

## **Electronic Supplementary Information**

for

### **Controlling the unpaired electron by electrostatic attraction in the solid state**

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## 1. Materials and General

All operations were carried out under an atmosphere of dry argon or nitrogen by using modified Schlenk line and glovebox techniques. All solvents were freshly distilled from Na/benzophenone and degassed prior to use. Elemental analyses were performed on an Elementar Vario EL III instrument at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. EPR spectra were obtained using Bruker plus-6/1 X-band variable-temperature apparatus. Commercially available reagents were purchased from Aldrich, Acros or Alfa-Assar, and used as received. Compound 2,7-*t*Bu<sub>2</sub>-PTO (**1**) was synthesized according to the reported literatures.<sup>1</sup>

### Procedure for X-ray diffraction measurement

In glove box under N<sub>2</sub> atmosphere, the crystal sample of **1K(cryp)** or **1K(18c6)** was coated with polybutylene. This sample was stable for several weeks in the glove box and suitable for X-ray diffraction measurements. The crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N<sub>2</sub> flow. The data were collected on a Bruker APEX-II CCD area detector with a radiation source of Ga(K $\alpha$ ) (1.34139 Å) or Mo(K $\alpha$ ) (0.71073 Å) at setting temperatures. Multiscan or empirical absorption corrections (SADABS) were applied. The structures were solved by direct methods and all refined on  $F^2$  with the SHELX-2018/3 software package.<sup>2</sup> The positions of the H atoms were calculated and considered isotropically according to a riding model.

### Procedure for EPR measurement

In glove box under N<sub>2</sub> atmosphere, the crystal sample of **1K(cryp)** or **1K(18c6)** was dissolved in THF and loaded into sealed paramagnetic tube for EPR measurements.

### Procedure for UV/Vis spectral measurement

All the sample solutions were prepared in glove box. The crystal sample of **1K(cryp)** or **1K(18c6)** was dissolved in THF. The prepared sample solution was injected into a sealed cuvette, the absorption was recorded at room temperature.

## 2. Synthesis

### Synthesis of **1K(cryp)**

A mixture of **1** (58.3 mg, 0.16 mmol), K (6.6 mg, 0.17 mmol) and cryptand[2.2.2] (64.1 mg, 0.17 mmol) in THF ( $\approx$  20 ml) was stirred at room temperature overnight, whereupon the color of the solution was changed from yellow to brown green. After filtration, the filtrate was concentrated to ca. 2 ml and stored at -20 °C for 1 day to afford black crystals of **1K(cryp)** (48.5 mg, 39.4%). M.p. 186-189 °C. Elemental analysis (%) Calcd for C<sub>42</sub>H<sub>58</sub>KN<sub>2</sub>O<sub>10</sub>•C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>: C, 62.77; H, 7.79; N, 3.18. Found: C, 62.59; H, 7.55; N, 3.55.

### Synthesis of **1K(18c6)**

A mixture of **1** (98.5 mg, 0.26 mmol), **K** (11.1 mg, 0.28 mmol) and 18-c-6 (69.5 mg, 0.26 mmol) in THF ( $\approx$  30 ml) was stirred at room temperature overnight, whereupon the color of the solution was changed from yellow to green. After filtration, the filtrate was concentrated to ca. 5 ml and stored at 5 °C for 1 day to afford green crystals of **1K(18c6)** (77.1 mg, 43.2%). M.p. 184-186 °C. Elemental analysis (%) Calcd for  $C_{36}H_{46}KO_{10} \cdot C_4H_8O$ : C, 63.79; H, 6.84. Found: C, 63.23; H, 6.98.

### Synthesis of **[1K(15c5)]<sub>4</sub>**

A mixture of **1** (81.5 mg, 0.22 mmol), **K** (9.0 mg, 0.23 mmol) and 15-c-5 (71.2 mg, 0.32 mmol) in DME ( $\approx$  30 ml) was stirred at room temperature overnight, whereupon the color of the solution was changed from yellow to dark green. After filtration, the filtrate was concentrated to ca. 5 mL and stored at 5 °C for 2 day to afford dark red solid of **[1K(15c5)]<sub>4</sub>** (25.6 mg, 17.4%). M.p. 163-165 °C. Elemental analysis (%) Calcd for  $C_{136}H_{168}K_4O_{36}$ : C, 64.43; H, 6.68; Found: C, 64.91; H, 7.32.

