Supplementary Information

A molecular descriptor of shallow potential energy surface for ground state to achieve narrowband thermally activated delayed fluorescence emission

Jiaqiang Zhao[1], Huanling Liu[2], Jianzhong Fan[2]*, Qingfang Mu[2]*

1. School of Physics and Electronic Information, Weifang University, Weifang 261061, China
2. Shandong Province Key Laboratory of Medical Physics and Image Processing Technology, Institute of Materials and Clean Energy, School of Physics and Electronics, Shandong Normal University, Jinan 250014, China.

Corresponding Author

*Author to whom correspondence should be addressed.

E-mail: fanjianzhongvip@163.com and qingfangmusdnu@163.com

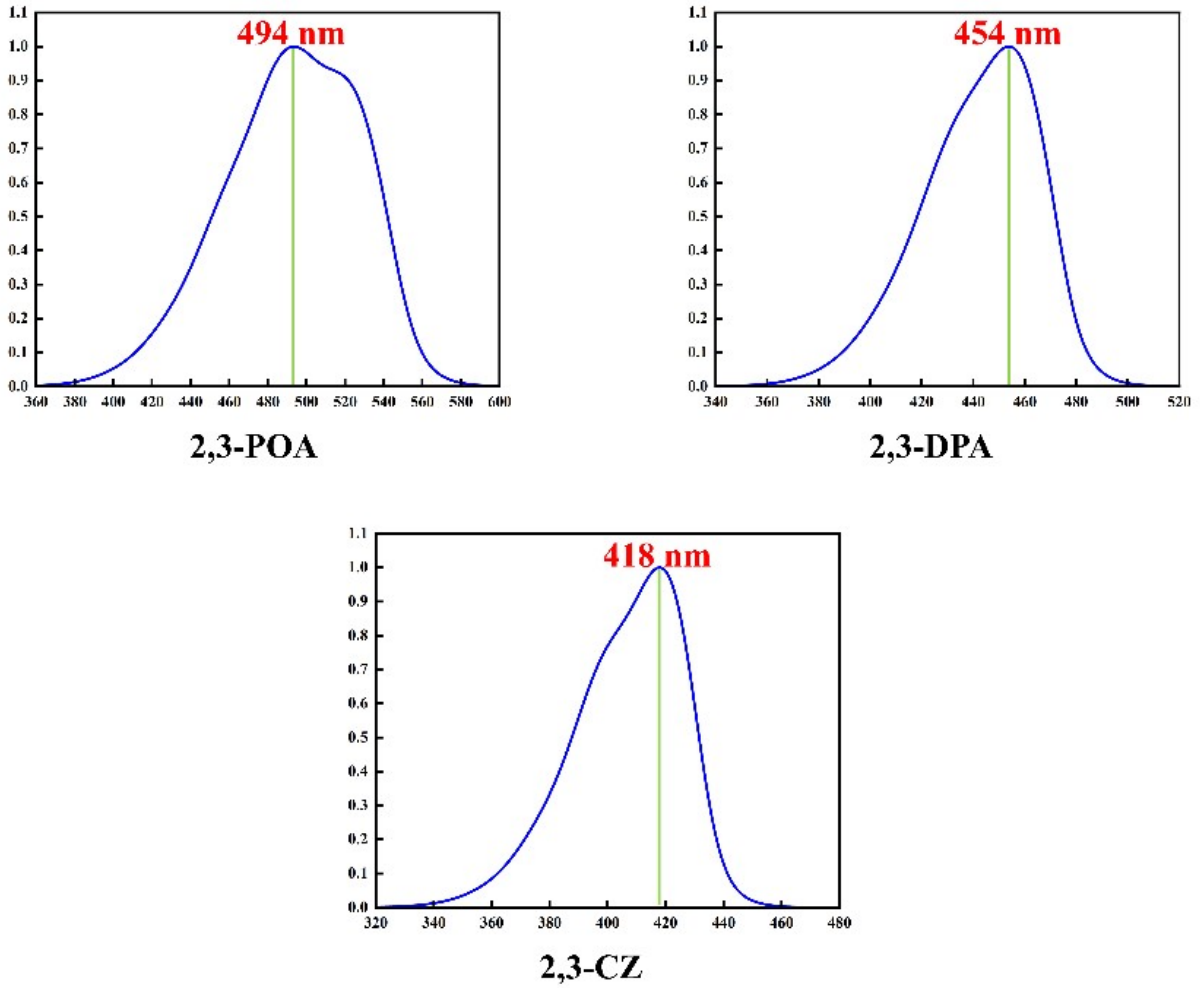

Figure S1. Calculated absorption spectra in toluene.

