



Supporting Information

for

Configuration–packing synergy enabling integrated crystalline-state RTP and amorphous-state TADF

Ruiyan Wang and Yunan Wu

Beilstein J. Org. Chem. **2026**, 22, 224–236. [doi:10.3762/bjoc.22.16](https://doi.org/10.3762/bjoc.22.16)

Copies of spectra, crystal data and structure refinement table for compound 1

Supporting Information

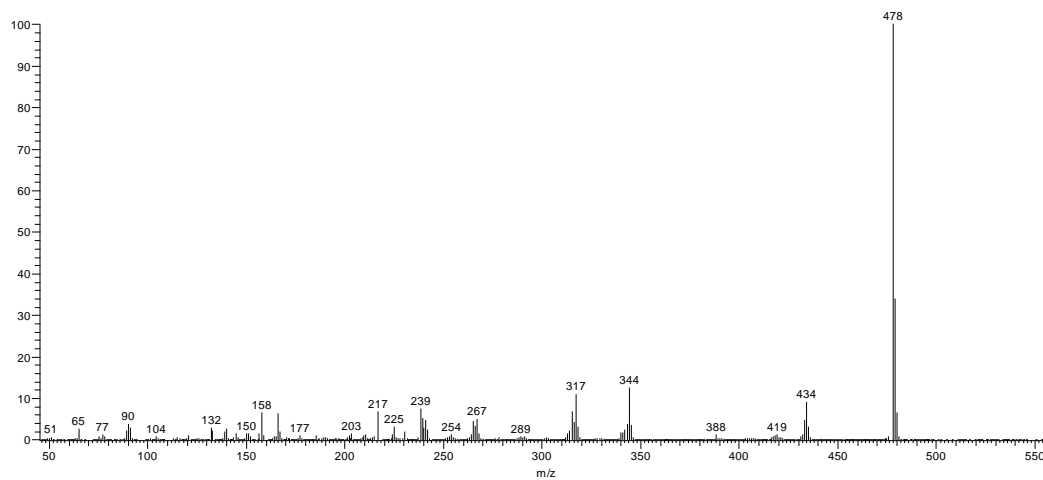


Figure S1. The mass spectrum of compound **1**

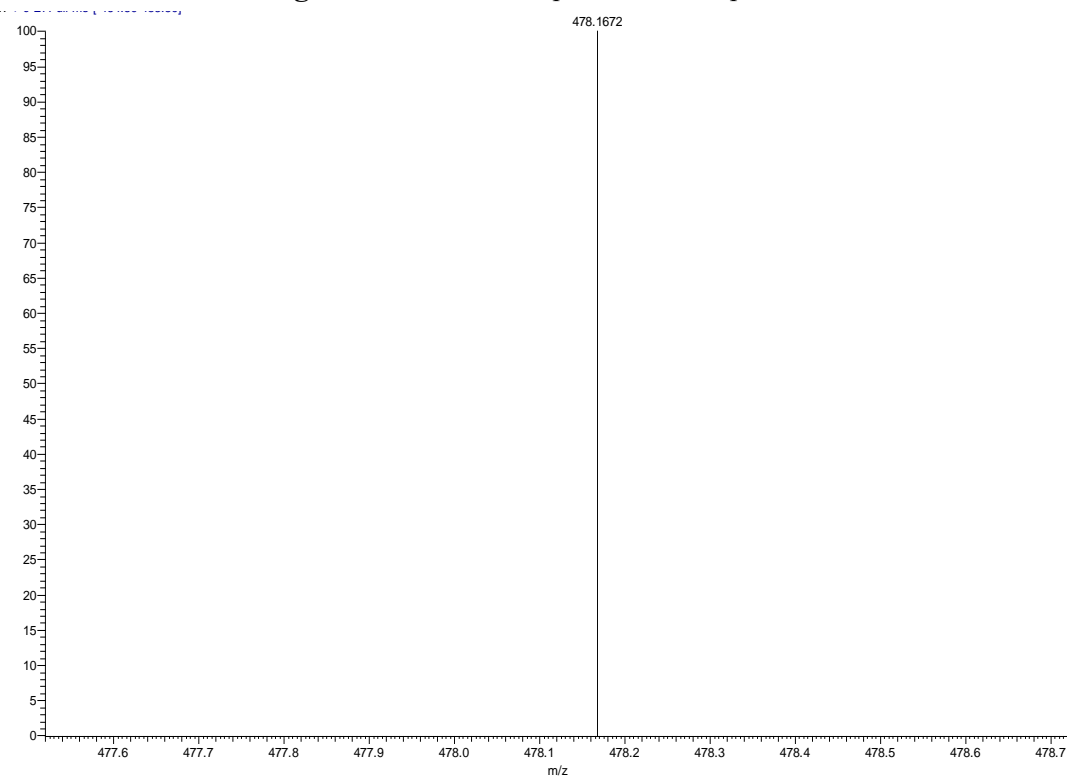


Figure S2. The high resolution mass spectrum of compound **1**

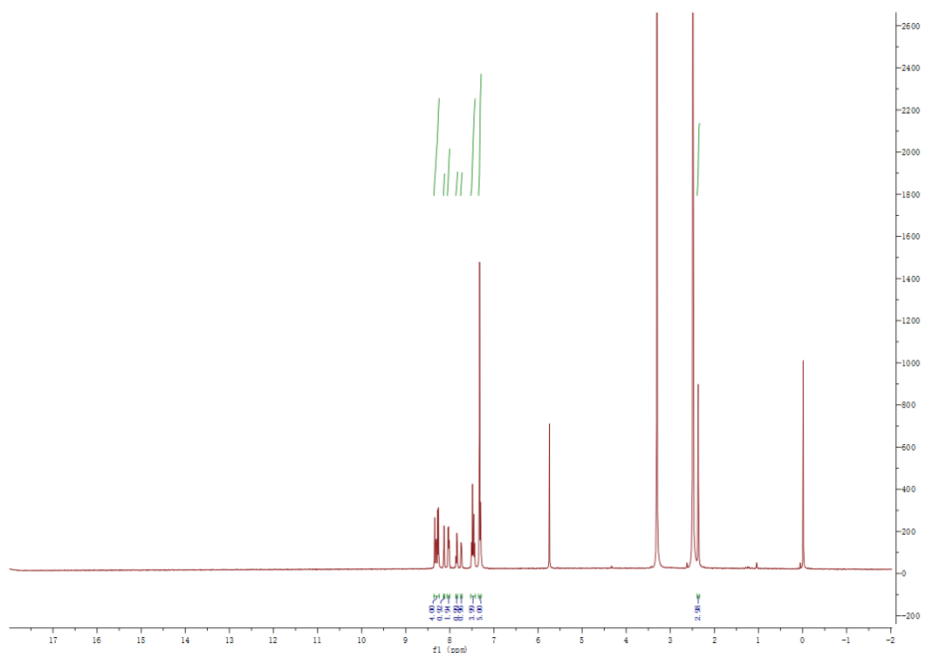


Figure S3. The ^1H NMR spectrum of compound **1** in DMSO-d_6 .

