

Electronic Supporting Information (ESI)

Deciphering the doublet luminescence mechanism in neutral organic radical: Spin-exchange coupling, reversed-quartet mechanism, excited-state dynamics

LingLing Lv,^{* a, b} YanYing Zhang,^a ZiYe Ning^a

^a*School of Chemical Engineering and Technology, Tianshui Normal University, Tianshui, Gansu 741001, China.*

^b*Key Laboratory of Advanced Optoelectronic Functional Materials of Gansu Province, Tianshui Normal University, Tianshui, Gansu 741001, China.*

* Corresponding author: e-mail: lvling002@tsnu.edu.cn/lvling002@163.com

Table S1 Vital transition active orbital at the ω B97X-D3 and CASSCF levels for the excited states of the TTM-1Cz-An compound.

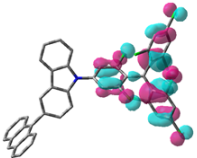
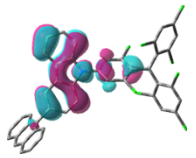
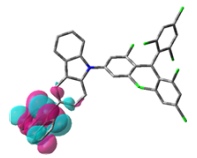
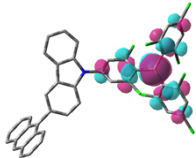
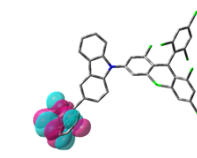
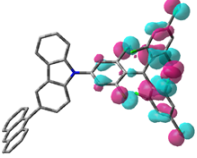
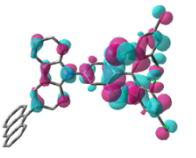
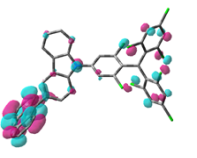
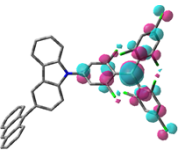
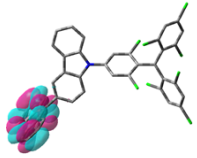
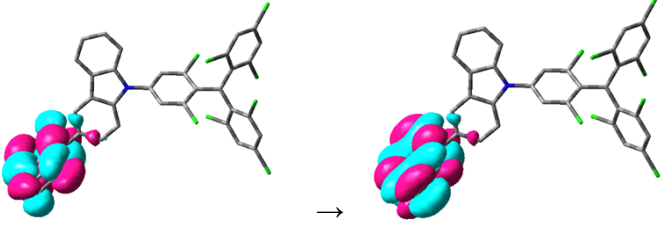
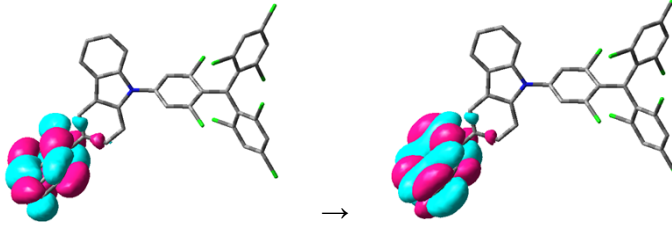
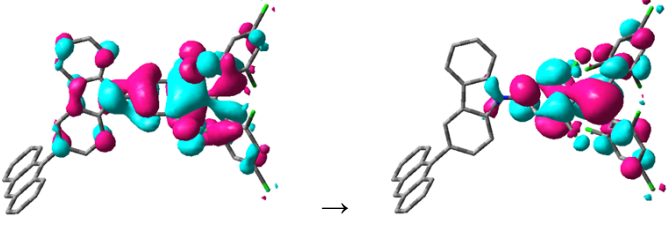
Method	HOMO-4	HOMO-1	HOMO	SOMO	LUMO
wB97X-D3					
Method	HOMO-2	HOMO-1	HOMO	SOMO	LUMO
CASSCF(7,5)					

Table S2 Natural transition orbital (NTO) pairs at the ω B97X-D3 level with Tamm-Dancoff approximation for the excited states of TTM-1Cz-An.

Excited state	Excited energy (eV)	Nature transition orbital	Orbital composition
D ₁	2.251	 217 α → 218 α	45.7%
		 216 β → 217 β	45.7%
D ₂	3.122	 216 β → 217 β	78.2%

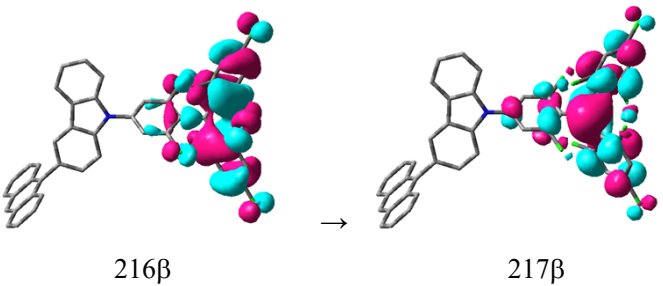
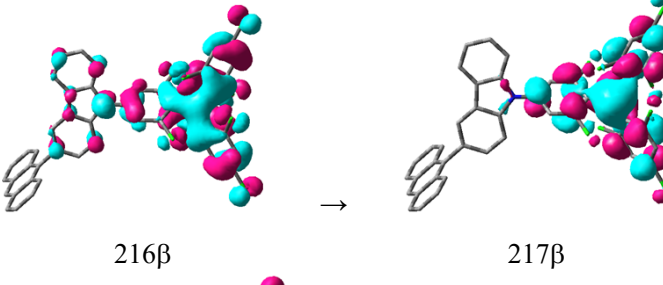
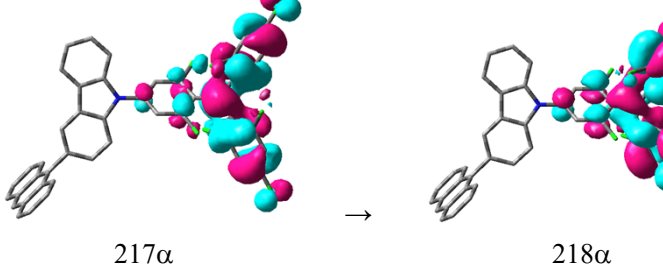
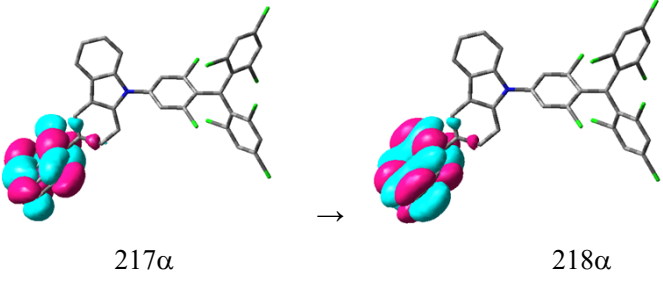
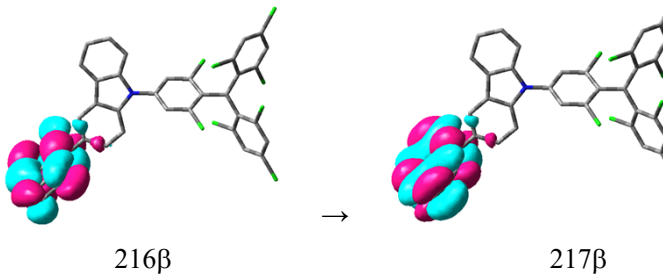
D ₃	3.202	 216β → 217β	71.5%
D ₄	3.548	 216β → 217β	50.9%
		 217α → 218α	11.5%