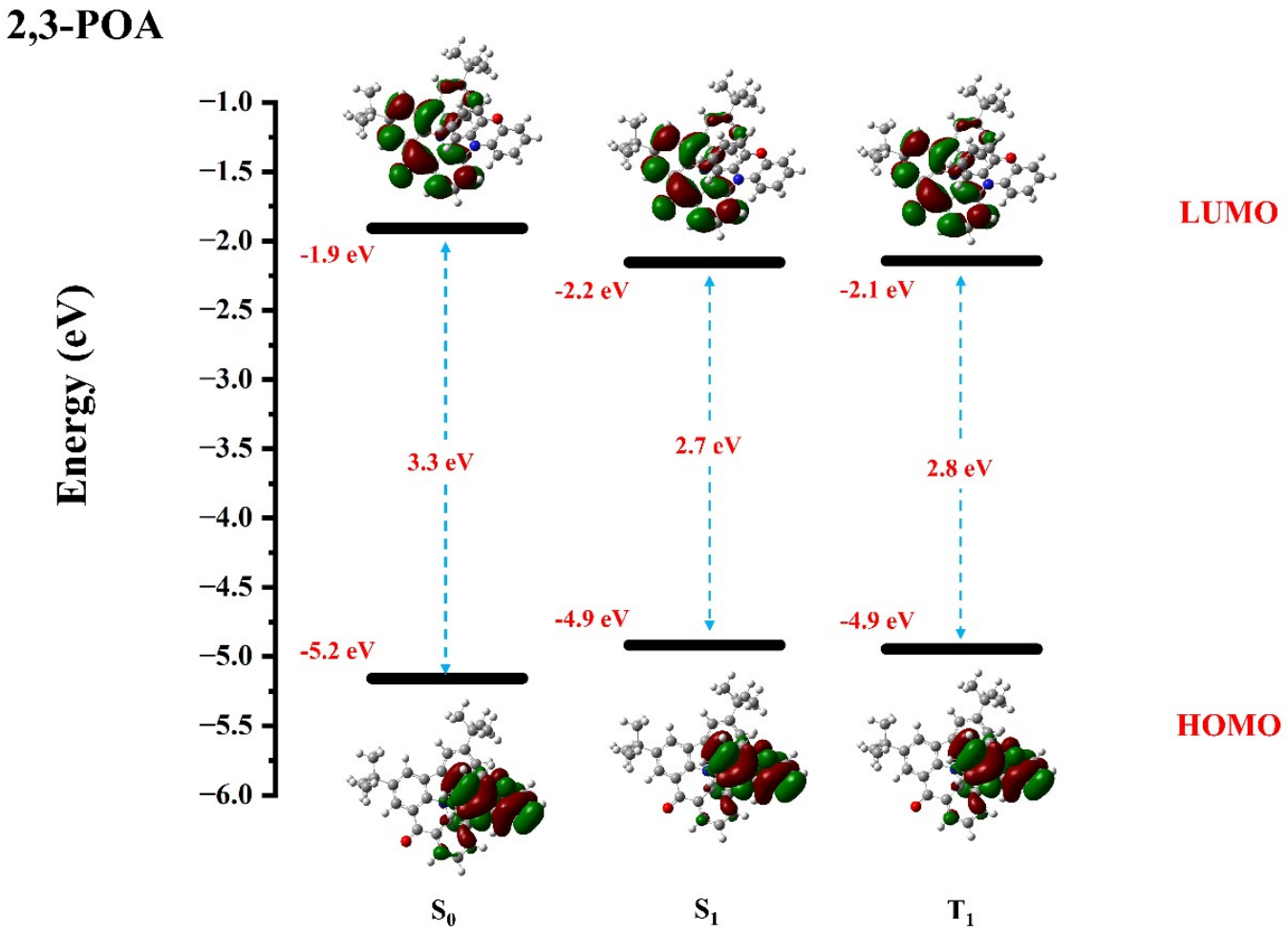

Figure S2. The orbital transition information for 2,3-POA of the S_0, S_1 and T_1 states in toluene.

