-0.94274400
H	3.62708600	-3.10493800	-1.17033800

H	7.45072000	-1.83888600	1.72297200
O	8.75132000	-3.91342500	1.38951100
O	7.92356000	-5.36393400	-0.11633800
S	1.66338600	-1.49065500	-0.00309200
C	-6.64223600	-3.32274100	-0.40483000
C	-6.61171400	-2.09217000	-1.08466400
C	-4.46069300	-2.81568800	0.53523500
C	-4.43586400	-1.57295200	-0.12786900
C	-5.52822400	-1.23187700	-0.95201900
C	-5.54927800	-3.67272400	0.40610600
C	-7.81982000	-4.22203800	-0.57122000
H	-7.45033600	-1.82696200	-1.72504900
H	-3.62283600	-3.10202500	1.16847400
H	-5.55569700	-4.62456000	0.93286600
O	-8.79167600	-3.96949800	-1.27862200
O	-7.76164100	-5.38976300	0.13105700
C	3.26226100	0.68524000	-0.00870000
C	3.26226000	-0.68524400	0.00857800
C	6.64971000	3.33177900	-0.40153000
C	6.61233600	2.09963800	-1.08023800
C	5.53201700	1.23597400	-0.94781900
C	4.43861700	1.57237900	-0.12384600
C	4.46391800	2.81509700	0.53781800
C	5.55243500	3.67351600	0.40832900
C	7.86013200	4.21228200	-0.60861600
H	5.52190100	-0.29821100	1.49898500
H	7.45080000	1.83890600	-1.72288500

H	5.52196500	0.29823000	-1.49901300
H	3.62705200	3.10489800	1.17030200
H	5.53268300	4.62447900	0.94282200
O	7.92343300	5.36406900	0.11626500
O	8.75155000	3.91325400	-1.38909100
C	-0.67763600	0.00000400	-0.00007000
C	0.68004700	0.00000200	-0.00009400
C	-3.25977800	-0.68504900	-0.01134000
C	-3.25977700	0.68505600	0.01127200
C	-6.64222200	3.32274400	0.40489400
C	-6.61166700	2.09217700	1.08473400
C	-5.52818200	1.23188500	0.95204600
C	-4.43586000	1.57295900	0.12784500
C	-4.46072000	2.81569100	-0.53526500
C	-5.54930100	3.67272400	-0.40609300
C	-7.81979900	4.22204300	0.57133400
H	-5.51529200	-0.29300100	-1.50112600
H	-7.45026100	1.82697100	1.72515800
H	-5.51522500	0.29301100	1.50115400
H	-3.62289100	3.10202500	-1.16854300
H	-5.55574600	4.62455700	-0.93285900
O	-7.76167300	5.38974200	-0.13099000
O	-8.79162300	3.96950300	1.27877900
S	-1.65956200	-1.49000600	-0.00196700
S	-1.65956200	1.49001300	0.00186800
S	1.66339100	1.49065700	0.00286900
H	7.15959900	5.46654100	0.70096900

H	7.15988000	-5.46626700	-0.70126800
H	-8.57223100	-5.89556100	-0.04700000
H	-8.57226200	5.89553400	0.04709100

1 Layer Zn_2TTFTB

C	7.80002100	6.12376600	3.46471300
C	12.25272400	2.28117300	-3.57949000
C	11.13310300	4.29878300	0.28922200
C	10.51345100	8.06818200	1.24287400
C	9.15314100	4.61209700	-5.18914300
C	6.78369700	3.07936700	-1.07097400
C	5.75736600	3.47570700	-0.19699800
C	4.66660400	2.64451600	0.03849200
C	4.57859700	1.38129600	-0.57847400
C	5.60653300	0.98835300	-1.45967800
C	6.69042800	1.82554800	-1.69948300
C	7.95268900	3.98401200	-1.33909000
H	5.82432500	4.44396000	0.29475500
H	3.87953000	2.96504700	0.71811700
H	7.47562700	1.51914700	-2.38738600
H	9.96645000	7.00869500	-1.51556500
H	8.70368200	6.41729400	-2.12825900
H	12.20728500	5.94824100	-4.25473100
H	12.17198200	6.86896400	-3.00992300
O	8.96825400	6.47089200	3.76821100
O	11.90897700	2.95355800	-2.59238700

O	7.41810000	5.79021300	2.27442400
O	11.88207100	2.50811200	-4.81153800
O	10.26919600	4.30187900	1.23040300
O	11.13831500	5.16396100	-0.64782100
O	9.71338000	7.45109300	0.49853500
O	8.90110200	4.13519400	-6.29147000
O	10.67073000	7.86697200	2.50728000
O	10.34330600	4.61376000	-4.61660600
O	8.87193600	3.57367000	-2.12155600
O	7.95669800	5.16978200	-0.80846900
O	9.60147900	6.70713600	-2.36221800
O	12.35107400	5.97160500	-3.30294900
S	1.79597400	1.33667600	-0.30258800
Zn	8.81373800	5.61624400	0.94209000
Zn	10.58107600	4.67655000	-2.58280100
C	-9.54114300	7.46685300	-3.48665800
C	-6.52719200	3.22998600	0.27842100
C	-6.46592700	2.05059400	1.03932600
C	-4.37282100	2.67155500	-0.69699700
C	-4.32201300	1.47556500	0.04540200
C	-5.38251000	1.18566200	0.92802600
C	-5.46323400	3.52924900	-0.58763400
C	-7.71518900	4.15295900	0.39477300
C	-8.82921400	3.72436600	5.35034100
C	-10.10098700	8.90003000	0.21416100
C	-11.68461900	5.59871800	0.07405300
C	-12.17964100	3.06163200	3.47949300

H	-11.57956200	5.31606100	4.40127900
H	-11.66643800	6.48515000	3.37866000
H	-8.76669300	7.09804300	1.91075900
H	-8.96487300	6.93445800	3.45350900
H	-7.28020400	1.82391600	1.72450700
H	-3.55761200	2.91588800	-1.37542800
H	-5.49970000	4.44475800	-1.17434700
O	-8.67040000	3.80191100	1.16020500
O	-7.69035900	5.22436600	-0.31748200
O	-9.94929100	3.49043200	5.98968500
O	-9.11832300	8.06455500	0.40324300
O	-8.72865200	4.06418500	4.16625900
O	-10.95553800	8.79783600	-0.69014400
O	-10.97578200	5.62196100	-0.98994200
O	-11.25516400	5.94105000	1.22221600
O	-11.36267600	3.25751400	2.51682000
O	-10.62876900	8.10441800	-3.17074300
O	-12.16595700	3.65739400	4.59931900
O	-8.75372800	6.93616200	-2.68001000
O	-11.05965100	6.03747100	3.98240800
O	-8.64241200	6.48886400	2.66339700
Zn	-9.18539100	6.42449900	-0.70613000
Zn	-9.96722300	4.73015600	2.42597800
C	3.39463800	-0.85197700	-0.26255400
C	3.40152400	0.51234300	-0.35549900
C	9.31904800	-7.45223400	2.40000600
C	9.20646700	-5.25665500	5.81510600

C	11.46950500	-4.21218900	-1.37884000
C	6.80880000	-3.45611000	0.05377600
C	6.79648200	-2.21015900	0.70427500
C	5.69840400	-1.36365000	0.59626900
C	4.57513400	-1.73910000	-0.16810900
C	4.57969900	-2.99878300	-0.79911600
C	5.68503000	-3.83783500	-0.69862100
C	8.00375300	-4.34616000	0.14667400
C	7.17225100	-2.62665900	3.97538300
C	9.58938900	-7.33552200	-2.97494400
H	5.54119400	0.03012200	-1.97006000
H	10.74126300	-2.59218500	4.09895000
H	9.47946900	-1.94650400	3.42436000
H	11.37385400	-5.98665400	2.27308200
H	11.56576500	-4.67217100	1.49078500
H	7.65506700	-1.91445400	1.30312200
H	5.69938400	-0.41038700	1.11961900
H	3.71718900	-3.30741300	-1.38654900
H	5.68635800	-4.80172600	-1.20307600
O	8.89174400	-6.46418200	3.06334400
O	9.97924700	-7.41530500	1.30483600
O	9.44363600	-5.44679000	7.11780000
O	11.52465300	-5.07922600	-0.40916000
O	9.99735400	-4.66369100	5.09422600
O	10.54840400	-4.15481900	-2.22284100
O	8.04832000	-5.42006400	-0.55882700
O	9.01014400	-4.01972900	0.88452500

