**Supporting Information**

**Preparation of anthracene-based tetra-perimidine hexafluorophosphate and selective recognition for chromium(III) ion**

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**1. CCDC number for compound 3.**

CCDC 1918752 contains the supplementary crystallographic data for compound The data can be obtained free of charge via http//www.ccdc.cam.ac.uk/conts/retrieving. html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK; fax: (+44) 223-336-033; or e-mail: deposit@ccdc.cam. ac. uk.

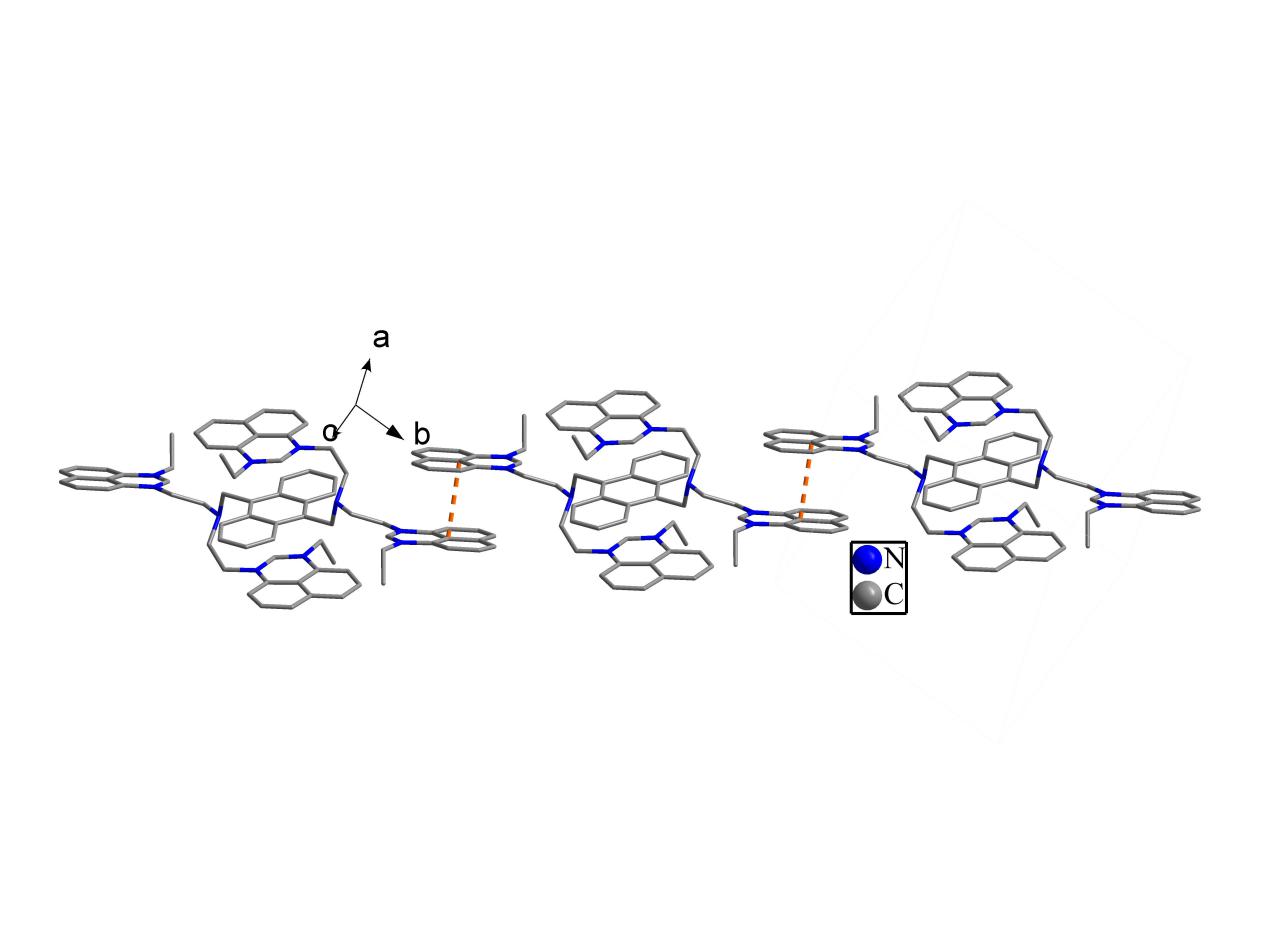
**2. Crystal data and structure refinements for 3**

