RSC Advances

Supporting Information

Accurate Description of Hybridized Local and Charge-transfer Excited-state in Donor-Acceptor Molecules Using Density Functional Theory

*Y. Y. Pan, *[ab] J. Huang,[a] Z. M. Wang,[a] S. T. Zhang,[b] D. W. Yu, [a] B. Yang *[b] and Y. G. Ma [c]*

[a]School of Petrochemical Engineering, Shenyang University of Technology, 30 Guanghua Street, Liaoyang, 111003, P. R. China

[b]State Key Laboratory of Supramolecular Structure and Materials, Jilin University, 2699 Qianjin Avenue, Changchun 130012, P.R. China.

[c]State Key Laboratory of Luminescent Materials and Devices, Institute of Polymer Optoelectronic Materials and Devices, South China University of Technology, Guangzhou, 510640, P. R. China.

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Part Ⅰ： The optimised ω of TPA-AC in ground and excited state.

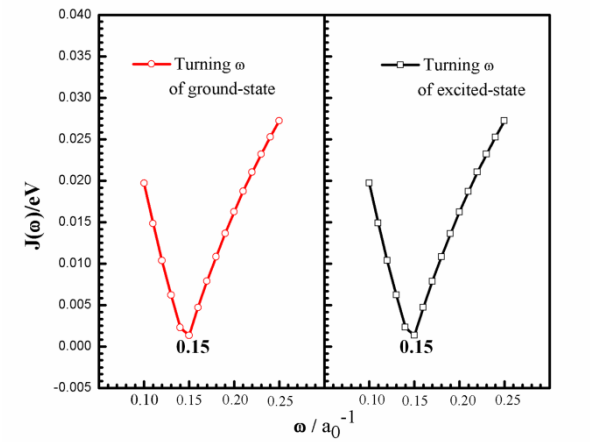


Figure S1 Tuning ω for TPA-AC in vacuum (the optimal ω are 0.15 in ground-state and 0.15 in excited-state for which $J(\omega)$ is at minimum).

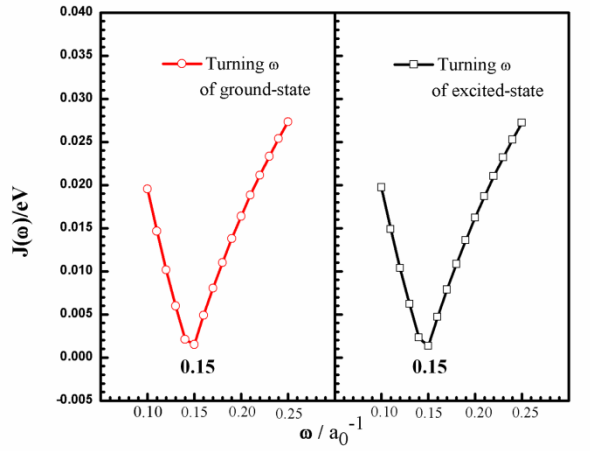


Figure S2 Tuning ω for TPA-AC in hexane (the optimal ω are 0.15 in ground-state and 0.15 in excited-state for which $J(\omega)$ is at minimum).

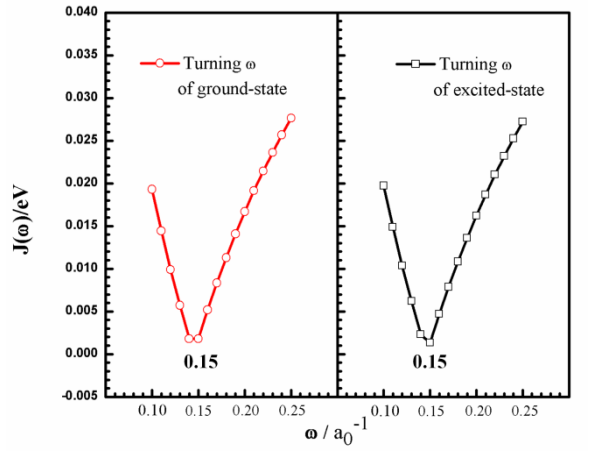


Figure S3 Tuning ω for TPA-AC in tetrahydrofuran (the optimal ω are 0.15 in ground-state and 0.15 in excited-state for which $J(\omega)$ is at minimum).