Table S3 Natural transition orbital (NTO) pairs at the CAM-B3LYP level with Tamm-Dancoff approximation for the excited states of TTM-1Cz-An.

Excited state	Excited energy (eV)	Nature transition orbital	Orbital composition
D ₁	2.169	 217α → 218α	46.2%
		 216β → 217β	46.2%

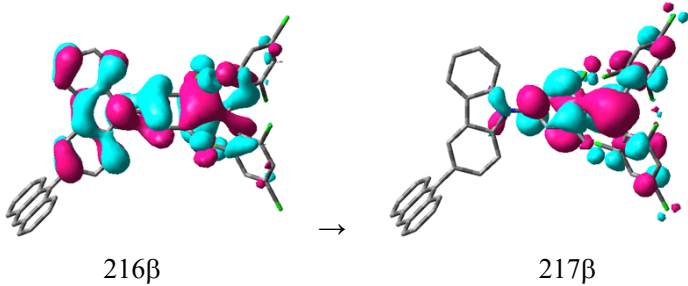
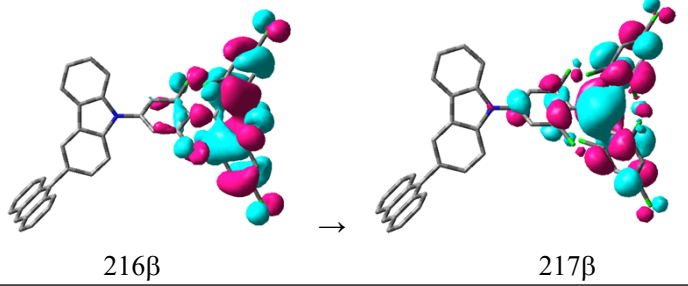
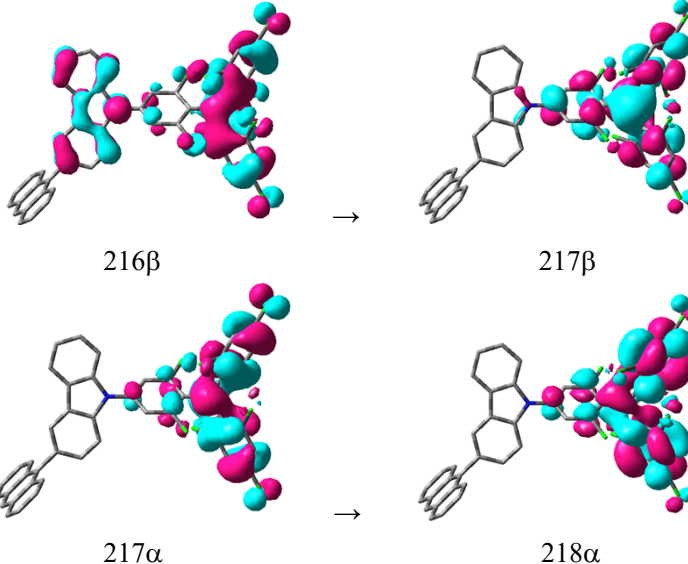
D ₂	2.904	 <p>216β → 217β</p>	88.1%
D ₃	3.122	 <p>216β → 217β</p>	74.1%
D ₄	3.400	 <p>216β → 217β</p> <p>217α → 218α</p>	60.9%
			14.1%

Table S4 Spin density and density difference for the key excited states of TTM-1Cz-An.