**Table S1**: Crystal data and structure refinements for **3**

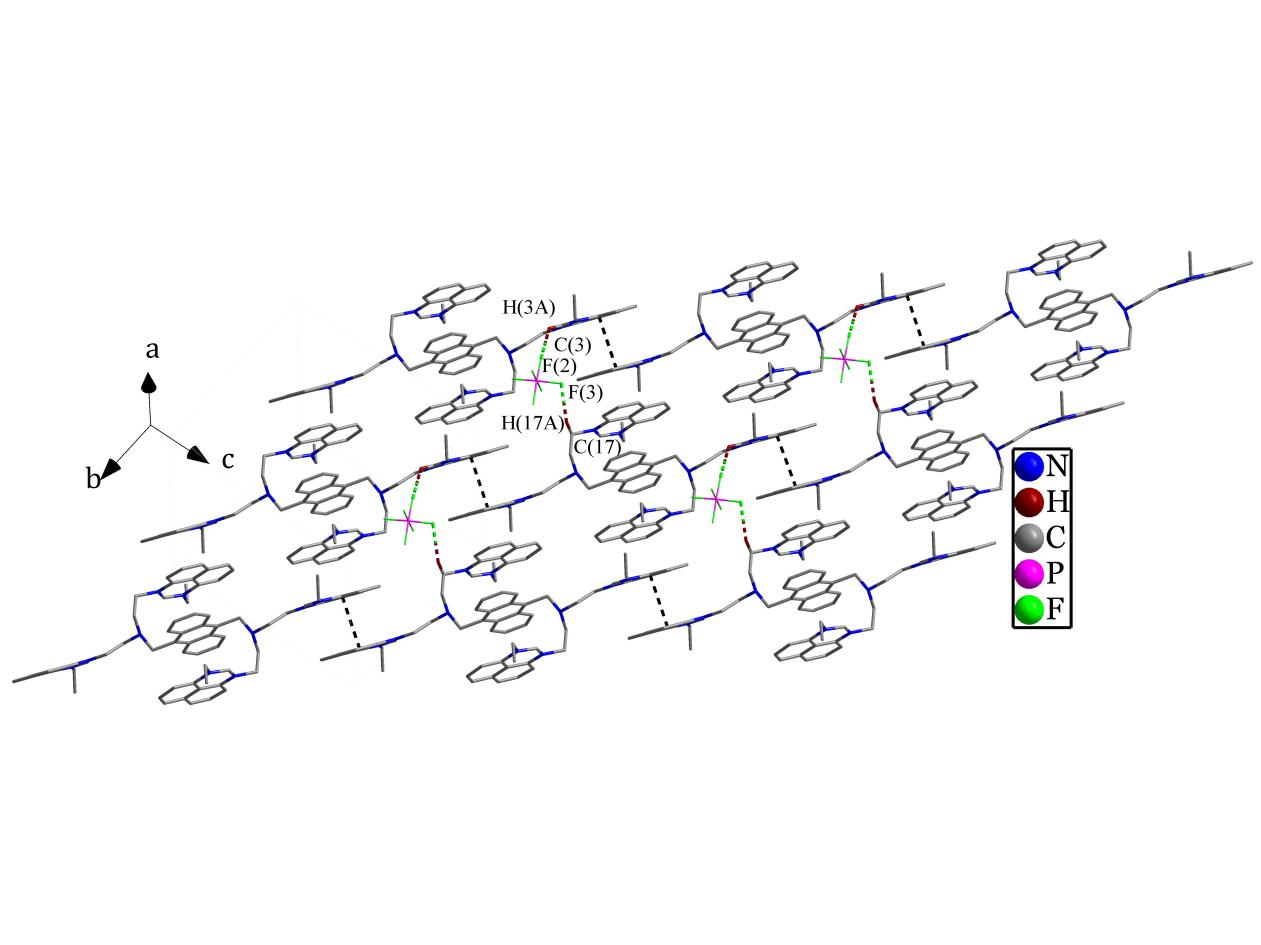
|  |  |  |  |
| --- | --- | --- | --- |
| Chemical formula | C84H90F24N14P4 | *F*(000) | 968 |
| Formula weight | 1875.57 | Cryst size, mm | 0.25 × 0.15 × 0.14 |
| Cryst syst | Triclinic | *θ*min*, θ*max*,* deg | 3.74, 67.06 |
| Space group | *P*ī | *T* /K | 172.9(1) |
| *a/*Å | 11.850(5) | No. of data collected | 14087 |
| *b*/Å | 12.401(6) | No. of unique data | 7439 |
| *c*/Å | 14.951(5) | No. of refined params | 579 |
| *α*/deg | 92.4(1) | Goodness-of-fit on *F*2 a | 1.048 |
| *β*/deg | 94.3(1) | Final *R* indicesb [*I* > 2*σ*(*I*)] |  |
| *γ*/deg | 107.3(4) | *R*1 | 0.0754 |
| *V/*Å3 | 2086.65(1) | *wR*2 | 0.1986 |
| *Z* | 1 | *R* indices (all data) |  |
| *D*calcd*,* Mg/m3 | 1.493 | *R*1 | 0.1117 |
| Abs coeff, mm-1 | 1.797 | *wR*2 | 0.2238 |

a *GOF* = [Σ*ω(F*o2*- F*c2*)*2/(*n* - *p*)]1/2, where *n* is the number of reflection and *p* is the number of parameters refined. b *R*1 *=* Σ(*||Fo| - |Fc||*)/Σ*|Fo|*; *wR*2 *=*[Σ[*w*(*F*o2 - *F*c2)2 ]/ Σ*w*(*F*o2)2]1/2.

**3. The crystal packings of compound 3**

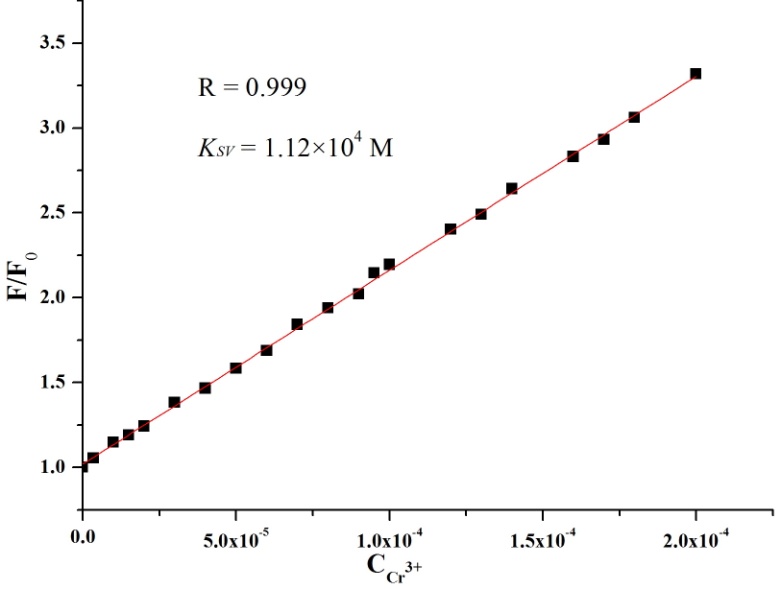
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**Figure S1(a):** 1D supermolecular chain of **3**.