O	7.52072300	-3.84079900	3.71905900
O	9.50542300	-6.15547000	-3.51853100
O	7.85791900	-1.59089100	3.81292200
O	9.90087200	-7.56293700	-1.79165200
O	10.28393000	-2.49943000	3.25559200
O	11.38015300	-5.02730100	2.37627900
Zn	9.89165200	-6.17370600	-0.22673400
Zn	9.30760000	-4.39627800	2.88640400
C	-10.67192500	-5.75897800	-5.11187800
C	-0.56141800	-0.13559100	-0.13293300
C	0.80165400	-0.14760200	-0.18714800
C	-3.15429700	0.57246900	-0.06009600
C	-3.16593800	-0.79464400	-0.02226600
C	-10.64500000	-8.05261200	2.41983100
C	-7.14141000	-3.54730400	-4.73377500
C	-6.60123600	-3.39085000	-0.13850300
C	-6.57566900	-2.20399900	-0.89088700
C	-5.47140400	-1.35982800	-0.85056700
C	-4.35458600	-1.67567800	-0.04969300
C	-4.37281200	-2.87795500	0.68427600
C	-5.48245500	-3.71637700	0.64676100
C	-7.80215300	-4.28391200	-0.16584300
C	-11.95441000	-5.41788000	1.87086500
C	-8.96108000	-7.54726600	-2.09521900
H	-11.31119100	-4.88361400	-0.96303000
H	-11.19862900	-6.17327600	-1.79218900
H	-10.88478900	-2.62311300	-3.54627600

H	-10.61172400	-2.34309000	-2.03950900
H	-5.34391200	0.28528200	1.53728300
H	-7.43109300	-1.95793300	-1.51612100
H	-5.46194900	-0.45390000	-1.45259100
H	-3.51575700	-3.14291200	1.30027000
H	-5.49193300	-4.63601200	1.22787500
O	-10.82394300	-5.99000700	-6.30825200
O	-10.09738800	-4.68454000	-4.61201400
O	-11.37563200	-8.59413500	1.43880700
O	-7.41006000	-3.77222800	-3.54202400
O	-9.54491300	-7.50906200	2.18260100
O	-7.95420200	-3.72483500	-5.73972800
O	-7.78132500	-5.35419400	0.54564500
O	-8.84268500	-3.94696600	-0.84597900
O	-11.13240000	-5.24453100	0.88150600
O	-11.98156200	-6.38354100	2.66792400
O	-8.52733100	-6.55289700	-2.74543100
O	-9.71363700	-7.50052100	-1.05712100
O	-11.26924300	-5.21171300	-1.87963000
O	-10.19232400	-2.49796700	-2.89022000
S	-1.53595300	1.36577000	-0.16385300
S	-1.55831400	-1.61899700	-0.02615900
S	1.77778600	-1.64819100	-0.15428500
Zn	-9.49338100	-6.32811500	0.54622500
Zn	-9.26403600	-4.61564500	-2.73901800
H	-9.33138600	7.42352100	-4.58636300
H	-10.14169400	9.76687700	0.94368700

H	-12.98093400	2.27569300	3.29663900
H	-12.73337600	-4.59641600	1.98768500
H	-11.05789800	-6.51069400	-4.33564100
H	-8.69146700	-8.57635300	-2.48139900
H	-10.89499900	-8.39173100	3.45899100
H	9.35914000	-8.18296700	-3.66986500
H	9.13464000	-8.48362900	2.83613500
H	8.23141900	-5.68189800	5.45046500
H	11.93228600	3.50511900	0.32914500
H	12.33456500	-3.48264300	-1.42534800
H	12.93534300	1.40087000	-3.45976800
H	11.16014800	8.87248100	0.80626500
H	-12.76077500	5.27434700	-0.03978000
H	6.99904200	6.09159100	4.26072300
H	-6.13230000	-3.15101400	-5.02465200
H	-7.91368400	3.58317300	5.98921700
H	6.11625400	-2.51540300	4.40052600
H	8.32213700	5.11611800	-4.58127200
H	9.98786300	7.20568400	2.94810700
H	11.25883900	3.30706000	-4.87548600
H	-10.76062200	8.23490400	-2.16373000
H	-10.77724200	3.59101300	5.41311800
H	-12.21909200	-8.93597900	1.76807700
H	-8.84952200	-4.09680500	-5.43358300
H	9.81771500	-5.39495200	-2.91051800
H	8.73083200	-5.93194200	7.55620200

1Layer Zn_2TTFTB Cation

C	7.80002100	6.12376600	3.46471300
C	12.25272400	2.28117300	-3.57949000
C	11.13310300	4.29878300	0.28922200
C	10.51345100	8.06818200	1.24287400
C	9.15314100	4.61209700	-5.18914300
C	6.78369700	3.07936700	-1.07097400
C	5.75736600	3.47570700	-0.19699800
C	4.66660400	2.64451600	0.03849200
C	4.57859700	1.38129600	-0.57847400
C	5.60653300	0.98835300	-1.45967800
C	6.69042800	1.82554800	-1.69948300
C	7.95268900	3.98401200	-1.33909000
H	5.82432500	4.44396000	0.29475500
H	3.87953000	2.96504700	0.71811700
H	7.47562700	1.51914700	-2.38738600
H	9.96645000	7.00869500	-1.51556500
H	8.70368200	6.41729400	-2.12825900
H	12.20728500	5.94824100	-4.25473100
H	12.17198200	6.86896400	-3.00992300
O	8.96825400	6.47089200	3.76821100
O	11.90897700	2.95355800	-2.59238700
O	7.41810000	5.79021300	2.27442400
O	11.88207100	2.50811200	-4.81153800
O	10.26919600	4.30187900	1.23040300
O	11.13831500	5.16396100	-0.64782100
O	9.71338000	7.45109300	0.49853500
O	8.90110200	4.13519400	-6.29147000

O	10.67073000	7.86697200	2.50728000
O	10.34330600	4.61376000	-4.61660600
O	8.87193600	3.57367000	-2.12155600
O	7.95669800	5.16978200	-0.80846900
O	9.60147900	6.70713600	-2.36221800
O	12.35107400	5.97160500	-3.30294900
S	1.79597400	1.33667600	-0.30258800
Zn	8.81373800	5.61624400	0.94209000
Zn	10.58107600	4.67655000	-2.58280100
C	-9.54114300	7.46685300	-3.48665800
C	-6.52719200	3.22998600	0.27842100
C	-6.46592700	2.05059400	1.03932600
C	-4.37282100	2.67155500	-0.69699700
C	-4.32201300	1.47556500	0.04540200
C	-5.38251000	1.18566200	0.92802600
C	-5.46323400	3.52924900	-0.58763400
C	-7.71518900	4.15295900	0.39477300
C	-8.82921400	3.72436600	5.35034100
C	-10.10098700	8.90003000	0.21416100
C	-11.68461900	5.59871800	0.07405300
C	-12.17964100	3.06163200	3.47949300
H	-11.57956200	5.31606100	4.40127900
H	-11.66643800	6.48515000	3.37866000
H	-8.76669300	7.09804300	1.91075900
H	-8.96487300	6.93445800	3.45350900
H	-7.28020400	1.82391600	1.72450700
H	-3.55761200	2.91588800	-1.37542800

H	-5.49970000	4.44475800	-1.17434700
O	-8.67040000	3.80191100	1.16020500
O	-7.69035900	5.22436600	-0.31748200
O	-9.94929100	3.49043200	5.98968500
O	-9.11832300	8.06455500	0.40324300
O	-8.72865200	4.06418500	4.16625900
O	-10.95553800	8.79783600	-0.69014400
O	-10.97578200	5.62196100	-0.98994200
O	-11.25516400	5.94105000	1.22221600
O	-11.36267600	3.25751400	2.51682000
O	-10.62876900	8.10441800	-3.17074300
O	-12.16595700	3.65739400	4.59931900
O	-8.75372800	6.93616200	-2.68001000
O	-11.05965100	6.03747100	3.98240800
O	-8.64241200	6.48886400	2.66339700
Zn	-9.18539100	6.42449900	-0.70613000
Zn	-9.96722300	4.73015600	2.42597800
C	3.39463800	-0.85197700	-0.26255400
C	3.40152400	0.51234300	-0.35549900
C	9.31904800	-7.45223400	2.40000600
C	9.20646700	-5.25665500	5.81510600
C	11.46950500	-4.21218900	-1.37884000
C	6.80880000	-3.45611000	0.05377600
C	6.79648200	-2.21015900	0.70427500
C	5.69840400	-1.36365000	0.59626900
C	4.57513400	-1.73910000	-0.16810900
C	4.57969900	-2.99878300	-0.79911600