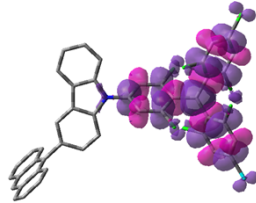
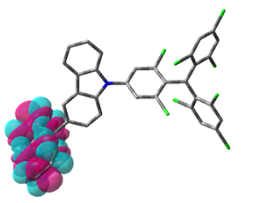
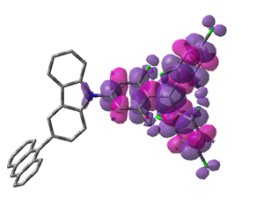
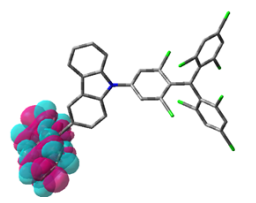
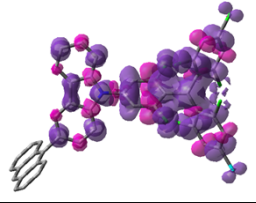
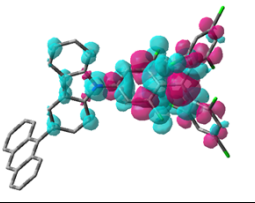
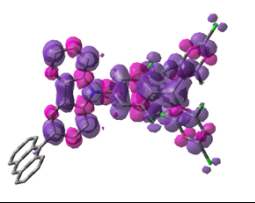
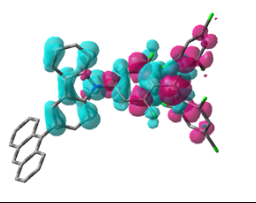
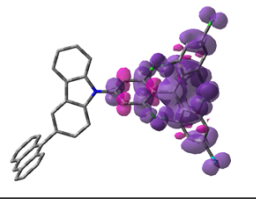
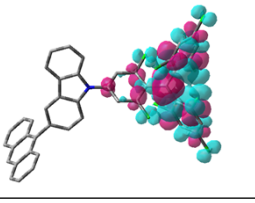
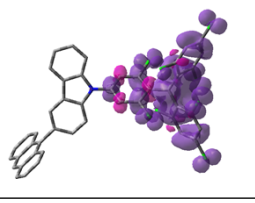
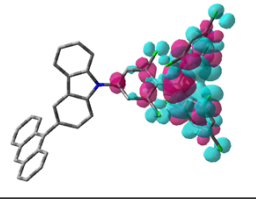
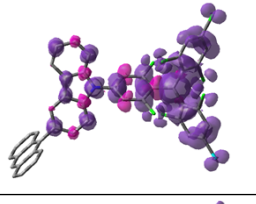
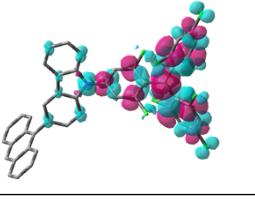
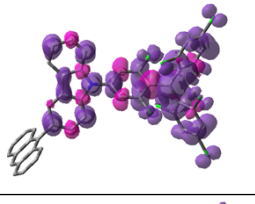
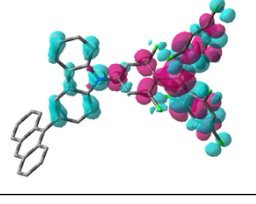
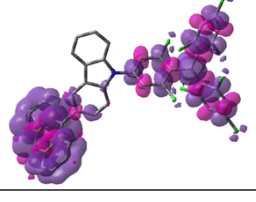
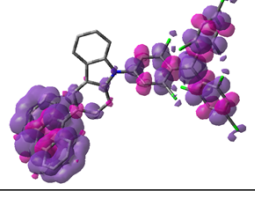
Excited state	wB97X-D3/def2-TZVP//def2/j		CAM-B3LYP/def2-TZVP//def2/J	
	Spin density	Density difference	Spin density	Density difference
D ₁				
D ₂				
D ₃				
D ₄				
Q ₁				

Table S5 Contributions to the ZFS tensors (D and E) from spin-orbit coupling and spin–spin dipolar (all values are in cm^{-1}) with the SOMF operator for the quartet Q_1 state.

Method	$\omega\text{B97X-D3}$		CAM-B3LYP	
	D	E	D	E
Spin-Spin	0.00373	-0.00211	0.00399	0.00025
SOC	-0.02927	-0.00295	-0.03002	-0.00536
$\alpha \rightarrow \alpha$	-0.31804	0.00908	-0.32683	-0.01103
$\beta \rightarrow \beta$	-0.31460	0.01260	-0.32384	-0.01367
$\alpha \rightarrow \beta$	0.45509	-0.02126	0.46807	0.01171
$\beta \rightarrow \alpha$	0.14828	-0.00337	0.15258	0.00764
Total	-0.02556	-0.00507	-0.02604	-0.00508

Table S6 The projections of the eigenfunctions on the model space at the vibration and non-vibration levels; here, $C^2 |S, M_S\rangle$: C^2 denotes the configuration weight coefficients, S is spin quantum number, and M_S denotes spin-sublevels.

Non-vibration coupling	Vibration coupling
$ \Phi_6\rangle = 0.99 1/2, +1/2\rangle$	$ \Phi_6\rangle = 0.88 1/2, +1/2\rangle + 0.12 3/2, \pm 1/2 \text{ or } +3/2\rangle$
$ \Phi_5\rangle = 0.99 1/2, -1/2\rangle$	$ \Phi_5\rangle = 0.88 1/2, -1/2\rangle + 0.12 3/2, \pm 1/2 \text{ or } -3/2\rangle$
$ \Phi_4\rangle = 0.61 3/2, +1/2\rangle + 0.19 3/2, -1/2\rangle$ + 0.20 $ 3/2, \pm 3/2\rangle$	$ \Phi_4\rangle = 0.49 3/2, +1/2\rangle + 0.12 3/2, -1/2\rangle$ + 0.39 $ 3/2, \pm 3/2\rangle$
$ \Phi_3\rangle = 0.61 3/2, -1/2\rangle + 0.19 3/2, +1/2\rangle$ + 0.20 $ 3/2, \pm 3/2\rangle$	$ \Phi_3\rangle = 0.49 3/2, -1/2\rangle + 0.12 3/2, +1/2\rangle$ + 0.39 $ 3/2, \pm 3/2\rangle$
$ \Phi_2\rangle = 0.73 3/2, -3/2\rangle + 0.06 3/2, +3/2\rangle$ + 0.21 $ 3/2, \pm 1/2\rangle$	$ \Phi_2\rangle = 0.51 3/2, +3/2\rangle + 0.35 3/2, \pm 1/2\rangle$ + 0.11 $ 1/2, +1/2\rangle$
$ \Phi_1\rangle = 0.73 3/2, +3/2\rangle + 0.06 3/2, -3/2\rangle$ + 0.21 $ 3/2, \pm 1/2\rangle$	$ \Phi_1\rangle = 0.51 3/2, -3/2\rangle + 0.35 3/2, \pm 1/2\rangle$ + 0.11 $ 1/2, -1/2\rangle$

Table S7 Spin-orbit coupling (SOC) matrix elements (cm^{-1}) between excited states of TTM-1Cz-An calculated at the CASSCF level. S is spin quantum number; M_S denotes spin-sublevels.