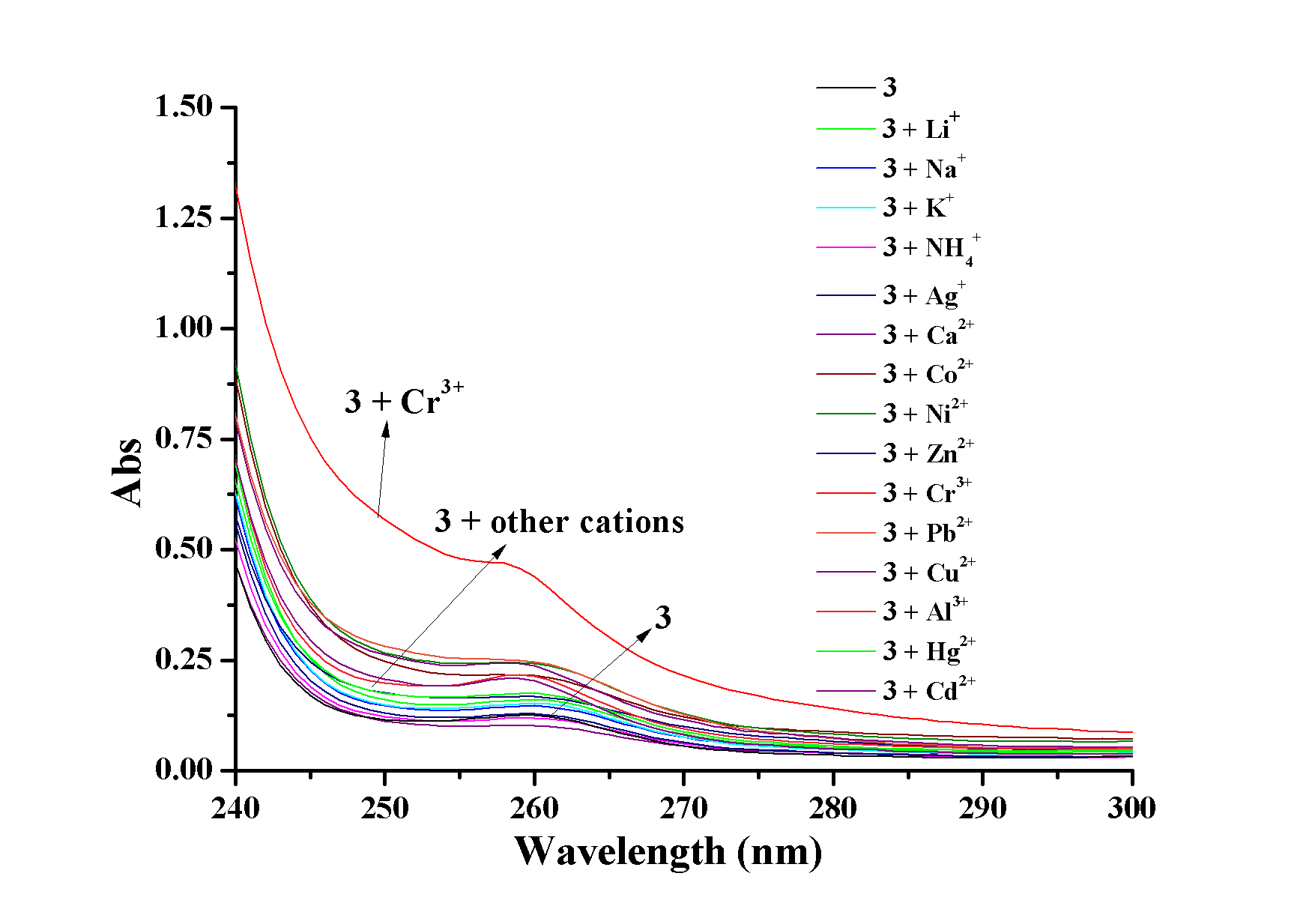
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**Figure S1(b):** 2D supermolecular layer of **3.**

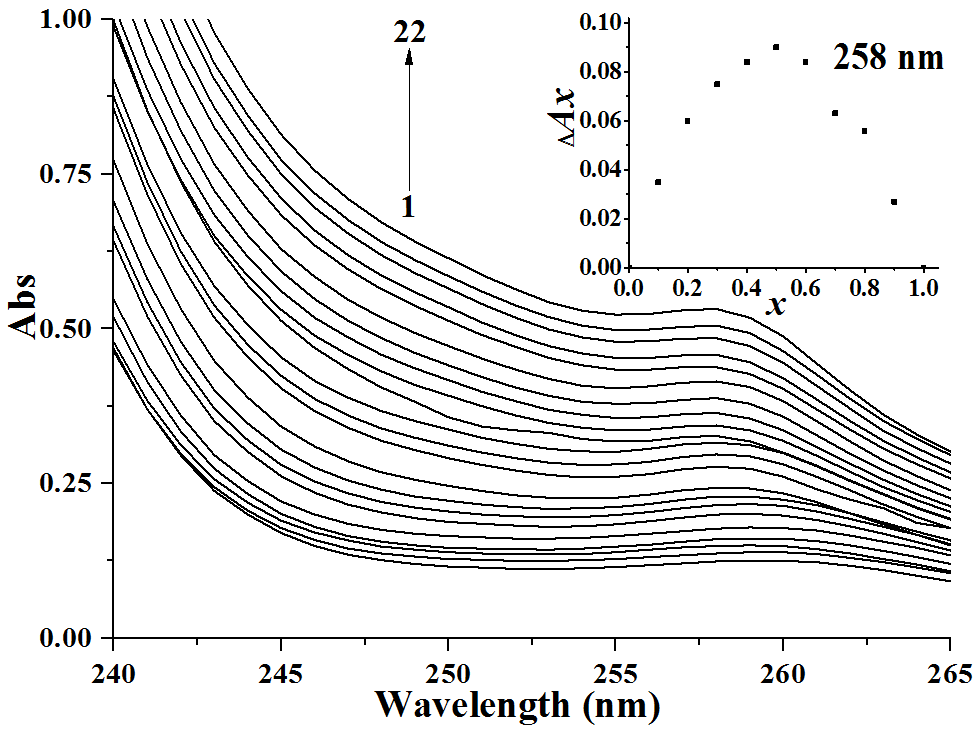
**4. The Figures of fluorescence and UV/vis spectroscopies for compound** **3**

