Electronic Supplementary Information for:

The fluorescence regulation mechanism of the paramagnetic metal in a biological HNO sensor

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Section 1.Computational details

Complete active space self-consistent field method.

It is a challenging task to accurately compute the electronic spectra and properties of transition metal complexes in the ground and excited states. In the past several years, the complete active space self-consistent field (CASSCF) method[S1-S2] has been applied successfully to adiabatically distinguish among different transitions of molecules containing transition metals, particularly for those excited states with charge-transfer (CT) character[S3-S5] and with the strong spin-orbit coupling effect.[S6] Since the multi-configurational self-consistent field (MCSCF) method at the CASSCF level takes account of the static correlation but not the dynamical correlation, the refined single-point energy calculation is done at the multi-configuration second-order perturbation theory level (CASPT2),[S7-S8] to obtain vertical/adiabatic excitation energies by comprehensive treatment of the electron correlation effect with reasonable computational errors as compared with the experimental data.[S3-S6] In this work the *ab initio* calculations of 1,3,5,7,8-pentamethylBODIPY (**1**) without symmetric constraint were performed primarily at the CASSCF level of theory with a total of 8 electrons in 8 orbitals (i.e. 8e/8o), using a 6-31G* basis set for all atoms. These orbitals originate from the highest occupied π orbitals and their corresponding π^* orbitals, which delocalize in the whole s-indacene ring of BODIPY. Substituent effects on 1,3,5,7,8-pentamethyl BODIPY were systematically examined to search for signaling moiety with relatively long-wavelength absorption and emission properties aiming to avoid unintended cellular damage by high energy radiation and to minimize innate biological autofluorescence.[S9] However, balanced strategies were adopted in the choice of active space for the rest of complicated and large systems of BOT1, $[Cu^{II}(BOT1)Cl]^+$, and $[Cu^{I}(BOT1)]Cl$, where some π/π^* orbitals of BODIPY moiety were replaced by π/π^* orbitals of triazole bridging unit or nonbonding orbital of d_z^2 and $d_{x^2-y^2}$ of Cu(II, I). As a result, 12e/10o, 11e/9o and 12e/9o active spaces were employed in the computations of BOT1, $[Cu^{II}(BOT1)Cl]^+$ and $[Cu^{I}(BOT1)]Cl$ molecules, respectively. The schematic orbitals in these active spaces have been depicted in supporting information (**SI**).The LANL2DZ basis set with relativistic effect core potential (ECP) was used for Cu(II, I) of $[Cu^{II}(BOT1)Cl]^+$ and $[Cu^{I}(BOT1)]Cl$, with the 6-31G basis set for all other elements in BOT1, $[Cu^{II}(BOT1)Cl]^+$, and $[Cu^{I}(BOT1)]Cl$ due to the limitation of computer memory for CASPT2 calculations of large systems with such large active space. The calculated results were found to have good agreement with available spectral data (*vide supra*).

Complete active space perturbation theory and relaxation pathways.

The radiative/nonradiative relaxation pathways were determined by using the first derivative of the energy at the Frank-Condon (FC) points of the corresponding excited states. These procedures were repeatedly validated to be reliable and feasible to describe the radiative/nonradiative relaxation mechanisms of molecules containing transition metals, which has been discussed in detail elsewhere.[S3-S5] The critical points in radiative/nonradiative pathways, i.e. minima, conical intersections, and singlet triplet state crossings, were explicitly optimized by using the state-averaged CASSCF method.[S10] A two-roots equally weighted (0.5:0.5) or three-roots differently weighted (0.0:0.5:0.5) state-averaged approach was used for critical points in the excited states, whereas single root optimization was adopted in

the ground state. The crossings between two electronic states were optimized using the gradient projection method, which is performed in the intersection space rather than the whole space. The single-point energies were then refined at the CASPT2 level of theory based on the zeroth-order five roots state averaged CASSCF wave function. The vertical excitation energies and the corresponding oscillator strengths (*f*) for different transitions of BODIPYs, BOT1, $[Cu^{II}(BOT1)Cl]^{+}$, and $[Cu^{I}(BOT1)]Cl$ were determined from the ground state CASSCF optimization followed by five roots state averaged CASSCF state interaction (CASSI) computations. In the present work, all *ab initio* calculations were performed using Gaussian[S11] and Molcas[S12] program packages.

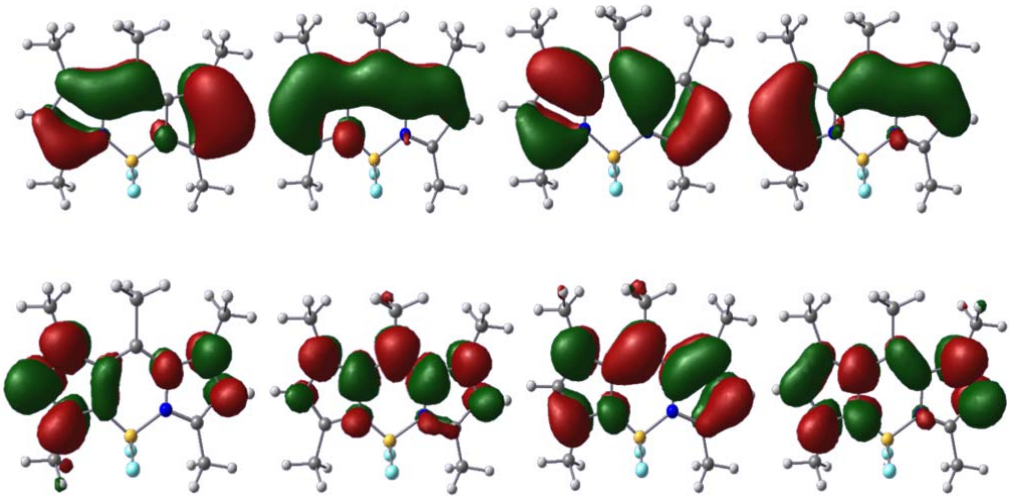
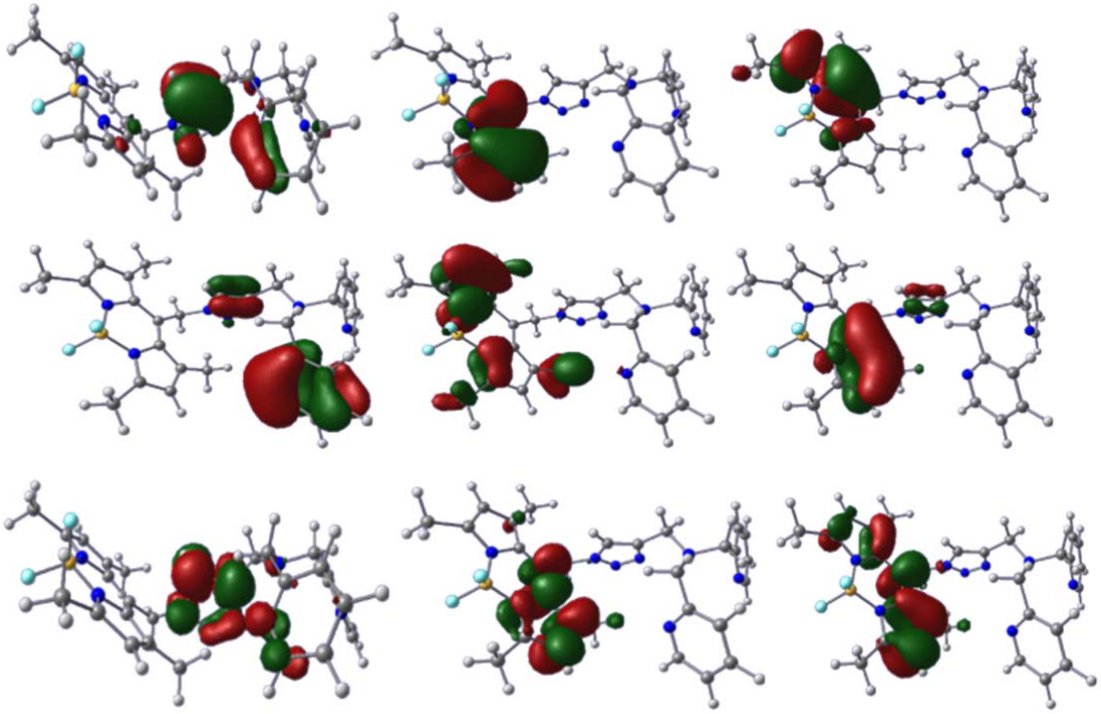


Figure S-1.1 Molecular orbitals of 1,3,5,7,8-pentamethylBODIPY(1) used in defining the active space for the CASSCF(8e/8o)/CASPT2 calculations.



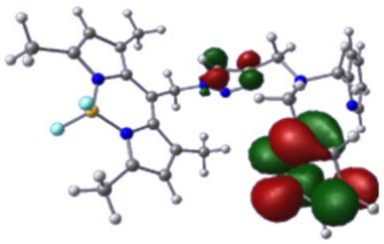


Figure S-1.2 Molecular orbitals of BOT1 used in defining the active space for the CASSCF(12e/10o)/CASPT2 calculations.

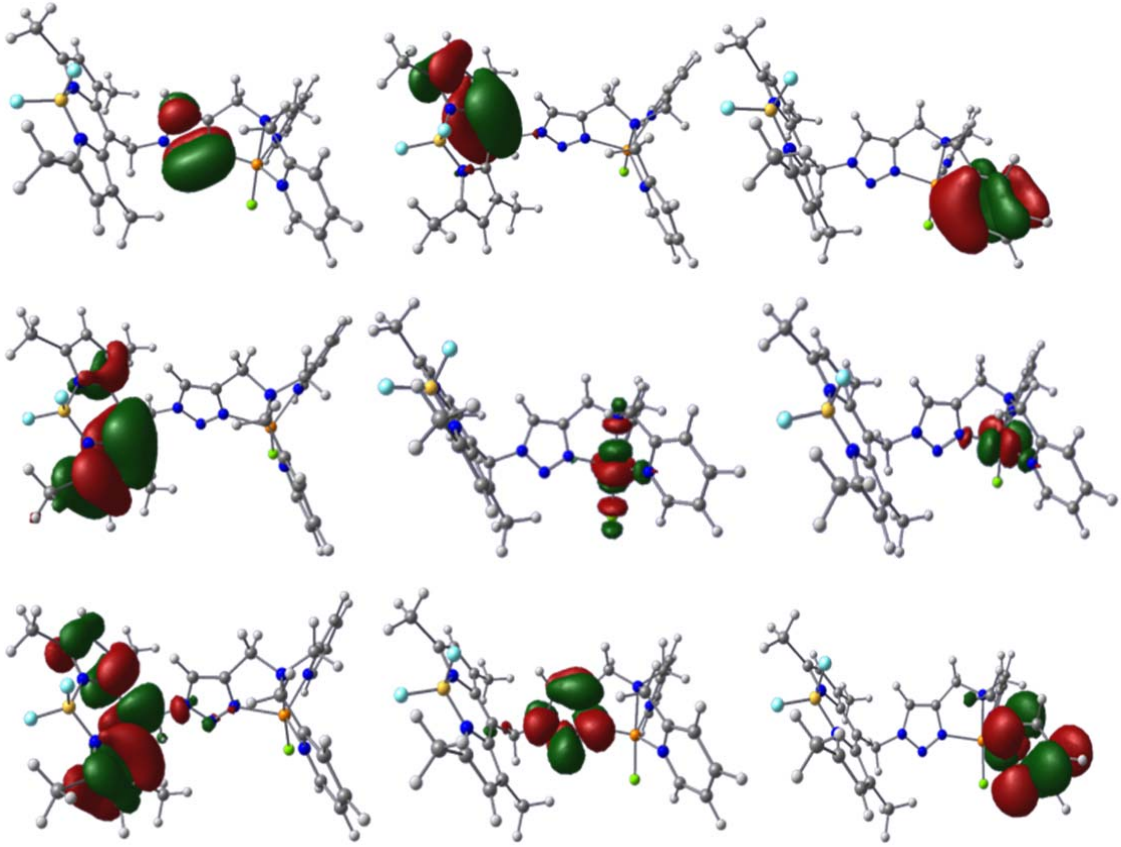


Figure S-1.3 Molecular orbitals of Cu^{I}(BOT1)Cl and Cu^{II}(BOT1)Cl^{+} used in defining the active space for the CASSCF(12e/9o)/CASPT2 and CASSCF(11e/9o)/CASPT2 calculation.

References

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Section 2. Schematic structures with selective parameters

Figure S-2.1 The schematic structures of pentamethyl BODIPY, BOT1, Cu^{I}(BOT1)Cl and Cu^{II}(BOT1)Cl^{+}.

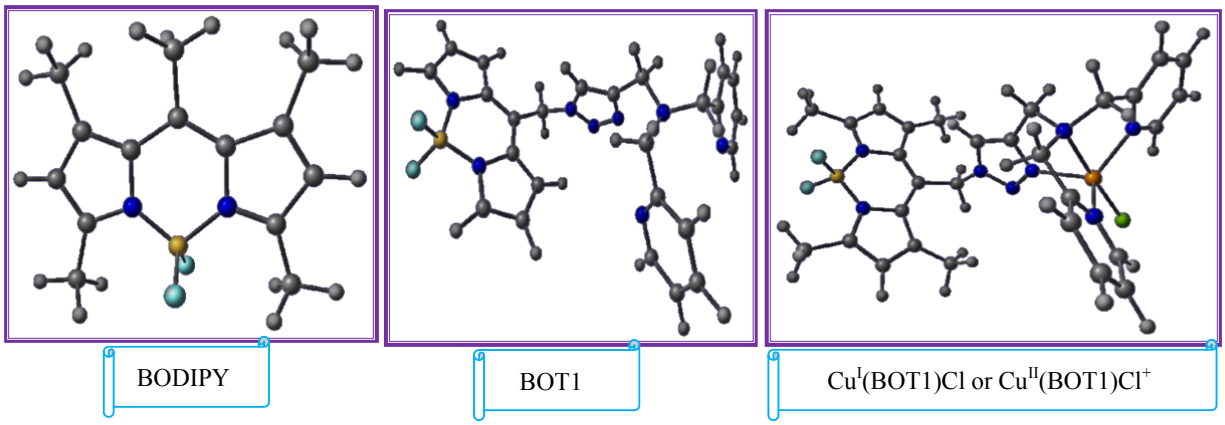
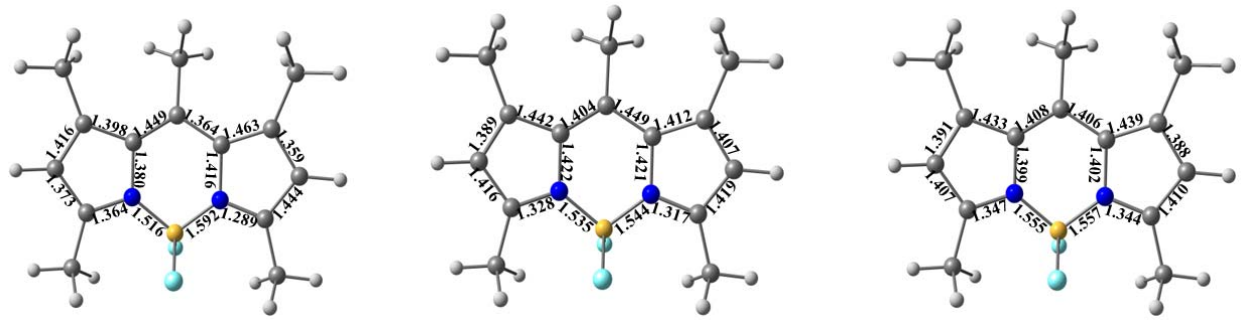
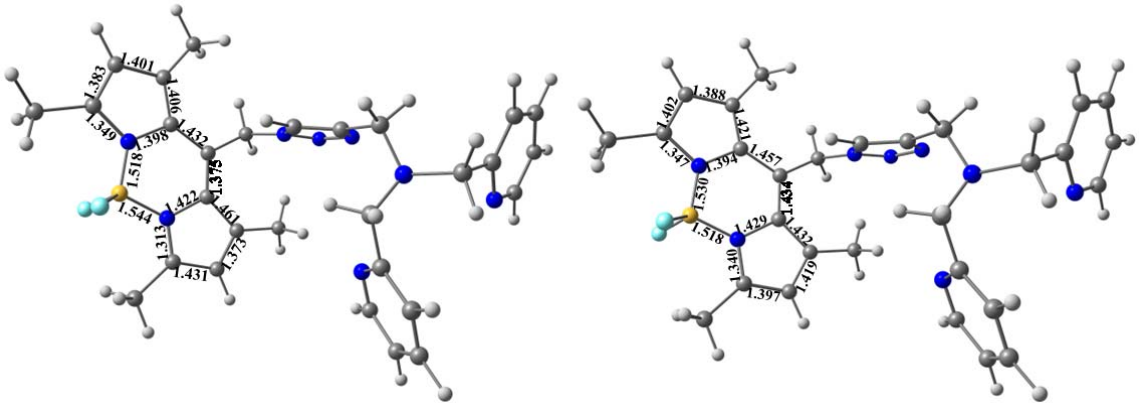


Figure S-2.2 Key structural parameters of the critical points for 1,3,5,7,8-pentamethylBODIPY(1) from the CASSCF(8e/8o) calculations.