C	5.68503000	-3.83783500	-0.69862100
C	8.00375300	-4.34616000	0.14667400
C	7.17225100	-2.62665900	3.97538300
C	9.58938900	-7.33552200	-2.97494400
H	5.54119400	0.03012200	-1.97006000
H	10.74126300	-2.59218500	4.09895000
H	9.47946900	-1.94650400	3.42436000
H	11.37385400	-5.98665400	2.27308200
H	11.56576500	-4.67217100	1.49078500
H	7.65506700	-1.91445400	1.30312200
H	5.69938400	-0.41038700	1.11961900
H	3.71718900	-3.30741300	-1.38654900
H	5.68635800	-4.80172600	-1.20307600
O	8.89174400	-6.46418200	3.06334400
O	9.97924700	-7.41530500	1.30483600
O	9.44363600	-5.44679000	7.11780000
O	11.52465300	-5.07922600	-0.40916000
O	9.99735400	-4.66369100	5.09422600
O	10.54840400	-4.15481900	-2.22284100
O	8.04832000	-5.42006400	-0.55882700
O	9.01014400	-4.01972900	0.88452500
O	7.52072300	-3.84079900	3.71905900
O	9.50542300	-6.15547000	-3.51853100
O	7.85791900	-1.59089100	3.81292200
O	9.90087200	-7.56293700	-1.79165200
O	10.28393000	-2.49943000	3.25559200
O	11.38015300	-5.02730100	2.37627900

Zn	9.89165200	-6.17370600	-0.22673400
Zn	9.30760000	-4.39627800	2.88640400
C	-10.67192500	-5.75897800	-5.11187800
C	-0.56141800	-0.13559100	-0.13293300
C	0.80165400	-0.14760200	-0.18714800
C	-3.15429700	0.57246900	-0.06009600
C	-3.16593800	-0.79464400	-0.02226600
C	-10.64500000	-8.05261200	2.41983100
C	-7.14141000	-3.54730400	-4.73377500
C	-6.60123600	-3.39085000	-0.13850300
C	-6.57566900	-2.20399900	-0.89088700
C	-5.47140400	-1.35982800	-0.85056700
C	-4.35458600	-1.67567800	-0.04969300
C	-4.37281200	-2.87795500	0.68427600
C	-5.48245500	-3.71637700	0.64676100
C	-7.80215300	-4.28391200	-0.16584300
C	-11.95441000	-5.41788000	1.87086500
C	-8.96108000	-7.54726600	-2.09521900
H	-11.31119100	-4.88361400	-0.96303000
H	-11.19862900	-6.17327600	-1.79218900
H	-10.88478900	-2.62311300	-3.54627600
H	-10.61172400	-2.34309000	-2.03950900
H	-5.34391200	0.28528200	1.53728300
H	-7.43109300	-1.95793300	-1.51612100
H	-5.46194900	-0.45390000	-1.45259100
H	-3.51575700	-3.14291200	1.30027000
H	-5.49193300	-4.63601200	1.22787500

O	-10.82394300	-5.99000700	-6.30825200
O	-10.09738800	-4.68454000	-4.61201400
O	-11.37563200	-8.59413500	1.43880700
O	-7.41006000	-3.77222800	-3.54202400
O	-9.54491300	-7.50906200	2.18260100
O	-7.95420200	-3.72483500	-5.73972800
O	-7.78132500	-5.35419400	0.54564500
O	-8.84268500	-3.94696600	-0.84597900
O	-11.13240000	-5.24453100	0.88150600
O	-11.98156200	-6.38354100	2.66792400
O	-8.52733100	-6.55289700	-2.74543100
O	-9.71363700	-7.50052100	-1.05712100
O	-11.26924300	-5.21171300	-1.87963000
O	-10.19232400	-2.49796700	-2.89022000
S	-1.53595300	1.36577000	-0.16385300
S	-1.55831400	-1.61899700	-0.02615900
S	1.77778600	-1.64819100	-0.15428500
Zn	-9.49338100	-6.32811500	0.54622500
Zn	-9.26403600	-4.61564500	-2.73901800
H	-9.33138600	7.42352100	-4.58636300
H	-10.14169400	9.76687700	0.94368700
H	-12.98093400	2.27569300	3.29663900
H	-12.73337600	-4.59641600	1.98768500
H	-11.05789800	-6.51069400	-4.33564100
H	-8.69146700	-8.57635300	-2.48139900
H	-10.89499900	-8.39173100	3.45899100
H	9.35914000	-8.18296700	-3.66986500

H	9.13464000	-8.48362900	2.83613500
H	8.23141900	-5.68189800	5.45046500
H	11.93228600	3.50511900	0.32914500
H	12.33456500	-3.48264300	-1.42534800
H	12.93534300	1.40087000	-3.45976800
H	11.16014800	8.87248100	0.80626500
H	-12.76077500	5.27434700	-0.03978000
H	6.99904200	6.09159100	4.26072300
H	-6.13230000	-3.15101400	-5.02465200
H	-7.91368400	3.58317300	5.98921700
H	6.11625400	-2.51540300	4.40052600
H	8.32213700	5.11611800	-4.58127200
H	9.98786300	7.20568400	2.94810700
H	11.25883900	3.30706000	-4.87548600
H	-10.76062200	8.23490400	-2.16373000
H	-10.77724200	3.59101300	5.41311800
H	-12.21909200	-8.93597900	1.76807700
H	-8.84952200	-4.09680500	-5.43358300
H	9.81771500	-5.39495200	-2.91051800
H	8.73083200	-5.93194200	7.55620200

3 Layer Zn_2TTFTB

C	-5.15639400	9.93510000	-6.49568800
C	6.32995300	11.73149300	-6.17014700
C	0.53158200	4.42767100	-3.21700100
C	-0.81990700	4.27446600	-3.13091400

C	-7.00566100	5.47436200	2.35134100
C	-7.70421100	4.59194400	3.19337900
C	-5.20165800	3.85278500	2.21947500
C	-5.90204900	2.96246900	3.05779900
C	-7.16513500	3.35635400	3.54199800
C	-5.74775500	5.08132400	1.86636000
C	2.41943600	8.27506900	6.25660900
C	-7.55693100	6.83360100	2.00734600
C	7.30813600	10.47519100	-0.95556800
C	-5.59441900	13.24988100	-4.46959400
C	-10.13856300	8.23072200	5.51065300
C	5.58060800	9.64780800	2.86903600
C	-6.54002600	11.28092200	-0.69984200
C	3.42610800	12.91932000	-3.72248100
C	2.90604600	8.00652800	-2.82801200
C	1.78986500	7.80254200	-1.99750900
C	1.00711400	6.65788500	-2.12024100
C	1.31837500	5.67423200	-3.08047300
C	2.44593000	5.87632400	-3.90134700
C	3.21810800	7.02550500	-3.78480400
C	2.64883700	11.79413900	4.66982500
C	-9.78396200	8.99027700	-0.18528100
C	3.74810800	9.23242000	-2.71308300
C	2.80979400	6.09416500	1.02202900
C	-3.90126600	7.24157000	-2.57424900
C	1.74109000	5.55027700	1.75346200
C	-3.97008000	5.99215600	-1.93687300

C	1.41007900	4.20589900	1.63420000
C	-2.96719500	5.04629600	-2.11551400
C	2.15549400	3.34974200	0.79991200
C	-1.84734100	5.32119600	-2.92604200
C	3.23204700	3.89352200	0.07239100
C	-1.77610400	6.57764000	-3.56045200
C	3.54861200	5.24564600	0.17931900
C	-2.78734800	7.51846600	-3.38603600
C	-12.24533300	9.13634500	3.51794300
C	3.12359700	7.55947800	1.14320200
C	-5.02866200	8.22961200	-2.42686200
H	1.16715600	6.20080900	2.41038500
H	-4.82942500	5.76829100	-1.30691700
H	0.57315400	3.80372600	2.20165200
H	-3.04319100	4.08089000	-1.61893800
H	-0.93423700	6.80598700	-4.21046900
H	4.37263300	5.66060800	-0.39792500
H	-2.72959200	8.48089800	-3.89146400
H	-9.11998500	11.06215000	4.42209200
H	2.49049100	11.13737000	1.75669200
H	-8.59082400	9.06821900	-2.90772200
H	2.82186100	10.46503600	-5.92889200
H	-10.62857100	10.77711500	4.20035700
H	1.94453200	9.92786600	0.99494400
H	-7.39758200	8.16477800	-3.21975500
H	3.84830900	9.43187100	-5.43702600
H	4.99891400	8.81788000	5.91479900