### Synthesis of **(1K)<sub>2n</sub>**

A mixture of **1** (63.2 mg, 0.17 mmol), **K** (8.2 mg, 0.21 mmol) in DME ( $\approx$  30 ml) was stirred at room temperature overnight, whereupon the color of the solution was changed from yellow to green. After filtration, the filtrate was concentrated to ca. 5 mL and stored at 5 °C for 1 day to afford black crystals of **(1K)<sub>2n</sub>** (20.3 mg, 23.8%). M.p. >300 °C. Elemental analysis (%) Calcd for  $C_{28}H_{32}KO_6$ : C, 66.77; H, 6.40. Found: C, 65.89; H, 7.63.

## 3. Reciprocal transformation

### From **1K(cryp)** to **1K(18c6)**

A mixture of **1** (60.1 mg, 0.16 mmol), **K** (6.6 mg, 0.17 mmol) and cryptand[2.2.2] (63.6 mg, 0.17 mmol) in THF ( $\approx$  30 ml) was stirred at room temperature overnight, whereupon the color of the solution was changed from yellow to brown green. After filtration, KI (36.3 mg, 0.22 mmol) and 18-c-6 (45.3 mg, 0.17 mmol) were added into the filtrate. The color soon changed to from brown green to green. The mixture was allowed to stir overnight and then concentrated to ca. 3 ml and stored at -20 °C for 1 day to afford green crystals of **1K(18c6)**. Cell parameters:  $a = 8.03 \text{ \AA}$ ,  $b = 22.37 \text{ \AA}$ ,  $c = 24.55 \text{ \AA}$ ,  $V = 4408 \text{ \AA}^3$ , Orthorhombic P.

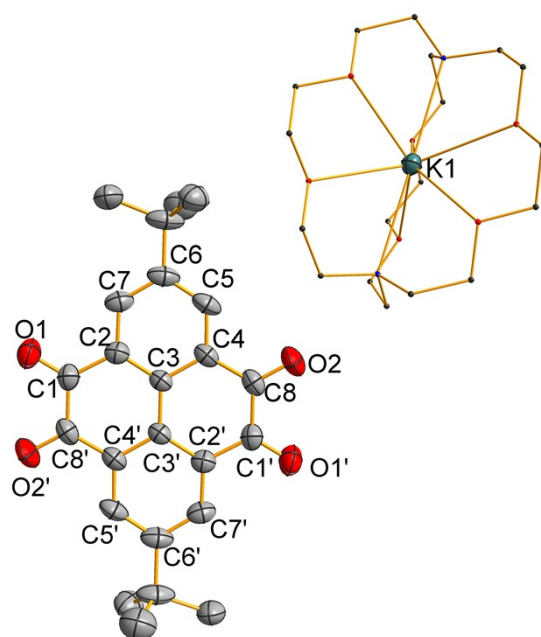
### From **1K(18c6)** to **1K(cryp)**

A mixture of **1** (64.8 mg, 0.17 mmol), **K** (7.1 mg, 0.18 mmol) and 18-c-6 (48.0 mg, 0.18 mmol) in THF ( $\approx$  30 ml) was stirred at room temperature overnight, whereupon the color of the solution was changed from yellow to green. After filtration, cryptand[2.2.2] (68.4 mg, 0.18 mmol) was added into the filtrate. The color changed to from green to brown green 5 min later. The mixture was allowed to stir overnight and then concentrated to ca. 3 mL and stored at -20 °C for 1 day to afford black crystals of **1K(cryp)**. Cell parameters:  $a = 13.01 \text{ \AA}$ ,  $b = 16.42 \text{ \AA}$ ,  $c = 20.60 \text{ \AA}$ ,  $\beta = 98.77^\circ$ ,  $V = 4349 \text{ \AA}^3$ , Monoclinic C.