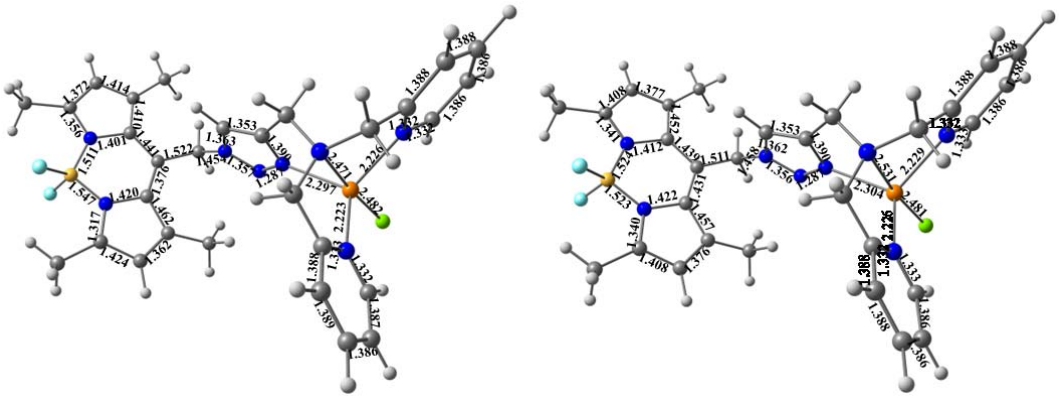
S_0-min $S_{CT}(^1\pi\pi^*)$-min(gas phase) $S_{CT}(^1\pi\pi^*)$-min(non-polar)

Figure S-2.3 Key structural parameters of the critical points for BOT1 obtained from the CASSCF(12e/10o) calculation.



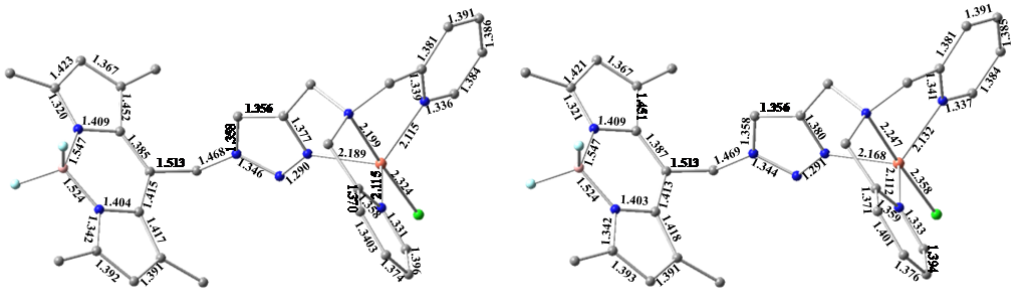
S_0-min $S_{CT}(^1\pi\pi^*)$-min

Figure S-2.4 Key structural parameters of the critical points for Cu^{I}(BOT1)Cl obtained from the CASSCF(12e/9o) calculation.

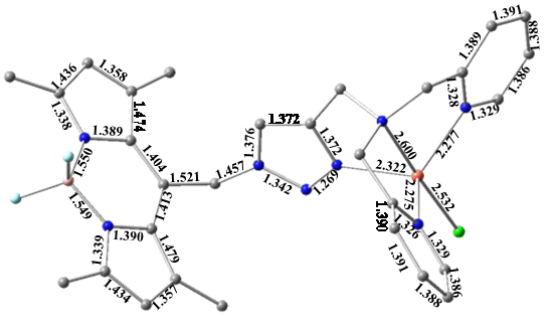


S_0-min $S_{CT}(^1\pi\pi^*)$-min

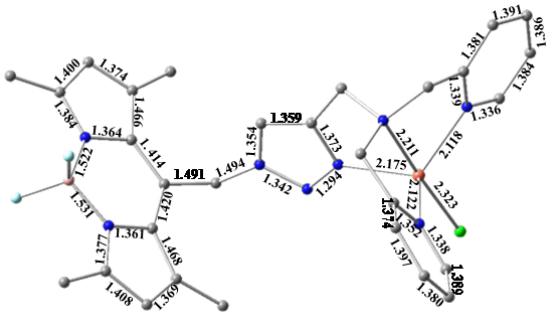
Figure S-2.5 Key structural parameters of the critical points for Cu^{II}(BOT1)Cl^{+} obtained from the CASSCF(11e/9o) calculation.The key geometric parameters of the critical stationary points along the nonradiative pathway of Figure 2 in main article



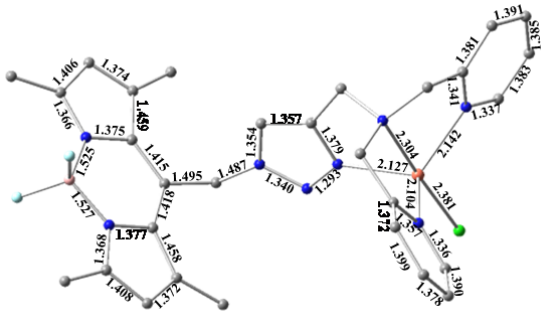
$^2D_0$-min $^2D_1$ (dd)-min



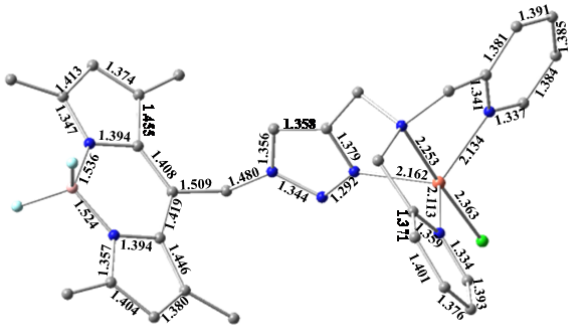
$^2D_{LMCT}(\pi d)$-min



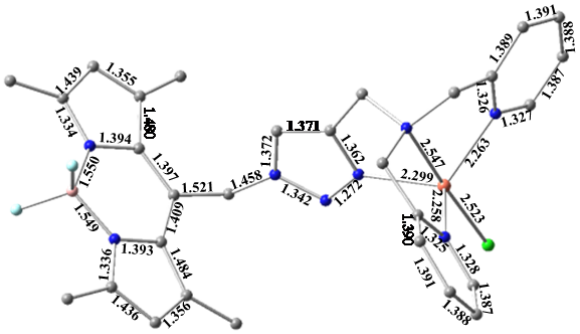
$^2D_2(^3\pi\pi^*)$-min



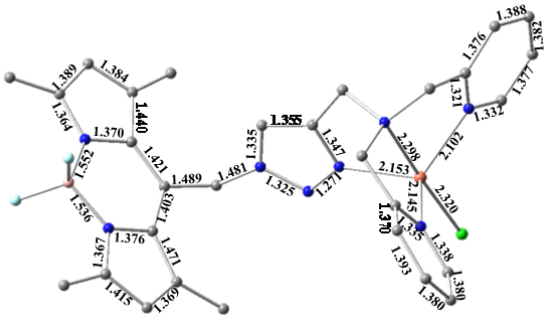
$^2D_{3'}(^3\pi\pi^*/dd)$-min



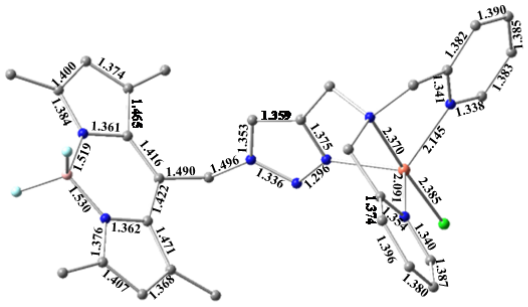
CI($^2D_{3'}/^2D_2$)



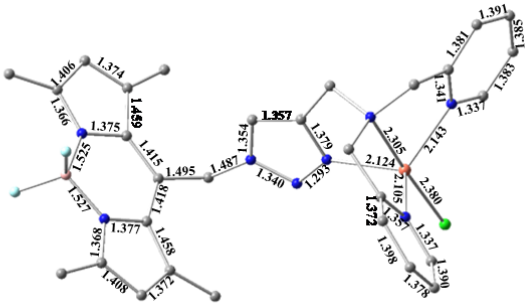
STC($^2D_{LMCT}$ /$^2D_2$)



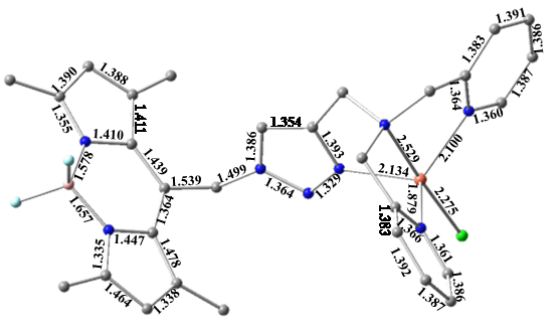
CI($^2D_1/^2D_0$)



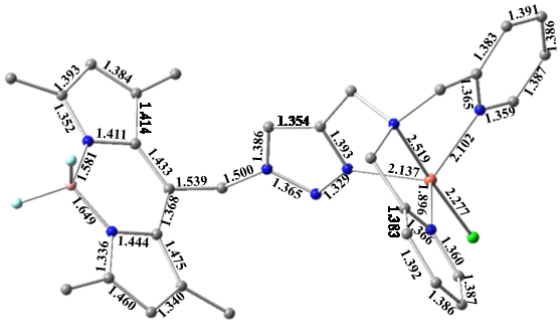
Path-$^2D_{3'}(^3\pi\pi^*/dd)$-1



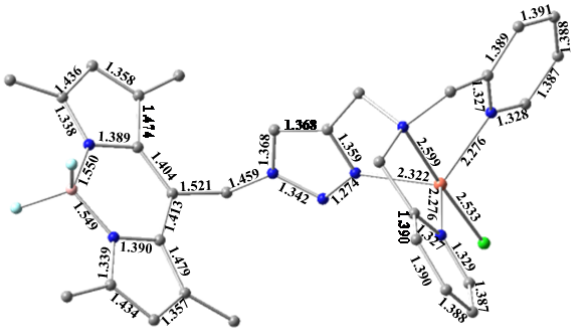
Path-$^2D_{3'}(^3\pi\pi^*/dd)$-2



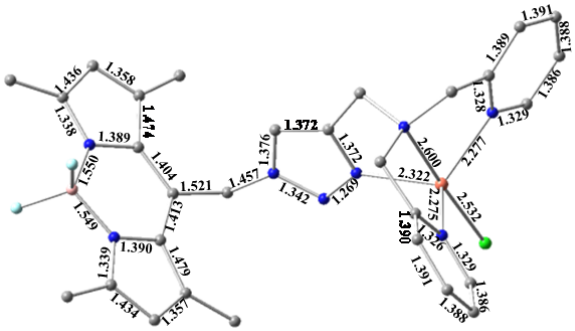
Path-$^2D_2(^3\pi\pi^*)$-1



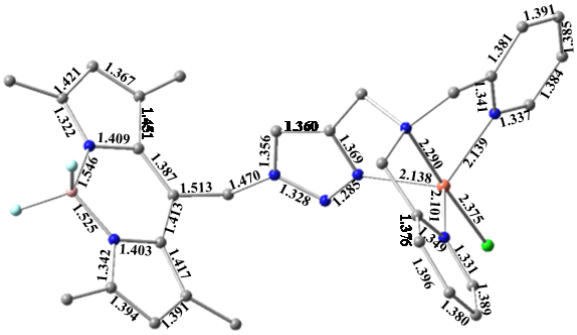
Path-$^2D_2(^3\pi\pi^*)$-2



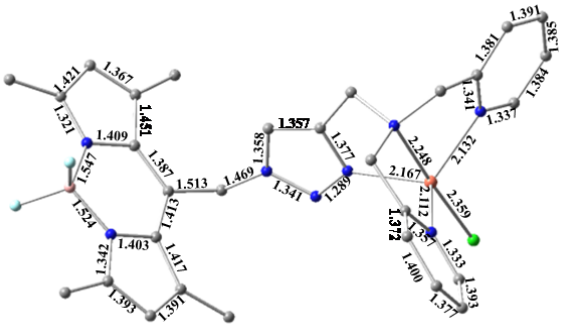
Path-$^2D_{LMCT}(\pi d)$-1



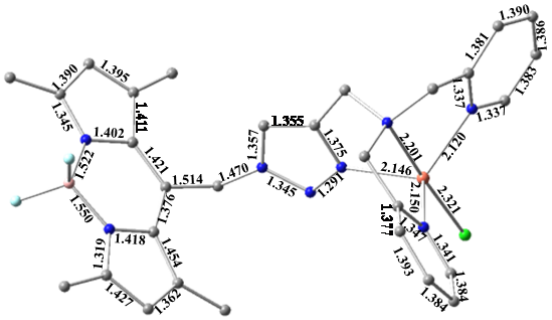
Path-$^2D_{LMCT}(\pi d)$-2



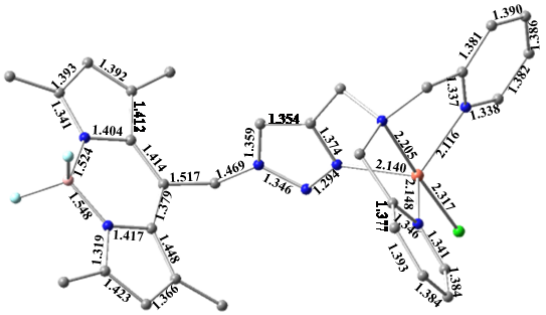
Path-$^2D_1$(dd)-1



Path-$^2D_1$(dd)-2



Path-$^2D_0$-1



Path-$^2D_0$-2

Figure S-2.6 The electron occupancy in the molecular orbitals of the active space during Cu^{2+} nonradiative relaxation path through five different electronic state.