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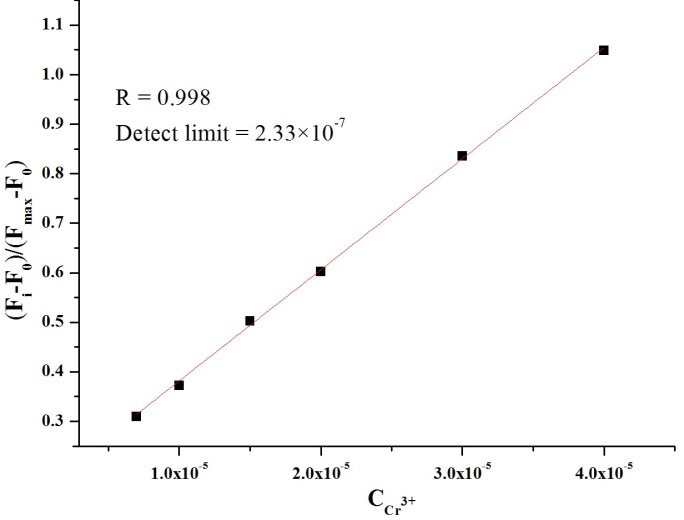
**Figure S2:** Stern-Volmer plot of **3** (5.0 × 10-6 mol/L)in the presence of Cr3+ in CH3CN/DMSO (v:v = 9:1) at 25 ˚C.

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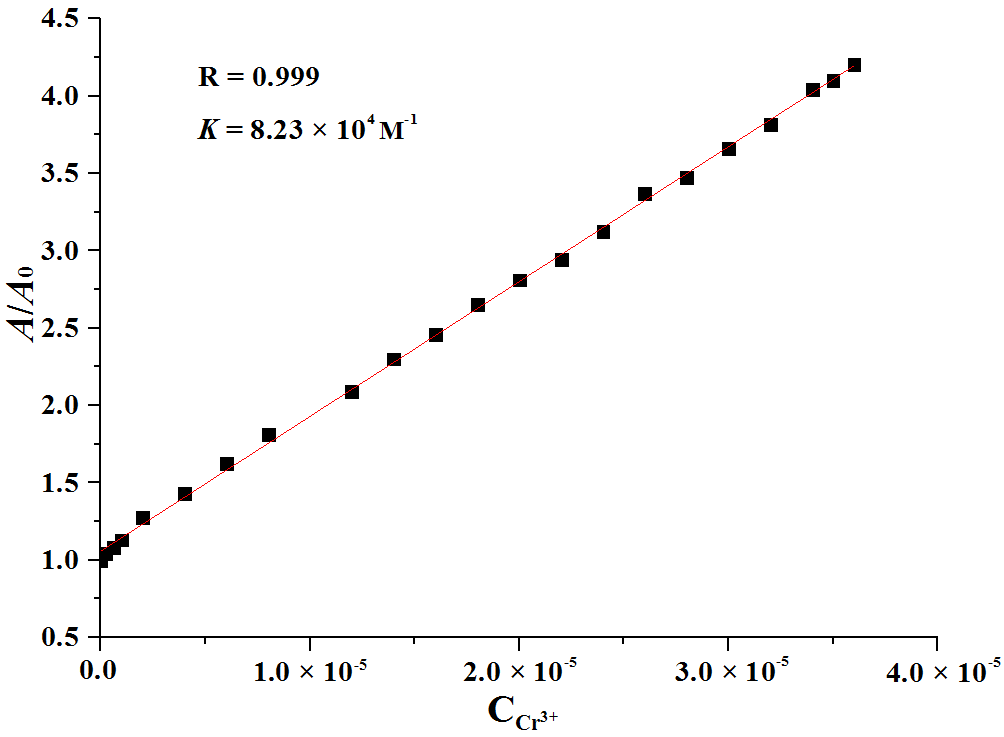
**Figure S3:** UV/vis absorption change of **3** (5.0 × 10-6 mol/L) upon the addition of the nitrate salts of Li+, Na+, K+, NH4+, Ca2+, Al3+, Zn2+, Cd2+, Ag+, Pb2+, Co2+, Hg2+, Al3+, Ni2+ and Cr3+ (5 × 10-5 mol/L) in acetonitrile at 25 ˚C.

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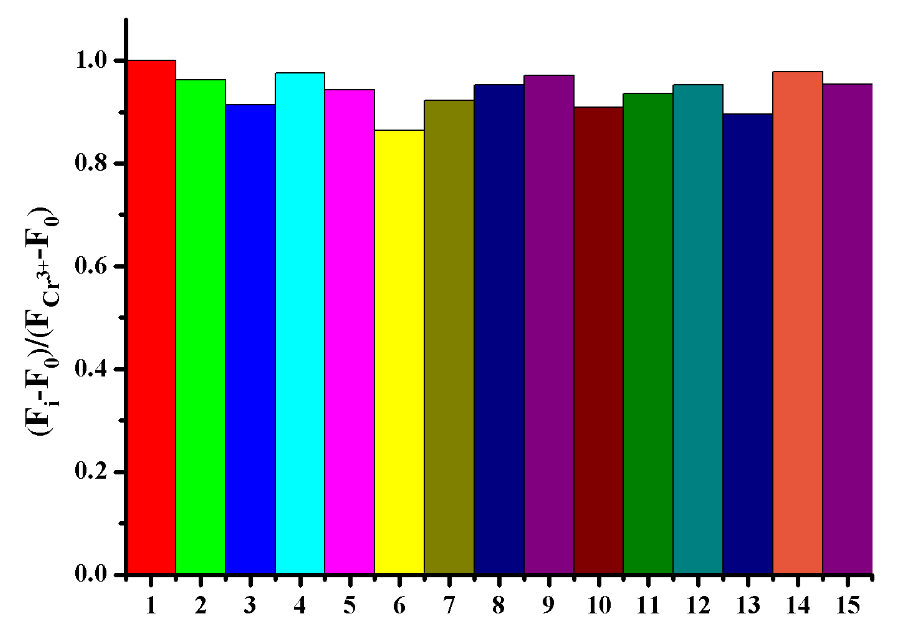
**Figure S4:** TheUV-Vis absorption spectra of **3** (5.0 × 10-6 mol/L) in CH3CN/DMSO (v:v = 9:1) at 25 ˚C. CCr3+ for curves 1-22 are 0, 0.02, 0.06, 0.1, 0.2, 0.4, 0.6, 0.8, 1.2, 1.4, 1.6, 1.8, 2.0, 2.2, 2.4, 2.6, 2.8, 3.0, 3.2, 3.4, 3.5 and 3.6 × 10-5. Inset: the Job’s plot for **3**·Cr3+ complex in CH3CN/DMSO (v:v = 9:1) at 258 nm.