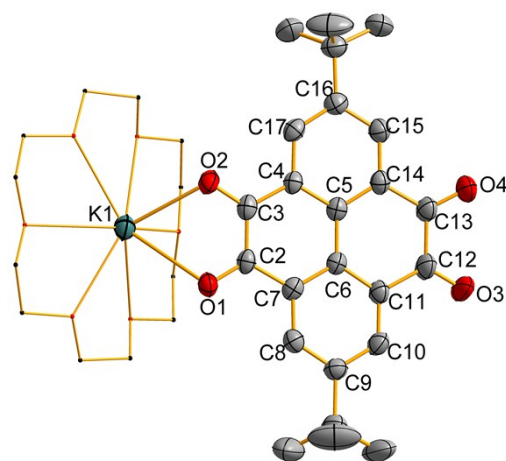
## 4. Crystal structures

**Table S1.** Crystal data and structure refinement. Crystals of **1K(cryp)** and **1K(18c6)** suitable for X-ray analysis were grown from THF. And crystals of **[1K(15c5)]<sub>4</sub>** and **(1K)<sub>2n</sub>** suitable for X-ray analysis were grown from DME. Two seriously disordered solvent molecules (THF) in **1K(18c6)** have been squeezed.

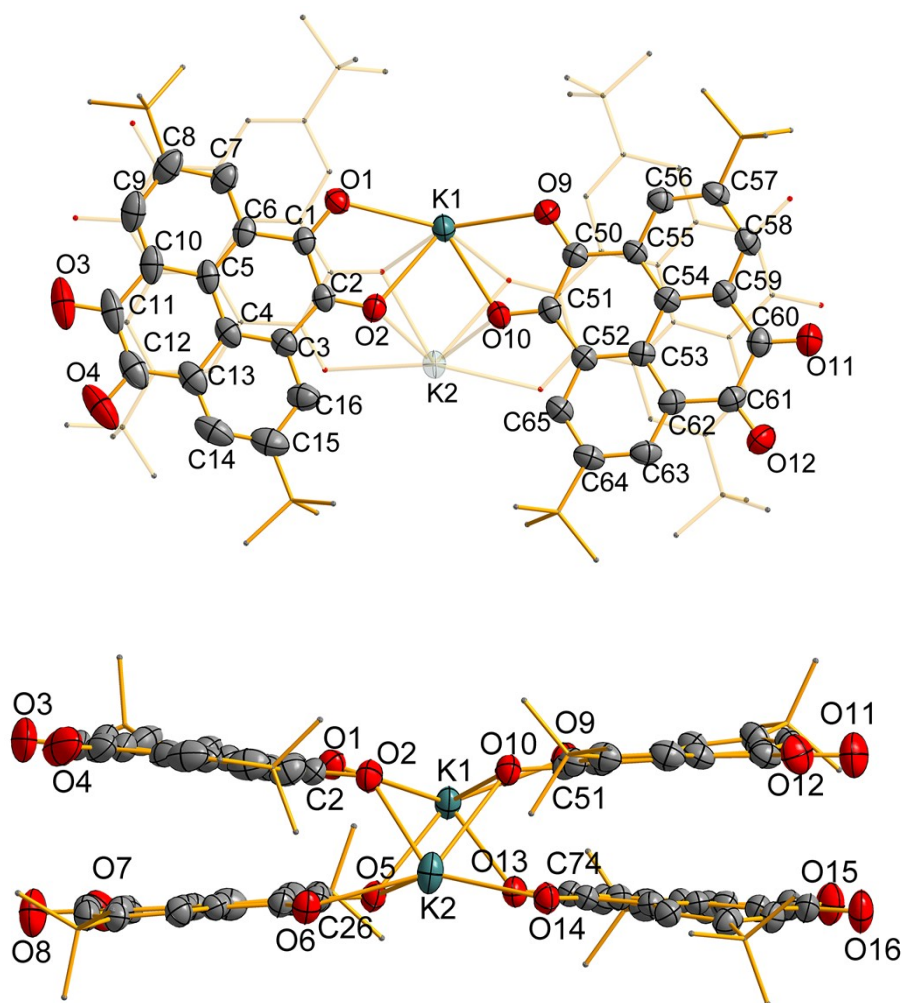
	<b>1K(cryp)</b>	<b>1K(18c6)</b>	<b>[1K(15c5)]<sub>4</sub></b>	<b>(1K)<sub>2n</sub></b>
CCDC No.	2061470	2061471	2061472	2061473
Formula	C <sub>42</sub> H <sub>58</sub> KN <sub>2</sub> O <sub>10</sub>	C <sub>36</sub> H <sub>46</sub> KO <sub>10</sub>	C <sub>144</sub> H <sub>188</sub> K <sub>4</sub> O <sub>40</sub>	C <sub>28</sub> H <sub>32</sub> KO <sub>6</sub>
Formula weight	790.00	677.83	2715.33	503.63
Temp. (K)	193(2) K	296(2)	296(2)	193(2) K
Crystal system	Monoclinic	Orthorhombic	Triclinic	Triclinic
Space group	<i>C2/c</i>	<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>	<i>P-1</i>	<i>P-1</i>
<i>a</i> (Å)	12.8968(4)	8.0229(5)	15.9555(13)	11.7079(6)
<i>b</i> (Å)	16.1529(6)	22.4041(14)	17.9505(14)	11.8131(6)