H	-6.80893500	9.13977400	2.60327000
H	4.52446200	12.52144900	-1.09672500
H	-7.60202700	12.13341400	-5.26505800
H	4.24104000	10.09443200	6.32103600
H	-7.24188500	10.51696000	2.10243000
H	3.63820400	12.61459000	0.17611200
H	-8.27433900	10.73870300	-5.46537300
H	-8.67563800	4.89223800	3.58229300
H	-4.22280300	3.56893800	1.83781800
H	-5.19882000	5.75908700	1.21482200
H	1.54460100	8.55386300	-1.24867100
H	0.15708400	6.51310400	-1.45690100
H	2.70555200	5.12803300	-4.64720900
H	4.07820900	7.17251900	-4.43459400
O	-4.72395800	11.12447600	-6.84699400
O	-6.06213600	9.72778200	-5.67900200
O	1.77968500	9.41261100	6.53193000
O	-8.68613600	7.16918400	2.49893800
O	6.45728100	9.88026800	-0.23398000
O	-5.57326000	12.41476800	-3.49881600
O	2.58010500	7.87352800	5.09684300
O	-6.81450600	7.60320700	1.27985100
O	7.09509300	11.12995200	-2.02958000
O	-6.06757800	13.01829800	-5.62428100
O	-10.43453900	8.48301000	6.79125600
O	5.13307500	8.91591400	3.81730900
O	-6.26135200	10.59240700	0.33428800

O	4.44924800	12.78610800	-2.93460600
O	-9.15702100	8.73560400	4.96334900
O	4.78704000	10.37580000	2.18070100
O	-7.27228000	10.78165900	-1.62984200
O	3.24544200	12.25263100	-4.76865600
O	2.21327700	10.96934900	3.74899800
O	-9.13167100	8.38181400	-1.09443800
O	4.66427800	9.42879500	-3.60780800
O	3.54417400	11.54726900	5.49269800
O	-9.16109300	9.65203200	0.72237300
O	3.54987800	10.10130900	-1.78928200
O	-11.42433400	8.81422600	2.58124100
O	4.00483000	8.06790200	0.37817800
O	-4.94534000	9.33575100	-3.05974200
O	5.13419100	12.06600700	-6.56322200
O	-11.92461900	9.54584100	4.66879100
O	2.42221600	8.24734200	1.99505300
O	-6.04327000	7.86473500	-1.71388500
O	6.65337900	11.43841600	-5.00694700
O	-9.80651400	11.05146800	3.74593900
O	2.35803500	10.79435400	0.85715300
O	-7.93445300	8.87789100	-3.59537900
O	3.27903500	9.65588200	-6.18556600
O	4.47258600	9.19375700	6.63720300
O	-7.33528900	9.91334200	2.85542200
O	4.49934500	12.32663900	-0.14259700
O	-8.12114300	11.43361700	-4.81628500

S	-0.02753500	1.65365300	0.49692200
S	-1.47002000	2.59392000	-3.34022000
Zn	3.11100000	9.25113300	3.56487100
Zn	-7.19627300	8.79772000	-0.32200600
Zn	5.55901200	11.16562300	-3.23690200
Zn	-9.42049000	9.10102400	2.73397500
Zn	4.43966500	10.10955700	0.10613200
Zn	-6.49129000	10.60183500	-3.57764900
C	-9.71944300	-1.98348200	-6.27006600
C	-5.27345800	1.67546900	3.43701400
C	-5.86343300	0.45261300	3.55001000
C	-7.80847900	-1.47046300	-0.82354300
C	-7.34027700	-2.32944500	0.18591400
C	-5.51138100	-0.85061000	-1.31104800
C	-5.03793800	-1.72703100	-0.31516600
C	-5.97671000	-2.46433600	0.43227800
C	-6.87229900	-0.73848500	-1.57234400
C	-15.15836000	-1.56479100	5.73334600
C	-9.27809200	-1.32417300	-1.10028300
C	-10.00481700	-0.57144000	2.92027900
C	-9.35012200	0.31036200	2.04254300
C	-8.01418000	0.64969100	2.23551900
C	-7.28486100	0.11131100	3.31426500
C	-7.93558700	-0.79661000	4.17356300
C	-9.27476500	-1.12045600	3.98802800
C	-11.44866000	-0.89655000	2.74757400
C	-13.02728200	-0.19322100	-4.94607300

C	-14.72609800	1.19051600	3.09000800
C	-12.07569900	-3.26094500	-2.62267100
C	-13.63506600	-3.84142200	1.19274000
H	-14.44403900	-0.27143200	0.62541000
H	-13.87194600	-2.83689600	-4.65053800
H	-14.80789800	-1.72109600	0.24707100
H	-13.53010600	-4.30708600	-4.94420500
H	-12.58794500	-0.94252200	5.63530700
H	-11.09051200	0.50031000	-1.44224700
H	-13.42760000	0.33220500	5.46564500
H	-12.53126500	0.40433800	-1.97427000
H	-8.06101400	-2.89109100	0.77712100
H	-4.79960900	-0.26908500	-1.89350800
H	-7.71536500	2.69768500	4.21059700
H	-7.22747000	-0.07255600	-2.35634100
H	-9.90612600	0.73168000	1.20707300
H	-7.52492200	1.32921300	1.54107000
H	-7.38662400	-1.23184500	5.00617400
H	-9.76971100	-1.80855100	4.67076900
O	-15.86813500	-0.46394600	5.47934100
O	-10.10758900	-1.82272500	-0.27541700
O	-14.75672400	-2.31487200	4.83766100
O	-9.61995100	-0.64314200	-2.15537400
O	-12.07542600	-1.50769700	3.69621600
O	-12.15645100	0.19114100	-4.07053200
O	-12.09856000	-0.52958900	1.69703000
O	-12.99434900	-1.30384400	-5.53771300

O	-14.98464300	0.06013200	2.47775700
O	-11.18753100	-3.25569700	-3.54199000
O	-13.96031200	1.33114600	4.05594100
O	-12.49456700	-2.14535400	-2.14064900
O	-12.62823600	-3.44981100	0.54025100
O	-10.89521500	-2.36237600	-6.69050200
O	-14.43344900	-3.10887400	1.87940800
O	-9.50223200	-1.33606200	-5.23220800
O	-14.34567400	-0.93713900	-0.07615800
O	-14.03460200	-3.74344100	-4.35113600
O	-13.22047700	-0.38032200	6.10910500
O	-12.01696700	0.48334900	-1.15829200
S	-3.50538000	1.77281100	3.82454500
S	-4.79410100	-0.93552200	4.02395600
Zn	-13.99226200	-1.53749200	3.00246900
Zn	-10.85503700	-1.22280400	-3.58874500
Zn	-12.18493100	-1.51494600	-0.14732600
C	9.60250100	3.46205600	-6.83800100
C	12.86744800	2.39587600	-4.88206000
C	0.26318600	0.43599000	-3.67392500
C	0.12611300	1.76918200	-3.52896600
C	2.55340300	0.82626500	0.67885900
C	1.75322800	1.92785100	0.68099300
C	6.89438000	1.20893800	10.22920800
C	10.76849900	-1.58973800	3.11431000
C	12.09366500	5.74080600	-2.72529300
C	9.05512700	-0.53208100	6.88809600

C	11.37312700	3.07397600	0.62562400
C	6.85100200	0.68452300	0.99663800
C	6.10887700	1.57999200	1.78661700
C	4.72162500	1.63635200	1.68822200
C	4.02832200	0.79056400	0.79962900
C	4.77411900	-0.12340400	0.02839600
C	6.16138600	-0.16482900	0.11466800
C	9.77544100	3.77546300	7.51489700
C	8.33837500	0.64802000	1.07010300
C	4.72484700	0.26523700	5.12048500
C	3.72763000	0.88920900	5.88776300
C	2.39697800	0.50198900	5.77219300
C	2.02209700	-0.54190400	4.90421600
C	3.02262100	-1.16562900	4.13359300
C	4.35099000	-0.76430000	4.23948800
C	12.82966000	5.40122600	-8.16705200
C	6.15801900	0.70382600	5.23084900
C	13.12204500	0.67572200	-1.08791000
H	4.00968600	1.68746200	6.57161800
H	1.63540400	0.99977900	6.36942900
H	3.80856800	3.25480300	-0.59357600
H	5.11742700	-1.24342200	3.63333600
H	8.98548500	3.17727100	5.09027600
H	9.52803400	0.83287400	-1.57321900
H	7.50113600	2.73732700	4.90331300
H	10.80483900	0.18570000	-2.08787100
H	11.24791600	2.10790500	3.43328500

H	9.51246500	3.81001200	-4.01774900
H	10.91672000	2.34312800	4.96596000
H	8.88300700	2.57210000	-3.33166400
H	6.63517100	2.23505100	2.47807700
H	4.16501500	2.33055900	2.31395200
H	4.25651400	-0.79115000	-0.65868300
H	6.72679100	-0.86432300	-0.49793600
O	9.81977100	4.26834500	-5.84116700
O	10.48273800	3.02343900	-7.60902900
O	13.28644900	3.29339800	-5.68098800
O	11.70747700	2.49888400	-4.34333800
O	12.41359700	5.84281200	-7.08255400
O	8.19859000	1.05610800	10.44849800
O	9.73938500	-1.18656200	3.73425200
O	11.93249000	4.69291700	-2.03776600
O	6.42898400	1.53393600	9.14931500
O	11.41549300	-0.99295200	2.19530000
O	12.00362100	5.87860800	-3.98994700
O	8.27334100	-0.42533600	7.88168500
O	11.75302500	2.30805600	1.57787800
O	9.34631700	0.51718800	6.19827800
O	10.61247300	2.64547400	-0.30526600
O	10.13974100	3.56083100	6.33737800
O	9.01761600	0.06130700	0.15185900
O	8.81486400	3.16857600	8.14224000
O	8.97790800	1.24606100	2.02418600
O	7.01508000	0.17916300	4.45347300