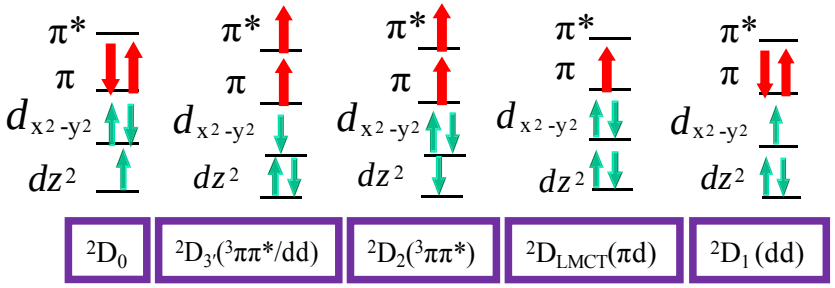
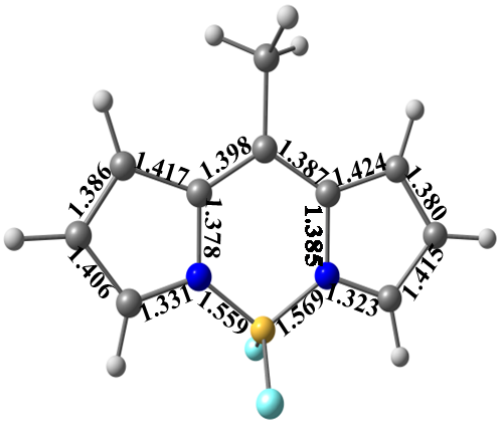
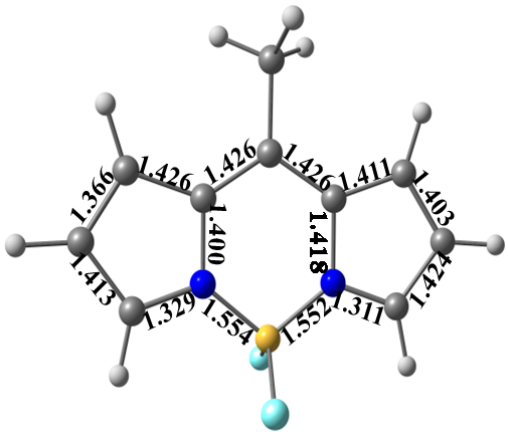
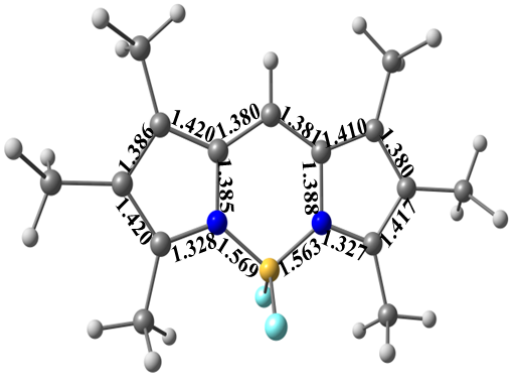
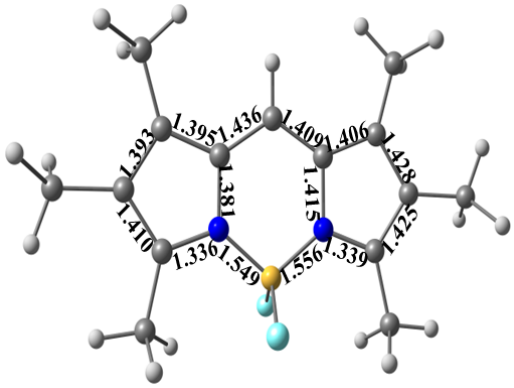
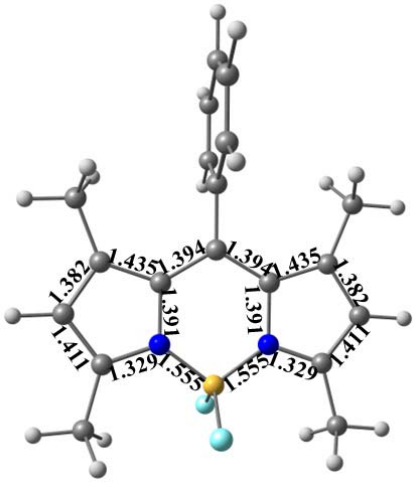
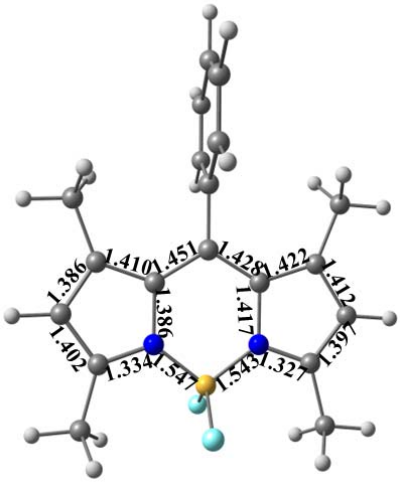
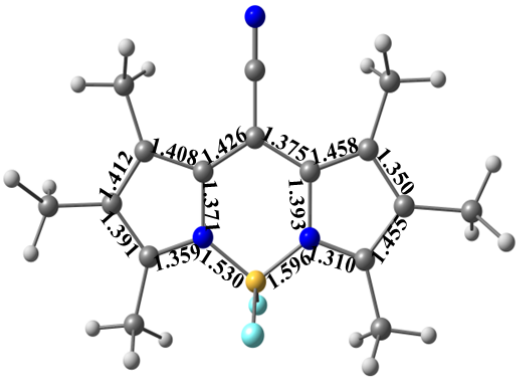
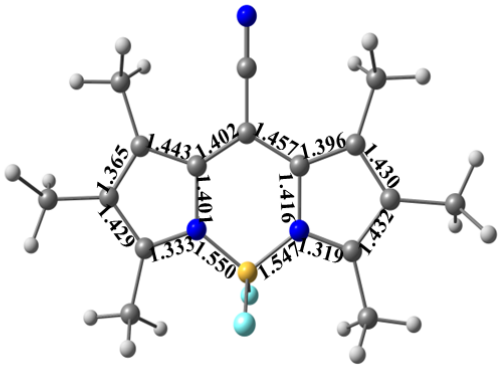
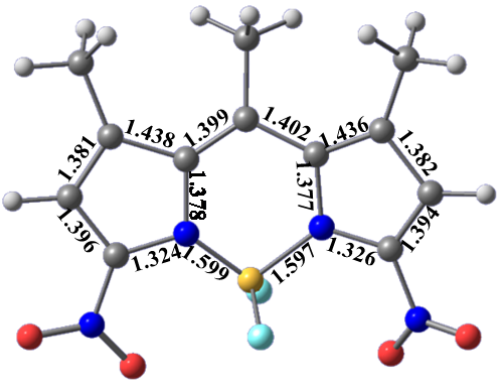
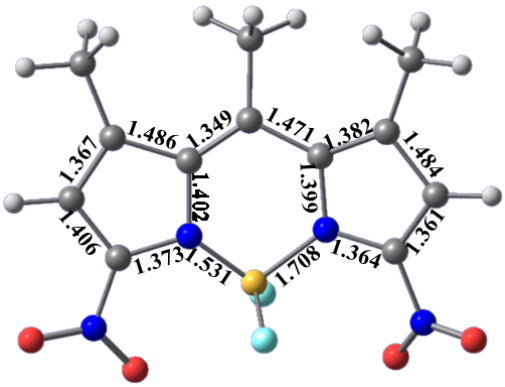
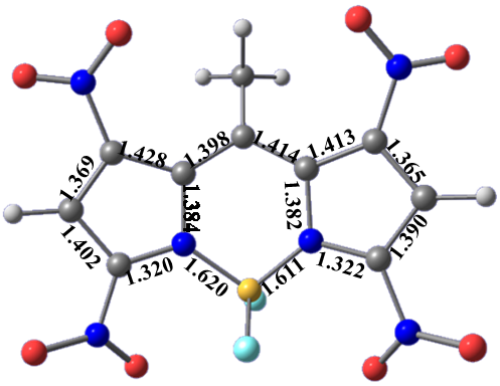
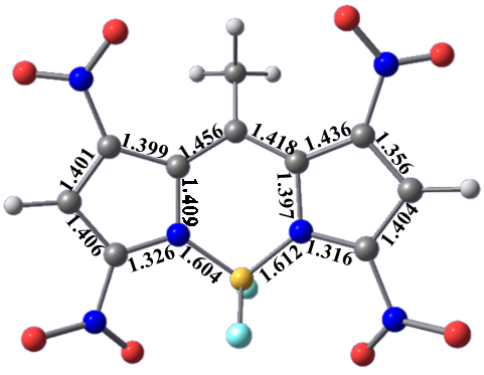
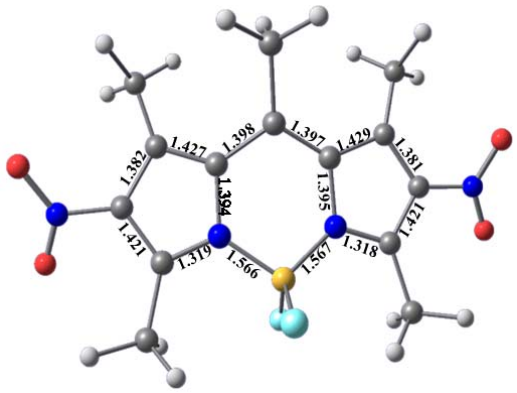
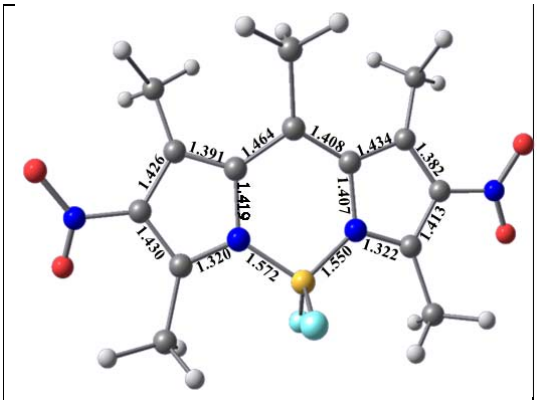
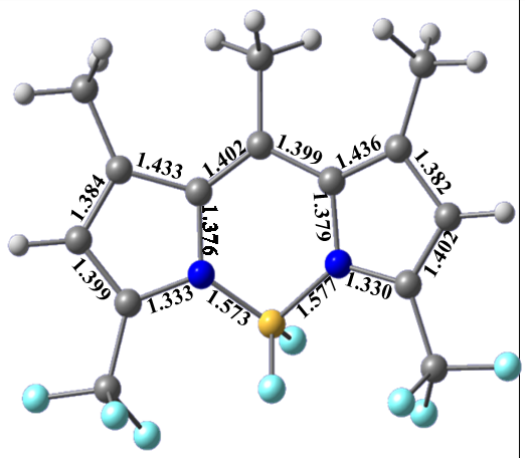
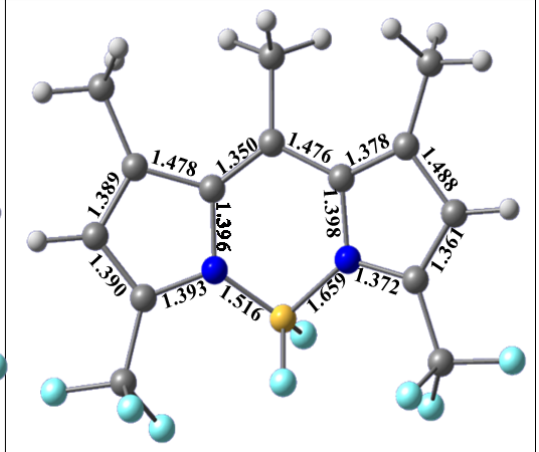


Figure S-2.7 Key structural parameters of the critical points for nine BODIPY substituents from the CASSCF(8e/8o) calculations.

Molecule	S_0-min	$S_{CT}(^1\pi\pi^*)$-min
2		
3		

4	 1.382 1.435 1.394 1.394 1.435 1.382 1.391 1.391 1.411 1.411 1.329 1.555 1.555 1.329	 1.386 1.410 1.451 1.428 1.422 1.412 1.386 1.417 1.402 1.397 1.334 1.547 1.543 1.327
5	 1.412 1.408 1.426 1.375 1.458 1.350 1.371 1.393 1.391 1.359 1.530 1.596 1.310 1.455	 1.365 1.443 1.402 1.457 1.396 1.430 1.401 1.416 1.429 1.333 1.550 1.547 1.319 1.432
6	 1.381 1.438 1.399 1.402 1.436 1.382 1.378 1.377 1.396 1.324 1.599 1.597 1.326 1.394	 1.367 1.486 1.349 1.471 1.382 1.484 1.402 1.399 1.406 1.373 1.531 1.708 1.364 1.361
7	 1.369 1.428 1.398 1.414 1.413 1.365 1.384 1.382 1.402 1.320 1.620 1.611 1.322 1.390	 1.401 1.399 1.456 1.418 1.436 1.356 1.409 1.397 1.406 1.326 1.604 1.612 1.316 1.404

8		
9		

Section 3. Charge Translocation Calculations

To further explore the properties of 1 in the excited state, a charge translocation calculation was performed based on Mulliken charge population and an appropriate fragment partition strategy. As shown in Figure S3-1, the dimethylpyrro ring is defined as part 1, while the rest moiety of the penta-methylsubstituted BODIPY is defined as part 2. The charge distributions were obtained using a full Mulliken population analysis at the CASPT2//CASSCF level of theory. Table S3-1 present the Mulliken charge distributions of parts 1 and 2 in the ground (S_0) and $S_{CT}(^1\pi\pi^*)$ state upon the photo-excitation of BODIPY. {Charge translocation: $S_{CT}(^1\pi\pi^*)$(part2-part1)-S_0(part2-part1)}

Figure S3-1. The scheme of fragment partition for charge translocation is shown in which the dimethylpyrro ring is defined as part 1, while the rest moiety of the penta-methyl substituted BODIPY is defined as part 2.

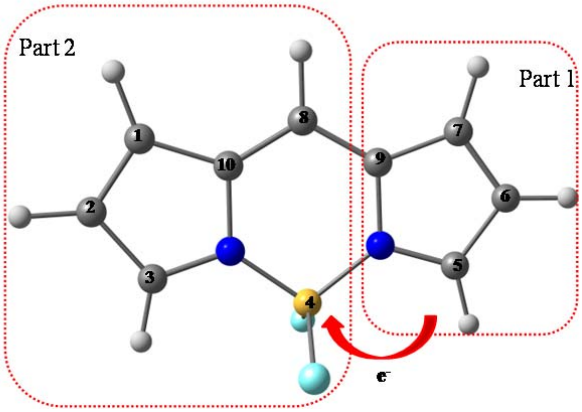


Table S3-1. Mulliken charge distribution of 1 and BOT1 fluorophores in parts1 and 2 in the ground (S_0) and the $S_{CT}(^1\pi\pi^*)$ state upon the photo-excitation. (unit: e)

		S_0	$S_{CT}(^1\pi\pi^*)$	Charge translocation
1	Part 1	-0.0395	-0.2803	0.481
	Part 2	0.0397	-0.2802	
BOT1	Part 1	-0.2661	-0.1611	0.210
	Part 2	0.2661	0.1608	

Section 4. Tables

Table S4-1 The absolute energies (A.E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of 1,3,5,7,8-pentamethyl BODIPY at theCAS(8,8)/6-31G/CASPT2 level of theory.The corresponding energy profiles are plotted in Figure 1 of the main article.*

1,3,5,7,8-penta methyl BODIPY	CASSCF	CASPT2	
	A.E.	A.E.	R.E.
S_0			
Root1	-872.766456	-875.246185	0
Root2		-875.154609	2.492
Root3		-875.115089	3.567
Root4		-875.108281	3.753
Root5		-875.081562	4.480
Path-$S_{CT}(^1\pi\pi^*)$-1			
Root1		-875.256411	-0.278
Root2	-872.650090	-875.169842	2.077
Root3		-875.127445	3.231
Root4		-875.117902	3.491
Root5		-875.104767	3.848

Path- $S_{CT}(^1\pi\pi^*)$-2			
Root1		-875.250669	-0.122
Root2	-872.650196	-875.169914	2.075
Root3		-875.119576	3.445
Root4		-875.113918	3.559
Root5		-875.101651	3.933
Path- $S_{CT}(^1\pi\pi^*)$-3			
Root1		-875.250639	-0.121
Root2	-872.650445	-875.169929	2.075
Root3		-875.119375	3.451
Root4		-875.114571	3.581
Root5		-875.102046	3.922
Path- $S_{CT}(^1\pi\pi^*)$-4			
Root1		-875.251189	-0.136
Root2	-872.650448	-875.169923	2.074
Root3		-875.119180	3.456
Root4		-875.114313	3.588
Root5		-875.102098	3.921
Path- $S_{CT}(^1\pi\pi^*)$-5			
Root1		-875.256494	-0.281
Root2	--872.650372	-875.169948	2.075
Root3		-875.127689	3.224
Root4		-875.117943	3.490
Root5		-875.104994	3.842
Path-$S_{CT}(^1\pi\pi^*)$-6			
Root1		-875.256325	-0.276
Root2	-872.650221	-875.169837	2.078
Root3		-875.127016	3.243
Root4		-875.118232	3.482
Root5		-875.104150	3.865

Table S4-2 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of BOT1 at the CAS(12,10)/6-31G/CASPT2 level of theory.*

BOT1	**CASSCF**	**CASPT2**	
	A.E.	**A.E.**	**R.E.**
S_0			
Root1	-1774.834232	-1778.473667	0
Root2		-1778.386483	2.372
Root3		-1778.360468	3.080
Root4		-1778.353591	3.267
Root5		-1778.307125	4.532
$S_{CT}(^1\pi\pi^*)$			

Root1		-1778.475001	-0.036
Root2	-1774.721464	-1778.394360	2.158
Root3		-1778.369760	2.827
Root4		-1778.327238	3.985
Root5		-1778.303823	4.622

Table S4-3 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of Cu^{I}(BOT1)Cl at the CAS(12,9)/6-31G/CASPT2 level of theory.

Cu^{I}(BOT1)Cl	**CASSCF**	**CASPT2**	
	A.E.	**A.E.**	**R.E.**
S_0			
Root1	-2429.366543	-2433.325216	0
Root2		-2433.236129	2.424
Root3		-2433.204391	3.288
Root4		-2433.166099	4.330
Root5		-2433.055770	7.332
$S_{CT}(^1\pi\pi^*)$			
Root1		-2433.331532	-0.172
Root2	-2429.317049	-2433.250823	2.024
Root3		-2433.206150	3.240
Root4		-2433.186484	3.775
Root5		-2433.067775	7.005

Table S4-4 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of BOT1 at the CAS(8,8)/6-31G/CASPT2 level of theory.*

BOT1	**CASSCF**	**CASPT2**	
	A.E.	**A.E.**	**R.E.**
S_0			
Root1	-1618.753906	-1621.996320	0
Root2		-1621.906869	2.434
Root3		-1621.870390	3.427
Root4		-1621.869041	3.463
Root5		-1621.830810	4.504
$S_{CT}(^1\pi\pi^*)$			
Root1		-1621.997878	-0.042
Root2	-1618.640717	-1621.916123	2.182
Root3		-1621.889182	2.915
Root4		-1621.844388	4.134
Root5		-1621.792980	5.533

Table S4-6 The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the optimized structures of $[Cu^{II}(BOT1)Cl]^+$ at the CAS(11,9)/6-31G/CASPT2 level of theory.The corresponding energy profiles are plotted in Figure 2 of main article.

$[Cu^{II}(BOT1)Cl]^+$	**CASSCF**	**CASPT2**	
	A.E.	**A.E.**	**R.E.**
$^2D_0$			
Root1	-2429.333377	-2433.147027	0
Root2		-2433.119068	0.761
Root3		-2433.089826	1.557
Root4		-2433.061866	2.317
Root5		-2433.063379	2.276
Min -$^2D_1$(dd)			
Root1		-2433.146361	0.018
Root2	-2429.317567	-2433.123248	0.647
Root3		-2433.089363	1.569
Root4		-2433.066319	2.196
Root5		-2433.062726	2.294
Min -$^2D_2$($^3\pi\pi^*$)			
Root1		-2433.150109	-0.084
Root2		-2433.123137	0.650
Root3	-2429.276867	-2433.104312	1.162
Root4		-2433.077333	1.896
Root5		-2433.072622	2.025
Min -$^2D_{3'}$($^3\pi\pi^*$/dd*)			
Root1		-2433.148922	-0.052
Root2		-2433.126374	0.562
Root3		-2433.096951	1.363
Root4	-2429.255847	-2433.074460	1.975
Root5		-2433.069345	2.114
Path-$^2D_{3'}$($^3\pi\pi^*$/dd*)-1			
Root1		-2433.138795	0.224
Root2		-2433.113628	0.909
Root3		-2433.087224	1.627
Root4	-2429.240957	-2433.062064	2.312
Root5		-2433.059286	2.388
Path-$^2D_{3'}$($^3\pi\pi^*$/dd*)-2			
Root1		-2433.137048	0.272
Root2		-2433.115576	0.856
Root3		-2433.088360	1.596
Root4	-2429.245389	-2433.066929	2.180
Root5		-2433.058533	2.408

CI($^2D_3$/ $^2D_2$)			
Root1		-2433.131420	0.425
Root2		-2433.128514	0.504
Root3	-2429.216768	-2433.071280	2.061
Root4	-2429.211901	-2433.068259	2.143
Root5		-2433.040816	2.890
Path-$^2D_2$($^3\pi\pi^*$)-1			
Root1		-2433.135854	0.304
Root2		-2433.127976	0.518
Root3	-2429.215407	-2433.074676	1.969
Root4		-2433.066861	2.181
Root5		-2433.043386	2.820
Path-$^2D_2$($^3\pi\pi^*$)-2			
Root1		-2433.136618	0.283
Root2		-2433.129759	0.470
Root3	-2429.217690	-2433.076497	1.919
Root4		-2433.069814	2.101
Root5		-2433.045849	2.753
Path-$^2D_2$($^3\pi\pi^*$)-3			
Root1		-2433.141988	0.137
Root2		-2433.131088	0.434
Root3	-2429.226681	-2433.083920	1.717
Root4		-2433.073184	2.009
Root5		-2433.054897	2.507
Path-$^2D_1$(dd)-1			
Root1		-2433.135444	0.315
Root2	-2429.306894	-2433.113152	0.922
Root3		-2433.078781	1.857
Root4		-2433.056540	2.462
Root5		-2433.051693	2.594
Path-$^2D_1$(dd)-2			
Root1		-2433.138617	0.229
Root2	-2429.306065	-2433.113320	0.917
Root3		-2433.081857	1.773
Root4		-2433.056591	2.461
Root5		-2433.054984	2.505
Path-$^2D_1$(dd)-3			
Root1		-2433.139002	0.22
Root2	-2429.305769	-2433.113564	0.91
Root3		-2433.082252	1.76
Root4		-2433.056845	2.45
Root5		-2433.055411	2.49
CI($^2D_1$(dd/$^2D_0$)			