State 1	State 2	$\langle S_1 = 3/2, M_{S_{1,k}} \hat{H}_{\text{SOC}} S_2 = 1/2, M_{S_{2,k}} \rangle$
Q ₁	D ₀	$\langle S_1 = 3/2, 3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = 0.013 + 0.006i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.000 + 0.005i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = 0.008 - 0.003i$
		$\langle S_1 = 3/2, -3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = 0.013 - 0.006i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.000 + 0.005i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = 0.008 + 0.003i$
	D ₁	$\langle S_1 = 3/2, 3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.001 + 0.001i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.000 - 0.000i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.000 - 0.000i$
		$\langle S_1 = 3/2, -3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = 0.001 - 0.001i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.000 - 0.000i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.000 + 0.000i$
	D ₂	$\langle S_1 = 3/2, 3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.003 + 0.003i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.000 - 0.002i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.002 - 0.002i$
		$\langle S_1 = 3/2, -3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.003 - 0.003i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.000 - 0.002i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.002 + 0.002i$
	D ₃	$\langle S_1 = 3/2, 3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = 0.027 - 0.044i$
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = -0.000 + 0.028i$
		$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, 1/2 \rangle = 0.015 + 0.026i$
$\langle S_1 = 3/2, -3/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = 0.027 + 0.044i$		
$\langle S_1 = 3/2, -1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = 0.015 + -0.026$		
		$\langle S_1 = 3/2, 1/2 \hat{H}_{\text{SOC}} S_2 = 1/2, -1/2 \rangle = -0.000 + 0.028i$

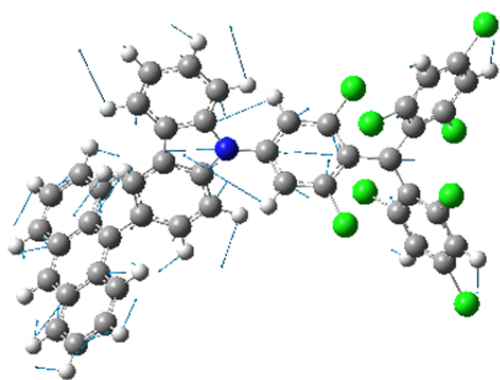
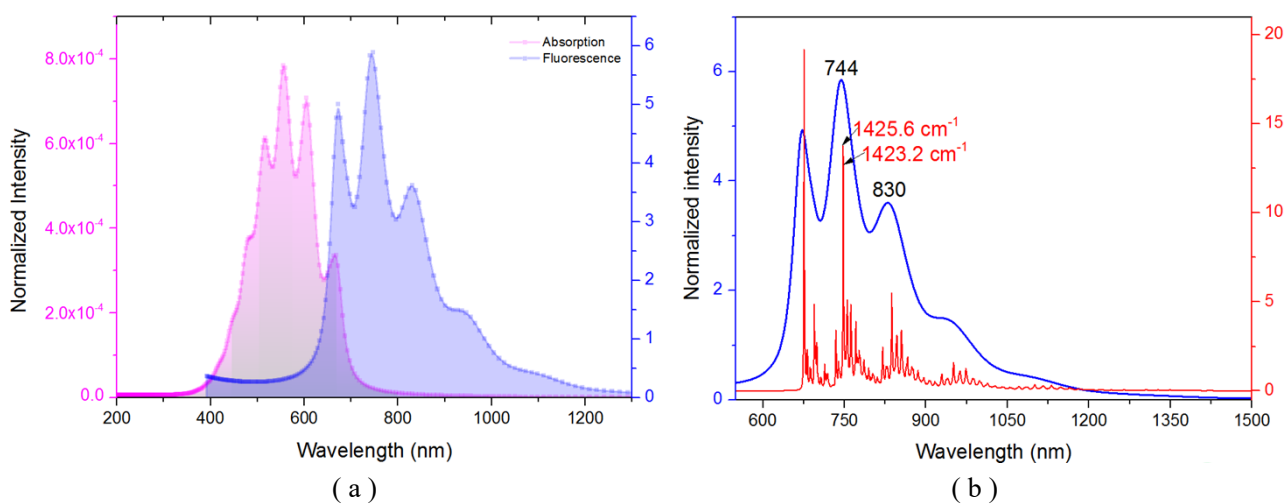
Table S8 Calculated Huang-Rhys factors (S_i), reorganization energies (λ_i), and derivatives of the SOC of the key normal modes on the corresponding Q₁ state potential surface

Vibration freq/ cm^{-1}	S_i	λ_i/cm^{-1}	$\partial\langle Q_1 \hat{H}_{\text{SOC}} D_1 \rangle / \partial Q_k$
1245	0.007	9.41	0.066
1423	0.019	27.19	0.062
1536	0.005	7.88	0.080
1551	0.007	11.02	0.066
1623	0.008	12.41	0.051
1684	0.008	5.51	0.228

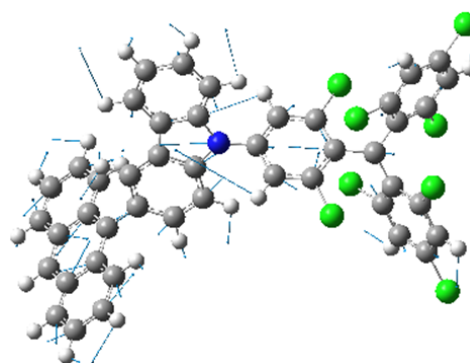
Table S9 The adiabatic and vertical excitation energies (eV) of the doublet ($D_1 - D_4$) of TTM-1Cz-An

State	SCS-wB2PLYP ^A	DLPNO-CCSD(T)	SCS-wB2PLYP	SCS-wB2GP-PLYP	wB97X-D3	CAM-B3LYP
D_0	0.0	0.0	0.0	0.0	0.0	0.0
D_1	2.506	2.650	2.316	2.504	2.251	2.169
D_2	2.814	2.745	3.422	3.448	3.122	2.904
D_3	3.082	3.034	3.496	3.512	3.202	3.123
D_4		3.071	3.632	3.573	3.548	3.400

^a the adiabatic excitation energy difference, $E(D_0) = -5453.9343158$; others are vertical excitation energies.