<i>c</i> (Å)	20.4741(8)	24.5984(16)	27.485(2)	12.0431(10)
$\alpha$ (°)	90	90	88.330(2)	109.702(4)
$\beta$ (°)	98.9680(10)	90	74.113(2)	98.730(3)
$\gamma$ (°)	90	90	86.647(3)	119.522(2)
<i>V</i> [Å <sup>3</sup> ]	4213.0(3)	4421.5(5)	7557.7(11)	1257.61(14)
<i>Z</i>	4	4	2	2
$\rho_{\text{calcd}}$ (g·cm <sup>-3</sup> )	1.245	1.018	1.193	1.330
$\mu$ (mm <sup>-1</sup> )	0.184	0.164	0.192	1.452
<i>F</i> (000)	1692	1444	2896.0	534
Collected data	18968	33362	65907	4067
Unique data	4831	7772	34259	4067
	[ <i>R</i> (int) = 0.0516]	[ <i>R</i> (int) = 0.0490]	[ <i>R</i> (int) = 0.0369]	[ <i>R</i> (int) = 0]
GOF on <i>F</i> <sup>2</sup>	0.872	1.025	0.943	1.165
Final <i>R</i> indexes	<i>R</i> <sub>1</sub> = 0.0528	<i>R</i> <sub>1</sub> = 0.0551	<i>R</i> <sub>1</sub> = 0.0828	<i>R</i> <sub>1</sub> = 0.0967
[ <i>I</i> > 2σ( <i>I</i> )]	$\omega R_2$ = 0.1449	$\omega R_2$ = 0.1542	$\omega R_2$ = 0.1973	$\omega R_2$ = 0.2112
<i>R</i> indexes (all data)	<i>R</i> <sub>1</sub> = 0.0643	<i>R</i> <sub>1</sub> = 0.0664	<i>R</i> <sub>1</sub> = 0.1421	<i>R</i> <sub>1</sub> = 0.1373
	$\omega R_2$ = 0.1571	$\omega R_2$ = 0.1649	$\omega R_2$ = 0.2325	$\omega R_2$ = 0.2297
Completeness	0.996	0.995	0.984	0.980