Root1		-2433.121760	0.688
Root2	-2429.309761	-2433.118255	0.783
Root3		-2433.072692	2.023
Root4		-2433.054877	2.508
Root5		-2433.040412	2.901
Path-$^2D_0$-1			
Root1	-2429.324712	-2433.142099	0.134
Root2		-2433.110126	1.004
Root3		-2433.084438	1.703
Root4		-2433.052499	2.572
Root5		-2433.055370	2.494
Path-$^2D_0$-2			
Root1	-2429.326128	-2433.144067	0.081
Root2		-2433.112191	0.948
Root3		-2433.086436	1.649
Root4		-2433.054625	2.514
Root5		-2433.058940	2.397
Path-$^2D_0$-3			
Root1	-2429.333375	-2433.147028	0
Root2		-2433.119072	0.761
Root3		-2433.089823	1.557
Root4		-2433.061865	2.317
Root5		-2433.063369	2.276

Table S4-7 *The absolute energies (A. E.) in Hartree and relative energies (R.E.) in eV for the $^2D_{LMCT}$ state optimized structures of [Cu^{II}(BOT1)Cl]$^+$ at the CAS(9,8)/6-31G/CASPT2 level of theory.The corresponding energy profiles are plotted in Figure 2 of main article.*

[Cu^{II}(BOT1)Cl]$^+$	**CASSCF**	**CASPT2**	
	A.E.	**A.E.**	**R.E.**
$^2D_0$			
Root1	-2429.309918	-2433.117071	0
Root2		-2433.056211	1.656
Root3		-2433.030302	2.361
Root4		-2433.009053	2.939
Root5		-2433.002200	3.126
STC($^2D_{LMCT}$/$^2D_2$)			
Root1		-2433.108207	0.241
Root2		-2433.104340	0.346
Root3	-2429.118423	-2433.060619	1.536
Root4	-2429.114055	-2433.055323	1.680
Root5		-2433.051696	1.779

Path-$^2D_{LMCT}$-1			
Root1		-2433.101029	0.437
Root2	-2429.142918	-2433.061188	1.521
Root3		-2433.044454	1.976
Root4		-2433.045485	1.948
Root5		-2433.041290	2.062
Path-$^2D_{LMCT}$-2			
Root1		-2433.101295	0.429
Root2	-2429.142768	-2433.061609	1.509
Root3		-2433.044648	1.971
Root4		-2433.059606	1.564
Root5		-2433.043609	1.999

Solvent effect on BODIPYs

The emission wavelengths for the $S_{CT}(^1\pi\pi^*)\rightarrow S_0^*$ transition of BODIPY are calculated to be blue shifted from 527 nm in gas phase to 505 nm in the non-polar tetrahydrofuran solvent. This further confirms the charge transfer feature for the excite state of BODIPY upon photoexcitation. The calculated value in gas phase (527 nm) is a little closer to the experimentally observed band in non-polar solvent peaking at 519 nm. Meanwhile, there is the negligible discrepancy in structural parameters between two minima of $S_{CT}(^1\pi\pi^*)$ state in gas phase and non-polar matrix (see Figure S2-2 in ESI), as well as in fluorescence parameters shown in Table S4-8. These results are consistent with the experimental observations, in which the optical properties of BODIPY dye are found to be affected only slightly by the solvent polarity and there is a relatively small Stokes shifts (*Chem. Rev*. **2007**, 107, 4891 and *Chem. Soc. Rev*. **2014**, *43*, 4778). Therefore, the solvent polarity may slightly alter the energy level of the fluorescence state, but may not fundamentally change the nature and structure of the excite state of BODIPY and its derivatives. These results suggest that the solvent polarity or microenvironment unlikely modifies the major mechanism of the radiative and non-radiative relaxation for the BODIPY-copper based HNO sensor. Considering that polarity microenvironment facilitates the separation of positive-negative charge, it may accelerate the PET from the fluorescence site to the metal center. However, as discussed in detail in the Text, the PET mechanism was found here to be only part of the full mechanism.

Computational accuracy for BODIPY derivatives

To further examine the computational accuracy, we examined nine BODIPY derivatives, 1,3,5,7,8-pentamethyl (**1**), *meso*-methyl (**2**), 1,2,3,5,6,7-hexamethyl (**3**), 1,3,5,7-tetramethyl-*meso*-phenyl (**4**), 1,2,3,5,6,7-hexamethyl-*meso*-cyano (**5**), 1,7,8-trimethyl-3,5-dinitro (**6**), 1,3,5,7-tetranitro-*meso*-methyl (**7**), 1,3,5,7,8-pentamethyl-2,6-dinitro (**8**), 3,5-trifluoromethyl- 1,7,8-trimethyl BODIPYs (**9**). The results are shown in the following Table S4-8. The calculated errors of absorption and emission wavelengths for BODIPY and their derivatives are within the acceptable range (< 0.17 eV) as compared with those of experimental observations. Even for BOT1 when the bridging and receptor units are introduced, the error is only 0.16 eV. This indicates that the computational protocol adopted in this work is appropriate to provide reasonable results.

Table S4-8 .Vertical excitation energies ($E_{\perp}$), oscillator strengths (f, f_{em}) for absorption and emission, wavelengths of absorption (λ_{ab}) and fluorescence emission (λ_{FE}), fluorescence quantum yield (Φ) and charge translocations from part 1 to 2 (δ_{CT}) for nine BODIPYs and BOT1.

	$E_{\perp}$(eV)	λ_{ab}^{calc}(expt)	*f*	λ_{FE}^{calc}(expt)	f_{em}	Φ	δ_{CT}(e)
1	2.49	498(493)	0.81	Non-polar 505(519)	0.74	0.99	0.399
				Gas phase 527	0.85		0.481
2	2.61	475	0.60	526	0.68	--	0.109
3	2.31	537(528)	0.84	587(552)	0.72	0.56	0.223
4	2.43	511(500)	0.66	549(510)	0.84	0.56	0.144
5	2.21	560(588)	0.60	656(612)	0.65	0.54	0.306
6	2.52	492	0.47	579	0.70	--	0.654
7	2.25	552	0.81	646	0.41	--	0.315
8	2.30	540	0.86	587	0.53	--	0.139
9	2.64	469	0.48	532	0.71	--	0.325
BOT1	2.43	509(518)	0.98	557(526)	0.67	0.12	0.210

Section 5. Cartesian Coordinates

BODIPY derivatives-1 S_0-min

C	2.424316095	-1.059589968	-0.054160595
C	3.363064856	0.037031993	-0.079580788
C	2.657355104	1.196814366	-0.021584440
C	1.245404966	0.815357702	0.026202514
C	-1.200363330	0.842742239	0.014561343
C	-2.573092713	-0.915611269	-0.036753134
C	-2.503986858	1.344814854	-0.046321289
C	-3.354656658	0.212895527	-0.076291028
C	0.078648547	1.521823390	0.059950718
C	0.078369790	3.029015119	0.136258085
C	3.284793561	2.562435130	-0.046491822
C	-3.026948221	2.758454147	-0.087667369
C	2.771781476	-2.513068148	-0.090491184
C	-3.001602854	-2.351856961	-0.043039642
N	1.220761213	-0.599916150	-0.003335238
N	-1.263936705	-0.536107936	0.010748270
F	-0.041641490	-2.208313891	1.255463503
F	-0.061078972	-2.368244294	-0.994545226

B	-0.092640906	-1.496363768	0.073913370
H	-4.425918922	0.233045007	-0.126484390
H	-0.220536824	3.463289149	-0.811230236
H	-0.622872611	3.362794113	0.888138000
H	1.043501286	3.426424756	0.395931162
H	2.893208731	3.170841205	-0.853056432
H	3.127148965	3.095313376	0.884680128
H	4.353738425	2.465175977	-0.192169502
H	2.246431163	-3.042283143	0.692380847
H	2.461727085	-2.938142553	-1.037006223
H	3.838922539	-2.646238936	0.029711115
H	-2.909790622	3.271401996	0.862469025
H	-2.552359363	3.363482123	-0.850688274
H	-4.087748338	2.739040888	-0.309792731
H	-2.642981104	-2.866067722	-0.927084599
H	-2.614551866	-2.879408265	0.821387883
H	-4.083613353	-2.409967481	-0.024835422
H	4.427109396	-0.073237987	-0.139621129

BODIPY derivatives-1 $S_{CT}(^1\pi\pi^*)$-min

C	2.461966109	-1.024639520	-0.093682139
C	3.348105359	0.078627543	-0.135604495
C	2.605555535	1.249669420	-0.061533974
C	1.227007288	0.838354555	0.032551130
C	-1.219650316	0.853932559	0.027278297
C	-2.487280102	-0.985328614	-0.054164729
C	-2.553327937	1.300766246	-0.092148522
C	-3.348105433	0.140286180	-0.133295108
C	0.034354914	1.572702454	0.129584382
C	0.020397594	3.068496568	0.314980632
C	3.188332291	2.633450283	-0.122818604
C	-3.105709762	2.697991958	-0.185967935
C	2.827185673	-2.469978864	-0.128447958
C	-2.886409428	-2.423609554	-0.066233354
N	1.212925098	-0.582976313	-0.002762074

N	-1.241145385	-0.566864676	0.034317738
F	-0.012528811	-2.186764565	1.319869529
F	-0.045174233	-2.410694343	-0.920054791
B	-0.013231285	-1.498158610	0.120300937
H	-4.416233020	0.095452512	-0.215072334
H	-0.107960406	3.600897993	-0.623700424
H	-0.787124392	3.361491168	0.972065972
H	0.935144381	3.414522179	0.769541647
H	2.687289454	3.255652871	-0.855444382
H	3.141836931	3.143273721	0.834658691
H	4.233410012	2.572644896	-0.404788763
H	2.413629308	-2.990241910	0.729150654
H	2.426490776	-2.948906410	-1.014822504
H	3.904614624	-2.580511455	-0.122457670
H	-3.088744276	3.213159837	0.768946032
H	-2.565746081	3.306180874	-0.901221182
H	-4.138858166	2.654689781	-0.510584493
H	-2.511247852	-2.917759793	-0.955524749
H	-2.466847637	-2.941740693	0.788552308
H	-3.965107505	-2.509775438	-0.040874166
H	4.413948964	0.003452677	-0.222137383

BODIPY derivatives-2 S_0-min

C	2.505265487	-0.925632177	-0.050142467
C	3.368036365	0.195426183	-0.053687502
C	2.557272186	1.310961608	-0.010311877
C	1.209316686	0.851705348	0.012457024
C	-1.209528870	0.835433375	0.013857012
C	-2.511643936	-0.936112019	-0.056402099
C	-2.548257699	1.298504680	-0.006329131
C	-3.366561887	0.180712276	-0.052339176
C	0.001712391	1.533652444	0.028844547
C	-0.021081484	3.039379489	0.026542041
N	1.242583319	-0.532882776	-0.014306242
N	-1.241458759	-0.542114728	-0.014995830

F	0.010195270	-2.203618601	1.194592774
F	0.010829978	-2.311786887	-1.060767065
B	-0.001636841	-1.487012904	0.029631632
H	-4.436386551	0.153449278	-0.080541253
H	-0.257986516	3.397648066	-0.969980691
H	-0.778061258	3.411106673	0.704553230
H	0.930310045	3.456089740	0.320784417
H	4.437578263	0.163462888	-0.083178499
H	-2.860664405	2.322892502	0.005355397
H	-2.764569896	-1.976207843	-0.083442400
H	2.756690288	-1.966322839	-0.072863048
H	2.876999619	2.332390747	-0.003092470

BODIPY derivatives-2 $S_{CT}(^1\pi\pi^*)$-min

C	2.489681868	-0.941751312	-0.073593463
C	3.354605376	0.175146058	-0.089222834
C	2.573924870	1.294258673	-0.035606323
C	1.214883139	0.863697938	0.008909454
C	-1.222516441	0.866201968	0.012050561
C	-2.470182126	-0.962941983	-0.078577160
C	-2.564779767	1.298007624	-0.032395386
C	-3.363498025	0.146140097	-0.088561847
C	-0.002958728	1.604422349	0.055213972
C	-0.023271441	3.107900206	0.064209090
N	1.225652689	-0.535966175	-0.017388529
N	-1.226526282	-0.551719782	-0.018515859
F	0.007778291	-2.198810158	1.226483312
F	0.006987252	-2.353847900	-1.017694614
B	0.004617379	-1.494760398	0.049977790
H	-4.431554617	0.087338744	-0.132507908
H	-0.242134306	3.508223600	-0.922651993
H	-0.777585575	3.481593024	0.748277548
H	0.929697729	3.510347400	0.381555439
H	4.423860449	0.131120696	-0.134099119
H	-2.897595002	2.313767703	-0.029117050

H	-2.706298236	-2.006223322	-0.108960200
H	2.731290114	-1.982856797	-0.098468213
H	2.905125454	2.311725455	-0.036241387

BODIPY derivatives-3 S_0-min

C	2.526749793	-0.826699034	-0.030632884
C	3.370584248	0.311380281	-0.005815125
C	2.544926391	1.416552138	0.014510816
C	1.217720269	0.940731937	0.007473215
C	-1.206190508	0.953381972	-0.006248740
C	-2.528110424	-0.805706176	-0.000362605
C	-2.538555700	1.445556624	-0.015657506
C	-3.370402999	0.337251498	-0.025128013
C	0.008267433	1.607627946	0.015194115
C	2.987214117	2.849897759	0.026145122
C	-2.952028211	2.890217176	-0.016728507
C	2.911921783	-2.275426949	-0.061316080
C	-2.942285016	-2.246348886	0.028338941
N	1.255519728	-0.446886923	-0.009531196
N	-1.254284311	-0.430873169	-0.038006987
F	-0.027892973	-2.101686935	1.186657131
F	0.003343962	-2.215144966	-1.065030514
B	-0.002116917	-1.374390190	0.020675610
H	2.151620004	3.537951857	-0.010190341
H	3.558441108	3.070879659	0.922854430
H	3.626954019	3.062541726	-0.824946870
H	2.424087496	-2.810368700	0.743357973
H	2.590174644	-2.728203047	-0.992032565
H	3.981444567	-2.398472296	0.034484541
H	-3.529501118	3.129732636	0.870551911
H	-2.098397352	3.556579811	-0.042106558
H	-3.571544600	3.116840302	-0.878517505
H	-2.574492254	-2.760683253	-0.851387148
H	-2.516125099	-2.743186156	0.891285118
H	-4.019883664	-2.335726135	0.064989850

H	0.014914635	2.680711130	0.037262926
C	-4.874658054	0.316102203	-0.032216404
C	4.874645036	0.336111737	-0.011863514
H	-5.267051181	-0.241705621	-0.877328084
H	-5.276970069	-0.132607753	0.871564428
H	-5.272895822	1.321651718	-0.097001016
H	5.268487585	0.835981523	0.869183167
H	5.295264848	-0.661010166	-0.030501980
H	5.259561100	0.863070149	-0.880929590

BODIPY derivatives-3 $S_{CT}(^1\pi\pi^*)$-min

C	2.515142888	-0.835399984	-0.008427176
C	3.368382045	0.286788182	-0.018027920
C	2.554351302	1.416945169	-0.007506521
C	1.237316534	0.957373001	0.006757446
C	-1.217160056	0.996550136	0.005954962
C	-2.514483480	-0.827702926	-0.030481871
C	-2.542869558	1.464786025	0.003560148
C	-3.377727072	0.306473659	-0.019803205
C	0.005972796	1.695764661	0.018754959
C	3.015831065	2.845633966	-0.010224545
C	-2.990829435	2.896092536	0.017994863
C	2.871459525	-2.286804688	-0.017352050
C	-2.900537614	-2.272263675	-0.057169408
N	1.244192578	-0.423926270	0.003415042
N	-1.239510227	-0.417898070	-0.005968010
F	-0.012364101	-2.094697403	1.201300926
F	-0.001709495	-2.190882231	-1.052990641
B	0.004168620	-1.351980396	0.039592443
H	2.183948099	3.538111097	-0.044884744
H	3.595393206	3.076984359	0.879662411
H	3.648252774	3.054196389	-0.868810214
H	2.386832497	-2.800266833	0.804808062
H	2.530887726	-2.756827663	-0.933820581
H	3.940152210	-2.425280934	0.067730427

H	-3.572062321	3.120831938	0.907588492
H	-2.147556145	3.574914914	0.000099736
H	-3.610699494	3.125234757	-0.843834482
H	-2.511414776	-2.756807226	-0.945052474
H	-2.492347112	-2.793336178	0.801099524
H	-3.977766118	-2.376320820	-0.047162639
H	0.020738211	2.764205007	0.028409396
C	-4.877403934	0.265491839	-0.028971894
C	4.868977701	0.291701096	-0.037865038
H	-5.255877932	-0.286026542	-0.884661697
H	-5.268102762	-0.214376505	0.864342248
H	-5.294686510	1.264140121	-0.072238069
H	5.271171699	0.810549005	0.828506550
H	5.280919086	-0.708645951	-0.040251392
H	5.246724208	0.803036175	-0.919571060