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**Figure S5:** Emission (at 423 nm) of **3** at different concentrations of Cr3+ (0.7, 1.0, 1.5, 2.0, 3.0, 4.0 × 10-5 mol/L) added, normalized between the minimum emission (0.0 M Cr3+) and the emission 4.0 × 10-5 mol/L Cr3+. The detection limit was determined to be 2.33 × 10-7 mol/L.

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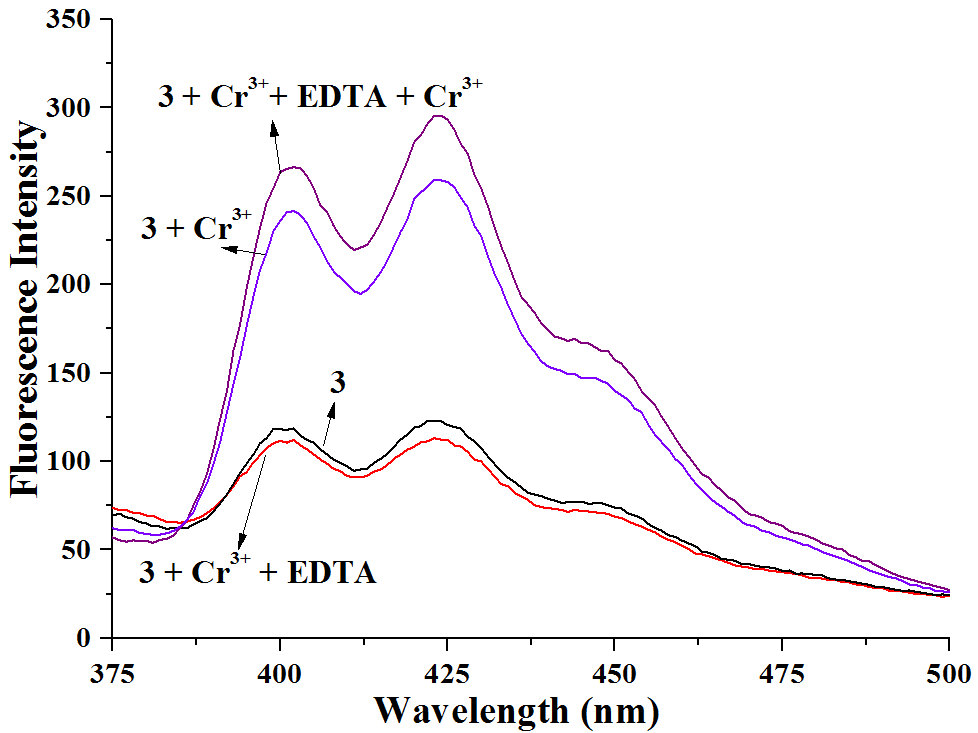
**Figure S6:** Benesi-Hildebrand plot of host **3** (5.0 × 10-6 mol/L) in the presence of Cr3+ in CH3CN/DMSO (v:v = 9:1) at 25 ˚C.

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**Figure S7:** Change ratio ((*F*i - *F*0)/(*F*Cr3+ - *F*0)) of fluorescence intensity of **3** (5.0 × 10-6 mol/L) at 423 nm upon the addition of 30 equiv. Cr3+ in the presence of 30 equiv. background cations. 1: Cr3+; 2: Cr3+ + Li+; 3: Cr3+ + Na+; 4: Cr3+ + K+; 5: Cr3+ + NH4+; 6: Cr3+ + Ag+; 7: Cr3+ + Ca2+; 8: Cr3+ + Co2+; 9: Cr3+ + Ni2+; 10: Cr3+ + Zn2+; 11: Cr3+ + Cu2+; 12: Cr3+ + Cd2+; 13: Cr3+ + Pb2+; 14: Cr3+ + Hg2+; 15: Cr3+ + Al3+ in CH3CN/DMSO (v:v = 9:1) at 25 ˚C.