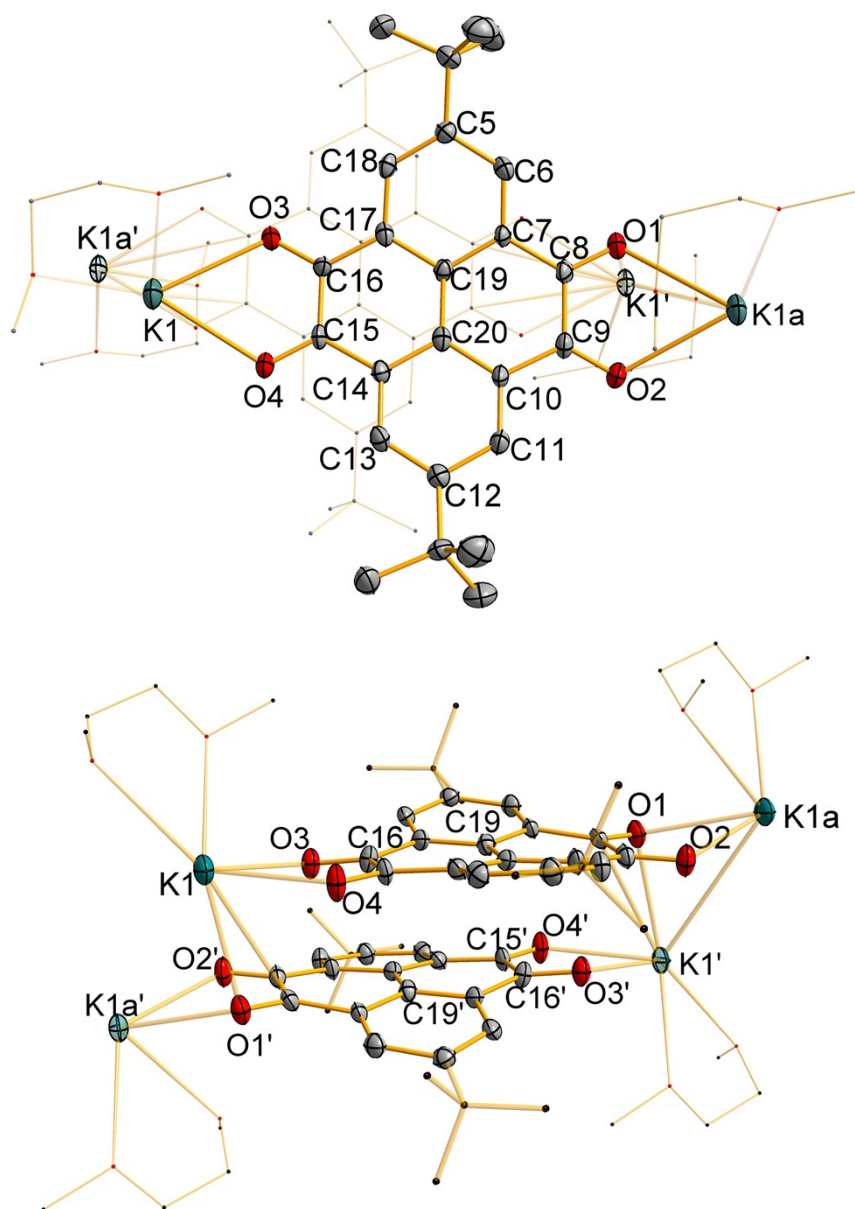
**Fig. S1** Thermal ellipsoid drawing of the molecular structure of **1K(cryp)** at 50% probability. Hydrogen atoms and K-cryptand cation are omitted for clarity. Selected bond lengths (Å) and angles (°): O1–C1 1.238(3), O2–C8 1.229(3), C1–C2 1.469(3), C1–C8' 1.490(3), C3–C3' 1.443(3), C2–C7 1.395(3), C2–C3 1.410(3), C3–C4 1.411(3), C4–C5 1.395(3), C4–C8 1.470(3), C5–C6 1.396(4), C6–C7 1.384(3); O1–C1–C2 121.9(2), O1–C1–C8' 119.9(2), O2–C8–C4 121.7(2), O2–C8–C1' 119.8(2).