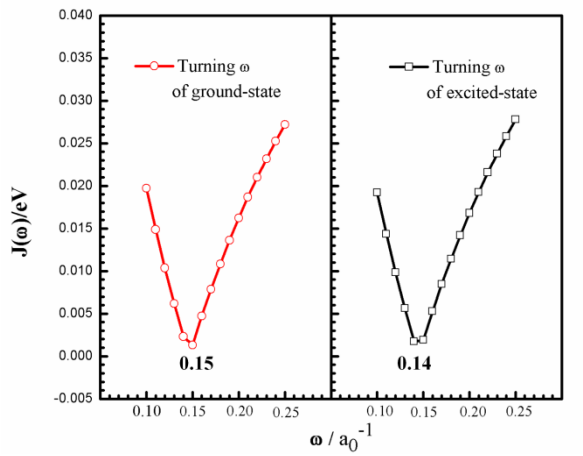
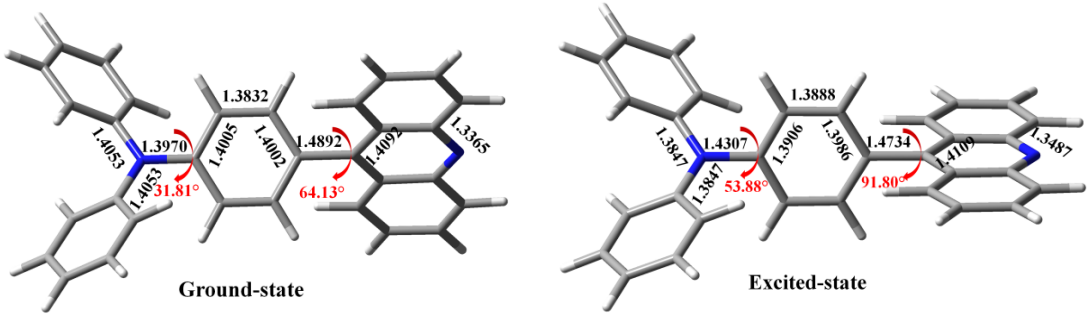


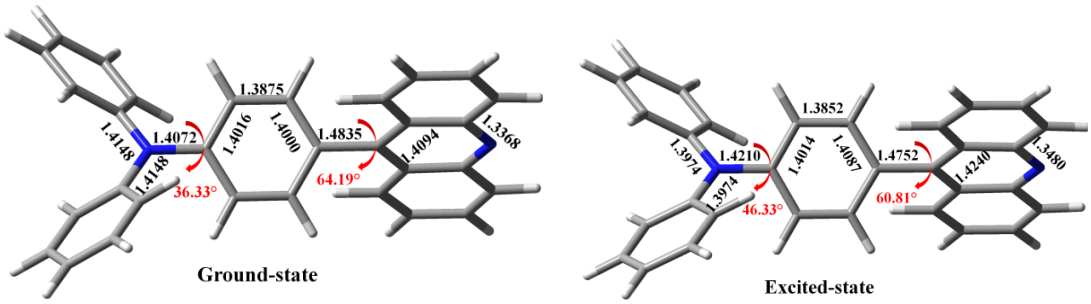
Figure S4 Tuning ω for TPA-AC in acetonitrile (the optimal ω are 0.15 in ground-state and 0.14 in excited-state for which $J(\omega)$ is at minimum).

Part Ⅱ: The optimised geometries of ground and excited state employed different functionals.