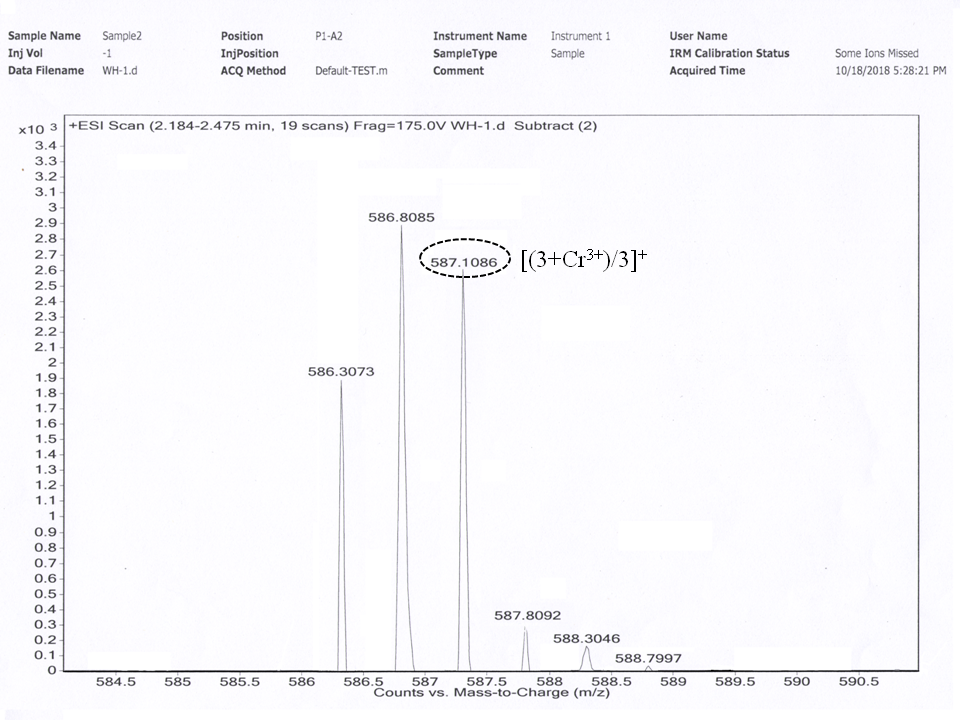
**1.tif**

**Figure S8:** Fluorescence intensity of **3** (5.0 × 10-6 mol/L) in various mixtures of different Cr3+ salts (1: CrCl3, 2: CrBr3, 3: Cr2(SO4)3, 4: Cr(NO3)3, 5: Cr(OAc)3; 3.0 × 10-6 mol/L) in CH3CN/DMSO (v:v = 9:1) at 25 ˚C.

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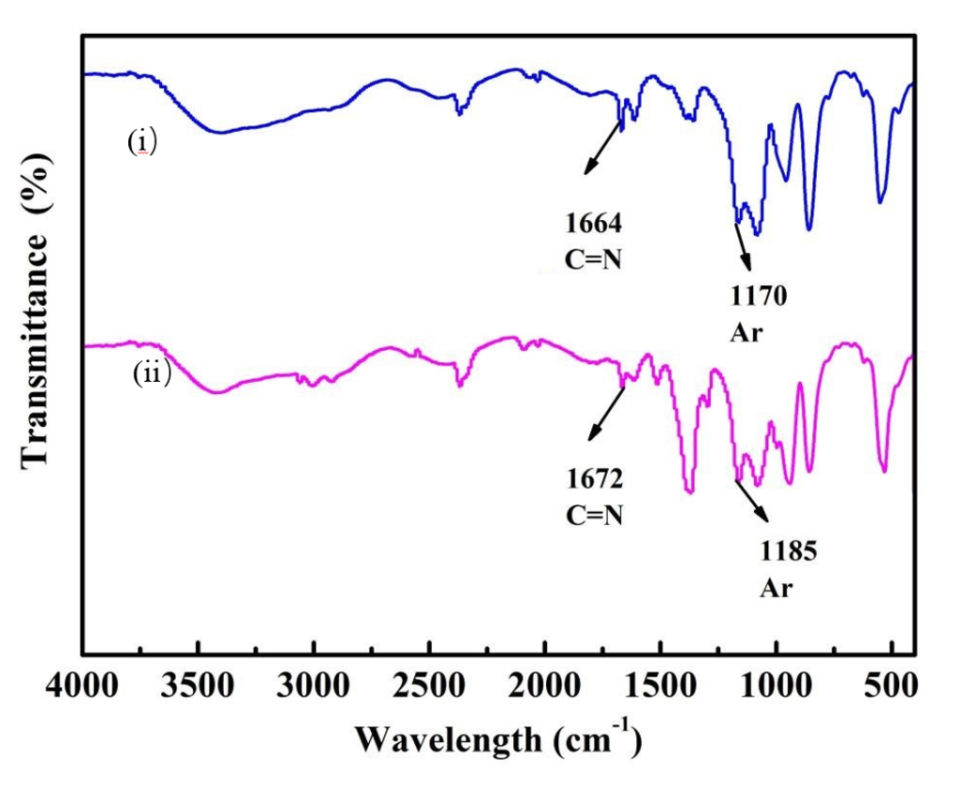
**Figure S9:** Fluorescence reversibility of **3** upon the detection of Cr3+. Fluorescent changes of **3** after the addition of Cr3+, EDTA, Cr3+ in that order in CH3CN/DMSO (v:v = 9:1) at 25 ˚C.

**5. The Figure of HRMS spectra for 3·Cr3+**



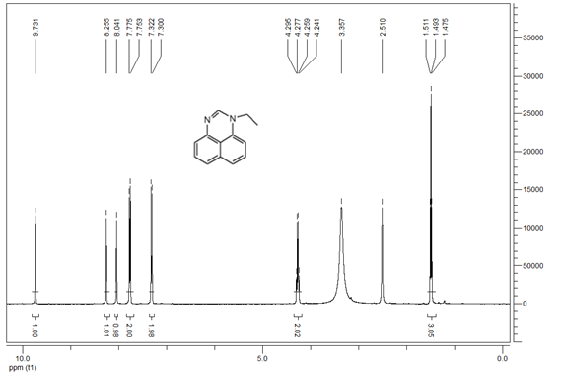
**Figure S10:** HRMS spectra for **3·Cr3+**

**6. Infrared spectraof 3 and 3·Cr3+**

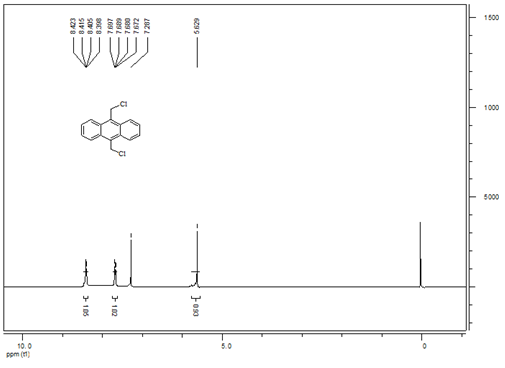


**Figure S11:** Infrared spectroscopy of **3** (top) and **3.Cr3+** (bottom).

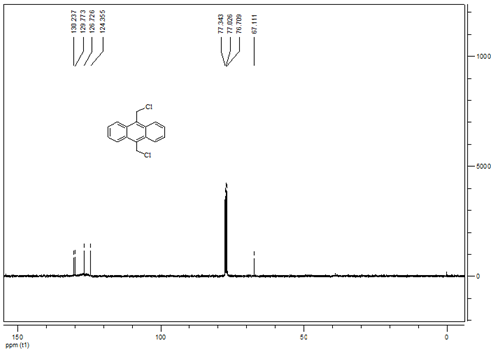
**7. The 1H NMR and 13C NMR spectra of intermediate and compound 3**