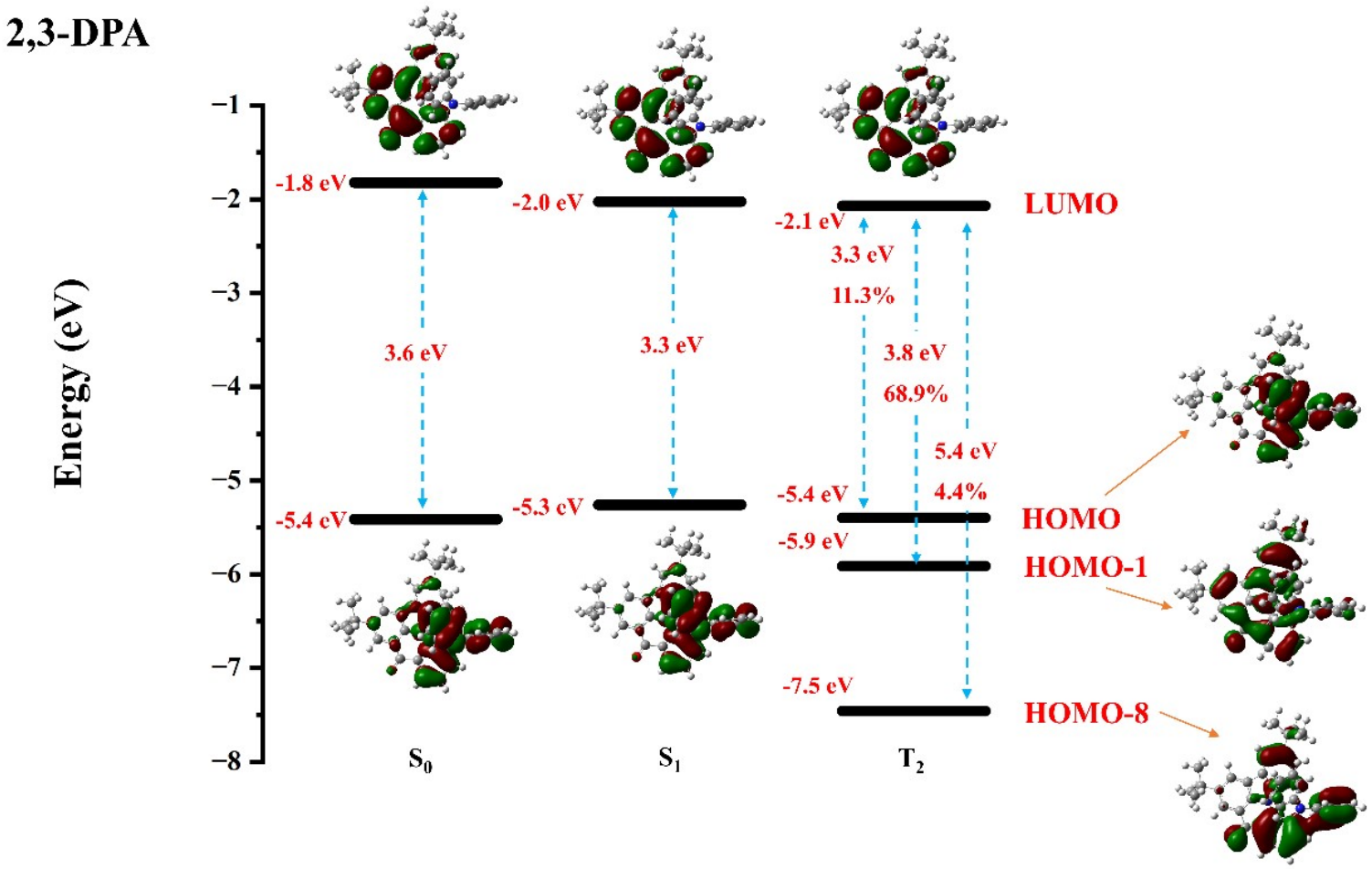

Figure S3. The orbital transition information for 2,3-DPA of the S_0, S_1 and T_2 states in toluene.

