

Electronic supplementary information

A Soluble Cryogenic Thermometer with High Sensitivity Based on Excited-state Configuration Transformations

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Supporting figures

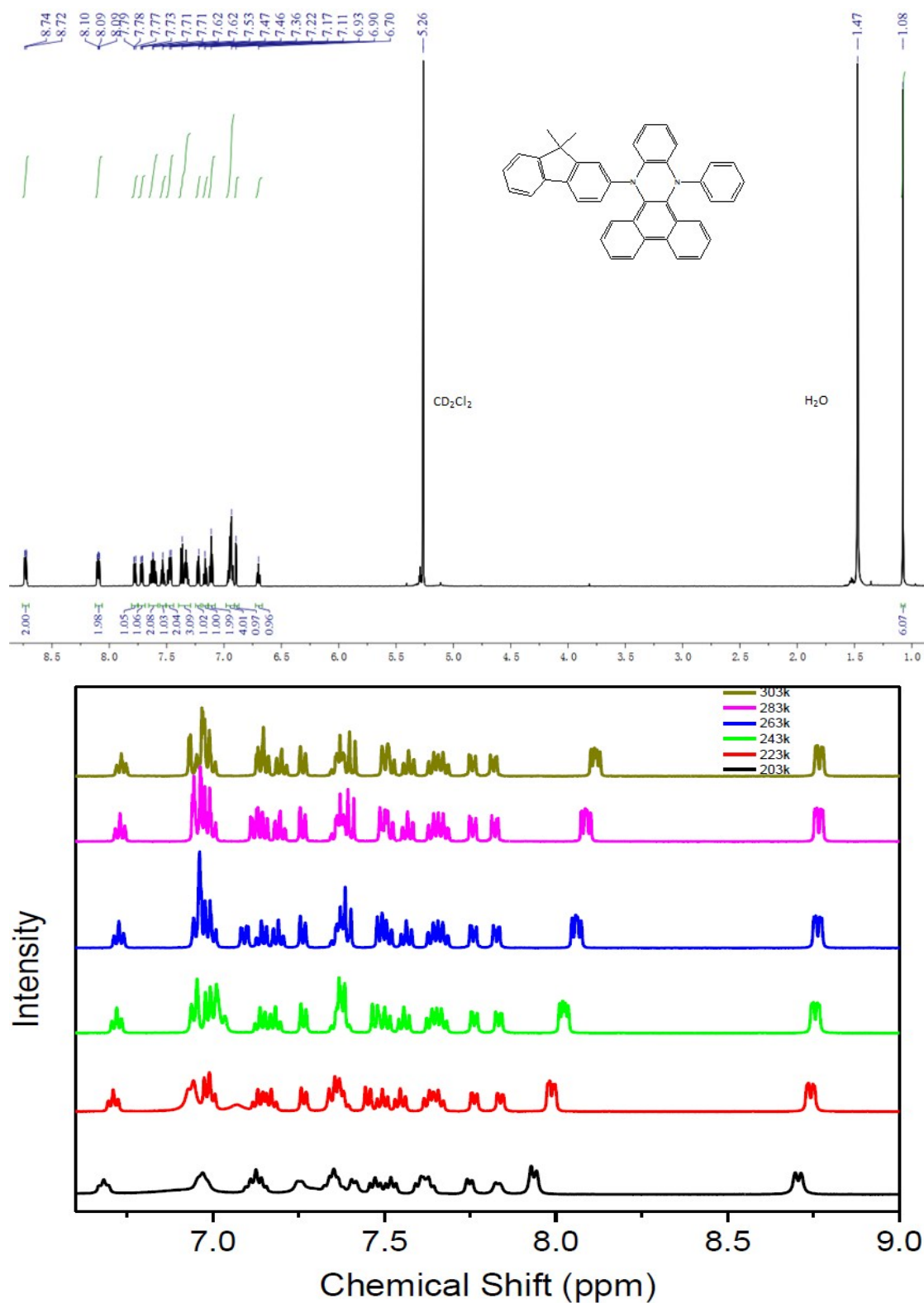


Fig. S1 The ^1H NMR spectra of FIPAC at room temperature (top) and the temperature-dependent ^1H NMR spectra for the aromatic part of FIPAC ranging from 203 K to 303 K for every 20 K (bottom) in CD_2Cl_2 .