**Fig. S2** Thermal ellipsoid drawing of the molecular structures of **1K(18c6)** at 50% probability. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): C2–O1 1.253(5), C3–O2 1.263(5), C12–O3 1.202(5), C13–O4 1.218(5), C2–C3 1.458(6), C2–C7 1.478(5), C3–C4 1.459(5), C4–C5 1.406(5), C5–C6 1.455(5), C6–C7 1.414(5), C4–C17 1.410(5), C5–C14 1.406(5), C6–C11 1.408(5), C7–C8 1.409(5), C8–C9 1.388(6), C9–C10 1.388(6), C10–C11 1.386(6), C11–C12 1.491(6), C12–C13 1.534(6), C13–C14 1.474(5), C14–C15 1.392(6), C15–C16 1.394(6), C16–C17 1.381(6), K1–O1 2.847(3), K1–O2 2.668(3); O1–C2–C3 121.6(3), O1–C2–C7 120.7(3), C3–C2–C7 117.8(3), O2–C3–C2 120.6(3), O2–C3–C4 120.4(4), O3–C12–C11 123.2(4), O3–C12–C13 118.7(4), O4–C13–C14 123.6(4), O4–C13–C12 117.8(4).



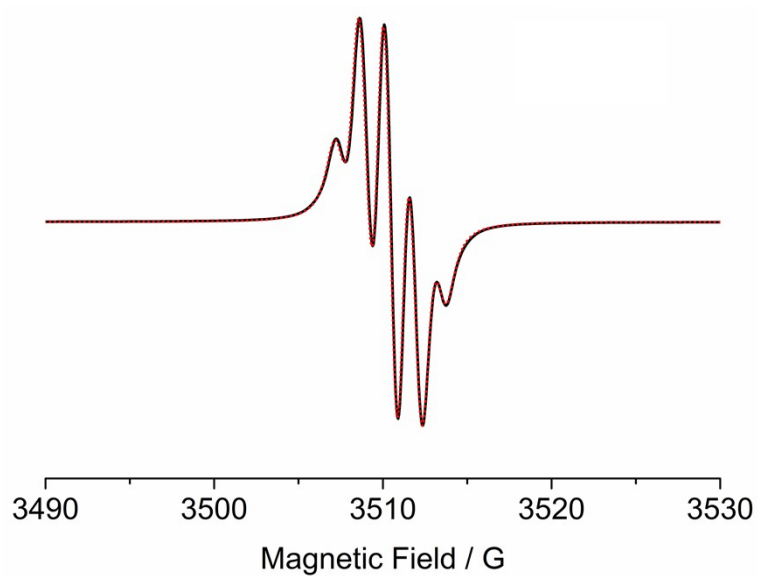
**Fig. S3** Thermal ellipsoid drawing of the molecular structures of  $(1_4K_2)^{2-}$  dianion in  $[1K(15c5)]_4$  at 50% probability (up: topview; down: side view). Two  $(15c5)_2K^+$  cations, solvent molecules and hydrogen atoms are omitted for clarity. Selected bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ ): C1–O1 1.256(4), C2–O2 1.260(4), C11–O3 1.219(4), C12–O4 1.223(5), C1–C2 1.457(4), C11–C12 1.515(7), C4–C5 1.438(5), C50–O9 1.255(4), C51–O10 1.256(3), C60–O11 1.218(4), C61–O12 1.220(4), C50–C51 1.464(4), C60–C61 1.534(5), C53–C54 1.449(4), K1–O1 2.760(2), K1–O2 2.670(2), K1–O9 2.749(2), K1–O10 2.692(2), C1–C6 1.480(4), C2–C3 1.462(4), C3–C4 1.391(5), C3–C16 1.404(5), C4–C13 1.428(5), C5–C6 1.409(5), C5–C10 1.409(5), C10–C11 1.482(6), C12–C13 1.451(6); C50–C55 1.479(4), C51–C52 1.460(4), C52–C65 1.395(4), C52–C53 1.415(4), C53–C62 1.402(4), C54–C55 1.402(4), C54–C59 1.412(4), C59–C60 1.458(5), C61–C62 1.464(5); O1–C1–C2 121.3(3), O1–C1–C6 121.2(3), O2–C2–C1 120.3(3), O2–C2–C3 120.1(3), O9–C50–C51 121.3(3), O9–C50–C55 120.9(3).



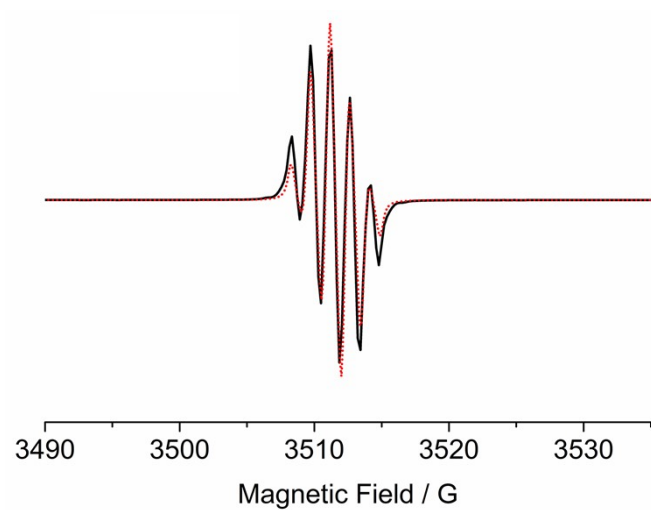
**Fig. S4** Thermal ellipsoid drawing of the molecular structures of one unit in **(1K)<sub>2n</sub>** at 50% probability (up: topview; down: side view). Two neighboring K atoms and two DME molecules were added, and hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): C8-O1 1.240(6), C9-O2 1.221(6), O3-C16 1.260(6), O4-C15 1.247(6), K1-O3 2.698(4), K1-O4 2.728(4), K1''-O2 2.751(4), K1''-O1 2.788(4), C8-C9 1.531(8), C15-C16 1.480(7), C14-C15 1.468(7), C5-C18 1.375(7), C5-C6 1.407(7), C6-C7 1.384(7), C7-C19 1.412(7), C7-C8 1.473(7), C9-C10 1.480(7), C10-C11 1.382(7), C10-C20 1.414(7), C11-C12 1.419(8), C12-C13 1.398(8), C12-C21 1.521(7), C13-C14 1.400(7), C14-C20 1.410(7), C16-C17 1.450(7), C17-C18 1.415(7), C17-C19 1.423(7), C19-C20 1.433(7); O1-C8-C7 123.5(5), O1-C8-C9 118.2(5), O2-C9-C10 123.5(5), O2-C9-C8 119.0(5), O4-C15-C14 121.6(5), O4-C15-C16 119.6(5), O3-C16-C17 122.8(5), O3-C16-C15 119.2(4).