O	13.06520000	1.72814100	-1.79135800
O	6.42434900	1.64867400	6.08876100
O	12.12223900	0.01569900	-0.63618900
O	8.34245300	2.83219300	4.42950000
O	10.10125700	0.79973900	-2.35809300
O	10.97804100	1.67845100	4.26139300
O	9.31955300	3.41053200	-3.15057300
S	1.51220900	2.92620400	-3.49361600
S	-0.55979200	0.46673000	4.63517400
Zn	11.73299800	4.64027700	-5.47311400
Zn	7.88724000	1.63354300	7.42263400
Zn	10.93389500	0.48816600	0.97547200
Zn	9.02336000	0.72374100	4.05036500
Zn	11.28988800	2.73878200	-2.29978100
C	2.90254900	-6.12879700	-7.69214500
C	-4.71574900	-9.61251500	-8.70190200
C	-2.77737000	-10.58747900	-4.94966600
C	7.87723500	-7.42410200	-5.67877000
C	-3.25848600	0.01003500	4.13583900
C	-1.06002800	-0.92002100	0.31594500
C	-2.05329300	-0.52712100	4.41193700
C	0.04070800	-0.15083300	0.43465900
C	-3.58137100	-1.81905100	-0.05656000
C	-0.16627600	-2.22308000	-3.82617600
C	-2.84259900	-2.94666000	0.13061700
C	1.18928100	-2.10164300	-3.78379800
C	0.06526400	-2.17532700	4.73744300

C	0.59366600	-0.92077600	4.78605300
C	-2.47742300	-5.85982600	-3.90418500
C	-1.49588000	-5.66280400	-2.91793200
C	-1.95588400	-3.66886500	-4.81542200
C	-0.95109400	-3.48340800	-3.84787900
C	-0.73535400	-4.49731900	-2.89484400
C	-2.69244500	-4.84827600	-4.85444600
C	3.46218900	-10.68372600	6.98285600
C	-6.26974400	-11.00315100	3.22659100
C	8.49286300	-8.36815400	-0.44859100
C	-3.29857700	-7.11703000	-3.94287800
C	-4.22016300	-7.03149300	0.07676500
C	4.02829700	-5.34456100	-3.69977200
C	-4.69463600	-6.10823500	-0.87114100
C	2.84503200	-5.45103900	-4.45179800
C	-4.26246700	-4.78530200	-0.85613100
C	1.93658300	-4.39953800	-4.50196700
C	-3.32824800	-4.34503000	0.10239400
C	2.16916000	-3.20763600	-3.78564600
C	-2.83641500	-5.27930800	1.03535400
C	3.37283900	-3.09203800	-3.06029000
C	-3.28737200	-6.59484400	1.03267400
C	4.28131600	-4.14337500	-3.01333700
C	6.52275100	-8.58065700	3.46296400
C	-4.69843800	-8.44277700	0.08236200
C	4.97307800	-6.48923000	-3.58644400
C	2.25420900	-5.88835200	4.81232700

C	2.62791700	-4.82626400	5.65489400
C	1.91600500	-3.63066900	5.65265300
C	0.80795200	-3.45313900	4.80000900
C	0.41185200	-4.53435000	3.98670100
C	1.12771500	-5.72552600	3.98641800
C	3.03924600	-7.15001900	4.75115000
C	-8.24034000	-10.93663700	0.84432400
C	5.19905500	-10.11552700	-1.99421300
C	-1.12748300	-7.73761200	-8.04510800
C	2.04639300	-5.86474200	8.71894800
C	4.90342900	-11.25126200	1.97373300
C	-3.13169500	-11.85054400	-1.11110900
H	2.75100300	-1.95611700	3.43711700
H	5.62430500	-6.11235800	8.96727000
H	3.33123800	-7.94630400	1.88865400
H	-6.66959500	-10.92678700	-1.89199000
H	5.40124400	-10.10246800	-4.99291600
H	4.38406000	-5.33993500	8.41886700
H	3.23800900	-9.39317300	1.42923500
H	-5.53367900	-11.95688000	-2.02676500
H	6.72008600	-9.61029900	-5.59343600
H	6.21039700	-8.75017700	6.31454100
H	5.60768100	-6.46232100	-0.89273800
H	-5.63025700	-8.08739100	-4.42919700
H	2.55158900	-8.38995600	-6.90634500
H	6.65469000	-7.42020200	6.97447000
H	4.22197400	-6.57446800	-0.21044000

H	-6.32759700	-9.46143800	-4.54256900
H	3.36569700	-9.68242900	-7.26829800
H	-1.33323800	-6.43751600	-2.17117600
H	-2.13896000	-2.88982700	-5.55288500
H	-5.63279200	-3.13088400	1.22032300
H	0.02530000	-4.36078700	-2.12872700
H	-3.44956400	-4.99780700	-5.62160300
H	-5.40931500	-6.44113200	-1.62117400
H	2.64264100	-6.36947500	-4.99818800
H	-4.63547500	-4.08797200	-1.60308300
H	1.03990500	-4.49935600	-5.10846100
H	-2.10780100	-4.95983000	1.77918500
H	3.58249800	-2.17543400	-2.51138000
H	-2.91170400	-7.30292800	1.76864600
H	5.20013300	-4.04551300	-2.43796000
H	3.48531000	-4.94498100	6.31312800
H	2.21604300	-2.82841500	6.32219100
H	-0.45043200	-4.42426300	3.33084000
H	0.82336800	-6.54609200	3.33945100
O	4.11006800	-6.24584600	-7.25249900
O	1.98921400	-6.98889900	-7.61804600
O	-5.01534400	-8.95071500	-7.62621700
O	-3.55595200	-9.93522200	-9.04272400
O	-2.17218100	-9.97099200	-5.88752500
O	-3.99085000	-10.31592000	-4.65041200
O	-2.05373100	-7.31613600	-7.31845000
O	3.71258500	-9.72445100	7.77227000

O	-6.87831200	-11.51274800	4.29873700
O	7.62584800	-8.31611300	0.47574400
O	-3.27361700	-7.89538900	-2.93554800
O	3.53185900	-10.70340000	5.71442400
O	-5.58468900	-11.72544000	2.48183200
O	8.30939600	-8.44647100	-1.70317300
O	-4.04890700	-7.32225000	-4.98642900
O	6.23244500	-9.26380900	4.51127400
O	-4.50963100	-9.16987300	1.12750000
O	5.94805400	-6.42181200	-2.74329400
O	5.61201500	-8.12740100	2.70016400
O	-5.34644800	-8.94110600	-0.91855700
O	4.80049500	-7.58153700	-4.25172200
O	2.76044900	-8.02520200	3.85157500
O	-7.25485200	-11.10062200	0.01414900
O	5.89952200	-10.23600600	-3.05014500
O	4.04634300	-7.37270400	5.53647200
O	-8.15216100	-10.67846300	2.06506000
O	5.13342300	-8.98919300	-1.38388900
O	2.30288400	-7.03873300	8.23474100
O	5.61353700	-10.69024900	1.08700400
O	-3.01482000	-10.85056500	-1.87050600
O	6.90943800	-7.11765000	-6.43630400
O	2.87007600	-4.94431000	8.92282700
O	3.98543800	-10.69142200	2.66874600
O	-4.14799900	-12.15134400	-0.38739500
O	7.85415700	-8.26899000	-4.71856500

O	5.19314200	-5.86288600	8.14010800
O	3.37707000	-8.49257000	1.08803100
O	-5.99340800	-11.25519600	-2.50605100
O	5.80788300	-9.84013400	-5.83305000
O	6.23132200	-8.26452900	7.15776700
O	5.16603000	-6.53709000	-0.02757100
O	-6.15337300	-8.74094000	-3.92685500
O	3.16218800	-9.08691800	-6.53866600
S	-2.71104900	-0.23484700	0.04355900
S	-1.13905500	-0.69885900	-3.80499300
S	-1.06180400	-2.72606000	0.40683600
S	1.85810100	-0.41533000	-3.73304300
S	-1.73809100	-2.30022700	4.56925600
S	1.72909900	-0.78680500	0.54623800
Zn	-3.51851200	-8.56337500	-6.46447400
Zn	4.17386300	-9.47051200	4.30824600
Zn	-5.36367200	-10.93778700	0.57278800
Zn	6.79291100	-8.31340400	-2.97942300
Zn	4.09534000	-7.69246800	7.57914400
Zn	5.60593800	-8.63568600	0.63668500
Zn	-4.48473100	-9.58720400	-2.71354400
Zn	4.92987700	-7.84482300	-6.30951600
H	-15.12615600	-1.87786100	6.81526900
H	-15.28471500	2.08572300	2.65884000
H	2.67556300	13.71238300	-3.41603900
H	-13.35045500	9.01966300	3.26125900
H	-6.15885400	12.33177300	-0.78354200