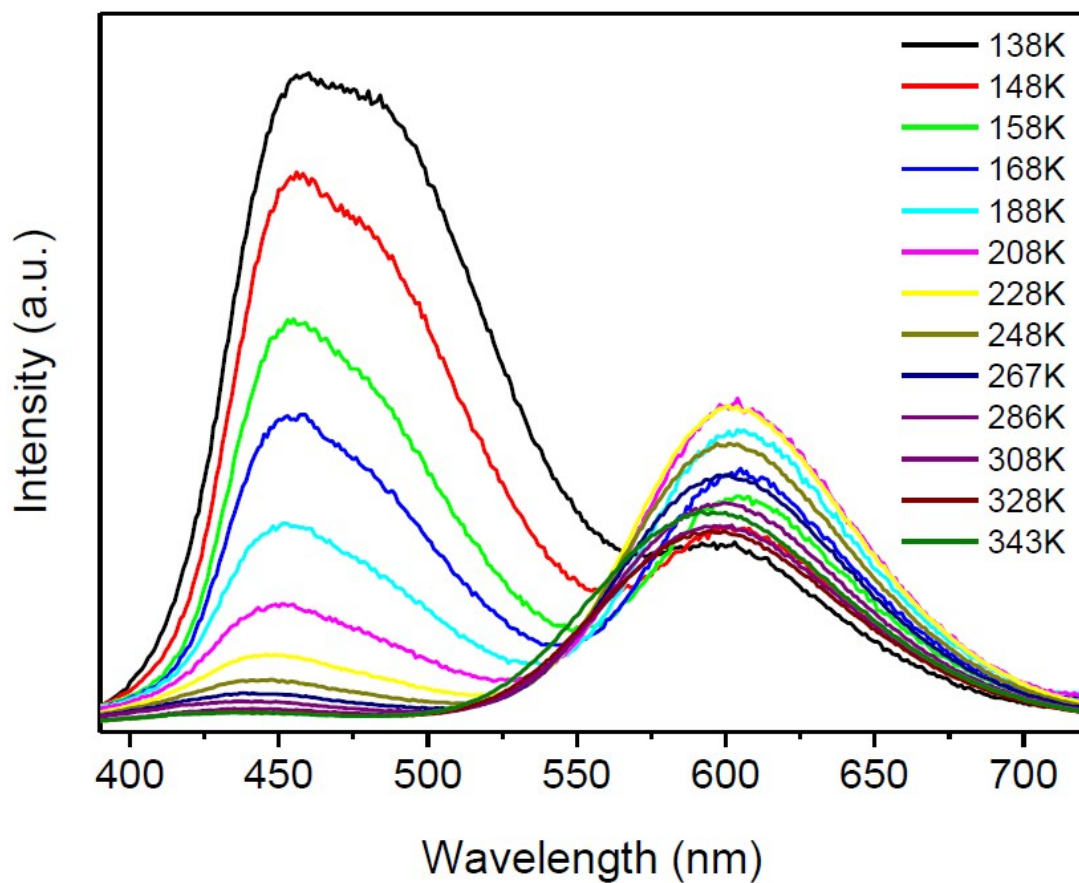


Fig. S2 The temperature-dependent emission spectra of FIPAC from 138 K to 343 K for every 10 K.

Table S1. Quantum yields of FIPAC ranges from 138 K to 343 K

T/K	138	148	158	168	188	208	228	248	268	288	298	308	328	343
$\Phi/\%$	17.7	14.6	11.8	10.5	9.4	8.6	7.8	6.7	5.9	5.2	5.0	3.9	3.8	4.3