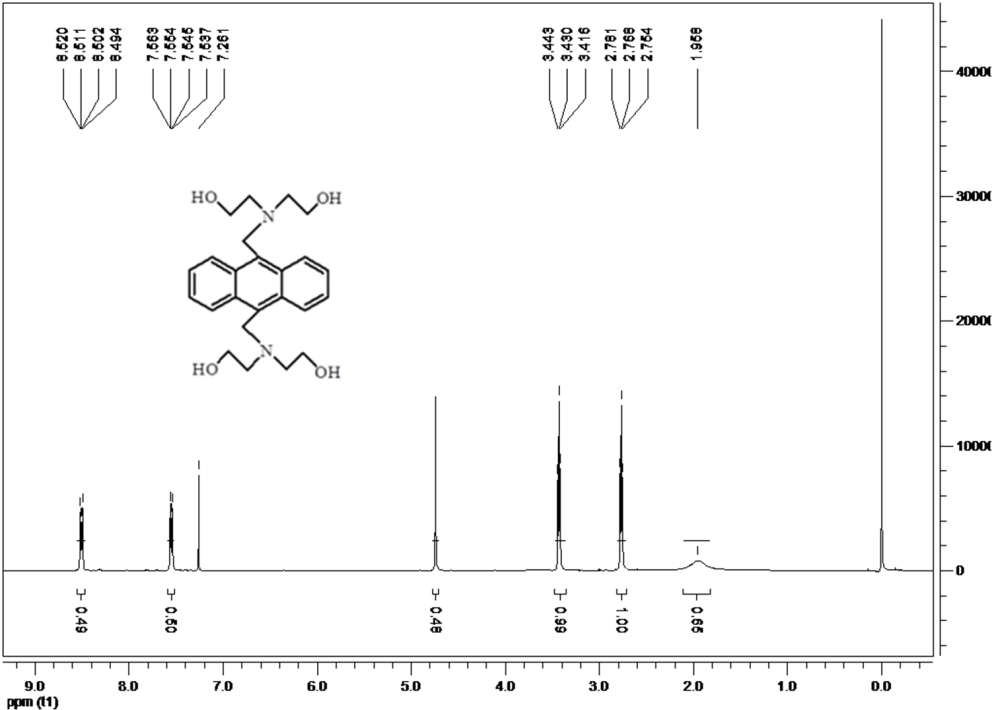
**Figure S12:** The 1H NMR (400 MHz, DMSO-*d*6) spectra of 1-ethylperimidine.

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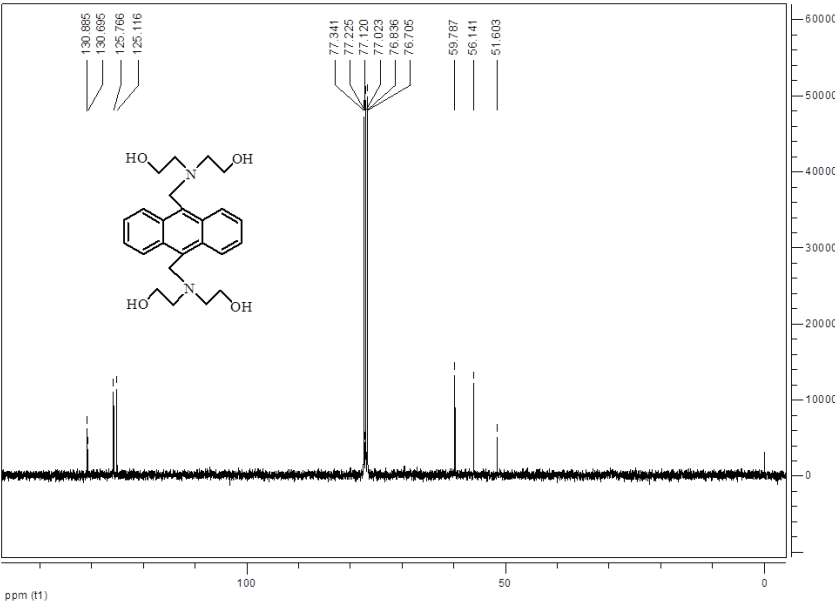
**Figure S13:** The 1H NMR (400 MHz, CDCl3) spectra of9,10-bis(chloromethyl)anthracene.

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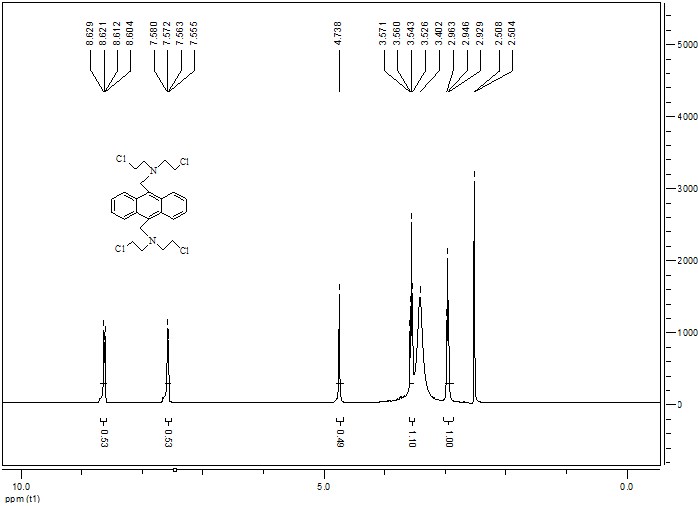
**Figure S14:** The 13C NMR (100 MHz, CDCl3) spectra of 9,10-bis(chloromethyl)anthracene.