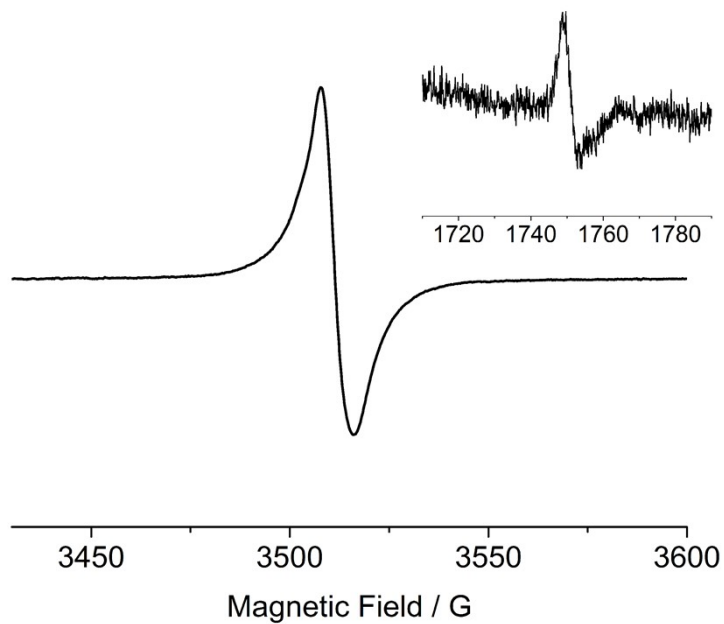
## 5. EPR and SQUID measurements



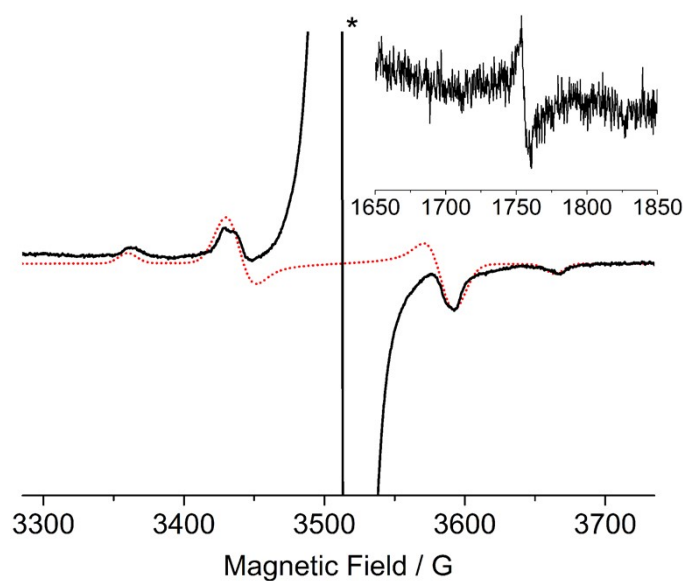
**Fig. S5** Experimental (black line) and simulated (red dotted line) EPR spectra of **1K(cryp)** in THF solution at room temperature.