BODIPY derivatives-4 S_0-min

C	1.893315423	2.507706942	-0.007256336
C	0.770682379	3.362001538	-0.013631750
C	-0.369473941	2.581819729	-0.007529481
C	0.084896708	1.220346470	0.000644757
C	0.084740037	-1.220150003	-0.001167847
C	1.892326709	-2.508540010	-0.008148174
C	-0.370499999	-2.581392127	-0.009262837
C	0.769210663	-3.362183083	-0.014443148
C	-1.766601158	3.142481500	-0.012007070
C	-1.768168803	-3.140567038	-0.014668299
C	3.340709816	2.902777833	-0.016568792
C	3.339576520	-2.904204230	-0.011100883
N	1.475738269	1.245915902	0.000767629
N	1.475390685	-1.246401359	-0.001055857
F	3.168290581	-0.002082760	1.163201154
F	3.210957206	0.001393278	-1.098658749
B	2.405632757	-0.000404682	0.017034352
H	-2.323246755	2.842268267	-0.891134498

H	-2.335614537	2.829227535	0.854225708
H	-1.715456770	4.225021738	-0.003831468
H	3.867562517	2.459121882	0.818569099
H	3.824854822	2.565377202	-0.925109032
H	3.428180064	3.980159238	0.045784768
H	-2.336655005	-2.828370643	0.852308377
H	-2.324635919	-2.838004865	-0.893103683
H	-1.718277851	-4.223193446	-0.008556043
H	3.837672702	-2.534265808	-0.898865280
H	3.853629343	-2.491425132	0.847871972
H	3.425929007	-3.983176829	0.014188940
C	-0.589613815	0.000075908	0.000908714
H	0.808431661	-4.433413860	-0.021502409
H	0.810334265	4.433208397	-0.020625562
C	-2.086782546	0.000210632	0.002805255
C	-2.783676783	0.000830075	1.203598640
C	-2.788993157	-0.000609180	-1.194658714
C	-4.169171879	0.000959655	1.206264841
H	-2.242455036	0.001258862	2.132896576
C	-4.174532751	-0.000519996	-1.191123911
H	-2.252018095	-0.001313610	-2.126437750
C	-4.866969680	0.000340207	0.009065088
H	-4.700869154	0.001518905	2.140804680
H	-4.710399838	-0.001111087	-2.123280859
H	-5.942104500	0.000431255	0.011440320

BODIPY derivatives-4 $S_{CT}(^1\pi\pi^*)$-min

C	-1.908186262	-2.503282533	-0.011861874
C	-0.791447500	-3.351237925	-0.024410743
C	0.353777496	-2.570058791	-0.016899683
C	-0.095465786	-1.233483962	0.001249025
C	-0.082943056	1.241351812	0.000935649
C	-1.930878001	2.490418848	-0.012800071
C	0.347257152	2.596931708	-0.018169810
C	-0.839075781	3.361675179	-0.033791454

C	1.755796195	-3.117313211	-0.030672737
C	1.734942579	3.171459199	-0.028708851
C	-3.352059827	-2.891395797	-0.022513474
C	-3.375862765	2.864626572	-0.013861233
N	-1.481841890	-1.238947696	0.005373559
N	-1.499666580	1.235079834	0.003343539
F	-3.186488780	-0.020510997	1.177161738
F	-3.243712140	-0.024326549	-1.076778222
B	-2.416290270	-0.006374855	0.029383039
H	2.310166006	-2.805339389	-0.908593585
H	2.327539504	-2.808177605	0.836675386
H	1.713327059	-4.200406502	-0.032259375
H	-3.874238569	-2.457726331	0.822593339
H	-3.840870985	-2.528725587	-0.920588043
H	-3.447068929	-3.969412860	0.018298290
H	2.306690968	2.875615890	0.842580395
H	2.297671893	2.865138027	-0.902464680
H	1.674518300	4.253779494	-0.034737453
H	-3.868387906	2.463741197	-0.891857312
H	-3.874925954	2.448021712	0.852685590
H	-3.482042735	3.941571283	-0.004936537
C	0.646368213	0.013840250	0.008315883
H	-0.906993310	4.430704838	-0.053066070
H	-0.829980039	-4.422711938	-0.038458061
C	2.139465861	0.006474925	0.010214115
C	2.845332811	0.001600357	1.208335057
C	2.849276886	-0.001536356	-1.185398007
C	4.231197342	-0.002945626	1.212657763
H	2.306486944	0.005300468	2.139306447
C	4.235235705	-0.005779095	-1.185050295
H	2.313566055	-0.000166265	-2.118202477
C	4.927459048	-0.006131969	0.014996166
H	4.763763040	-0.002900554	2.146963118
H	4.770921707	-0.007881501	-2.117543805
H	6.022533991	-0.009218601	0.016825808

BODIPY derivatives-5 S_0-min

C	2.468923076	-1.144490785	-0.004243045
C	3.381262706	-0.010699643	-0.014684209
C	2.627266376	1.109164521	0.000609733
C	1.234679347	0.676074879	0.012752936
C	-1.223521237	0.691446288	0.003549561
C	-2.571869371	-1.063227575	-0.013756889
C	-2.538990012	1.193695591	-0.007132307
C	-3.386771304	0.064308630	-0.018693163
C	3.134724027	2.521461105	0.002090743
C	-2.971948105	2.637087287	-0.006942771
C	2.811836167	-2.602171500	-0.024700116
C	-2.974983322	-2.506917838	-0.017976535
N	1.230508086	-0.717327961	0.010858764
N	-1.268735872	-0.678374573	-0.001717199
F	-0.042036659	-2.383995922	1.181037676
F	-0.025232854	-2.445383351	-1.077897342
B	-0.075238177	-1.634438040	0.029184611
H	2.790330361	3.068600435	-0.867348102
H	2.797135686	3.063197323	0.877448979
H	4.216238136	2.526647852	-0.001339726
H	2.236190392	-3.129782696	0.722465796
H	2.561128010	-3.023540241	-0.990862946
H	3.864055421	-2.757588826	0.163323984
H	-2.616767706	3.166050013	0.869787498
H	-2.606671782	3.169672411	-0.877371185
H	-4.050874643	2.708651567	-0.012815806
H	-2.586863767	-3.016392919	-0.892443825
H	-2.590446943	-3.019690561	0.856306052
H	-4.053483323	-2.596019730	-0.019919691
C	-4.893564938	0.033962030	-0.033141213
C	4.884250942	-0.094027892	-0.040400070
H	-5.271344735	-0.492200932	-0.904384742
H	-5.289403464	-0.463963558	0.846820221

H	-5.315951181	1.029856319	-0.053934650
H	5.317857330	0.312098559	0.867810778
H	5.227285580	-1.115372103	-0.134491338
H	5.292244093	0.460394614	-0.878526723
C	0.039275916	1.354802842	0.012202567
C	0.072057732	2.800954055	0.014824061
N	0.110397927	3.935338845	0.015020387

BODIPY derivatives-5 $S_{CT}(^1\pi\pi^*)$-min

C	2.475801539	-1.143154231	-0.004734611
C	3.366443372	-0.026399887	-0.019957777
C	2.612103622	1.111482052	-0.004786627
C	1.230920575	0.694728880	0.011952536
C	-1.241855308	0.731060529	0.005378390
C	-2.508579100	-1.098183114	-0.016411364
C	-2.555556720	1.202116362	-0.009123780
C	-3.382517946	0.036044824	-0.024738215
C	3.122712910	2.524328188	-0.005297223
C	-3.021665821	2.632606648	-0.009305662
C	2.804571293	-2.601769500	-0.023389351
C	-2.899387902	-2.538763159	-0.018517270
N	1.216596895	-0.705880423	0.011783651
N	-1.256466686	-0.685185380	0.000203081
F	-0.042313965	-2.385365284	1.185130238
F	-0.023650438	-2.451290715	-1.068274079
B	-0.029583338	-1.627455456	0.034436536
H	2.783476865	3.078198832	-0.874055509
H	2.794816906	3.072866879	0.871019037
H	4.205201917	2.528202077	-0.011277219
H	2.236110333	-3.131531177	0.730641298
H	2.554438670	-3.040315276	-0.984624163
H	3.856650617	-2.760868862	0.163713305
H	-2.677380763	3.165466341	0.868353412
H	-2.663014903	3.170602175	-0.878115711
H	-4.102362108	2.679156931	-0.017875681

H	-2.492639482	-3.038566557	-0.889822630
H	-2.495874766	-3.038769993	0.854570774
H	-3.975797928	-2.645433571	-0.020069612
C	-4.880320711	-0.049343127	-0.042825132
C	4.869087802	-0.098621667	-0.047209344
H	-5.231678714	-0.594399610	-0.913995728
H	-5.254889307	-0.565491133	0.836548150
H	-5.335364683	0.930577470	-0.065156998
H	5.301810718	0.308644366	0.862004460
H	5.220668758	-1.116168435	-0.147332237
H	5.273842197	0.465828518	-0.881181859
C	0.036611993	1.428977908	0.018356967
C	0.057850218	2.856908537	0.023951695
N	0.072193087	3.994932506	0.026971754

BODIPY derivatives-6 S_0-min

C	2.520942062	-0.484831040	-0.126250851
C	3.359289330	0.623731709	-0.234961152
C	2.555037513	1.737244431	-0.081506931
C	1.220703744	1.237806160	0.101000674
C	-1.224804588	1.236898706	0.101888134
C	-2.519434065	-0.490077203	-0.123158904
C	-2.562876925	1.731985309	-0.077079115
C	-3.362829044	0.617087036	-0.230192053
C	-0.003777831	1.915319905	0.178941819
C	3.074944487	3.147433054	-0.159741386
C	-3.086477524	3.140819212	-0.153387323
N	1.255623093	-0.138358501	0.065647109
N	-1.256311108	-0.140636596	0.064805679
F	-0.000306990	-1.521599611	1.575947464
F	0.000403613	-2.044608003	-0.665680462
B	0.002090736	-1.099226350	0.298467964
H	-4.416358192	0.578618909	-0.404214416
H	2.540933907	3.743772331	-0.889459911
H	3.019429951	3.655393317	0.796953875

H	4.116294519	3.125368252	-0.454403192
H	-3.028124429	3.649005767	0.802993841
H	-2.556348973	3.737927944	-0.885309749
H	-4.128921123	3.116420373	-0.443942516
H	4.412816371	0.589237025	-0.409874081
N	-2.996650136	-1.855047404	-0.149514661
N	3.001890499	-1.847910174	-0.151290719
O	-2.413040524	-2.671195787	0.478611025
O	-3.985990596	-2.031015260	-0.797931991
O	4.002797626	-2.018445157	-0.783372695
O	2.423354919	-2.664007301	0.481859408
C	-0.004873011	3.413709257	0.340977766
H	0.862339254	3.741100351	0.888110324
H	-0.001701433	3.902552097	-0.628268107
H	-0.875585831	3.740821422	0.882629191

BODIPY derivatives-6 $S_{CT}(^1\pi\pi^*)$-min

C	2.528635611	-0.576457538	-0.230228568
C	3.387920682	0.535553591	-0.276782869
C	2.635591721	1.654865038	-0.055158912
C	1.229590588	1.201740455	0.101744126
C	-1.203518258	1.312525930	0.101961731
C	-2.595510275	-0.434791141	-0.095286901
C	-2.455534600	1.831867758	-0.166994822
C	-3.368278236	0.668454092	-0.289126082
C	0.115238517	1.950155124	0.236619203
C	3.181360185	3.053345429	-0.071512732
C	-2.935041198	3.238851414	-0.371151981
N	1.227622388	-0.195191220	-0.012409086
N	-1.298557751	-0.082713336	0.139114680
F	-0.016277994	-1.578365815	1.537654997
F	-0.204056316	-2.012140936	-0.715525795
B	0.046261945	-1.127567855	0.271311735
H	-4.419322500	0.694127756	-0.484567029
H	2.636620812	3.695683857	-0.753399111

H	3.160678334	3.510799497	0.911655076
H	4.214513119	3.027731488	-0.395813404
H	-3.045343015	3.760127988	0.573633959
H	-2.259204025	3.810348740	-0.992133411
H	-3.903198440	3.226195807	-0.854751710
H	4.441485538	0.479415474	-0.446306396
N	-3.105641191	-1.785980555	-0.044281423
N	2.995911806	-1.909389251	-0.203183669
O	-2.546571344	-2.572654083	0.635912549
O	-4.086673045	-1.977602352	-0.704126290
O	4.131371007	-2.076740413	-0.566459522
O	2.261891584	-2.766885750	0.180998691
C	0.112939847	3.436569799	0.510630462
H	1.018590357	3.757627176	0.995726810
H	-0.011503358	4.033400163	-0.388559010
H	-0.697477670	3.684843645	1.185229919

BODIPY derivatives-7 S_0-min

C	2.520571865	-0.994725538	-0.103111736
C	3.390047975	0.104243712	-0.138333860
C	2.570649332	1.189218545	0.021362325
C	1.218904685	0.742892043	0.134196766
C	-1.216910655	0.749069483	0.126868580
C	-2.544424794	-0.965364207	-0.095998373
C	-2.547822223	1.207110779	-0.001787481
C	-3.386068223	0.139251471	-0.147946692
C	0.011492203	1.424713808	0.311783945
C	0.015337312	2.866459732	0.753418103
N	1.259485399	-0.637679324	0.051090113
N	-1.274266266	-0.630069913	0.055375503
F	-0.006065398	-2.073566000	1.496525082
F	-0.007920746	-2.488748072	-0.778007356
B	-0.016318978	-1.618638246	0.240700073
H	-4.442842386	0.138270607	-0.295856683
H	-0.003739531	3.531134307	-0.095479155

H	-0.847381170	3.063162498	1.369962527
H	0.896598369	3.072471800	1.338782228
H	4.445841583	0.084338677	-0.293122288
N	-3.043366962	2.559975287	-0.129285351
N	3.087969740	2.531793259	-0.119545731
N	2.989629134	-2.367140716	-0.165295537
N	-3.031101310	-2.328466151	-0.154983513
O	-4.110639715	2.778837610	0.346906988
O	-2.376127252	3.338162526	-0.737468627
O	2.423454616	3.321103127	-0.714277053
O	4.161349840	2.733466561	0.350847043
O	4.006139126	-2.514452015	-0.771099291
O	2.372713376	-3.196102470	0.408168512
O	-2.390733512	-3.173414461	0.371000137
O	-4.079921431	-2.464034134	-0.706408256

BODIPY derivatives-7 $S_{CT}(^1\pi\pi^*)$-min

C	2.499995041	-0.973275253	-0.094386970
C	3.341385935	0.135894951	-0.279210876
C	2.534979790	1.211048741	-0.099223229
C	1.201375392	0.761631199	0.187418793
C	-1.226499320	0.752179617	0.227299570
C	-2.493778023	-1.006260517	-0.185836433
C	-2.528284237	1.202890389	-0.018357837
C	-3.355815334	0.101229915	-0.271878327
C	0.012693616	1.454535608	0.530987527
C	0.018174441	2.798208773	1.215118771
N	1.253395346	-0.634300315	0.158898948
N	-1.251978728	-0.652456498	0.116720483
F	-0.031262670	-2.052036890	1.640976046
F	0.025074449	-2.535258211	-0.611403789
B	-0.001659339	-1.623041012	0.373857032
H	-4.400571289	0.088933301	-0.488135273
H	-0.072883953	3.617340668	0.521195683
H	-0.805329508	2.847268436	1.918292669

H	0.933213964	2.921998418	1.777671975
H	4.382064940	0.110943877	-0.515467471
N	-3.006536691	2.553620149	-0.139770741
N	2.977297594	2.559512596	-0.313500250
N	2.995742919	-2.326095088	-0.107389826
N	-2.961205552	-2.363862844	-0.328639237
O	-4.147736766	2.733125660	0.152729452
O	-2.242572921	3.382601937	-0.523624387
O	2.155189935	3.364955130	-0.624488961
O	4.148910751	2.755710395	-0.227058071
O	4.006295604	-2.486551981	-0.724836637
O	2.409570640	-3.141020738	0.519557314
O	-2.410362829	-3.213696106	0.285613501
O	-3.924903354	-2.491255583	-1.023494037

BODIPY derivatives-8 S_0-min

C	2.492787033	-1.020650153	0.018862646
C	3.329309989	0.126193622	-0.051402928
C	2.565015124	1.276519429	-0.018746248
C	1.218944182	0.809156041	0.083227411
C	-1.220171228	0.805770963	0.085883916
C	-2.492962042	-1.023788307	0.016823488
C	-2.565027845	1.273372655	-0.007289427
C	-3.329470060	0.122376787	-0.049570393
C	-0.001034930	1.487370855	0.146630226
C	3.066030946	2.686542541	-0.185471778
C	-3.064009589	2.685692942	-0.159858042
C	2.873270544	-2.471275263	0.042850832
C	-2.871156111	-2.475183385	0.035171110
N	1.250346190	-0.585680182	0.089333882
N	-1.250071409	-0.587886676	0.091601478
F	0.003083213	-2.118614838	1.453778837
F	0.000862308	-2.429547409	-0.791219907
B	0.000297428	-1.521301753	0.225343589
H	2.403028332	3.266020972	-0.811234094

H	3.157853486	3.182831737	0.774838823
H	4.044495925	2.687195260	-0.636016612
H	2.135128815	-3.047779760	0.576888489
H	2.946850434	-2.849694391	-0.969463002
H	3.836041730	-2.598039128	0.512901988
H	-3.163175051	3.169697155	0.806008733
H	-2.394682127	3.272676556	-0.771971084
H	-4.038541157	2.693368034	-0.618734117
H	-2.939806143	-2.851126403	-0.978410860
H	-2.134058284	-3.051892293	0.570563847
H	-3.835433107	-2.605157748	0.501046437
N	-4.755797404	0.057119127	-0.180697613
O	-5.216923390	-0.919085725	-0.693247136
O	-5.399610929	0.978024497	0.227487700
N	4.755845040	0.059398974	-0.179449485
O	5.217135553	-0.924045137	-0.677859593
O	5.399722532	0.980179429	0.228978462
C	-0.006822246	2.990229247	0.295507801
H	0.853053919	3.322089090	0.850876026
H	0.001122528	3.479584728	-0.672965990
H	-0.881945996	3.314984034	0.831818136