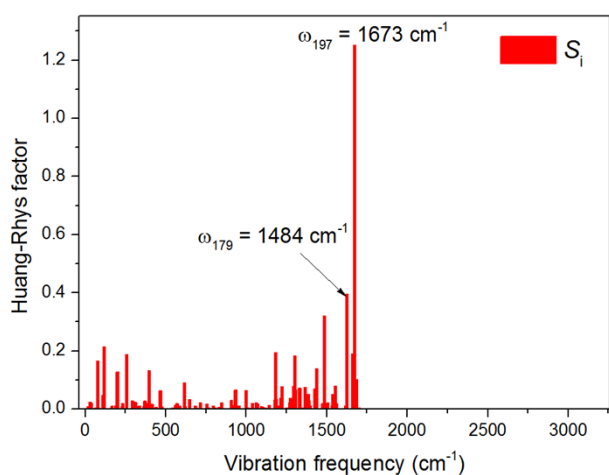


$$\omega_{170} = 1423.2 \text{ cm}^{-1}$$

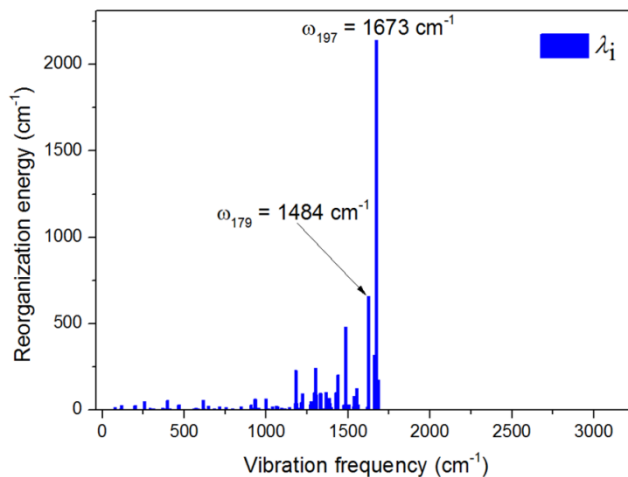


$$\omega_{171} = 1425.6 \text{ cm}^{-1}$$

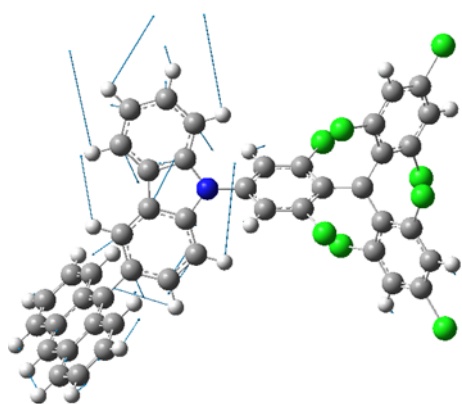
Fig. S1 Calculated absorption and fluorescence spectrum of the excited D_1 state for the TTM-1Cz-An compound. The decisive promoting vibration modes for fluorescence are listed at the bottom of Figure.



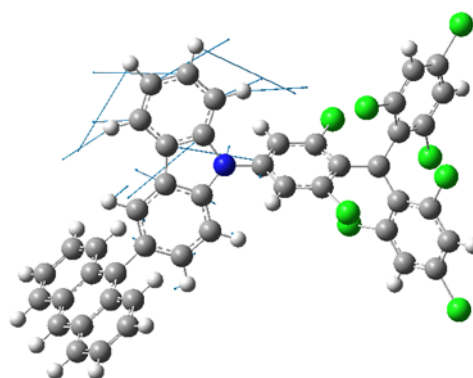
(a)



(b)



$\omega_{179} = 1484 \text{ cm}^{-1}$



$\omega_{197} = 1673 \text{ cm}^{-1}$

Fig. S2 Calculated Huang–Rhys factors (a) and reorganization energy (b) versus the normal vibration frequency between D₁ and D₂ on the D₁ potential energy surface, respectively; The vital promoting vibration modes are listed at the bottom of figure.

Out file of the J_{TR} calculation

```
=====
QD-NEVPT2 Results
(Van Vleck)
=====
```

```
*****
```

```
MULT 4
```

```
*****
```

```
Total Hamiltonian to be processed
```

```
0
```

```
0 -5456.561894
```

ROOT = 0

--- Reading QDVector (MULT= 4, ROOT= 0) Norm = 1.00000000e+00
[uuu] 1.000000000

Total Energy Correction : dE = -8.68025142065108
Zero Order Energy : E0 = -5447.88164262696955
Total Energy (E0+dE) : E = -5456.56189404762063

MULT 2

Total Hamiltonian to be processed

	0	1	2	3	4
0	-5456.649051	-0.000001	0.002694	0.000225	0.030522
1	0.000001	-5456.561896	-0.000001	-0.000346	0.000002
2	0.002530	-0.000001	-5456.555530	-0.000397	-0.004245
3	0.000203	-0.000356	-0.000330	-5456.609830	0.000108
4	0.021418	-0.000000	-0.003460	0.000066	-5456.510765

ROOT = 0

--- Reading QDVector (MULT= 2, ROOT= 0) Norm = 1.00000000e+00
[u20] 0.521703070
[duu] -0.000006039
[udu] 0.502058698
[uud] -0.502052659
[u02] 0.472941281