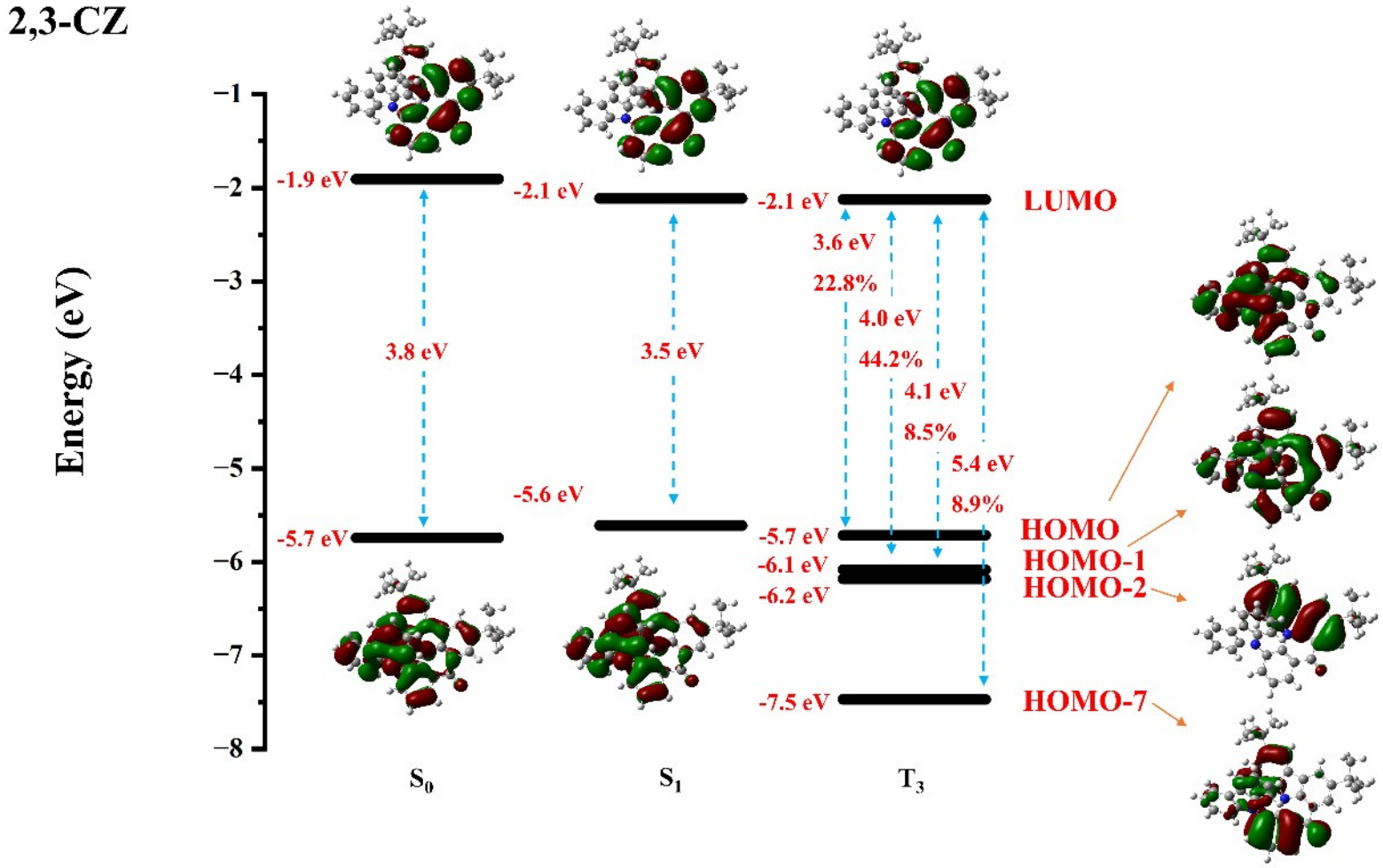

Figure S4. The orbital transition information for 2,3-CZ of the S_0, S_1 and T_3 states in toluene.