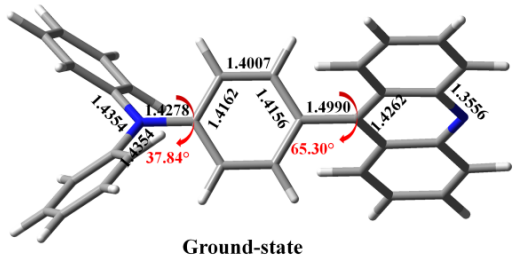
SVWN



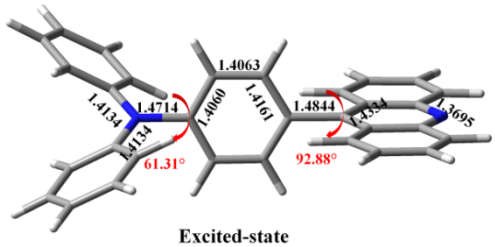
PBE



BLYP

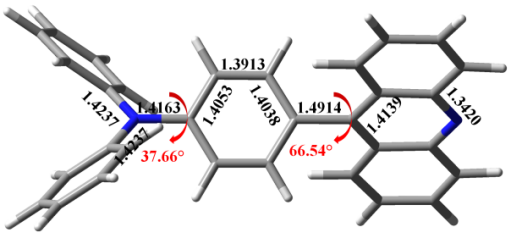


Ground-state

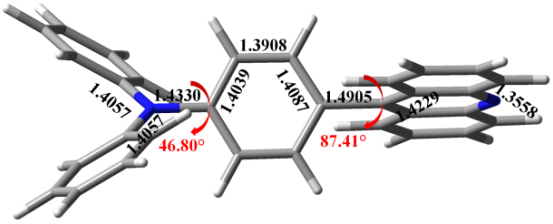


Excited-state

B3LYP

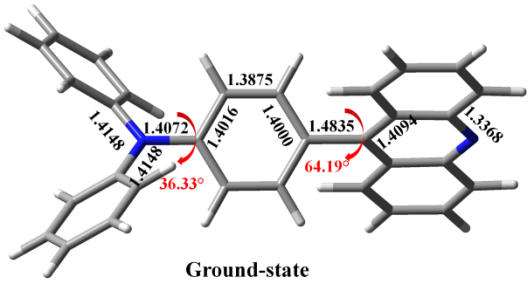


Ground-state

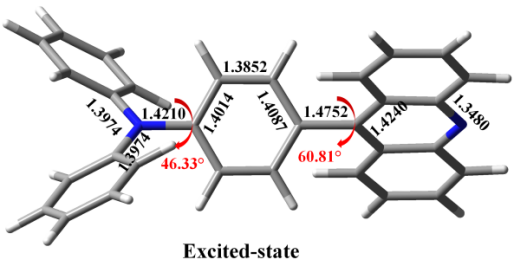


Excited-state

PBE0

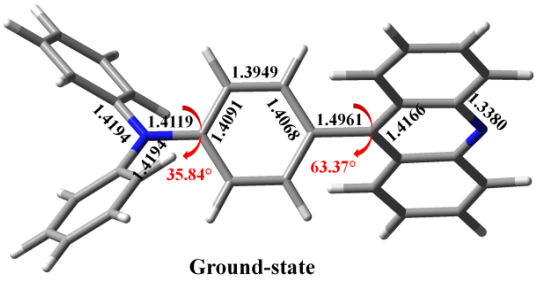


Ground-state

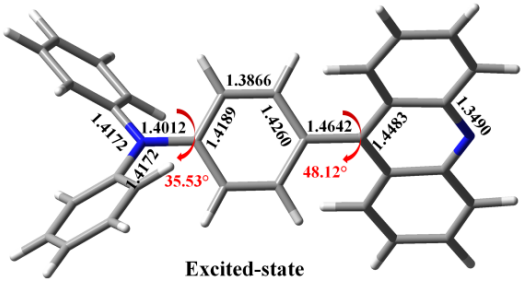


Excited-state

BMK

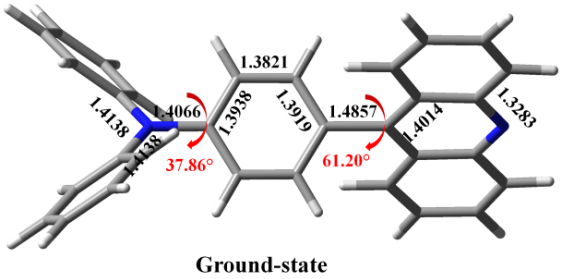


Ground-state

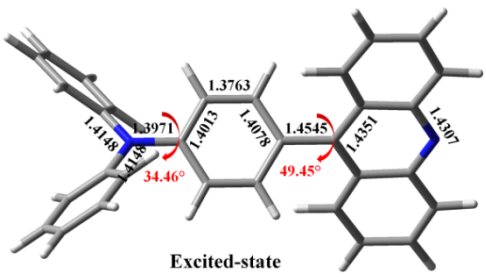


Excited-state

BHHLYP

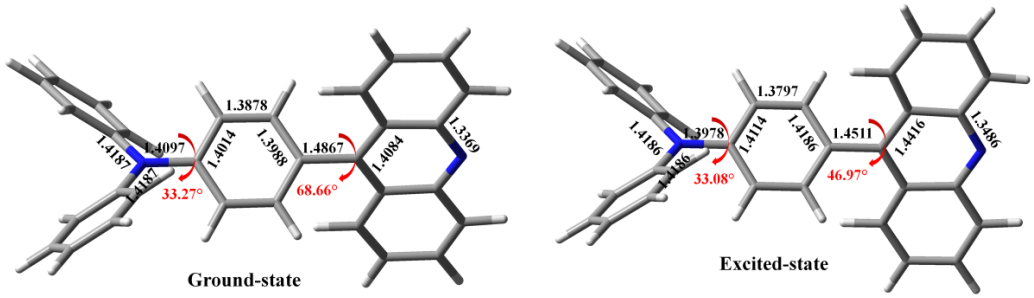


Ground-state

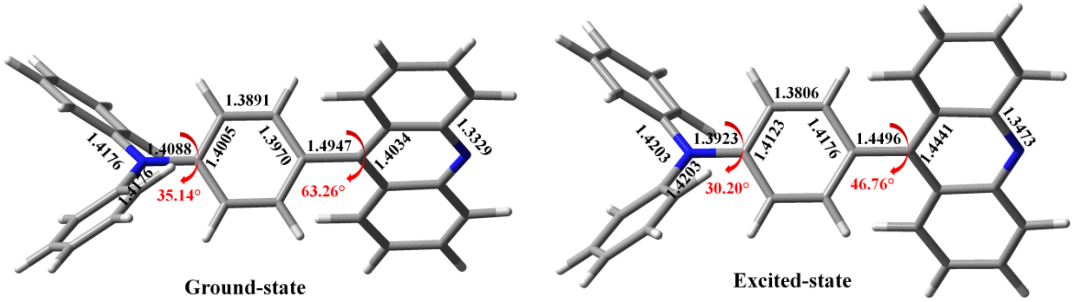


Excited-state

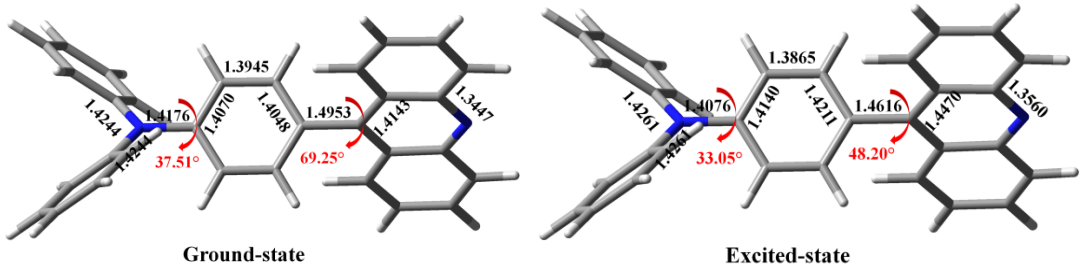
M06-2X



M06HF



ωB97X



Part Ⅲ: The excited-state properties of TPA-AC in different solvents employed different functionals.