H	-10.75464000	7.41488100	5.03588300
H	-5.14482800	14.27242000	-4.25491400
H	-10.90428000	8.96011500	-0.19489400
H	-4.64011500	9.09127700	-7.03264700
H	-8.87338600	-2.28095000	-6.94297100
H	-13.85769900	0.54216400	-5.17140300
H	-13.88603900	-4.94751400	1.14806900
H	-9.27345900	-11.04074800	0.37413300
H	-5.59973900	-9.89668100	-9.35284600
H	-2.22192700	-11.39635000	-4.39899400
H	-2.26742600	-12.58632800	-1.08152100
H	-6.21314500	-9.87910400	3.19818400
H	5.06409000	-12.36917400	2.12155400
H	4.61488600	-10.99779700	-1.61643800
H	3.13150900	-11.65909300	7.47076100
H	7.60792300	-8.37814800	3.24731800
H	9.58063900	-8.33765200	-0.11254300
H	8.88064700	-6.94067300	-5.91470500
H	13.51155000	1.49993700	-4.67668900
H	14.16132400	0.25351100	-0.88849500
H	11.16820100	-2.61366200	3.41221200
H	0.94775700	-5.69430900	8.98574200
H	6.23888600	1.02423300	11.13209600
H	9.50908600	-1.52057300	6.62396400
H	10.29918400	4.57880600	8.12879300
H	6.68500700	9.65567600	2.66785400
H	11.71535900	4.14548200	0.63503400

H	8.39126200	10.42464100	-0.61897700
H	12.35247500	6.68854200	-2.15224600
H	7.09915300	11.73570900	-6.98536200
H	8.51731500	3.15935300	-6.98402900
H	2.12388400	12.80562900	4.66955200
H	-12.46191700	-4.23439400	-2.23306500
H	2.67411600	-5.12898800	-8.19816800
O	-1.19112000	-8.82980800	-8.75484800
H	-0.17048000	-7.17229600	-8.13530700
O	12.52363400	4.24121500	-8.67671600
H	13.51548600	6.01836800	-8.80624800
H	2.60389100	7.59809000	7.13760800
C	5.85153000	-7.72658700	-9.20950500
O	5.32647000	-8.59239000	-8.51270900
O	6.15943900	-7.95169300	-10.49329900
H	6.11654100	-6.70288400	-8.86384600
C	3.78649400	-8.54663900	10.50152600
O	3.89015700	-8.77129800	11.82148400
O	4.65788000	-7.96795900	9.87289500
H	2.83471400	-8.93238600	10.04200600
H	3.12030900	-9.24153200	12.17071100
H	5.90865700	-8.85707200	-10.74200300
H	-2.10239800	-9.28246500	-8.72037800
H	-7.46097100	-10.86153200	4.71290800
H	-16.02028500	0.06553500	6.27412500
H	-11.66297400	-2.00991400	-6.12134500
H	-5.23962400	11.85982600	-6.37570800

H	-11.29567000	8.11400000	7.03179500
H	1.83036300	9.64549400	7.46932900
H	4.43674800	12.05291900	-5.82216100
H	11.81713800	3.73901900	-8.13661600
H	8.39920800	0.76964200	11.34947600

3Layer Cation Zn_2TTFTB

C	-5.15639400	9.93510000	-6.49568800
C	6.32995300	11.73149300	-6.17014700
C	0.53158200	4.42767100	-3.21700100
C	-0.81990700	4.27446600	-3.13091400
C	-7.00566100	5.47436200	2.35134100
C	-7.70421100	4.59194400	3.19337900
C	-5.20165800	3.85278500	2.21947500
C	-5.90204900	2.96246900	3.05779900
C	-7.16513500	3.35635400	3.54199800
C	-5.74775500	5.08132400	1.86636000
C	2.41943600	8.27506900	6.25660900
C	-7.55693100	6.83360100	2.00734600
C	7.30813600	10.47519100	-0.95556800
C	-5.59441900	13.24988100	-4.46959400
C	-10.13856300	8.23072200	5.51065300
C	5.58060800	9.64780800	2.86903600
C	-6.54002600	11.28092200	-0.69984200
C	3.42610800	12.91932000	-3.72248100
C	2.90604600	8.00652800	-2.82801200
C	1.78986500	7.80254200	-1.99750900

C	1.00711400	6.65788500	-2.12024100
C	1.31837500	5.67423200	-3.08047300
C	2.44593000	5.87632400	-3.90134700
C	3.21810800	7.02550500	-3.78480400
C	2.64883700	11.79413900	4.66982500
C	-9.78396200	8.99027700	-0.18528100
C	3.74810800	9.23242000	-2.71308300
C	2.80979400	6.09416500	1.02202900
C	-3.90126600	7.24157000	-2.57424900
C	1.74109000	5.55027700	1.75346200
C	-3.97008000	5.99215600	-1.93687300
C	1.41007900	4.20589900	1.63420000
C	-2.96719500	5.04629600	-2.11551400
C	2.15549400	3.34974200	0.79991200
C	-1.84734100	5.32119600	-2.92604200
C	3.23204700	3.89352200	0.07239100
C	-1.77610400	6.57764000	-3.56045200
C	3.54861200	5.24564600	0.17931900
C	-2.78734800	7.51846600	-3.38603600
C	-12.24533300	9.13634500	3.51794300
C	3.12359700	7.55947800	1.14320200
C	-5.02866200	8.22961200	-2.42686200
H	1.16715600	6.20080900	2.41038500
H	-4.82942500	5.76829100	-1.30691700
H	0.57315400	3.80372600	2.20165200
H	-3.04319100	4.08089000	-1.61893800
H	-0.93423700	6.80598700	-4.21046900

H	4.37263300	5.66060800	-0.39792500
H	-2.72959200	8.48089800	-3.89146400
H	-9.11998500	11.06215000	4.42209200
H	2.49049100	11.13737000	1.75669200
H	-8.59082400	9.06821900	-2.90772200
H	2.82186100	10.46503600	-5.92889200
H	-10.62857100	10.77711500	4.20035700
H	1.94453200	9.92786600	0.99494400
H	-7.39758200	8.16477800	-3.21975500
H	3.84830900	9.43187100	-5.43702600
H	4.99891400	8.81788000	5.91479900
H	-6.80893500	9.13977400	2.60327000
H	4.52446200	12.52144900	-1.09672500
H	-7.60202700	12.13341400	-5.26505800
H	4.24104000	10.09443200	6.32103600
H	-7.24188500	10.51696000	2.10243000
H	3.63820400	12.61459000	0.17611200
H	-8.27433900	10.73870300	-5.46537300
H	-8.67563800	4.89223800	3.58229300
H	-4.22280300	3.56893800	1.83781800
H	-5.19882000	5.75908700	1.21482200
H	1.54460100	8.55386300	-1.24867100
H	0.15708400	6.51310400	-1.45690100
H	2.70555200	5.12803300	-4.64720900
H	4.07820900	7.17251900	-4.43459400
O	-4.72395800	11.12447600	-6.84699400
O	-6.06213600	9.72778200	-5.67900200

O	1.77968500	9.41261100	6.53193000
O	-8.68613600	7.16918400	2.49893800
O	6.45728100	9.88026800	-0.23398000
O	-5.57326000	12.41476800	-3.49881600
O	2.58010500	7.87352800	5.09684300
O	-6.81450600	7.60320700	1.27985100
O	7.09509300	11.12995200	-2.02958000
O	-6.06757800	13.01829800	-5.62428100
O	-10.43453900	8.48301000	6.79125600
O	5.13307500	8.91591400	3.81730900
O	-6.26135200	10.59240700	0.33428800
O	4.44924800	12.78610800	-2.93460600
O	-9.15702100	8.73560400	4.96334900
O	4.78704000	10.37580000	2.18070100
O	-7.27228000	10.78165900	-1.62984200
O	3.24544200	12.25263100	-4.76865600
O	2.21327700	10.96934900	3.74899800
O	-9.13167100	8.38181400	-1.09443800
O	4.66427800	9.42879500	-3.60780800
O	3.54417400	11.54726900	5.49269800
O	-9.16109300	9.65203200	0.72237300
O	3.54987800	10.10130900	-1.78928200
O	-11.42433400	8.81422600	2.58124100
O	4.00483000	8.06790200	0.37817800
O	-4.94534000	9.33575100	-3.05974200
O	5.13419100	12.06600700	-6.56322200
O	-11.92461900	9.54584100	4.66879100