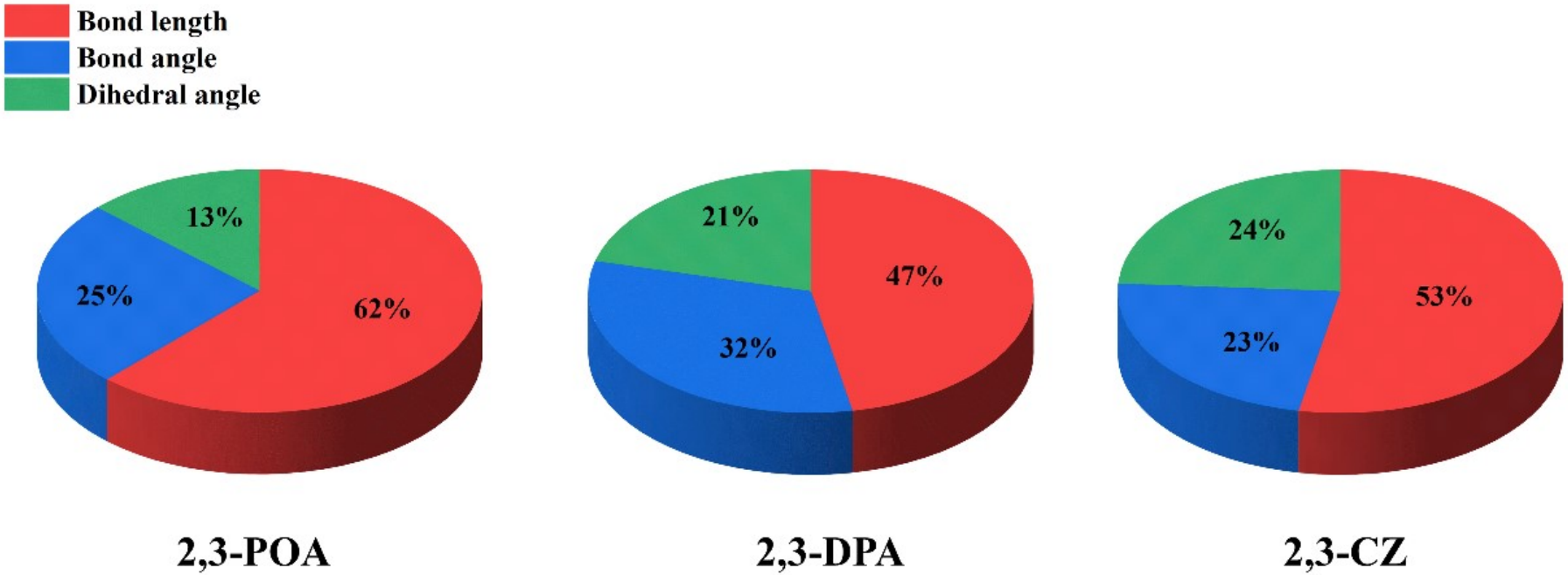

Figure S5. Contribution to the reorganization energy from bond length (red), bond angle (blue) and dihedral angle (green) in toluene for 2,3-POA, 2,3-DPA and 2,3-CZ, respectively.