BODIPY derivatives-8 $S_{CT}(^1\pi\pi^*)$-min

C	2.469676132	-1.023141657	-0.017974973
C	3.302803035	0.109724154	-0.151149951
C	2.555532918	1.268839035	-0.057980319
C	1.212577762	0.814663184	0.154919317
C	-1.234155964	0.819075781	0.174097154
C	-2.482873850	-1.042875841	0.027574675
C	-2.515274854	1.288348763	-0.098053479
C	-3.311260377	0.106488677	-0.163629383
C	0.025033720	1.534281207	0.388295958
C	3.001000973	2.687187630	-0.251310116
C	-2.966713547	2.701011517	-0.354745982
C	2.840538196	-2.472293130	-0.005401654

C	-2.863790032	-2.491935449	0.058429667
N	1.231154730	-0.592565233	0.150382678
N	-1.253485666	-0.599235226	0.213562582
F	0.021856062	-2.052185790	1.647575410
F	-0.027204867	-2.496789306	-0.569802118
B	0.010430443	-1.517800114	0.386766577
H	2.206255793	3.280956053	-0.681899126
H	3.293309272	3.139947122	0.691257599
H	3.859771461	2.731583135	-0.902525567
H	2.157274226	-3.030989633	0.614439885
H	2.794156302	-2.870069228	-1.013632935
H	3.849070693	-2.598731901	0.353337054
H	-3.320416530	3.178790103	0.551547291
H	-2.160363621	3.291445732	-0.765522705
H	-3.783452635	2.712442688	-1.060684677
H	-2.804250046	-2.913362992	-0.938175238
H	-2.196064078	-3.040449470	0.704060667
H	-3.878324056	-2.602688353	0.407077589
N	-4.724777594	0.065706659	-0.346396028
O	-5.200118509	-0.940024586	-0.787521910
O	-5.345444028	1.043719297	-0.047573321
N	4.715730865	0.046600695	-0.351770720
O	5.174447517	-0.967911894	-0.790998880
O	5.360079536	1.015866486	-0.073041058
C	0.012216948	2.965725081	0.856790810
H	0.894428626	3.181065258	1.443859261
H	-0.030676214	3.684743001	0.045262065
H	-0.848671379	3.137758504	1.491267727

BODIPY derivatives-9 S_0-min

C	2.506447638	-0.250356738	-0.079846311
C	3.353752601	0.860316067	-0.198033131
C	2.569823291	1.993722308	-0.100654773
C	1.223260893	1.525302381	0.068527758
C	-1.219264832	1.525197329	0.068599774

C	-2.509626538	-0.245216688	-0.079586796
C	-2.561465149	1.998760504	-0.099555492
C	-3.351088183	0.866344486	-0.196532148
C	0.004102248	2.208318860	0.128013483
C	3.114915223	3.391437668	-0.216120059
C	-3.102075484	3.398472963	-0.214175299
C	2.952732451	-1.685599235	-0.139579144
C	-2.959022971	-1.678584366	-0.140348045
N	1.245382142	0.146908888	0.065801791
N	-1.244545005	0.149107071	0.065604580
F	0.000576048	-0.984840142	1.770761312
F	-0.001556865	-1.868518722	-0.325633239
B	-0.002769395	-0.744525200	0.431485677
H	-4.410194737	0.831851527	-0.342375827
H	2.601468133	3.972651170	-0.972798819
H	3.052349994	3.931430707	0.722870891
H	4.160834162	3.344808559	-0.492818693
H	-3.038122154	3.937885770	0.725086530
H	-2.587148428	3.978854223	-0.970483864
H	-4.148125409	3.355290618	-0.490995411
H	4.412549142	0.820968981	-0.344736547
F	2.590191842	-2.269856485	-1.261795056
F	4.277290681	-1.722979273	-0.089878234
F	2.498860744	-2.397732628	0.866015671
F	-2.596174329	-2.264714189	-1.261872734
F	-4.283807493	-1.713974079	-0.092483740
F	-2.507837495	-2.392476945	0.865766582
C	0.003703245	3.712715279	0.220408782
H	-0.005656687	4.154119808	-0.771626611
H	-0.861536344	4.065440099	0.755305292
H	0.876514558	4.068060108	0.740663418

BODIPY derivatives-9 $S_{CT}(^1\pi\pi^*)$-min

C	2.531480246	-0.300417423	-0.101088347
C	3.379853137	0.796351545	-0.193753752

C	2.626876441	1.956337878	-0.066208261
C	1.221174580	1.527502869	0.090422906
C	-1.211598763	1.589313005	0.040730123
C	-2.563329625	-0.229303465	-0.096078547
C	-2.484258680	2.057641417	-0.205718989
C	-3.361359112	0.858065434	-0.278591889
C	0.094051911	2.266856569	0.159229919
C	3.190607525	3.342579479	-0.158558607
C	-3.017989753	3.446463122	-0.403555742
C	2.935470811	-1.736201798	-0.203375073
C	-2.997243216	-1.665730989	-0.114135302
N	1.219214401	0.131456239	0.076187009
N	-1.273085444	0.194126841	0.099501511
F	-0.067466497	-0.909948659	1.851354472
F	-0.054124472	-1.877683586	-0.206638930
B	0.046030738	-0.727313932	0.503883005
H	-4.418648736	0.864814253	-0.444442561
H	2.699152587	3.931413499	-0.925142026
H	3.110381148	3.881331460	0.779832541
H	4.243067137	3.285802798	-0.409490483
H	-2.990424752	4.018298153	0.517681986
H	-2.459942393	3.992904884	-1.151730575
H	-4.049979757	3.399522914	-0.727297512
H	4.437419256	0.746378538	-0.350219250
F	2.590151498	-2.281838238	-1.353552036
F	4.254719821	-1.831483380	-0.112121305
F	2.425318421	-2.478627626	0.759280197
F	-2.587909861	-2.297125772	-1.191530001
F	-4.326370860	-1.698532713	-0.118544424
F	-2.584351922	-2.327065557	0.939996423
C	0.077659883	3.768251775	0.318521653
H	-0.027343471	4.292694110	-0.627599185
H	-0.747723653	4.068015996	0.952276479
H	0.972918762	4.130804771	0.795655793

BOT1 S_0-min

C	-3.163022150	2.622805438	0.605334571
C	-1.981227359	2.680675749	1.409739341
C	-1.582280705	1.399846510	1.700388373
C	-2.546124692	0.512961967	1.053460667
C	-3.758451613	-1.445836283	0.223435371
C	-5.586621322	-1.402290330	-1.077130490
C	-4.117702152	-2.778429265	-0.047297458
C	-5.259354769	-2.728178260	-0.857722791
C	-2.693727948	-0.851813586	0.974996503
C	-1.723372954	-1.769869553	1.691463672
N	-3.479479422	1.364857204	0.401211944
N	-4.684633568	-0.631838244	-0.435626257
F	-4.565268469	1.416756332	-1.760142365
F	-5.893290386	1.411550710	0.126392289
B	-4.687021782	0.885705769	-0.433565023
H	-5.788440793	-3.571555168	-1.245144944
H	-1.619768743	-1.491759079	2.726743592
H	-2.093134319	-2.775070916	1.678233452
H	-1.498681051	3.582004709	1.717770052
N	-0.394960743	-1.747836496	1.105876218
C	-0.001439242	-1.645013022	-0.198956762
C	1.364037318	-1.722074634	-0.162655520
H	-0.686001245	-1.503288920	-1.001370390
N	0.685012911	-1.923099784	1.889908575
N	1.729639535	-1.904680066	1.159536940
C	2.374429360	-1.644139023	-1.255453851
H	3.088222639	-2.439066996	-1.096101198
H	1.883635888	-1.842387606	-2.212048474
N	3.114706585	-0.386494361	-1.289444086
C	2.350891995	0.797098976	-1.674694130
H	1.320908087	0.631545926	-1.396664366
H	2.376894580	0.953761287	-2.755443816
C	4.466567873	-0.481112392	-1.834752234
H	4.478774749	-1.056043507	-2.763532021
H	4.804796910	0.516542951	-2.066952703

C	2.815176021	2.047750210	-0.975046214
C	3.583477267	3.002137661	-1.604609006
N	2.422360246	2.204515626	0.310731625
C	4.000492090	4.132916315	-0.897581464
H	3.860809754	2.875231527	-2.632742927
C	2.822456849	3.280237425	0.982982872
C	3.623078659	4.272514126	0.418331170
H	4.606432262	4.876860225	-1.377203497
H	2.490967467	3.353879879	1.998974826
H	3.924013489	5.120551291	1.000265754
C	5.450129893	-1.067823389	-0.855058627
C	5.904169053	-2.374552352	-0.942985185
N	5.880482074	-0.249060200	0.112020722
C	6.797424483	-2.850444436	0.010140392
H	5.569634891	-3.010489375	-1.739288336
C	6.731942238	-0.700187666	1.023219515
C	7.217067015	-2.002055585	1.017525669
H	7.152535437	-3.861557154	-0.038646784
H	7.037340906	-0.001010546	1.774957767
H	7.901238852	-2.328426363	1.774783101
C	-3.499083528	-4.087648335	0.365114833
C	-6.742210499	-0.855060347	-1.850269865
H	-4.026065554	-4.896651433	-0.123225927
H	-2.455948343	-4.168228451	0.081924857
H	-3.571778957	-4.262857212	1.433027072
H	-7.609693726	-0.745632011	-1.208457371
H	-6.517774468	0.113122680	-2.268520895
H	-7.001128777	-1.530739804	-2.654903367
C	-0.337244047	1.092894109	2.482153904
C	-3.935742068	3.771422700	0.059515154
H	-0.284277670	0.091059102	2.865871482
H	0.534955155	1.230767484	1.851647467
H	-0.257873990	1.776464043	3.318980121
H	-4.963204272	3.722010277	0.394376184
H	-3.497023352	4.706494864	0.374597683

H	-3.952530666	3.726233873	-1.021370776

BOT1 $S_{CT}(^1\pi\pi^*)$-min

C	-3.255198900	2.669490561	0.480880147
C	-2.082390634	2.775133322	1.232595542
C	-1.635584312	1.473035740	1.575187873
C	-2.588743421	0.574613477	0.996367633
C	-3.800229649	-1.458658470	0.239553369
C	-5.654987371	-1.447386879	-1.015324228
C	-4.153965563	-2.813906430	-0.001393635
C	-5.305900570	-2.783926168	-0.776004711
C	-2.704101733	-0.854504499	0.984954941
C	-1.719123698	-1.708193113	1.731691700
N	-3.566710608	1.375038585	0.330384392
N	-4.742856850	-0.663324518	-0.409598633
F	-4.721897902	1.330143939	-1.801824037
F	-5.994297252	1.349054898	0.120259978
B	-4.769977470	0.866152045	-0.443512943
H	-5.842021260	-3.635409393	-1.137255276
H	-1.625042926	-1.381639352	2.754568478
H	-2.053783503	-2.726970519	1.763773081
H	-1.603561717	3.693251970	1.498630070
N	-0.385086917	-1.680612771	1.148224755
C	0.014372201	-1.539547118	-0.153258817
C	1.376389622	-1.652996159	-0.119948142
H	-0.664692589	-1.359012204	-0.951945214
N	0.689698527	-1.895381114	1.927237267
N	1.736009226	-1.876717842	1.201100199
C	2.387812851	-1.585408397	-1.213177875
H	3.085247499	-2.394560284	-1.053074563
H	1.888986711	-1.778714338	-2.167167179
N	3.160104108	-0.349063512	-1.263506400
C	2.430735539	0.860643659	-1.633483488
H	1.392896497	0.717129869	-1.371912836
H	2.475337921	1.037670367	-2.710250598

C	4.495417125	-0.486418435	-1.839747641
H	4.466340994	-1.051781534	-2.774196900
H	4.862198671	0.501631208	-2.069974559
C	2.925920029	2.083578928	-0.907228657
C	3.724802084	3.026617115	-1.509656250
N	2.531421576	2.222812273	0.382143280
C	4.173102247	4.129679963	-0.773368345
H	4.005485137	2.916331687	-2.538900009
C	2.958292834	3.268203304	1.080317434
C	3.793641498	4.250541416	0.541481620
H	4.804460295	4.864516425	-1.233807332
H	2.622524043	3.329347534	2.095777903
H	4.116524637	5.074981118	1.145052422
C	5.482423781	-1.116068008	-0.890162881
C	5.887706296	-2.439009818	-1.003958432
N	5.965618438	-0.326042665	0.072250879
C	6.787477220	-2.955643328	-0.081026126
H	5.509529298	-3.052834070	-1.798017496
C	6.824771463	-0.816709766	0.957385410
C	7.263454058	-2.133042195	0.924871828
H	7.106567080	-3.977656510	-0.148886655
H	7.172628827	-0.136634322	1.708054464
H	7.955342727	-2.492834024	1.659583918
C	-3.494908077	-4.091754941	0.431020581
C	-6.832124857	-0.927496452	-1.764139770
H	-4.002306226	-4.927528830	-0.031850922
H	-2.453010748	-4.144968666	0.136773031
H	-3.546882681	-4.243317083	1.503578951
H	-7.660847756	-0.749609922	-1.085663642
H	-6.606543052	0.006247876	-2.254137539
H	-7.149218025	-1.650142623	-2.504404066
C	-0.360118411	1.222680661	2.326100158
C	-4.068944290	3.775731753	-0.093180113
H	-0.299550150	0.252543030	2.786162836
H	0.496120524	1.312446648	1.667416630

H	-0.251600542	1.963256839	3.110352382
H	-5.086363371	3.727186223	0.273409823
H	-3.639906442	4.731780620	0.169415179
H	-4.116582910	3.689105162	-1.171208076

[Cu^{I}(BOT1)]Cl S_0-min

C	-4.211662113	2.676717276	0.026083989
C	-3.037986965	2.976764247	0.774274016
C	-2.529142515	1.818059507	1.277833847
C	-3.396776484	0.741781914	0.801981424
C	-4.464360993	-1.430467785	0.420438297
C	-6.379763666	-1.765567813	-0.714399018
C	-4.715230607	-2.818082183	0.401098280
C	-5.921882415	-2.995898677	-0.314876635
C	-3.386935349	-0.627286912	0.939886074
C	-2.220970006	-1.369199162	1.576569682
N	-4.425990440	1.377344539	0.059157655
N	-5.512158780	-0.818286757	-0.279229158
F	-5.819312994	0.981002321	-1.893382041
F	-6.831480161	1.189176512	0.166099937
B	-5.678874644	0.666807044	-0.505240239
H	-6.402840556	-3.931028988	-0.502937571
H	-2.087477451	-1.123544367	2.617723739
H	-2.414102355	-2.419342792	1.527545955
H	-2.651360473	3.958594894	0.936476172
N	-0.954219109	-1.142875101	0.898791174
C	-0.643715225	-1.340461641	-0.413517875
C	0.680110216	-1.086470797	-0.528123469
H	-1.372632533	-1.632675990	-1.133497625
N	0.161158034	-0.782488768	1.581778093
N	1.132857437	-0.738580508	0.739701564
C	1.619659669	-1.173816058	-1.686977651
H	2.102783988	-2.142420523	-1.680867464
H	1.059212744	-1.104049499	-2.620013610
N	2.672606897	-0.157142417	-1.612830970

C	2.222171360	1.198264507	-1.924169362
H	1.195250424	1.287019359	-1.590163769
H	2.219810780	1.379153579	-2.999548953
C	3.918992629	-0.542713794	-2.272149685
H	3.739024675	-0.892936341	-3.289279122
H	4.536238307	0.344220872	-2.349319217
C	3.026255232	2.280892995	-1.235836012
C	3.219164253	3.521391101	-1.826854052
N	3.495958954	2.024740133	-0.015204491
C	3.902164681	4.502654751	-1.120175794
H	2.847031804	3.716834071	-2.813545087
C	4.156377537	2.954882414	0.673020648
C	4.378137217	4.219984812	0.150093820
H	4.061859786	5.468647181	-1.558579131
H	4.496330331	2.657207680	1.644082099
H	4.910725394	4.952780343	0.721147388
C	4.709896394	-1.586764165	-1.513012880
C	5.506117428	-2.511315195	-2.173833040
N	4.670530036	-1.545087731	-0.182187419
C	6.279892996	-3.386957468	-1.423919937
H	5.526011265	-2.543785569	-3.245632969
C	5.412860945	-2.374055142	0.550241075
C	6.238516362	-3.318286407	-0.040387233
H	6.904785603	-4.108088795	-1.914080656
H	5.335963447	-2.249776627	1.610812381
H	6.827935626	-3.974045050	0.567286404
C	-3.981601092	-3.994007335	0.995263489
C	-7.605572600	-1.449062444	-1.508488287
C	-5.077303820	3.668289234	-0.670835421
C	-1.333854445	1.783204571	2.180038643
H	-3.867920098	-3.917820718	2.070764695
H	-4.549912269	-4.894258621	0.802910236
H	-2.998646277	-4.146110287	0.561294784
H	-7.367036271	-1.358367025	-2.562084064
H	-8.333961482	-2.239875567	-1.389984027

H	-8.050162453	-0.517400564	-1.193405093
H	-4.520006647	4.123724523	-1.482168985
H	-5.968094617	3.221826480	-1.072700096
H	-5.353456354	4.454993989	0.020787334
H	-0.413077521	1.785136798	1.610930753
H	-1.335380180	2.669101420	2.801228486
H	-1.300160814	0.925817738	2.827650952
Cl	4.247489799	0.108453128	3.066639256
Cu	3.324168841	-0.048865150	0.768641453