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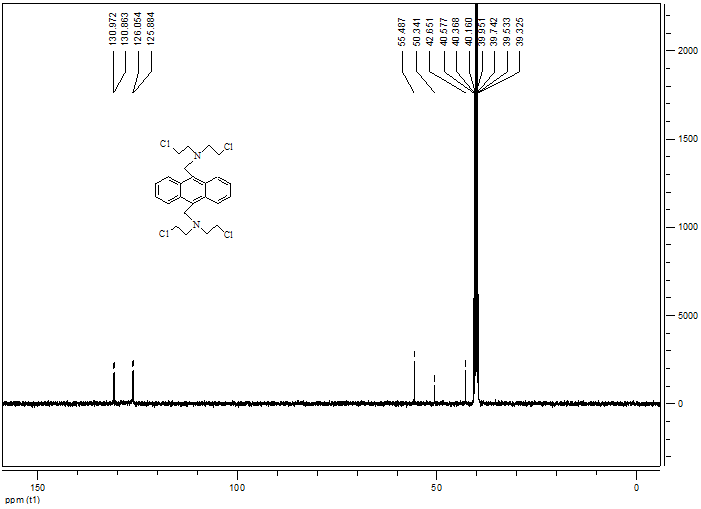
**Figure S15:** The 1H NMR (600 MHz, CDCl3) spectra of 9,10-bis[bi(2-hydoxylethyl)aminemethyl]anthracene.

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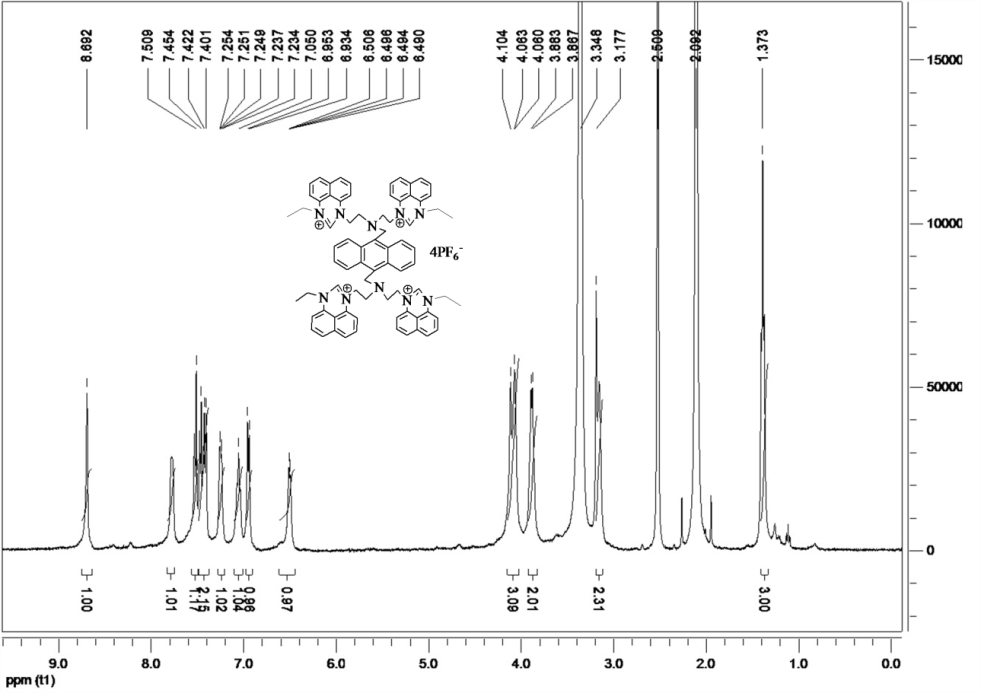
**Figure S16:** The 13C NMR (150 MHz, CDCl3) spectra of 9,10-bis[bi(2-hydoxylethyl)aminemethyl]anthracene

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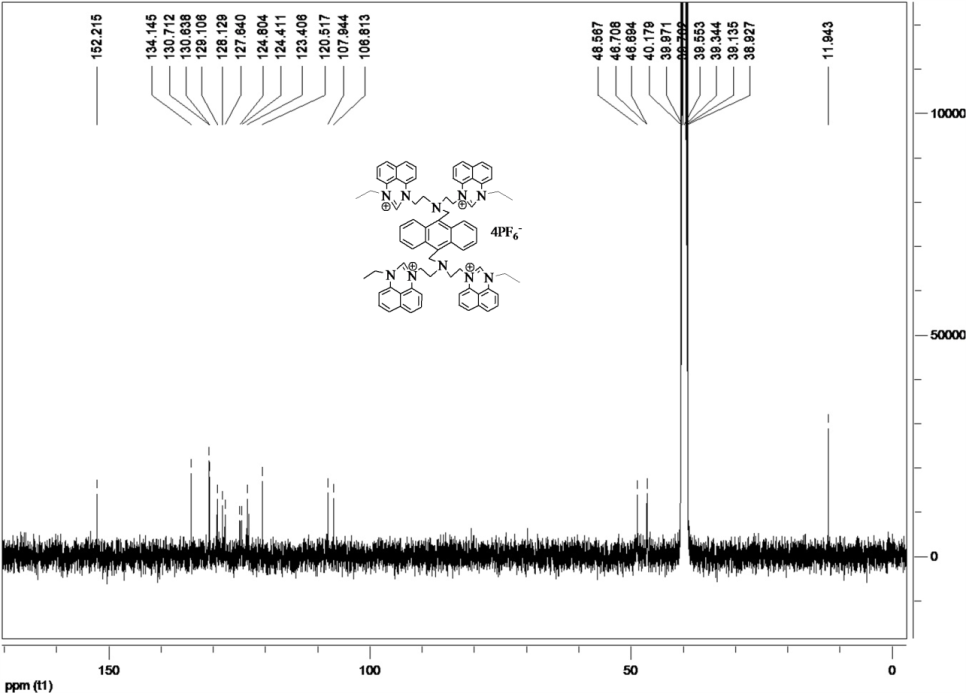
**Figure S17:** The 1H NMR (600 MHz, DMSO-*d*6) spectra of 9,10-bis[bi(2-chloroethyl)aminemethyl]anthracene.

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**Figure S18:** The 13C NMR (150 MHz, DMSO-*d*6) spectra of 9,10-bis[bi(2-chloroethyl)aminemethyl]anthracene.



**Figure S19:** The 1H NMR (600 MHz, DMSO-*d*6) spectrum of **3.**



**Figure S20:** The 13C NMR (150 MHz, DMSO-*d*6) spectrum of **3**.