Electronic Supplementary Information

Deciphering Novel Mechanism for Single-Component White Light Emission: Synergistic Effects of ESIPT and Excimer

Siqi Wang, Hongyan Mu, Jialin Liang, Xinlin Yang, Jiaan Gao, Hui Li* and Guangyong Jin*

Jilin Key Laboratory of Solid-State Laser Technology and Application, School of Physics, Changchun University of Science and Technology, Changchun 130022, China

* Corresponding author: E-mail address: huili@cust.edu.cn and jgycust@163.com

Tel: +86-431-85582465 Fax: +86-431-85582465

Table of contents

Table S1 Calculated the maximum fluorescence peaks (nm) of CF_3-HTTH based on the TD-DFT method with different functionals at 6-311+G (d, p) basis set.

WB97XD	CAM-B3LYP	M062X	PBE0-D3BJ	B3LYP-D3BJ	Exp.
407	413	409	430	436	450

Table S2 Calculated bond lengths (Å) and angles (°) of CF_3-HTTH and CF_3-MTTH for different electronic states.

	CF_3-HTTH						CF_3-MTTH		
	O_1-H_1	N_1-H_1	O_2-H_2	N_2-H_2	δ（O_1-H_1…N_1）	δ（O_2-H_2…N_2）	O_1-H_1	N_1-H_1	δ（O_1-H_1…N_1）
S_0-Enol	0.984	1.789	0.984	1.789	145.538	145.538	0.988	1.707	148.193
S_1-Enol	0.989	1.773	0.989	1.773	146.569	146.569	0.994	1.684	149.301
S_1-Keto	1.791	1.037	0.981	1.817	133.820	146.436	1.662	1.041	139.030

Table S3 Calculated absorption and emission peak (nm).

	$\lambda_{abs.}$	$\lambda_{flu.}$(Enol*)	$\lambda_{flu.}$(Keto*)	$\lambda_{flu.}$(exp.)
HTTH-CF_3	395	436	551	450 520 600
MTTH-CF_3	388	431	529	450 520
MTTM-CF_3	384	441	-	470 600

xyz coordinates for models (high layer)

CF_3-HTTH

S	1.397389	1.300619	0.811515
F	6.999944	2.654522	0.104073
F	6.004122	2.589712	2.029843
F	7.823339	1.439439	1.698691
O	3.602876	2.374320	1.035164
H	2.641930	2.164655	1.001572
N	1.406446	0.992352	0.455105
C	0.115690	0.601327	0.319894
C	2.216634	0.099598	0.081937
C	3.659719	0.228652	0.086813
C	4.285551	1.375585	0.463984
C	5.680938	1.484360	0.412713
H	6.129655	2.374013	0.830135
C	6.450916	0.478085	0.137058
H	7.525866	0.571485	0.174698
C	5.840556	0.672617	0.649929
C	4.464955	0.781533	0.624433
H	4.002145	1.666487	1.030437
C	6.663912	1.828337	1.127321
S	1.397522	1.300362	0.811695
F	6.999431	2.654996	0.104061
F	6.003752	2.589918	2.029906
F	7.823231	1.440092	1.698641
O	3.603309	2.374504	1.034921
H	2.642343	2.164940	1.001394
N	1.406602	0.992621	0.454920
C	0.115547	0.600989	0.320190
C	2.216769	0.099844	0.082119
C	3.659863	0.228734	0.086902
C	4.285841	1.375650	0.463778
C	5.681233	1.484266	0.412435
H	6.130046	2.373886	0.829810
C	6.451085	0.477880	0.137314
H	7.526037	0.571192	0.175080
C	5.840580	0.672824	0.649992
C	4.464969	0.781627	0.624354
H	4.002058	1.666601	1.030212
C	6.663697	1.828719	1.127334

CF_3-MTTH

S	0.111095	0.339246	0.663073
S	3.110505	0.318918	1.873343
F	3.921091	3.570032	2.084897
F	5.151927	4.682971	0.672558
F	5.277313	2.516370	0.763760
F	5.759713	4.789160	3.268777
F	3.710324	5.209058	2.688792
F	5.338678	6.428109	1.913422
O	0.441048	3.015186	3.120317
H	0.230475	2.353994	2.825116
O	5.443897	1.642008	2.148621
N	0.751146	1.247891	1.633528
N	2.232602	1.245540	0.420152
C	1.344072	3.140570	2.145925
C	2.352474	4.095595	2.309609
H	2.331722	4.703260	3.204592
C	3.334194	4.255062	1.350962
H	4.098446	5.007265	1.478861
C	3.328306	3.456342	0.202804
C	2.320631	2.525129	0.017845
H	2.310431	1.931270	0.883631
C	1.308818	2.348396	0.965446
C	0.231449	1.395068	0.764147
C	1.632837	0.307603	1.216670
C	1.361967	0.311420	0.009489
C	3.216722	1.383269	0.443486
C	4.274426	2.371762	0.249111
C	4.160862	3.255374	0.830651
H	3.297076	3.165121	1.473688
C	5.116365	4.233658	1.057614
C	6.224692	4.341322	0.216956
H	6.971028	5.106376	0.390178
C	6.358723	3.477134	0.859825
H	7.211910	3.569690	1.513940
C	5.389251	2.501398	1.104021
C	4.413352	3.563525	0.821919
C	6.447218	1.810190	3.147725
H	6.251657	1.041521	3.890315
H	7.446941	1.666525	2.732539
H	6.375308	2.798735	3.609080
C	4.975527	5.161620	2.226160

CF_3-MTTM

S	0.687242	0.675419	1.837461
O	0.032431	2.177990	4.004646
N	1.408286	1.042206	0.302056
C	0.590631	0.169745	0.321214
C	0.892847	1.414017	1.453752
C	1.583201	2.371680	2.316722
C	2.764393	2.953133	1.843318
H	3.101705	2.674829	0.858067
C	3.477198	3.864134	2.606909
C	3.015607	4.222602	3.872137
H	3.563286	4.942435	4.462716
C	1.841774	3.669549	4.362474
H	1.481673	3.960863	5.337390
C	1.124366	2.748052	3.595643
C	4.772538	4.425552	2.101415
C	0.625007	2.596616	5.229610
H	0.028728	2.374146	6.076916
H	1.543632	2.023657	5.315863
H	0.857078	3.665432	5.206840
F	5.845142	3.788928	2.638573
F	4.924696	5.732870	2.417857
F	4.889936	4.321797	0.761849
S	0.687270	0.675500	1.837314
O	0.032050	2.177551	4.004820
N	1.408294	1.042216	0.301948
C	0.590679	0.169645	0.321052
C	0.892909	1.413949	1.453691
C	1.583357	2.37149	2.316721
C	2.764487	2.953001	1.843238
H	3.101663	2.674844	0.857900
C	3.477394	3.863906	2.606848
C	3.015989	4.222182	3.872198
H	3.563750	4.941924	4.462813
C	1.842230	3.669047	4.362627
H	1.482281	3.960220	5.337642
C	1.124708	2.747660	3.595766
C	4.772611	4.425469	2.101185
C	0.624581	2.596125	5.229823
H	0.029204	2.373659	6.077092
H	1.543185	2.023133	5.316106
H	0.856682	3.664935	5.207094
F	5.845378	3.788901	2.638090
F	4.924691	5.732779	2.417701

F	4.889788	4.321831	0.761590