[Cu^{I}(BOT1)]Cl S_{CT}(^{1}ππ*)-min

C	-4.147972578	2.702750002	0.006774629
C	-3.000768997	2.983605445	0.773017553
C	-2.510315802	1.816381730	1.311273701
C	-3.384281715	0.751121839	0.838945963
C	-4.478234438	-1.429415421	0.460892500
C	-6.385102852	-1.699593941	-0.703790797
C	-4.812372061	-2.842757528	0.472696395
C	-5.974985140	-2.969046515	-0.253432669
C	-3.373636331	-0.672254024	0.988370950
C	-2.211106491	-1.410658247	1.611007521
N	-4.379846629	1.383840867	0.045101855
N	-5.496826875	-0.789612875	-0.277681528
F	-5.677962924	0.935774261	-1.970726826
F	-6.802419069	1.238166535	0.015377738
B	-5.601089980	0.704090412	-0.559299166
H	-6.498720542	-3.881523313	-0.436691453
H	-2.044409847	-1.134208506	2.639252606
H	-2.405350399	-2.465131082	1.598418669
H	-2.595536787	3.960787344	0.924986998
N	-0.952806492	-1.183337576	0.910932834
C	-0.661127924	-1.331411160	-0.411241753
C	0.664670417	-1.090495211	-0.533340747
H	-1.401191065	-1.579316387	-1.135918045
N	0.173167618	-0.853404562	1.591031064

N	1.137173211	-0.794848888	0.740168484
C	1.584451004	-1.144148815	-1.709031187
H	2.078633354	-2.107103783	-1.729787477
H	1.004393553	-1.065801514	-2.629924629
N	2.625949482	-0.119525796	-1.634507155
C	2.163199540	1.243230740	-1.877293979
H	1.144179851	1.313171902	-1.515877306
H	2.134665361	1.471591636	-2.943565196
C	3.868888402	-0.472205685	-2.312409273
H	3.688624220	-0.787241896	-3.341361091
H	4.480048288	0.421011059	-2.360459970
C	2.978509479	2.299662886	-1.162323238
C	3.167817025	3.558794397	-1.714586024
N	3.461822846	2.002219339	0.043167218
C	3.860213790	4.515265452	-0.984296782
H	2.784034268	3.786677912	-2.689723029
C	4.132091429	2.909113984	0.754045491
C	4.349916443	4.190145782	0.270654332
H	4.016220154	5.495194363	-1.392079924
H	4.484073189	2.579572218	1.710403593
H	4.889846812	4.903100511	0.859643223
C	4.672155245	-1.536561188	-1.596037213
C	5.457840429	-2.441078510	-2.296547402
N	4.655973815	-1.532835108	-0.264164434
C	6.247053473	-3.335340572	-1.586147261
H	5.457838048	-2.443144206	-3.368984937
C	5.414258819	-2.380138262	0.430861986
C	6.231254145	-3.305007608	-0.200716924
H	6.864438113	-4.040816714	-2.107686508
H	5.358007013	-2.285649304	1.495801601
H	6.833887018	-3.975035717	0.377736881
C	-4.127714704	-4.002469964	1.132432084
C	-7.576988720	-1.367494296	-1.529448633
C	-4.986905947	3.689294894	-0.731631453
C	-1.320812904	1.763818966	2.221804201

H	-4.022778406	-3.865439050	2.203801056
H	-4.717079499	-4.896174284	0.978799006
H	-3.140507061	-4.197374153	0.725178602
H	-7.297602501	-1.265052396	-2.573404181
H	-8.316826617	-2.152057671	-1.447524491
H	-8.014884111	-0.430410112	-1.221001417
H	-4.418216096	4.122791742	-1.548797369
H	-5.876597331	3.243299477	-1.139173088
H	-5.275142730	4.498693864	-0.070241030
H	-0.388989673	1.706152119	1.671551463
H	-1.287992928	2.667470036	2.817821717
H	-1.334154991	0.929821419	2.903420942
Cl	4.351604439	0.012473036	3.055020873
Cu	3.329534355	-0.088687561	0.796666114

$[Cu^{II}(BOT1)Cl]^{+}$ D_0-min

C	-4.613748058	2.650620487	0.096415154
C	-3.688248409	3.131900099	1.018381486
C	-3.038155365	2.050593098	1.605083964
C	-3.577779933	0.883861020	1.008395816
C	-4.064479171	-1.457349984	0.488355693
C	-5.696196890	-2.130931211	-0.886570275
C	-4.055519761	-2.909039159	0.469843442
C	-5.058561642	-3.294978721	-0.374342924
C	-3.310384441	-0.498861933	1.144607987
C	-2.116158932	-0.952890414	1.955858311
N	-4.552663842	1.309806625	0.092706702
N	-5.108037111	-1.066373200	-0.374355125
F	-5.256924427	0.590163165	-2.129462353
F	-6.832076967	0.642382804	-0.440498984
B	-5.458044797	0.398776280	-0.727712578
H	-5.342781367	-4.297568102	-0.605516221
H	-1.938543293	-0.322345488	2.802967733
H	-2.247252806	-1.951581659	2.323618136
H	-3.527939987	4.161331567	1.253813216

N	-0.890149958	-0.897627381	1.150510414
C	-0.672553009	-1.294676781	-0.130069851
C	0.640731020	-1.056461372	-0.370640745
H	-1.446318200	-1.686922670	-0.746674723
N	0.247322064	-0.425137702	1.693255175
N	1.158702671	-0.513961870	0.784502658
C	1.561199575	-1.287599580	-1.520606208
H	2.040508795	-2.252432932	-1.421360719
H	1.026186168	-1.285490428	-2.464660077
N	2.632996614	-0.253939830	-1.517197571
C	2.154332070	1.041981653	-2.054825141
H	1.116368898	1.149630070	-1.766222119
H	2.188993396	1.044440174	-3.139334753
C	3.863430732	-0.732725198	-2.185708904
H	3.632886467	-1.192973221	-3.141033809
H	4.489484905	0.128740087	-2.385484577
C	2.927381030	2.210428181	-1.495761294
C	3.093474253	3.389184463	-2.173285151
N	3.393333641	2.064587736	-0.228654753
C	3.734597372	4.459890281	-1.531888521
H	2.730996923	3.497912877	-3.175907474
C	4.001805429	3.074214651	0.389160071
C	4.185702360	4.305396422	-0.242875886
H	3.866171754	5.388433753	-2.050708009
H	4.340428242	2.891776979	1.387504377
H	4.675965052	5.100789325	0.278598985
C	4.626669243	-1.690866162	-1.301952772
C	5.430392375	-2.694729257	-1.805648444
N	4.528259489	-1.481420125	0.016751908
C	6.155465009	-3.479395933	-0.914630989
H	5.498579298	-2.860286006	-2.862078350
C	5.223658070	-2.223874046	0.882889281
C	6.054409565	-3.241674876	0.446578468
H	6.788928224	-4.261925919	-1.282460063
H	5.108148572	-1.979552862	1.917672013

H	6.604276374	-3.825109880	1.155136127
C	-3.204240936	-3.886691195	1.227920500
C	-6.815489853	-2.083749286	-1.866761722
C	-5.531819197	3.454503822	-0.765865373
C	-2.001145914	2.250272423	2.676185394
H	-3.305526207	-3.765095687	2.299651069
H	-3.517177189	-4.893762549	0.990749448
H	-2.152033011	-3.807871053	0.977101877
H	-6.423698554	-1.906810300	-2.862411854
H	-7.349456262	-3.023034585	-1.868544102
H	-7.498162160	-1.280653875	-1.638512789
H	-4.958904231	4.022727690	-1.490241594
H	-6.235415913	2.839282993	-1.298554015
H	-6.085522541	4.159695150	-0.158397119
H	-1.011447126	2.389736908	2.254319084
H	-2.242520384	3.144329234	3.235380297
H	-1.938117347	1.447409305	3.392148861
Cl	3.997305163	0.465539677	2.733113383
Cu	3.245827505	0.108846995	0.563539469

$[Cu^{II}(BOT1)Cl]^{+}$ $^{2}D_{1}$(dd)-min

C	-4.461438230	2.679243150	-0.016587482
C	-3.494288235	3.148376604	0.869359907
C	-2.894783510	2.059806021	1.493805751
C	-3.511281567	0.899948612	0.960334594
C	-4.125273049	-1.431345055	0.541606908
C	-5.802783507	-2.075683281	-0.792339571
C	-4.194885157	-2.879797655	0.587216272
C	-5.221676338	-3.247675810	-0.237252392
C	-3.312902229	-0.486253833	1.150601623
C	-2.118733813	-0.963487416	1.947688269
N	-4.476626797	1.338346096	0.040734212
N	-5.156228855	-1.022166040	-0.327027322
F	-5.225036958	0.566520504	-2.148731496
F	-6.789799938	0.769556459	-0.461408345

B	-5.431532911	0.442598851	-0.740044297
H	-5.559160145	-4.242858504	-0.424879405
H	-1.925237046	-0.343506269	2.798611996
H	-2.257739829	-1.964511936	2.306395343
H	-3.271647036	4.176445695	1.054549454
N	-0.897062114	-0.906727489	1.134190540
C	-0.697863054	-1.247564951	-0.165306109
C	0.615602551	-1.016182924	-0.412079206
H	-1.484133651	-1.594932296	-0.792566647
N	0.249094463	-0.469187205	1.684151305
N	1.153679482	-0.541909095	0.766297515
C	1.507623696	-1.203437569	-1.594048787
H	1.969376339	-2.181209919	-1.555370931
H	0.952890478	-1.142086103	-2.524905980
N	2.594340375	-0.191694750	-1.551806583
C	2.136892504	1.143862149	-1.995012416
H	1.102009578	1.249721856	-1.694327045
H	2.167012130	1.225298993	-3.076870126
C	3.813928079	-0.647810438	-2.251954493
H	3.574383091	-1.053381433	-3.229858285
H	4.448176757	0.216531422	-2.410096891
C	2.931353473	2.258042021	-1.355367776
C	3.114462666	3.475506237	-1.957525357
N	3.401953081	2.026035919	-0.101986292
C	3.774116471	4.493475182	-1.255691886
H	2.750243750	3.651562323	-2.949990974
C	4.028815503	2.988893667	0.574476499
C	4.228314585	4.252049709	0.020298055
H	3.918613807	5.450414855	-1.716134921
H	4.367416684	2.737520525	1.557835246
H	4.732524580	5.006233553	0.587708645
C	4.580029598	-1.660084573	-1.429196876
C	5.364669249	-2.640558203	-2.004155932
N	4.509686230	-1.527570281	-0.096851007
C	6.097574606	-3.483636098	-1.174917498

H	5.412029078	-2.744254110	-3.069559505
C	5.213851934	-2.327718361	0.710180358
C	6.024258315	-3.326524638	0.199672850
H	6.715947749	-4.248897432	-1.600280759
H	5.120834670	-2.143009873	1.759748265
H	6.580611356	-3.956085869	0.862199954
C	-3.391032683	-3.869268224	1.381773154
C	-6.925865908	-2.008648054	-1.767396527
C	-5.343805642	3.494989660	-0.904476210
C	-1.826218764	2.246573459	2.536039864
H	-3.493169772	-3.710019639	2.448375483
H	-3.747023279	-4.868532213	1.174467094
H	-2.334866000	-3.845179065	1.136934187
H	-6.533955650	-1.876796288	-2.770000414
H	-7.499643327	-2.923653643	-1.739055090
H	-7.571904915	-1.170655959	-1.558381410
H	-4.749901311	3.989029545	-1.665358014
H	-6.094154798	2.899560520	-1.393940199
H	-5.840879560	4.263030486	-0.324905010
H	-0.835394364	2.255067817	2.094154070
H	-1.972198182	3.202742507	3.020580780
H	-1.828311687	1.503412324	3.316495295
Cl	4.020374131	0.245744761	2.803852644
Cu	3.235457446	0.037283578	0.590069680

$[Cu^{II}(BOT1)Cl]^{+}$ $^{2}D_{2}(^{3}\pi\pi^{*})$-min

C	-4.667144106	2.686375438	0.010061902
C	-3.734090891	3.186019897	0.938220991
C	-3.103672424	2.140987886	1.557819598
C	-3.656146204	0.920259175	0.957359559
C	-4.160412360	-1.413957466	0.527156841
C	-5.789161744	-2.170541351	-0.832138722
C	-4.183400053	-2.877563236	0.602437643
C	-5.184072008	-3.288386421	-0.244336039

C	-3.342578394	-0.449245099	1.160511007
C	-2.136547809	-0.844656394	1.943401590
N	-4.597734525	1.311957636	0.055354196
N	-5.143975904	-1.047267234	-0.344308534
F	-5.136435647	0.534685741	-2.187117781
F	-6.836162744	0.674366521	-0.633273367
B	-5.451044788	0.371810224	-0.799667285
H	-5.478773623	-4.299669888	-0.420946239
H	-1.932481853	-0.200269183	2.776375158
H	-2.215153581	-1.839869553	2.336351120
H	-3.583823068	4.223448541	1.145194183
N	-0.885695334	-0.797065415	1.128406046
C	-0.689545467	-1.143554776	-0.165512995
C	0.634750195	-0.953744295	-0.404742240
H	-1.480284563	-1.481363783	-0.791944853
N	0.267160625	-0.386672123	1.678696059
N	1.178583103	-0.481633094	0.764632957
C	1.541465386	-1.181301534	-1.565458997
H	1.977773102	-2.169617317	-1.505630741
H	1.006557623	-1.118109950	-2.507658591
N	2.657464627	-0.196383309	-1.523840418
C	2.234634505	1.137247581	-2.008542044
H	1.202268389	1.277691737	-1.714040104
H	2.269144842	1.182223737	-3.092235142
C	3.867420173	-0.698180915	-2.210526587
H	3.620179656	-1.110159019	-3.183638208
H	4.529620512	0.143425625	-2.375349933
C	3.056028041	2.249021015	-1.404122484
C	3.276789337	3.445484334	-2.041844708
N	3.517506871	2.032710887	-0.152391206
C	3.970061832	4.455028026	-1.369862586
H	2.916612691	3.604406385	-3.038713996
C	4.182203895	2.993345863	0.500274424
C	4.421706105	4.229268327	-0.085498819
H	4.147755530	5.395177535	-1.852663932

H	4.513706475	2.751841696	1.488029670
H	4.954140858	4.981450177	0.458401901
C	4.589492573	-1.720954990	-1.365670814
C	5.347961324	-2.739266053	-1.908210382
N	4.499745943	-1.557580129	-0.040123522
C	6.036259314	-3.589531287	-1.049493848
H	5.408932968	-2.866281394	-2.970402934
C	5.160709568	-2.363965753	0.795830056
C	5.944502837	-3.400456716	0.319999147
H	6.634051643	-4.384932990	-1.448096384
H	5.056244364	-2.154470127	1.839303688
H	6.466403899	-4.035134192	1.005196410
C	-3.364814533	-3.805614144	1.447535551
C	-6.883256344	-2.106568965	-1.835072582
C	-5.572778468	3.453348512	-0.887650908
C	-2.115451369	2.287187723	2.675612459
H	-3.510359867	-3.628794530	2.507820350
H	-3.667106793	-4.825611668	1.251568769
H	-2.301724899	-3.744196499	1.239787601
H	-6.487451765	-1.831799309	-2.807414610
H	-7.370834599	-3.067469302	-1.919209675
H	-7.612350249	-1.358034903	-1.563459675
H	-4.999609577	3.935552257	-1.673071519
H	-6.315113234	2.823815411	-1.344988287
H	-6.077192868	4.230777191	-0.326105116
H	-1.120358895	1.949891552	2.406794894
H	-2.044402222	3.330933468	2.950745073
H	-2.418885758	1.752535749	3.565609036
Cl	4.078080598	0.317227621	2.748215425
Cu	3.277823763	0.056422230	0.583323845

$[Cu^{II}(BOT1)Cl]^{+}$ $^{2}D_{3}(^{3}\pi\pi^{*}/dd)$-min

C	-4.659230477	2.658660430	0.019069428

C	-3.707427141	3.172974408	0.913859618
C	-3.058253093	2.120627649	1.526715972
C	-3.616473394	0.910069566	0.966477299
C	-4.129881616	-1.438905051	0.519848497
C	-5.785183495	-2.165219854	-0.821514150
C	-4.131594357	-2.893579748	0.547840844
C	-5.145956180	-3.304151220	-0.282924125
C	-3.326976365	-0.467055091	1.146573388
C	-2.108125995	-0.893363800	1.926977790
N	-4.599783674	1.303338333	0.060681984
N	-5.168058602	-1.071328665	-0.335183351
F	-5.314240403	0.545691532	-2.134750225
F	-6.878748230	0.653123991	-0.441503390
B	-5.511484450	0.372980406	-0.729465636
H	-5.434074973	-4.313103677	-0.480587117
H	-1.910015284	-0.264862067	2.770570756
H	-2.217608233	-1.891835600	2.303370185
H	-3.540838460	4.209458021	1.109384949
N	-0.867417118	-0.842146703	1.121173230
C	-0.652757197	-1.225691383	-0.162138332
C	0.665080000	-1.006672534	-0.404679319
H	-1.431024834	-1.600940141	-0.782949035
N	0.274002249	-0.387516540	1.664826895
N	1.190517241	-0.487848082	0.759539319
C	1.569519966	-1.246301381	-1.568113635
H	2.028935371	-2.222243222	-1.482711847
H	1.026266640	-1.223847856	-2.507612246
N	2.657367814	-0.235679016	-1.555230519
C	2.208093335	1.079478534	-2.059822643
H	1.169586005	1.198390647	-1.777201166
H	2.252672406	1.116232021	-3.143743763
C	3.886163642	-0.720564959	-2.218370227
H	3.660308808	-1.166312356	-3.182022778
H	4.523909171	0.136024595	-2.403038619
C	2.995756429	2.218172119	-1.455423298