Table S1. Absorption and emission properties of TPA-AC with an increasing solvent polarities were estimated using different functional with PCM-TD-DFT/ 6-31+G (d, p) solvation model.

	vacuum		n-hexane		tetrahydrofuran		acetonitrile	
	Abs(nm)	PL (nm)	Abs(nm)	PL (nm)	Abs(nm)	PL (nm)	Abs(nm)	PL (nm)
SVWN	632.26	806.09	661.11	853.16	693.02	887.36	704.17	904.53
PBE	430.90	482.61	443.83	615.09	458.11	778.74	463.12	804.65
BLYP	649.78	791.43	677.15	847.16	710.04	872.24	721.9	887.20
B3LYP	458.31	523.10	472.37	788.04	488.6	1293.02	494.32	1114.43
PBE0	430.90	481.33	443.83	615.09	458.11	778.74	463.12	804.65
BMK	372.60	435.92	381.67	470.81	389.35	609.41	391.99	585.76
M062X	336.38	418.42	358.65	439.64	366.46	529.69	367.99	542.34
BHHLP	354.58	424.77	341.48	426.16	343.86	466.20	344.35	494.12
M06HF	302.70	341.60	307.20	395.92	308.83	420.36	308.99	437.02
ωB97X	364.06	442.20	369.75	450.91	372.49	501.42	373.13	555.06
Experiment	-	-	384	440	386	518	384	564