Total Energy Correction : dE = -8.67988758603860
Zero Order Energy : E0 = -5447.97398840918231
Total Energy (E0+dE) : E = -5456.65387599522091

ROOT = 1

--- Reading QDVector (MULT= 2, ROOT= 1) Norm = 1.00000000e+00
[duu] 0.816482670
[udu] -0.408264816
[uud] -0.408217854

Total Energy Correction : dE = -8.78828704372154

Zero Order Energy : E0 = -5447.77360661343391
 Total Energy (E0+dE) : E = -5456.56189365715545

 ROOT = 2

--- Reading QDVector (MULT= 2, ROOT= 2) Norm = 1.00000000e+00

[u20] -0.722293945
 [duu] 0.000177578
 [udu] 0.051238822
 [uud] -0.051416400
 [u02] 0.687760044

Total Energy Correction : dE = -8.82266079685451
 Zero Order Energy : E0 = -5447.73298112410066
 Total Energy (E0+dE) : E = -5456.55564192095517

Table S10 Cartesian coordinate parameters of the optimized ground and excited state geometric structures at the ω B97X-D3 and CAM-B3LYP levels.

At the ω B97X-D3 level			
The D ₀ state			
C	2.65702012955539	-1.38559386787443	0.65860020966321
C	2.06867138219777	-0.05368600119287	0.44031300884330
C	0.83550309431510	0.12302364670585	-0.22424060843182
C	2.70627536778375	1.13053696321869	0.86950379232836
C	0.27866454419742	1.37466343529844	-0.44812751654005
C	2.17491934236133	2.39298163129306	0.64017299452703
C	0.95458264123804	2.51759401326355	-0.02245503283443
H	-0.69418795809601	1.45766599987475	-0.93421226940761
H	2.72773106467784	3.28017489484118	0.95188657278499
C	3.13820639656721	-1.76950528398502	1.99599978142106
C	2.35422985004427	-1.59337337794332	3.15722871592971
C	4.41432238770819	-2.33815059108349	2.20064271724040
C	2.79610734329105	-1.95380829116494	4.42477317397492
C	4.87772003459458	-2.71550325838193	3.45557081976176
C	4.05960298803822	-2.51789117010717	4.56247838153529
H	2.14974430703986	-1.81102004374482	5.29091038423589
H	5.87452155134471	-3.14297256136425	3.56573641045467

C	2.75201982942624	-2.33060807349735	-0.46717632512151
C	3.27483551888879	-1.95099287329213	-1.72333363954616
C	2.30675168880174	-3.66737230008518	-0.37009020117899
C	3.33867050729983	-2.82014436726622	-2.80609308718815
C	2.36621722787060	-4.55936608076242	-1.43451996193520
C	2.87907150522250	-4.12318520141405	-2.65124820256997
H	3.75632444811572	-2.48264621701264	-3.75482704363147
H	1.99382879537650	-5.57718827493659	-1.31717097659038
Cl	0.73368897184722	-0.98147119734284	3.04607301429358
Cl	5.52052373017869	-2.52186166453460	0.87583821939689
Cl	4.62067079991456	-2.98150099403099	6.13387992862336
Cl	1.56842354048855	-4.25073755012146	1.08867499619183
Cl	3.94929517425836	-0.36883074131269	-1.96042828122169
Cl	2.94533781147775	-5.21628827811184	-3.99296013431071
Cl	-0.11120392682756	-1.24927151420725	-0.70981762819333
Cl	4.26982415461070	1.06689529595377	1.62216872814966
C	0.10341161356405	4.74817535746621	0.70486633105042
C	0.05279059446361	4.30062901519299	-1.51424759286223
C	0.24429036248594	4.68055183668232	2.09377193457474
C	-0.44734414588270	5.88467095027203	0.07479978728870
C	0.19730865650357	3.72010465984761	-2.77831131194766
C	-0.47799004854407	5.59883368700030	-1.35061509204334
C	-0.16055218578857	5.78227830904570	2.83779307117967
H	0.65271012673888	3.79421157556299	2.58362676612494
C	-0.84572238811024	6.98078690488331	0.84567250144612
C	-0.22115100254653	4.46158856575086	-3.87788495598862
H	0.62970937902585	2.72483759769240	-2.90168197251721
C	-0.89096004356938	6.32581442322824	-2.47274651362576
C	-0.70188398930505	6.93462625373679	2.23165125200154
H	-0.06175566008994	5.75711853419613	3.92635101941938
H	-1.27349651859709	7.86806981557058	0.37118071894344
C	-0.76438115493540	5.74961102300234	-3.73145715447574
H	-0.12114108900670	4.03099978558405	-4.87747307432012
H	-1.30418417725538	7.33118443684218	-2.35891318068005
H	-1.08381635021463	6.30318718722164	-4.61749997311668
N	0.40438453540438	3.79323165237586	-0.26404327151813
C	-1.12374229924934	8.09572462321178	3.07511734431344
C	-0.17974851557792	9.07570182863336	3.44573085038222
C	-2.46459679406510	8.20602867171892	3.49848506732210
C	1.19543660053047	9.01006934099411	3.03168664403983
C	-0.58824370051117	10.18736730507753	4.25906154344885
C	-2.86514365912779	9.32177681026093	4.31038309719007
C	-3.46183257758293	7.23132824466045	3.14831448724618
C	2.09028936204301	9.97204501429031	3.40235672696628