C	3.190160117	3.409361621	-2.105326028
N	3.448317280	2.038303729	-0.186898805
C	3.843159397	4.454228439	-1.438362618
H	2.840577339	3.543932311	-3.109513255
C	4.069270194	3.027674025	0.456788169
C	4.279799103	4.265538374	-0.147105177
H	3.997161724	5.390490453	-1.936729733
H	4.393970872	2.816426552	1.454216340
H	4.779103867	5.041576682	0.394630398
C	4.640789285	-1.697864007	-1.343478121
C	5.432675511	-2.700914398	-1.867350807
N	4.552503528	-1.511797862	-0.018306580
C	6.153228653	-3.510274156	-0.994846682
H	5.494285713	-2.847720994	-2.926941844
C	5.244499038	-2.279529702	0.829846755
C	6.060948873	-3.298283507	0.371195477
H	6.776481340	-4.292429055	-1.380524502
H	5.136591971	-2.053142113	1.869821223
H	6.607098847	-3.901274621	1.066137907
C	-3.275556100	-3.843287352	1.339127173
C	-6.914011015	-2.135127582	-1.793033033
C	-5.587235908	3.432647405	-0.854461694
C	-2.008117326	2.345886259	2.580113635
H	-3.380602849	-3.701063759	2.408570373
H	-3.584621512	-4.857019354	1.125387036
H	-2.220335067	-3.772161744	1.094833771
H	-6.537772288	-1.972175629	-2.797842302
H	-7.446459426	-3.075145071	-1.774429976
H	-7.598578147	-1.331547576	-1.570437062
H	-5.022262861	3.967336426	-1.610372810
H	-6.304121588	2.800796259	-1.348058536
H	-6.122679145	4.166050659	-0.263691934
H	-1.014259550	2.417419228	2.150299173
H	-2.212659997	3.281744606	3.082986542
H	-1.976742122	1.588752580	3.345355977

Cl	4.032381370	0.384773783	2.805592770
Cu	3.269145457	0.081666305	0.589733012

$[Cu^{II}(BOT1)Cl]^{+}$ $^{2}D_{LMCT}(\pi d)$-min

C	-4.522834015	2.678467551	0.311461448
C	-3.451225770	3.032125030	1.196336746
C	-2.863352355	1.900937470	1.662341709
C	-3.583665728	0.781500079	1.018260071
C	-4.284669518	-1.460350086	0.371142152
C	-6.037035723	-1.934990455	-0.929232942
C	-4.369528567	-2.927756560	0.259763759
C	-5.439344573	-3.180710551	-0.537074050
C	-3.386536455	-0.617513151	1.044625248
C	-2.165662363	-1.192628706	1.746257240
N	-4.587206173	1.342809511	0.237127696
N	-5.337063448	-0.940415770	-0.371696424
F	-5.442350458	0.858806049	-1.986391552
F	-6.927025335	0.887011784	-0.208228880
B	-5.617836641	0.564059518	-0.618018949
H	-5.801849880	-4.143858034	-0.830830940
H	-1.937122272	-0.649863730	2.644985580
H	-2.304139318	-2.218386361	2.038681403
H	-3.185210166	4.036169220	1.454078447
N	-0.962716405	-1.067831221	0.934313657
C	-0.642145638	-1.442064790	-0.350954303
C	0.690560392	-1.143021757	-0.482900171
H	-1.325763505	-1.883603333	-1.029992735
N	0.125130937	-0.560691135	1.534399504
N	1.089362216	-0.596347040	0.710568282
C	1.666373548	-1.398092504	-1.598482419
H	2.167144292	-2.335237101	-1.395900880
H	1.122680051	-1.518358083	-2.534838346
N	2.700820252	-0.375463558	-1.696210964
C	2.272097551	0.914301899	-2.224489103
H	1.229569760	1.041050804	-1.965197861

H	2.335291818	0.935123849	-3.311511620
C	3.994260695	-0.842612146	-2.185590289
H	3.897917357	-1.348698068	-3.145020249
H	4.605450210	0.035609010	-2.347488010
C	3.022520489	2.114286126	-1.675263646
C	3.241519097	3.238977623	-2.462600207
N	3.408213254	2.101348690	-0.406202849
C	3.862456723	4.345268748	-1.892994731
H	2.946582893	3.249429884	-3.492421748
C	4.011615396	3.143156090	0.156824019
C	4.254015724	4.303746135	-0.561833248
H	4.046285052	5.220541994	-2.483442980
H	4.292886820	3.009759597	1.181465960
H	4.743310313	5.134095905	-0.097669129
C	4.752580424	-1.743534168	-1.229429126
C	5.581940484	-2.752983380	-1.700539475
N	4.675386846	-1.492931667	0.072864122
C	6.340501148	-3.478981921	-0.787933679
H	5.646262614	-2.960186013	-2.749633842
C	5.395578386	-2.169394677	0.961695839
C	6.252488917	-3.184632701	0.565353674
H	6.992586798	-4.256928210	-1.131120979
H	5.272666307	-1.860516049	1.979080021
H	6.830869437	-3.717039270	1.290846120
C	-3.512044942	-3.990944717	0.883281645
C	-7.200550441	-1.738325900	-1.834897044
C	-5.404618850	3.624491133	-0.424240445
C	-1.733049638	1.898039277	2.651281472
H	-3.561709952	-3.975699475	1.966096208
H	-3.861394204	-4.963710452	0.564183599
H	-2.470166108	-3.912641486	0.591900221
H	-6.849285546	-1.427618018	-2.815740172
H	-7.753000641	-2.660535697	-1.944634091
H	-7.859974774	-0.964284902	-1.468170850
H	-4.819102063	4.142572356	-1.179309320

H	-6.235002996	3.138494568	-0.906193327
H	-5.783718786	4.374910495	0.260637350
H	-0.777769999	1.677959175	2.184737504
H	-1.657212532	2.878919697	3.100656759
H	-1.868253504	1.195734003	3.460544370
Cl	3.995128297	0.699906710	3.149142493
Cu	3.282089571	0.164200793	0.779666131

$[Cu^{II}(BOT1)Cl]^{+}$ Cl($^2D_{3'}$/ $^2D_2$)

C	-4.676074591	2.665817791	0.195548475
C	-3.698689219	3.157310402	1.162959457
C	-3.019746733	2.116521720	1.663165575
C	-3.552289978	0.893380776	1.033170344
C	-4.078421812	-1.451560256	0.487084954
C	-5.664264642	-2.186415721	-0.913763472
C	-4.112862604	-2.862840588	0.573216396
C	-5.093327815	-3.300008365	-0.300778503
C	-3.315639552	-0.446972934	1.167440604
C	-2.147891639	-0.909609314	2.056412984
N	-4.583647694	1.334474165	0.124335857
N	-5.069334670	-1.067805858	-0.440935662
F	-4.841568341	0.611162564	-2.167108594
F	-6.705644933	0.674100133	-0.860756051
B	-5.394576283	0.390728270	-0.958045167
H	-5.382962536	-4.322373476	-0.472407739
H	-1.941285949	-0.214145574	2.864712055
H	-2.331198897	-1.893216684	2.484162280
H	-3.575080949	4.197751699	1.416129098
N	-0.891189712	-0.973249308	1.240393451
C	-0.663029179	-1.598797878	0.025260616
C	0.631149758	-1.337827751	-0.276001708
H	-1.435982209	-2.148929085	-0.493711492
N	0.231879709	-0.329970105	1.672904468
N	1.160654091	-0.557536503	0.749610498
C	1.525146242	-1.730466406	-1.438050932

H	2.060227067	-2.652175236	-1.198668449
H	0.936640339	-1.901409126	-2.344217192
N	2.539930868	-0.649199396	-1.613867020
C	1.976835521	0.571026803	-2.251379134
H	0.923555611	0.646745850	-1.972953133
H	2.035573561	0.535584199	-3.341720391
C	3.794917731	-1.107929500	-2.270527815
H	3.608031445	-1.902758380	-2.996097817
H	4.222115295	-0.260362285	-2.810715883
C	2.709609378	1.806657823	-1.717869908
C	2.827280649	2.960813152	-2.469809749
N	3.197701432	1.731044220	-0.443982043
C	3.453719333	4.077050888	-1.921799262
H	2.428107211	2.986866818	-3.475714913
C	3.804951572	2.828946711	0.080908975
C	3.948404930	4.011755231	-0.628229652
H	3.550369599	4.989175874	-2.504924771
H	4.170769142	2.728109049	1.100652509
H	4.439574822	4.857918908	-0.163995495
C	4.823241515	-1.567756637	-1.229459903
C	5.815764966	-2.472626666	-1.560621068
N	4.748452053	-0.998864868	0.008546408
C	6.772548178	-2.817024131	-0.611454786
H	5.839801731	-2.900700066	-2.554210478
C	5.691056780	-1.345317917	0.924824271
C	6.711543460	-2.242778760	0.648482149
H	7.556588620	-3.527008111	-0.858896861
H	5.591981093	-0.875126082	1.900126776
H	7.435922872	-2.482195487	1.416553059
C	-3.323566913	-3.822557849	1.453879053
C	-6.762287748	-2.155650446	-1.962876217
C	-5.638899377	3.498483674	-0.634330134
C	-1.940476007	2.250290405	2.726999820
H	-3.553449135	-3.679439253	2.507746165
H	-3.594896398	-4.841524589	1.197141376

H	-2.249006721	-3.726991909	1.325500329
H	-6.342236849	-1.969546618	-2.949839111
H	-7.278836817	-3.109796534	-1.982370636
H	-7.477015126	-1.366866152	-1.744281605
H	-5.104990024	3.982893465	-1.449171841
H	-6.424955032	2.871867902	-1.044391611
H	-6.084132287	4.268538306	-0.010196662
H	-1.002822045	1.793582747	2.422263782
H	-1.757224804	3.303429374	2.913701110
H	-2.254981985	1.797114370	3.665012521
Cl	3.659043000	0.655341768	2.849516926
Cu	3.156983899	0.201359947	0.675881190

$[Cu^{II}(BOT1)Cl]^{+}$ STC($^{2}D_{LMCT}/^{2}D_{2}$)

C	-4.666981850	2.666219161	0.229905923
C	-3.617457293	3.091353977	1.113513595
C	-2.981536225	2.001591941	1.609123100
C	-3.639074163	0.830454579	0.978660717
C	-4.242660141	-1.449314359	0.400342918
C	-5.978910100	-2.033576589	-0.881502138
C	-4.266489358	-2.927477805	0.323245804
C	-5.328121199	-3.245199377	-0.457146705
C	-3.384781084	-0.553988508	1.043151490
C	-2.150312693	-1.061794923	1.773321265
N	-4.668987252	1.330590226	0.185513348
N	-5.321660156	-0.998082284	-0.357424062
F	-5.508782471	0.749681239	-2.020623198
F	-6.987972955	0.762698697	-0.239305671
B	-5.667134423	0.485170999	-0.644374405
H	-5.652048956	-4.229735855	-0.724353736
H	-1.936938578	-0.478245742	2.651152548
H	-2.265907415	-2.076535579	2.107362075
H	-3.405441095	4.112479009	1.353930811
N	-0.945942809	-0.966736009	0.957287994
C	-0.637200894	-1.362653255	-0.319788896

C	0.697932779	-1.083720636	-0.460875577
H	-1.332553241	-1.796477696	-0.993289128
N	0.153820364	-0.475092220	1.549737294
N	1.112135729	-0.537398176	0.716177889
C	1.658721359	-1.349813198	-1.584489004
H	2.139439339	-2.299341956	-1.392597274
H	1.109844021	-1.447452766	-2.520129828
N	2.717018685	-0.350215836	-1.675390829
C	2.314237729	0.946760229	-2.206325719
H	1.272596844	1.090960585	-1.953535741
H	2.386026348	0.966420206	-3.292556279
C	3.991505549	-0.848681280	-2.182304855
H	3.867843658	-1.358158186	-3.136503830
H	4.620887315	0.013756087	-2.357943938
C	3.080491444	2.132788205	-1.650270864
C	3.305648659	3.265316071	-2.424634396
N	3.470876360	2.101576908	-0.384926658
C	3.937404616	4.358818178	-1.842402635
H	3.006279966	3.292213653	-3.452755135
C	4.086150848	3.128348234	0.190668148
C	4.333971343	4.296823851	-0.513375476
H	4.125477470	5.240460384	-2.421910445
H	4.368478716	2.977216186	1.212485103
H	4.831318220	5.117468167	-0.040682384
C	4.740367553	-1.761593803	-1.230744078
C	5.553993734	-2.783003622	-1.704248198
N	4.668517681	-1.513893716	0.069592840
C	6.299285225	-3.522391230	-0.791646773
H	5.616148407	-2.989936496	-2.753467366
C	5.375336192	-2.199645465	0.959572034
C	6.215252725	-3.229389248	0.562173689
H	6.938544678	-4.310591572	-1.135701198
H	5.255666631	-1.887844784	1.976434474
H	6.784392911	-3.772994700	1.286611194
C	-3.361550007	-3.939053035	0.965378188

C	-7.152733561	-1.912733164	-1.786650097
C	-5.591293163	3.553904254	-0.525409047
C	-1.868249779	2.075298749	2.613967385
H	-3.397143839	-3.891927726	2.047990642
H	-3.677941327	-4.933468882	0.680600610
H	-2.327549770	-3.830233380	0.655743186
H	-6.815673319	-1.626210344	-2.780138529
H	-7.672485423	-2.857309818	-1.859834770
H	-7.837382716	-1.148710915	-1.445609023
H	-5.026883319	4.089999178	-1.284364757
H	-6.392678184	3.019395349	-1.005099370
H	-6.011820639	4.294770098	0.145847065
H	-0.892330687	1.941382545	2.159138740
H	-1.879432093	3.051744414	3.078860732
H	-1.954379472	1.349084420	3.409065213
Cl	4.031524907	0.655631365	3.114020723
Cu	3.303036338	0.157161679	0.750927462

$[Cu^{II}(BOT1)Cl]^{+}$ Cl($^2D_1/^2D_0$)

C	-4.746614575	2.695255175	0.040215022
C	-3.775959384	3.210964440	0.930923102
C	-3.098998773	2.164294715	1.497056545
C	-3.659834718	0.937645850	0.909516443
C	-4.201140037	-1.389990155	0.486234407
C	-5.920886609	-2.145822042	-0.767570303
C	-4.217770300	-2.828332162	0.549041356
C	-5.282884508	-3.254620055	-0.225552860
C	-3.357746932	-0.419990696	1.091376434
C	-2.140778480	-0.843882478	1.836659543
N	-4.663033934	1.330937842	0.053968955
N	-5.249013984	-1.044314843	-0.325451850
F	-5.206312619	0.552746735	-2.182774998
F	-6.910942157	0.730988005	-0.591910513
B	-5.541274218	0.403975376	-0.800097733
H	-5.588406078	-4.257090699	-0.389431941

H	-1.930651815	-0.251362579	2.694415302
H	-2.238101950	-1.848780464	2.162135778
H	-3.624433982	4.239579309	1.144660683
N	-0.901216277	-0.799212674	1.027838042
C	-0.712152068	-1.096962191	-0.259885355
C	0.612524793	-0.936892587	-0.493892019
H	-1.504778257	-1.387390059	-0.885491251
N	0.259807424	-0.457510781	1.567027372
N	1.157336695	-0.537319556	0.671126114
C	1.514625484	-1.132590700	-1.642566424
H	1.914895330	-2.130904811	-1.627831463
H	0.981038871	-1.003197888	-2.571929057
N	2.650511969	-0.197032673	-1.548383267
C	2.288945427	1.163861228	-1.980272305
H	1.278829208	1.347177758	-1.656769870
H	2.309022306	1.242678015	-3.056505226
C	3.849650671	-0.717545061	-2.219960442
H	3.584440205	-1.219906809	-3.136829295
H	4.474967049	0.119304936	-2.479175689
C	3.174799858	2.214412833	-1.387571995
C	3.444581272	3.412389547	-1.995130941
N	3.664673361	1.923601052	-0.180659081
C	4.234612250	4.346588426	-1.329403699
H	3.049389946	3.623343496	-2.960273169
C	4.422334307	2.811541219	0.473428617
C	4.727195871	4.039050829	-0.077401912
H	4.452801063	5.281790789	-1.782224407
H	4.765166317	2.525755537	1.431529135
H	5.330111593	4.723279827	0.464798492
C	4.647214751	-1.652978913	-1.363540903
C	5.451743249	-2.636656060	-1.891094138
N	4.580153198	-1.454110102	-0.059162494
C	6.211283896	-3.417656194	-1.031099520
H	5.490758905	-2.787761454	-2.943498170
C	5.301804791	-2.191473433	0.782560064

C	6.135997954	-3.188640616	0.329827463
H	6.840454531	-4.181278353	-1.416578216
H	5.199516512	-1.968621902	1.810389210
H	6.698945179	-3.761553962	1.022944052
C	-3.308872666	-3.742507974	1.307228347
C	-7.077093865	-2.144551271	-1.690668165
C	-5.694726995	3.467197112	-0.788104878
C	-2.052485881	2.347043750	2.542039623
H	-3.381586028	-3.605512334	2.377780608
H	-3.591241281	-4.761599647	1.099194662
H	-2.268401311	-3.635921579	1.027056315
H	-6.737795150	-2.056143601	-2.714767131
H	-7.623240135	-3.067588473	-1.593004974
H	-7.738407837	-1.324913144	-1.493746960
H	-5.163470317	3.933754960	-1.606933406
H	-6.475147653	2.855957675	-1.190026709
H	-6.141882246	4.247518169	-0.190808881
H	-1.078940535	2.008589697	2.230410951
H	-1.978018180	3.397807216	2.771825943
H	-2.303040534	1.839778027	3.462434035
Cl	3.799568246	0.152539004	2.910995781
Cu	3.243292005	-0.002538734	0.663569220