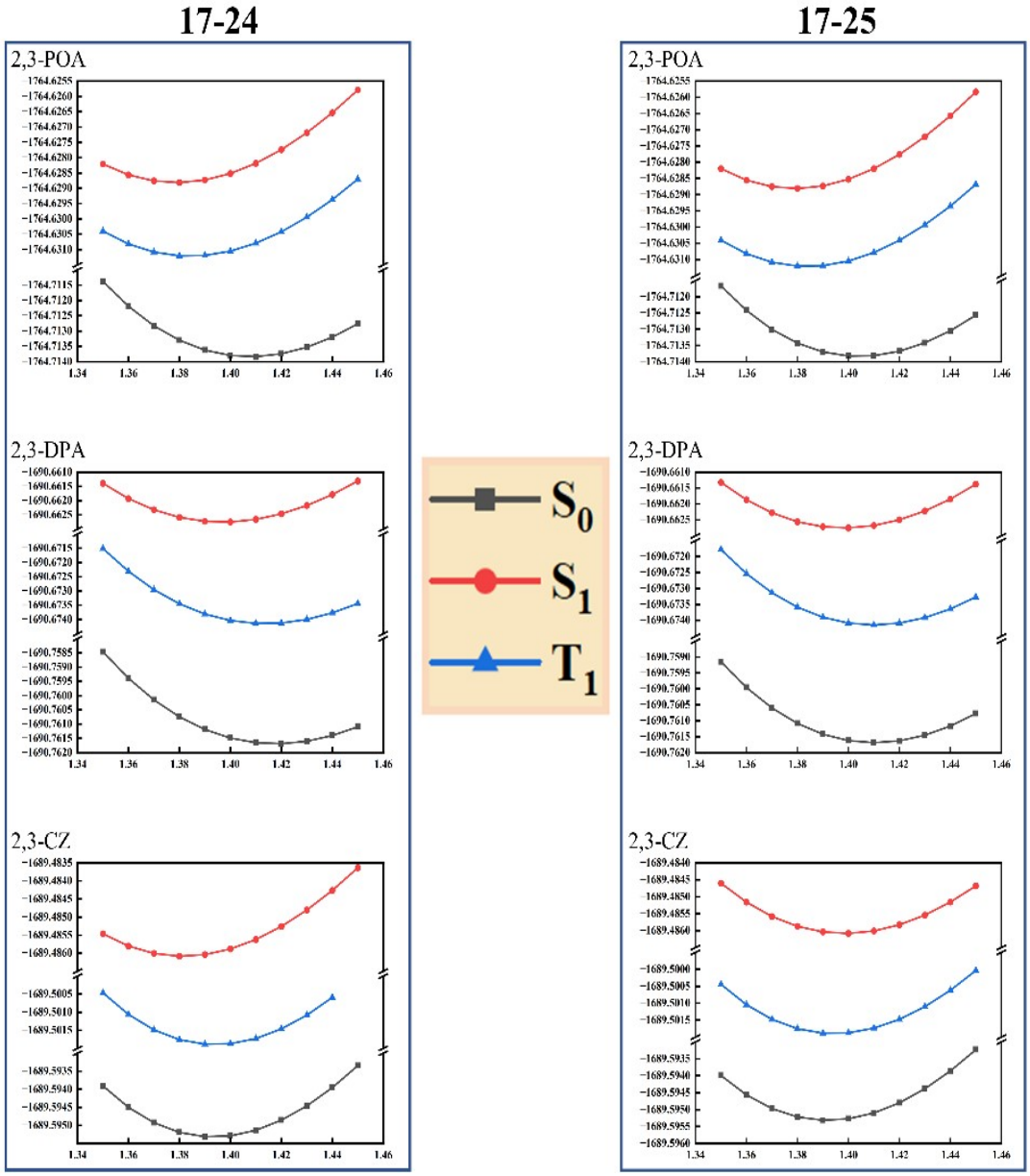

Figure S6. Potential energy curve of bond length between atom 17 and atom 24 as well as between atom 17 and atom 25 of S_0, S_1 and T_1 for 2,3-POA, 2,3-DPA and 2,3-CZ in toluene.

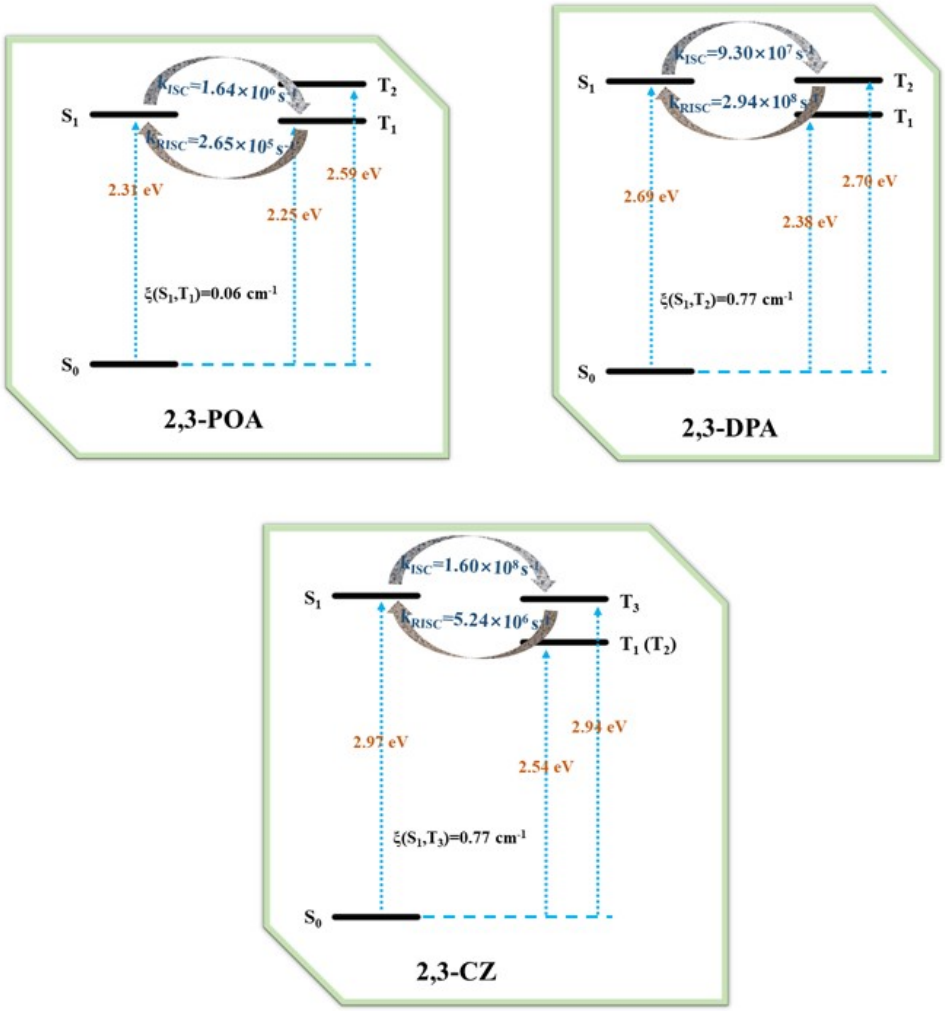

Figure S7. Adiabatic excitation energy diagrams for 2,3-POA, 2,3-DPA and 2,3-CZ in toluene. Corresponding SOC constants are also listed.