H	1.51676735170031	8.17276624653136	2.40853384070863
C	0.38486863650846	11.17613202360532	4.62785193353747
C	-1.91960389972417	10.28479976720097	4.67260714001456
C	-4.23334554804805	9.41947859346569	4.73395635285503
H	-3.16969307464220	6.37768969327240	2.53302137495181
C	-4.75338252285146	7.36075729818165	3.57135022049027
C	1.68109112551802	11.07386126569681	4.21503913220918
H	3.13086745841566	9.90419373353182	3.07504372316153
H	0.06155119138685	12.01613595384064	5.24896575328501
H	-2.22768811071495	11.13210904671831	5.29236681352378
C	-5.14827847945574	8.47273714523755	4.37720466417565
H	-4.52499765997537	10.27323308437435	5.35194873640875
H	-5.49570902673555	6.60813535105358	3.29401047603382
H	2.41276110660298	11.83332854767680	4.50172701472356
H	-6.18701272259366	8.55766173393176	4.70619783342403

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C	2.68519486517794	-1.34969349539651	0.63056759990808
C	2.09678097787983	-0.02394005864348	0.38398948997497
C	0.81526488892786	0.13435932635299	-0.18994313206421
C	2.77510507398125	1.17193660090864	0.70966693579957
C	0.24861511470504	1.38114317051264	-0.42062869992812
C	2.22704278417538	2.42757227024562	0.48124547036119
C	0.95780306589514	2.53335991239517	-0.08513873811947
H	-0.75690578059025	1.45612316254391	-0.83684370387460
H	2.79930322542090	3.32455152117714	0.72186679279649
C	3.27901051037726	-1.65673616664957	1.94323791270818
C	2.60061815159305	-1.39707438656673	3.15458927163147
C	4.56619868598088	-2.22356046849681	2.07134641630465
C	3.15160779381030	-1.67833783173671	4.39982559535040
C	5.13807590253590	-2.51973790346611	3.30360897766293
C	4.42104331970217	-2.24352257285165	4.46290649064508
H	2.58555667061204	-1.47177157719507	5.30830826963508
H	6.14072843583961	-2.94451052610687	3.35511194627263
C	2.67912031402854	-2.36805996676893	-0.43367580534834
C	3.11766216272278	-2.08634061375753	-1.74641856868300
C	2.22942840448713	-3.68772046860135	-0.20829850317353
C	3.11287536328515	-3.03713458746879	-2.76086307799349
C	2.21885765320165	-4.65891198572246	-1.20321420717132
C	2.66272890225755	-4.32247336077613	-2.47772120532440
H	3.47372376967947	-2.77800903599830	-3.75643094751218
H	1.84943317221408	-5.66144058134546	-0.98635665766476
Cl	0.97987508983237	-0.77328181736514	3.14545806271215
Cl	5.54944948236815	-2.50484801850221	0.66866493492116
Cl	5.12020285363946	-2.60666280887310	6.00596912531869

Cl	1.57481177566093	-4.14635156939682	1.33293377800450
Cl	3.77205607710151	-0.52770596616591	-2.14505712147091
Cl	2.65383189765879	-5.52013156721109	-3.72942290611297
Cl	-0.17338037608171	-1.24903788223167	-0.54352222359085
Cl	4.39766475733934	1.13153075289924	1.32808602427968
C	0.08204433329310	4.74073743633372	0.67101170005053
C	0.02196524571881	4.32402750822617	-1.55312502202448
C	0.24096418920150	4.65463372519082	2.05725165948884
C	-0.49073320384212	5.87804171252677	0.06176500770647
C	0.16494793706122	3.76021210423452	-2.82489486913968
C	-0.52562132923426	5.61283852665103	-1.36783035495013
C	-0.16837027928063	5.74099464024465	2.82063836554194
H	0.66575269698195	3.76588444963482	2.52896030266610
C	-0.89794546784102	6.95627411595607	0.85243060384873
C	-0.26438206016071	4.51362808312840	-3.91235603752481
H	0.60288770711392	2.76888945604018	-2.96175583127318
C	-0.95121748573621	6.35066772047677	-2.47822698975375
C	-0.73471229924481	6.89565442554316	2.23757540021334
H	-0.05559006859995	5.70270494216223	3.90751352226538
H	-1.34283591084299	7.84363930039172	0.39409002580394
C	-0.81926065382555	5.79461010930155	-3.74571595124765
H	-0.16322698941084	4.09906024418877	-4.91861874209911
H	-1.37593237997756	7.34931355519614	-2.34821417479933
H	-1.14389932892901	6.35881814967892	-4.62315478876850
N	0.38955634937596	3.80565438345895	-0.31307937265238
C	-1.15412824953274	8.03721630838212	3.09392619067997
C	-0.15148913759296	8.92672252151797	3.63217680372446
C	-2.55653483008052	8.24477481551483	3.36982780950601
C	1.21569666172359	8.76036418416592	3.37178983810760
C	-0.56150312024368	10.03568736821472	4.44556787582637
C	-2.95360903794252	9.36321975438438	4.17682624651308
C	-3.55134452954296	7.38170780623782	2.88987059620103
C	2.17702550926213	9.64479134916856	3.90309236931865
H	1.54307187609780	7.93074173190870	2.74162787357125
C	0.41080392408352	10.90313706508421	4.96209864426467
C	-1.95161613155048	10.23487945493092	4.69915075225852
C	-4.31469882810200	9.56745373123623	4.44190075747926
H	-3.26463696118963	6.51579102392360	2.28952794379740
C	-4.91512007348161	7.60564307672754	3.17047792256555
C	1.77935377083752	10.70771444619327	4.69460431720544
H	3.23470906134367	9.48370465721961	3.68135976250307
H	0.09148234573453	11.74685493713533	5.58013973533787
H	-2.25927171037968	11.08351635857855	5.31602446773959
C	-5.29584379689809	8.69150012581654	3.93886966281667