O	2.42221600	8.24734200	1.99505300
O	-6.04327000	7.86473500	-1.71388500
O	6.65337900	11.43841600	-5.00694700
O	-9.80651400	11.05146800	3.74593900
O	2.35803500	10.79435400	0.85715300
O	-7.93445300	8.87789100	-3.59537900
O	3.27903500	9.65588200	-6.18556600
O	4.47258600	9.19375700	6.63720300
O	-7.33528900	9.91334200	2.85542200
O	4.49934500	12.32663900	-0.14259700
O	-8.12114300	11.43361700	-4.81628500
S	-0.02753500	1.65365300	0.49692200
S	-1.47002000	2.59392000	-3.34022000
Zn	3.11100000	9.25113300	3.56487100
Zn	-7.19627300	8.79772000	-0.32200600
Zn	5.55901200	11.16562300	-3.23690200
Zn	-9.42049000	9.10102400	2.73397500
Zn	4.43966500	10.10955700	0.10613200
Zn	-6.49129000	10.60183500	-3.57764900
C	-9.71944300	-1.98348200	-6.27006600
C	-5.27345800	1.67546900	3.43701400
C	-5.86343300	0.45261300	3.55001000
C	-7.80847900	-1.47046300	-0.82354300
C	-7.34027700	-2.32944500	0.18591400
C	-5.51138100	-0.85061000	-1.31104800
C	-5.03793800	-1.72703100	-0.31516600
C	-5.97671000	-2.46433600	0.43227800

C	-6.87229900	-0.73848500	-1.57234400
C	-15.15836000	-1.56479100	5.73334600
C	-9.27809200	-1.32417300	-1.10028300
C	-10.00481700	-0.57144000	2.92027900
C	-9.35012200	0.31036200	2.04254300
C	-8.01418000	0.64969100	2.23551900
C	-7.28486100	0.11131100	3.31426500
C	-7.93558700	-0.79661000	4.17356300
C	-9.27476500	-1.12045600	3.98802800
C	-11.44866000	-0.89655000	2.74757400
C	-13.02728200	-0.19322100	-4.94607300
C	-14.72609800	1.19051600	3.09000800
C	-12.07569900	-3.26094500	-2.62267100
C	-13.63506600	-3.84142200	1.19274000
H	-14.44403900	-0.27143200	0.62541000
H	-13.87194600	-2.83689600	-4.65053800
H	-14.80789800	-1.72109600	0.24707100
H	-13.53010600	-4.30708600	-4.94420500
H	-12.58794500	-0.94252200	5.63530700
H	-11.09051200	0.50031000	-1.44224700
H	-13.42760000	0.33220500	5.46564500
H	-12.53126500	0.40433800	-1.97427000
H	-8.06101400	-2.89109100	0.77712100
H	-4.79960900	-0.26908500	-1.89350800
H	-7.71536500	2.69768500	4.21059700
H	-7.22747000	-0.07255600	-2.35634100
H	-9.90612600	0.73168000	1.20707300

H	-7.52492200	1.32921300	1.54107000
H	-7.38662400	-1.23184500	5.00617400
H	-9.76971100	-1.80855100	4.67076900
O	-15.86813500	-0.46394600	5.47934100
O	-10.10758900	-1.82272500	-0.27541700
O	-14.75672400	-2.31487200	4.83766100
O	-9.61995100	-0.64314200	-2.15537400
O	-12.07542600	-1.50769700	3.69621600
O	-12.15645100	0.19114100	-4.07053200
O	-12.09856000	-0.52958900	1.69703000
O	-12.99434900	-1.30384400	-5.53771300
O	-14.98464300	0.06013200	2.47775700
O	-11.18753100	-3.25569700	-3.54199000
O	-13.96031200	1.33114600	4.05594100
O	-12.49456700	-2.14535400	-2.14064900
O	-12.62823600	-3.44981100	0.54025100
O	-10.89521500	-2.36237600	-6.69050200
O	-14.43344900	-3.10887400	1.87940800
O	-9.50223200	-1.33606200	-5.23220800
O	-14.34567400	-0.93713900	-0.07615800
O	-14.03460200	-3.74344100	-4.35113600
O	-13.22047700	-0.38032200	6.10910500
O	-12.01696700	0.48334900	-1.15829200
S	-3.50538000	1.77281100	3.82454500
S	-4.79410100	-0.93552200	4.02395600
Zn	-13.99226200	-1.53749200	3.00246900
Zn	-10.85503700	-1.22280400	-3.58874500

Zn	-12.18493100	-1.51494600	-0.14732600
C	9.60250100	3.46205600	-6.83800100
C	12.86744800	2.39587600	-4.88206000
C	0.26318600	0.43599000	-3.67392500
C	0.12611300	1.76918200	-3.52896600
C	2.55340300	0.82626500	0.67885900
C	1.75322800	1.92785100	0.68099300
C	6.89438000	1.20893800	10.22920800
C	10.76849900	-1.58973800	3.11431000
C	12.09366500	5.74080600	-2.72529300
C	9.05512700	-0.53208100	6.88809600
C	11.37312700	3.07397600	0.62562400
C	6.85100200	0.68452300	0.99663800
C	6.10887700	1.57999200	1.78661700
C	4.72162500	1.63635200	1.68822200
C	4.02832200	0.79056400	0.79962900
C	4.77411900	-0.12340400	0.02839600
C	6.16138600	-0.16482900	0.11466800
C	9.77544100	3.77546300	7.51489700
C	8.33837500	0.64802000	1.07010300
C	4.72484700	0.26523700	5.12048500
C	3.72763000	0.88920900	5.88776300
C	2.39697800	0.50198900	5.77219300
C	2.02209700	-0.54190400	4.90421600
C	3.02262100	-1.16562900	4.13359300
C	4.35099000	-0.76430000	4.23948800
C	12.82966000	5.40122600	-8.16705200

C	6.15801900	0.70382600	5.23084900
C	13.12204500	0.67572200	-1.08791000
H	4.00968600	1.68746200	6.57161800
H	1.63540400	0.99977900	6.36942900
H	3.80856800	3.25480300	-0.59357600
H	5.11742700	-1.24342200	3.63333600
H	8.98548500	3.17727100	5.09027600
H	9.52803400	0.83287400	-1.57321900
H	7.50113600	2.73732700	4.90331300
H	10.80483900	0.18570000	-2.08787100
H	11.24791600	2.10790500	3.43328500
H	9.51246500	3.81001200	-4.01774900
H	10.91672000	2.34312800	4.96596000
H	8.88300700	2.57210000	-3.33166400
H	6.63517100	2.23505100	2.47807700
H	4.16501500	2.33055900	2.31395200
H	4.25651400	-0.79115000	-0.65868300
H	6.72679100	-0.86432300	-0.49793600
O	9.81977100	4.26834500	-5.84116700
O	10.48273800	3.02343900	-7.60902900
O	13.28644900	3.29339800	-5.68098800
O	11.70747700	2.49888400	-4.34333800
O	12.41359700	5.84281200	-7.08255400
O	8.19859000	1.05610800	10.44849800
O	9.73938500	-1.18656200	3.73425200
O	11.93249000	4.69291700	-2.03776600
O	6.42898400	1.53393600	9.14931500

O	11.41549300	-0.99295200	2.19530000
O	12.00362100	5.87860800	-3.98994700
O	8.27334100	-0.42533600	7.88168500
O	11.75302500	2.30805600	1.57787800
O	9.34631700	0.51718800	6.19827800
O	10.61247300	2.64547400	-0.30526600
O	10.13974100	3.56083100	6.33737800
O	9.01761600	0.06130700	0.15185900
O	8.81486400	3.16857600	8.14224000
O	8.97790800	1.24606100	2.02418600
O	7.01508000	0.17916300	4.45347300
O	13.06520000	1.72814100	-1.79135800
O	6.42434900	1.64867400	6.08876100
O	12.12223900	0.01569900	-0.63618900
O	8.34245300	2.83219300	4.42950000
O	10.10125700	0.79973900	-2.35809300
O	10.97804100	1.67845100	4.26139300
O	9.31955300	3.41053200	-3.15057300
S	1.51220900	2.92620400	-3.49361600
S	-0.55979200	0.46673000	4.63517400
Zn	11.73299800	4.64027700	-5.47311400
Zn	7.88724000	1.63354300	7.42263400
Zn	10.93389500	0.48816600	0.97547200
Zn	9.02336000	0.72374100	4.05036500
Zn	11.28988800	2.73878200	-2.29978100
C	2.90254900	-6.12879700	-7.69214500
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C	7.87723500	-7.42410200	-5.67877000
C	-3.25848600	0.01003500	4.13583900
C	-1.06002800	-0.92002100	0.31594500
C	-2.05329300	-0.52712100	4.41193700
C	0.04070800	-0.15083300	0.43465900
C	-3.58137100	-1.81905100	-0.05656000
C	-0.16627600	-2.22308000	-3.82617600
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C	1.18928100	-2.10164300	-3.78379800
C	0.06526400	-2.17532700	4.73744300
C	0.59366600	-0.92077600	4.78605300
C	-2.47742300	-5.85982600	-3.90418500
C	-1.49588000	-5.66280400	-2.91793200
C	-1.95588400	-3.66886500	-4.81542200
C	-0.95109400	-3.48340800	-3.84787900
C	-0.73535400	-4.49731900	-2.89484400
C	-2.69244500	-4.84827600	-4.85444600
C	3.46218900	-10.68372600	6.98285600
C	-6.26974400	-11.00315100	3.22659100
C	8.49286300	-8.36815400	-0.44859100
C	-3.29857700	-7.11703000	-3.94287800
C	-4.22016300	-7.03149300	0.07676500
C	4.02829700	-5.34456100	-3.69977200
C	-4.69463600	-6.10823500	-0.87114100
C	2.84503200	-5.45103900	-4.45179800
C	-4.26246700	-4.78530200	-0.85613100