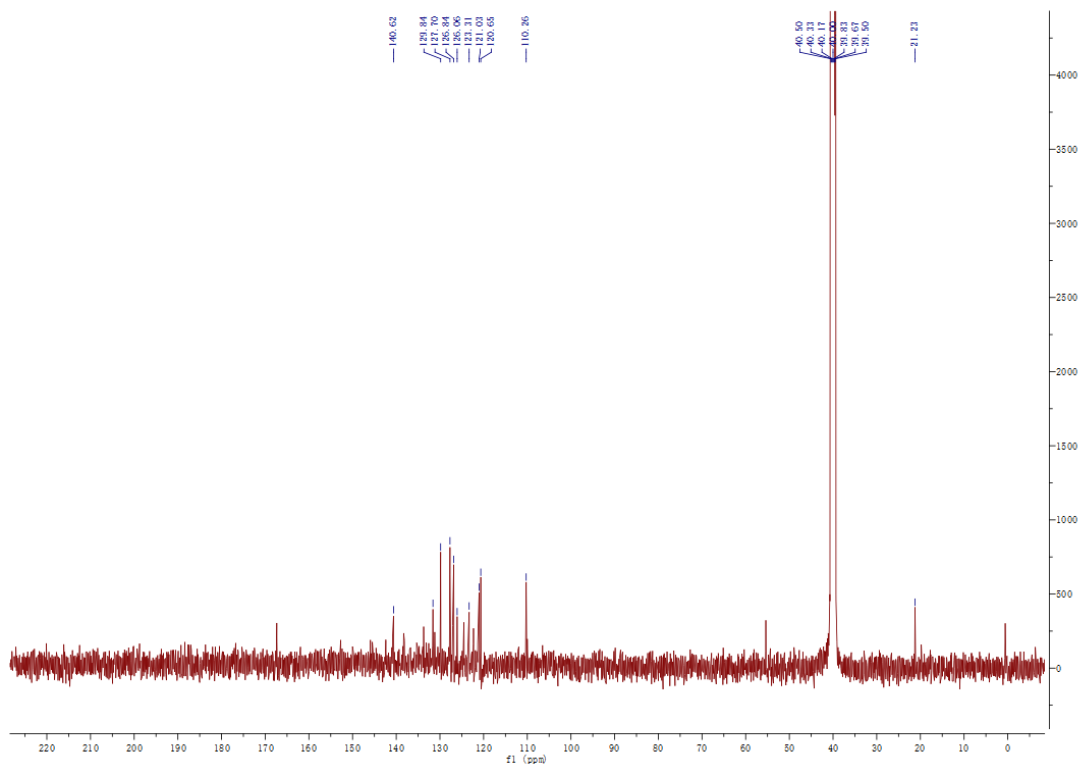


Figure S4. The ^{13}C NMR spectrum of compound **1** in DMSO-d_6 .

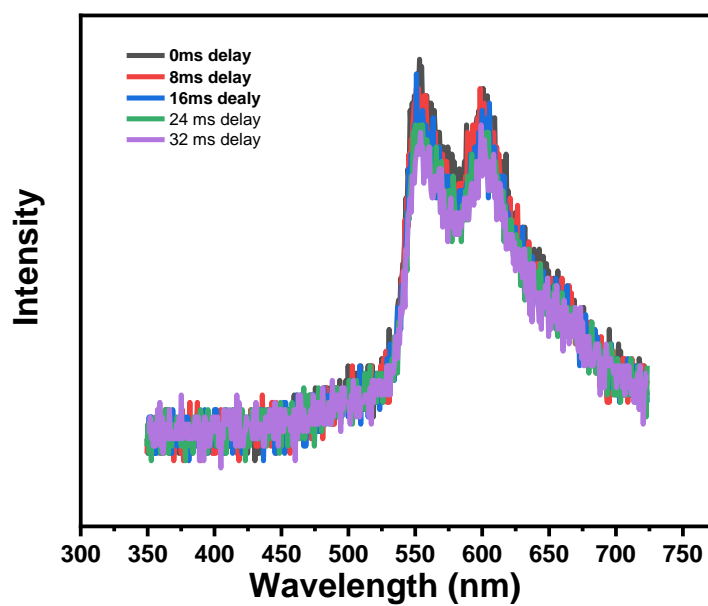


Figure S5. The TRES spectra of 1 powder.

Table S1. The lifetime of 1 powder

Temperature (K)	Lifetime (s)
100	1.13
200	1.12
300	0.47

Table S2. The lifetime of 1 film

Temperature(K)	$\tau_1(\mu\text{s})$	$B_1(\%)$	$\tau_2(\mu\text{s})$	$B_2(\%)$	Lifetime($\mu\text{s})$
100	0.446	30.86	14.69	69.14	10.3
200	1.334	31.85	19.9	68.15	14
300	0.854	36.28	16.48	63.72	16.48

Table S3. Crystal data and structure refinement for **1**

Compound	1
Empirical formula	C ₃₃ H ₂₂ N ₂ O ₂
Formula weight	478.52
Temperature/K	220.00(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	8.6894(2)
b/Å	35.8672(5)
c/Å	8.10020(10)
α/°	90
β/°	107.351(2)
γ/°	90
Volume/Å ³	2409.67(8)
Z	4
ρ _{calc} /cm ³	1.319
μ/mm ⁻¹	0.653
F(000)	1000.0
Crystal size/mm ³	0.23 × 0.15 × 0.04
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	9.864 to 146.646
Index ranges	-10 ≤ h ≤ 9, -43 ≤ k ≤ 40, -9 ≤ l ≤ 6
Reflections collected	7798
Independent reflections	4617 [R _{int} = 0.0301, R _{sigma} = 0.0400]
Data/restraints/parameters	4617/0/335
Goodness-of-fit on F ²	0.997
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0489, wR ₂ = 0.1351
Final R indexes [all data]	R ₁ = 0.0544, wR ₂ = 0.1427