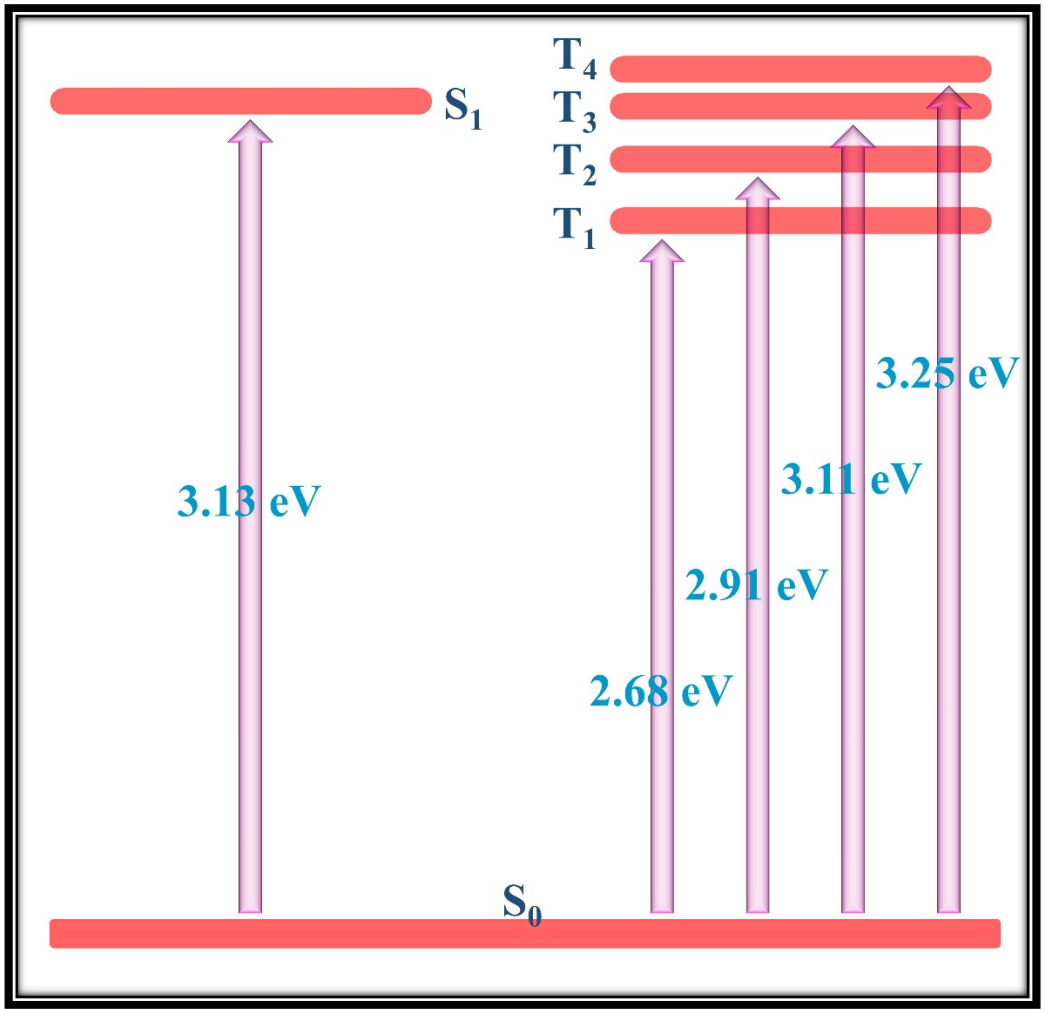

Figure S8. The vertical excitation energies of 2,3-CZ are being calculated.