C	1.93658300	-4.39953800	-4.50196700
C	-3.32824800	-4.34503000	0.10239400
C	2.16916000	-3.20763600	-3.78564600
C	-2.83641500	-5.27930800	1.03535400
C	3.37283900	-3.09203800	-3.06029000
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C	4.28131600	-4.14337500	-3.01333700
C	6.52275100	-8.58065700	3.46296400
C	-4.69843800	-8.44277700	0.08236200
C	4.97307800	-6.48923000	-3.58644400
C	2.25420900	-5.88835200	4.81232700
C	2.62791700	-4.82626400	5.65489400
C	1.91600500	-3.63066900	5.65265300
C	0.80795200	-3.45313900	4.80000900
C	0.41185200	-4.53435000	3.98670100
C	1.12771500	-5.72552600	3.98641800
C	3.03924600	-7.15001900	4.75115000
C	-8.24034000	-10.93663700	0.84432400
C	5.19905500	-10.11552700	-1.99421300
C	-1.12748300	-7.73761200	-8.04510800
C	2.04639300	-5.86474200	8.71894800
C	4.90342900	-11.25126200	1.97373300
C	-3.13169500	-11.85054400	-1.11110900
H	2.75100300	-1.95611700	3.43711700
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H	5.40124400	-10.10246800	-4.99291600
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H	-5.53367900	-11.95688000	-2.02676500
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H	6.21039700	-8.75017700	6.31454100
H	5.60768100	-6.46232100	-0.89273800
H	-5.63025700	-8.08739100	-4.42919700
H	2.55158900	-8.38995600	-6.90634500
H	6.65469000	-7.42020200	6.97447000
H	4.22197400	-6.57446800	-0.21044000
H	-6.32759700	-9.46143800	-4.54256900
H	3.36569700	-9.68242900	-7.26829800
H	-1.33323800	-6.43751600	-2.17117600
H	-2.13896000	-2.88982700	-5.55288500
H	-5.63279200	-3.13088400	1.22032300
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H	-3.44956400	-4.99780700	-5.62160300
H	-5.40931500	-6.44113200	-1.62117400
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H	3.48531000	-4.94498100	6.31312800

H	2.21604300	-2.82841500	6.32219100
H	-0.45043200	-4.42426300	3.33084000
H	0.82336800	-6.54609200	3.33945100
O	4.11006800	-6.24584600	-7.25249900
O	1.98921400	-6.98889900	-7.61804600
O	-5.01534400	-8.95071500	-7.62621700
O	-3.55595200	-9.93522200	-9.04272400
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O	-3.99085000	-10.31592000	-4.65041200
O	-2.05373100	-7.31613600	-7.31845000
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O	-6.87831200	-11.51274800	4.29873700
O	7.62584800	-8.31611300	0.47574400
O	-3.27361700	-7.89538900	-2.93554800
O	3.53185900	-10.70340000	5.71442400
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O	5.61201500	-8.12740100	2.70016400
O	-5.34644800	-8.94110600	-0.91855700
O	4.80049500	-7.58153700	-4.25172200
O	2.76044900	-8.02520200	3.85157500
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O	-8.15216100	-10.67846300	2.06506000
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O	5.61353700	-10.69024900	1.08700400
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O	3.98543800	-10.69142200	2.66874600
O	-4.14799900	-12.15134400	-0.38739500
O	7.85415700	-8.26899000	-4.71856500
O	5.19314200	-5.86288600	8.14010800
O	3.37707000	-8.49257000	1.08803100
O	-5.99340800	-11.25519600	-2.50605100
O	5.80788300	-9.84013400	-5.83305000
O	6.23132200	-8.26452900	7.15776700
O	5.16603000	-6.53709000	-0.02757100
O	-6.15337300	-8.74094000	-3.92685500
O	3.16218800	-9.08691800	-6.53866600
S	-2.71104900	-0.23484700	0.04355900
S	-1.13905500	-0.69885900	-3.80499300
S	-1.06180400	-2.72606000	0.40683600
S	1.85810100	-0.41533000	-3.73304300
S	-1.73809100	-2.30022700	4.56925600
S	1.72909900	-0.78680500	0.54623800
Zn	-3.51851200	-8.56337500	-6.46447400
Zn	4.17386300	-9.47051200	4.30824600

Zn	-5.36367200	-10.93778700	0.57278800
Zn	6.79291100	-8.31340400	-2.97942300
Zn	4.09534000	-7.69246800	7.57914400
Zn	5.60593800	-8.63568600	0.63668500
Zn	-4.48473100	-9.58720400	-2.71354400
Zn	4.92987700	-7.84482300	-6.30951600
H	-15.12615600	-1.87786100	6.81526900
H	-15.28471500	2.08572300	2.65884000
H	2.67556300	13.71238300	-3.41603900
H	-13.35045500	9.01966300	3.26125900
H	-6.15885400	12.33177300	-0.78354200
H	-10.75464000	7.41488100	5.03588300
H	-5.14482800	14.27242000	-4.25491400
H	-10.90428000	8.96011500	-0.19489400
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H	-8.87338600	-2.28095000	-6.94297100
H	-13.85769900	0.54216400	-5.17140300
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H	-9.27345900	-11.04074800	0.37413300
H	-5.59973900	-9.89668100	-9.35284600
H	-2.22192700	-11.39635000	-4.39899400
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H	7.60792300	-8.37814800	3.24731800

H	9.58063900	-8.33765200	-0.11254300
H	8.88064700	-6.94067300	-5.91470500
H	13.51155000	1.49993700	-4.67668900
H	14.16132400	0.25351100	-0.88849500
H	11.16820100	-2.61366200	3.41221200
H	0.94775700	-5.69430900	8.98574200
H	6.23888600	1.02423300	11.13209600
H	9.50908600	-1.52057300	6.62396400
H	10.29918400	4.57880600	8.12879300
H	6.68500700	9.65567600	2.66785400
H	11.71535900	4.14548200	0.63503400
H	8.39126200	10.42464100	-0.61897700
H	12.35247500	6.68854200	-2.15224600
H	7.09915300	11.73570900	-6.98536200
H	8.51731500	3.15935300	-6.98402900
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H	-12.46191700	-4.23439400	-2.23306500
H	2.67411600	-5.12898800	-8.19816800
O	-1.19112000	-8.82980800	-8.75484800
H	-0.17048000	-7.17229600	-8.13530700
O	12.52363400	4.24121500	-8.67671600
H	13.51548600	6.01836800	-8.80624800
H	2.60389100	7.59809000	7.13760800
C	5.85153000	-7.72658700	-9.20950500
O	5.32647000	-8.59239000	-8.51270900
O	6.15943900	-7.95169300	-10.49329900
H	6.11654100	-6.70288400	-8.86384600

C	3.78649400	-8.54663900	10.50152600
O	3.89015700	-8.77129800	11.82148400
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H	2.83471400	-8.93238600	10.04200600
H	3.12030900	-9.24153200	12.17071100
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H	-2.10239800	-9.28246500	-8.72037800
H	-7.46097100	-10.86153200	4.71290800
H	-16.02028500	0.06553500	6.27412500
H	-11.66297400	-2.00991400	-6.12134500
H	-5.23962400	11.85982600	-6.37570800
H	-11.29567000	8.11400000	7.03179500
H	1.83036300	9.64549400	7.46932900
H	4.43674800	12.05291900	-5.82216100
H	11.81713800	3.73901900	-8.13661600
H	8.39920800	0.76964200	11.34947600