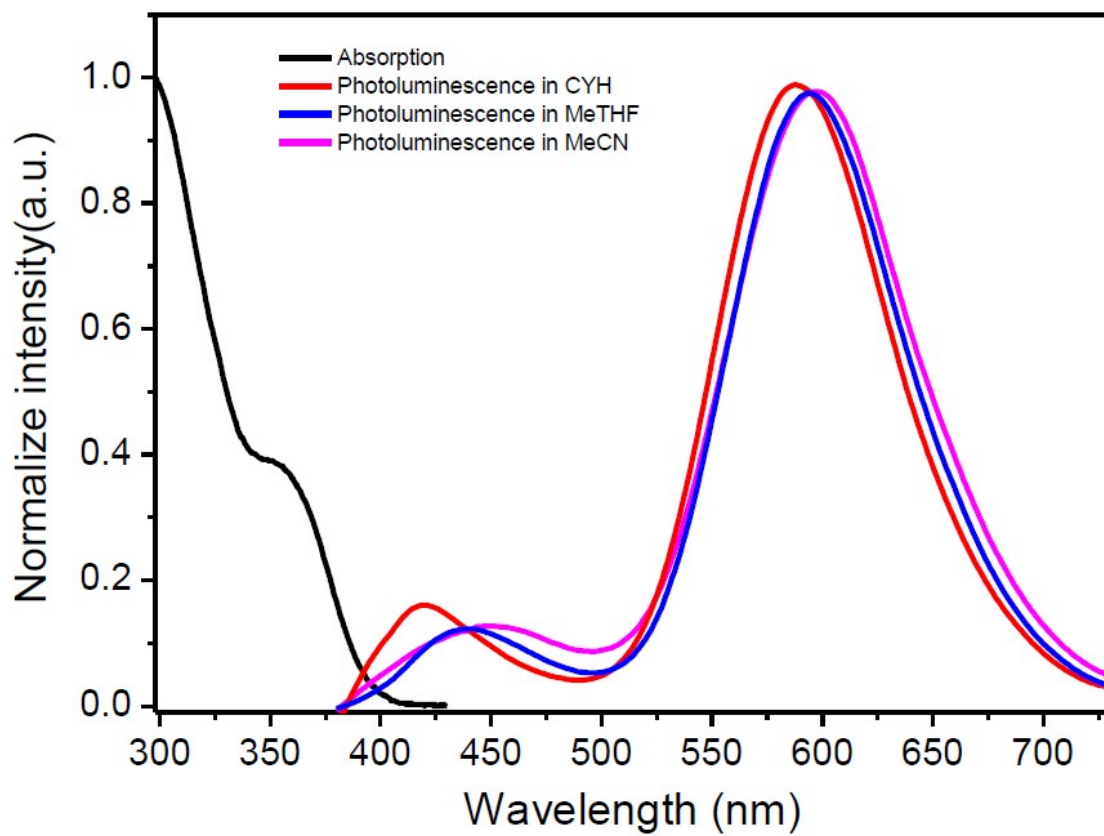


Fig. S3 Absorption (black line) and emission spectra of FIPAC in CYH (red line), MeTHF (blue line) and MeCN (magenta line).

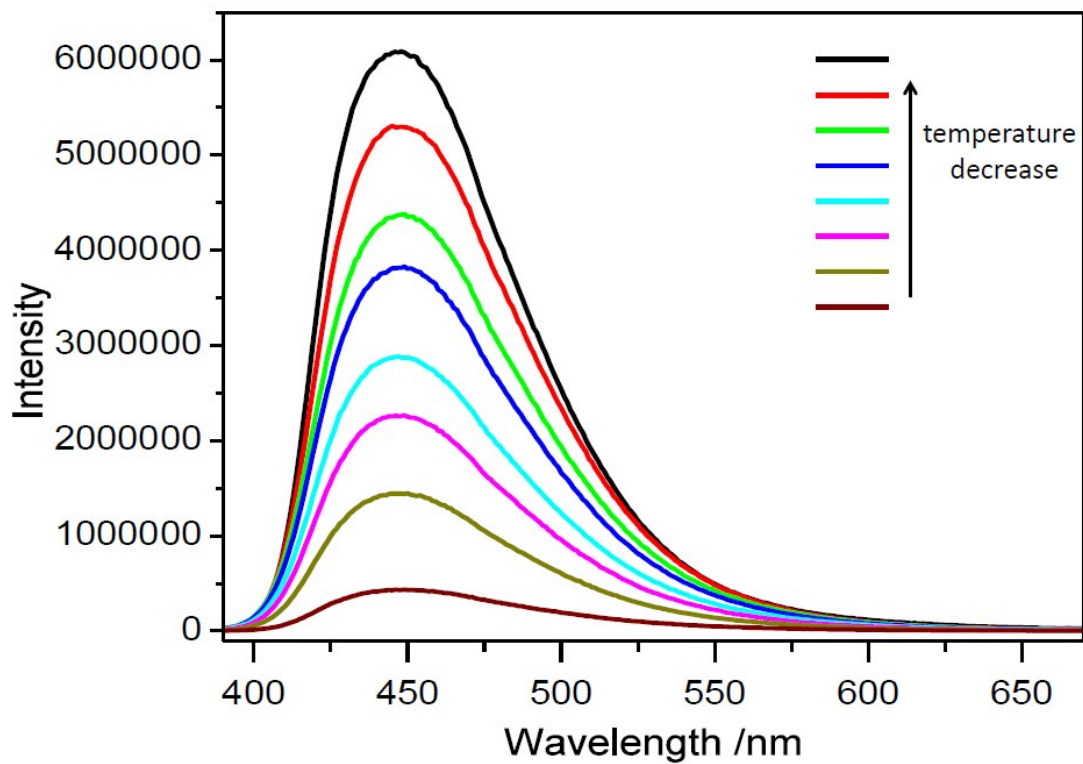


Fig. S4 The temperature-dependent PL spectra of FIPAC film at different temperature (the wine solid line was performed at room temperature).