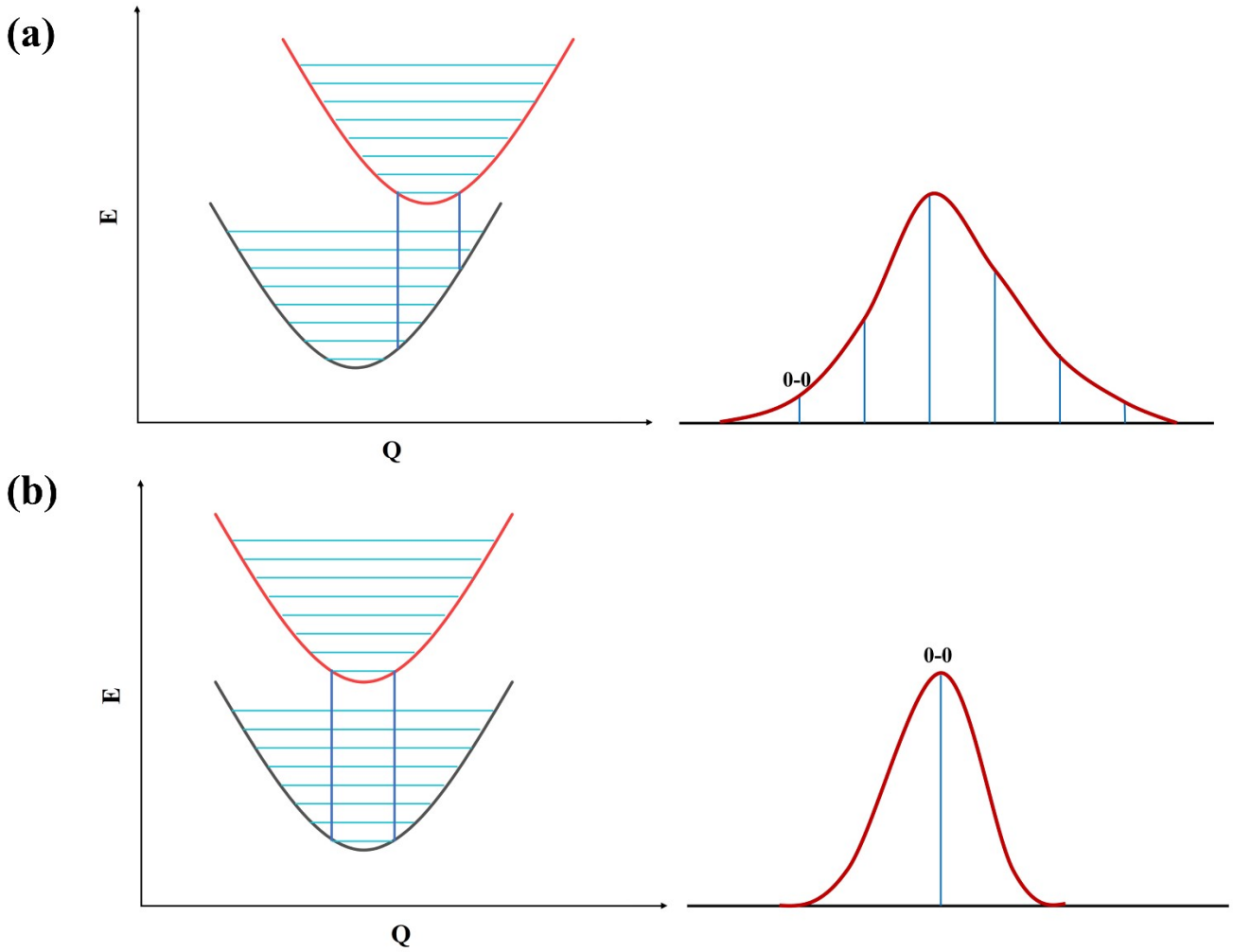

Figure S9. The vibrational energy levels and spectral diagrams.

Table S1. Reorganization energy contributions (cm^{-1}) from bond length in donor of 2,3-POA, 2,3-DPA and 2,3-CZ.

2,3-POA			2,3-DPA			2,3-CZ		
Atomic number		reorganization energies	Atomic number		reorganization energies	Atomic number		reorganization energies
17	**24**	**122.460**	**17**	**24**	**64.232**	**17**	**24**	**19.066**
17	**25**	**92.516**	**17**	**25**	**25.189**	34	50	16.453
35	53	68.732	34	51	12.818	50	58	15.821
37	53	54.643	24	35	10.261	24	35	8.294
55	62	46.800	24	34	9.658	36	53	7.081
34	51	35.337	51	60	8.475	53	61	6.934
36	55	29.718	37	56	4.301	**17**	**25**	**4.218**
24	35	28.779	25	37	4.152	24	34	3.775
52	59	17.420	36	55	3.754	55	61	2.330
56	62	15.861	35	52	3.712	34	36	1.802
25	37	12.384	25	36	2.584	35	52	1.283
24	34	12.099	56	63	1.858	25	36	0.898
25	36	9.094	52	60	0.448	37	55	0.309
37	56	1.548	51	59	0.327	52	59	0.231
35	52	1.253	52	61	0.311	37	54	0.150
34	50	0.463	36	54	0.200	35	51	0.146
36	54	0.251	56	64	0.180	50	57	0.135
52	60	0.211	34	50	0.123	55	62	0.098
55	61	0.206	35	53	0.088	61	67	0.038
59	67	0.167	60	68	0.082	53	60	0.034
56	63	0.149	63	69	0.040	25	37	-0.008
62	68	0.115	37	57	-0.004	52	58	-0.042