H	-4.61054560869710	10.42381203580986	5.05421156546115
H	-5.66389292237741	6.91385326302602	2.77730541993247
H	2.51722726885343	11.39840800864717	5.10980806977602
H	-6.35015646756517	8.87277888786956	4.16125432580680
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C	2.70803825574413	-1.37086713891624	0.63913656741971
C	2.07094339508816	-0.10723238749929	0.43185917252394
C	0.85929763619957	0.05972419089765	-0.36829527940824
C	2.56655172340597	1.14657141118841	0.99392307217295
C	0.26848649102298	1.27356491482044	-0.59764565051303
C	1.94222338085484	2.35096310296965	0.81246368726089
C	0.78795188880759	2.44765134123804	-0.00311765002286
H	-0.65634614615210	1.31923936590219	-1.17426852433170
H	2.39342331619592	3.25539035486281	1.22278468076468
C	3.21557307462603	-1.72906491927917	1.95999106126900
C	2.46275892851533	-1.49805639420215	3.14090004387382
C	4.48995347260418	-2.31487906526243	2.18395752403883
C	2.92139766273989	-1.78695863505858	4.42042432123918
C	4.96385108459090	-2.63947349999088	3.44763021448329
C	4.17487548137065	-2.37010279612724	4.56424142368603
H	2.29641012003167	-1.58136457725447	5.28972523671817
H	5.95741302323131	-3.07345941594402	3.56318057007570
C	2.85781792062088	-2.30389223834067	-0.47355494922990
C	3.26975524995941	-1.87367189617832	-1.76178424318010
C	2.59244924693123	-3.69574990906893	-0.37882325192696
C	3.38830273635893	-2.71781940507406	-2.85917727198286
C	2.72672489657239	-4.56782313966104	-1.45044005104110
C	3.12329197186759	-4.07181011405742	-2.69103419015348
H	3.70758163674898	-2.32479353886526	-3.82465759107589
H	2.49434084529209	-5.62563230539366	-1.32432052616894
Cl	0.85488576149109	-0.84927672536463	3.01057264525301
Cl	5.58698089883077	-2.57001786816913	0.85958982275343
Cl	4.76667667459135	-2.76249029902509	6.14720333705651
Cl	1.98253636349806	-4.37650965403041	1.09970647931866
Cl	3.69094498599833	-0.20452324246149	-2.00711379772016
Cl	3.27934174815059	-5.15372784386260	-4.03825111942340
Cl	0.06777765015507	-1.34454006485490	-0.99100392459522
Cl	4.07292488275178	1.14900580939209	1.84240540257661
C	-0.07353581387559	4.65566567998808	0.74453739324098
C	-0.18431161324440	4.19618029116578	-1.48112656206773
C	0.06109813928862	4.58235733743061	2.13325393473099
C	-0.61059364380640	5.79834510152204	0.11778771913718
C	-0.04735812081025	3.62610753745228	-2.74941380065143
C	-0.68573283401775	5.50308419835139	-1.30726406405488

C	-0.29861793905251	5.70300432715610	2.87591727767383
H	0.42130424869976	3.67976518022403	2.63020303161110
C	-0.96457686134092	6.90956475965182	0.88159312521711
C	-0.46765533881059	4.38093431666512	-3.84179365886432
H	0.38808473256254	2.63555089754671	-2.89149461913438
C	-1.10050497529230	6.24277580342385	-2.41577145670305
C	-0.79645107860672	6.87176652758998	2.26864460723033
H	-0.19592228852331	5.67713886685013	3.96382999468913
H	-1.37273688466829	7.80527341936226	0.40618000156549
C	-0.99596968178047	5.67042230527597	-3.68114152603159
H	-0.37401273404006	3.95875227415426	-4.84519279289234
H	-1.49124373855902	7.25565491534170	-2.29170409676468
H	-1.31415807196486	6.23572510130663	-4.56007344999648
N	0.18951657451084	3.68000776414924	-0.22857045243925
C	-1.14234170525691	8.06824018448904	3.09605636607427
C	-0.11608901245679	8.93120813822374	3.53588950990504
C	-2.48817533605693	8.34033519645425	3.41971410221922
C	1.26843052401988	8.70168417804147	3.22301874290161
C	-0.44821355529765	10.09183187358439	4.31453596747991
C	-2.81103675457476	9.50822961796602	4.19200936032105
C	-3.56700306287745	7.48249728474090	3.00989064611404
C	2.24156385294694	9.55307544130770	3.66112489119257
H	1.53626726271784	7.82964474025517	2.62289655186195
C	0.60563758291731	10.96143059177538	4.75554301920614
C	-1.78593261332928	10.35545299002530	4.62122960461406
C	-4.18525901881068	9.77887843719873	4.50736245117136
H	-3.33575352613840	6.58328360758515	2.43506427890594
C	-4.86144829640081	7.77409058610278	3.33202106657069
C	1.90788187608362	10.70134091244629	4.44325410195659
H	3.28756670892131	9.35871034648799	3.41118521526858
H	0.33861991768036	11.84037816238008	5.34875738366727
H	-2.03578931552741	11.24372050036634	5.20893041685294
C	-5.17905710738790	8.94255784984596	4.09083203668459
H	-4.41676461680659	10.67362208782017	5.09185491141465
H	-5.66618972440530	7.10831296458459	3.01032872242886
H	2.70145514937984	11.36983848949937	4.78610208416846
H	-6.22137256470425	9.15932479688166	4.33734172181345
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C	2.70461358349180	-1.38972079346873	0.66657739093537
C	2.09068783953493	-0.06232300260145	0.49644045727573
C	0.81537057392725	0.10196853620266	-0.08682548939737
C	2.74850117928574	1.12819380693182	0.87395975698630
C	0.24544013423612	1.34920877540240	-0.29926416534150
C	2.20225543057784	2.38697644077181	0.65618407957930

C	0.94753133698423	2.49936348342850	0.05938008911465
H	-0.75339253679353	1.42524848423009	-0.73089388566443
H	2.77142510036123	3.27942572841179	0.91981574615501
C	3.28284010092847	-1.78260224195426	1.96178514290752
C	2.57958271940818	-1.62912674067021	3.17658262542878
C	4.57458696069396	-2.34314306967633	2.06939497323504
C	3.11128431947968	-2.00225901074582	4.40555048021858
C	5.12761470821294	-2.73132086677508	3.28395092112248
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At the CAM-B3LYP level

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