Calculated for the energy barrier of excited-state configuration transforms

From the body text, it is easy to know that $\frac{A_s}{A_l} \propto e^{\frac{\Delta E}{kT} - 1}$

From Figure 5a, the relationship between A_s/A_l and $1/T$ can be fitted as $A_s/A_l = -0.0947 + 0.0044 \exp(1/0.00104 T)$

Then, it should be noted that $\frac{\Delta E}{kT} = \frac{1}{0.00104T}$

As a consequence, $\Delta E = 7.988 \text{ kJ/mol} = 0.08279 \text{ eV}$.

Geometries (in a.u.) of the different states investigated in this work.

Ground state/F* state

C	-7.42696000	-4.47777900	0.87287900
C	-6.07267800	-4.63171400	0.52155800
C	-5.29626900	-3.52026600	0.24070300
C	-5.83166000	-2.21020600	0.28442200
C	-7.21520800	-2.06732100	0.60473200
C	-7.98579600	-3.21380900	0.91311000
C	-5.01605500	-1.01933600	0.06761400
C	-3.62689900	-1.08515100	-0.19911400
C	-2.85722100	0.05844400	-0.32830700
H	-1.79285900	-0.02803600	-0.53089800
C	-3.44760500	1.32797300	-0.18385400
C	-4.80397100	1.42961600	0.06475600
C	-5.61215400	0.27299600	0.17674600
C	-7.03481400	0.37061100	0.40347400
C	-7.80038700	-0.74797400	0.60689500
H	-8.03231300	-5.34821900	1.11165900
H	-5.62945400	-5.62329000	0.48027500
H	-9.02862000	-3.08530500	1.18151800
H	-2.84084400	2.22582900	-0.26670200
H	-5.26717200	2.40375200	0.17626100
N	-7.67013300	1.64305700	0.57289900
N	-9.17360700	-0.54899000	0.96591900
C	-8.52921200	1.65248100	1.71978400
C	-8.52997100	2.67871500	2.66872600
C	-9.31504900	0.50619500	1.92514700
C	-9.35469100	2.58335700	3.79269000
H	-7.87750700	3.53588700	2.53241900
C	-10.10123600	0.39290400	3.07490400
C	-10.13905800	1.44367800	3.99514700
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H	-10.66753100	-0.51737300	3.24840400
H	-10.75936800	1.35900000	4.88327600
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C	-9.94067300	-1.50706300	-1.16677200
C	-11.55479300	-0.50055800	0.32134900
C	-10.96890400	-1.82924500	-2.05343300
H	-8.92031200	-1.76409900	-1.42567800

C	-12.57228100	-0.82180600	-0.57787500
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H	-10.72045000	-2.33992200	-2.98074700
H	-13.59345400	-0.53563600	-0.33755100
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C	-7.92221000	2.48764200	-0.54655700
C	-7.45519000	2.12738400	-1.82800300
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C	-7.67291700	2.97521600	-2.90600900
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C	-8.85484900	4.53921500	-1.48910400
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C	-8.44192300	4.86092700	-4.05112300
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H	-7.55430000	0.61020300	-4.45787600
H	-8.99451800	1.55584400	-4.88533500
H	-7.64579900	1.41999400	-6.03322400
C	-5.71116300	2.68445600	-4.49514100
H	-5.22636000	3.57229300	-4.07511600
H	-5.32784300	1.80308400	-3.96755200
H	-5.41886800	2.60155900	-5.54898000

S* state

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C	-5.89109400	-2.28007300	0.25916200
C	-7.30039200	-2.11904100	0.54293700
C	-8.06691900	-3.28046100	0.86767300

C	-5.03315100	-1.08860000	0.09045800
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P* state

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C	6.47807800	1.51770600	0.81918500
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C	7.75833100	1.14691700	0.39811200
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C	7.92591200	0.19781300	-0.61882300
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H	8.92753900	-0.08104700	-0.93609500
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H	-1.00194500	-4.58895200	1.98229700
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H	3.02062100	-2.39007000	-1.37894800
H	4.75595400	-2.61772600	-1.66528100