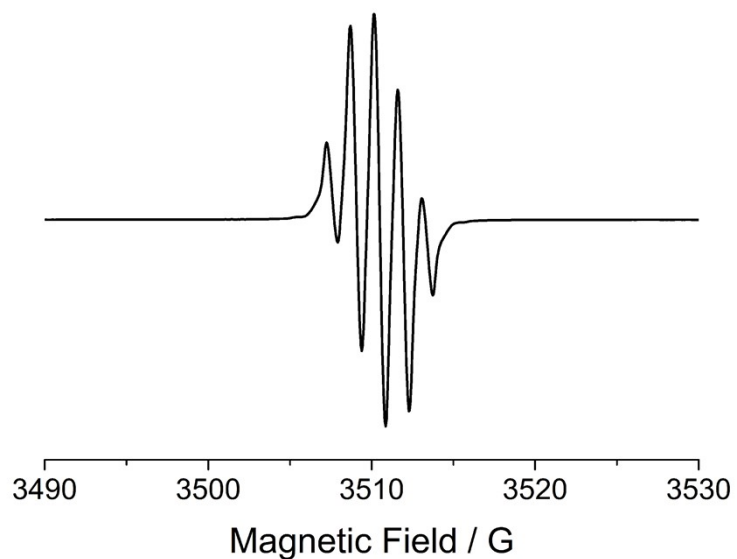
**Fig. S6** Experimental (black line) and simulated (red dotted line) EPR spectra of **1K(18c6)** in THF solution at room temperature.



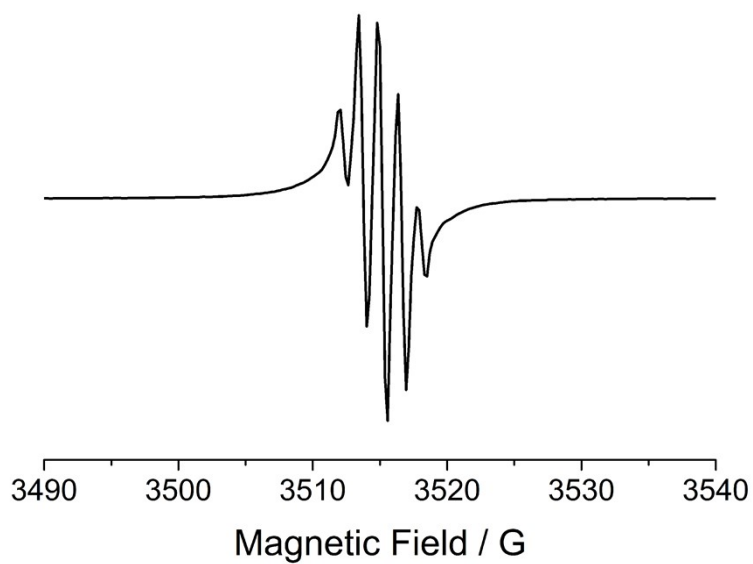
**Fig. S7** EPR spectrum of  $[1\mathbf{K}(15\mathbf{c5})]_4$  in powder at room temperature with inset showing the half-field signal.



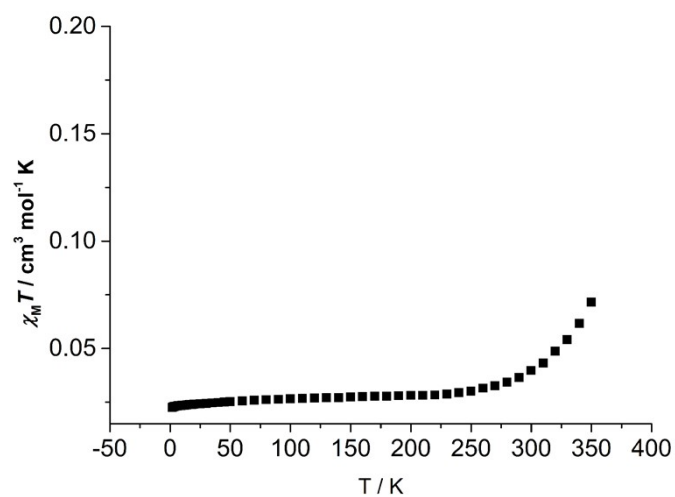
**Fig. S8** EPR spectrum (black line) of  $(1\mathbf{K})_{2n}$  in powder at room temperature with simulation (red dotted line) with inset showing the half-field signal. The central signals labelled with star belongs to the monoradical.



**Fig. S9** EPR spectrum of  $[1K(15c5)]_4$  in THF solution at room temperature.

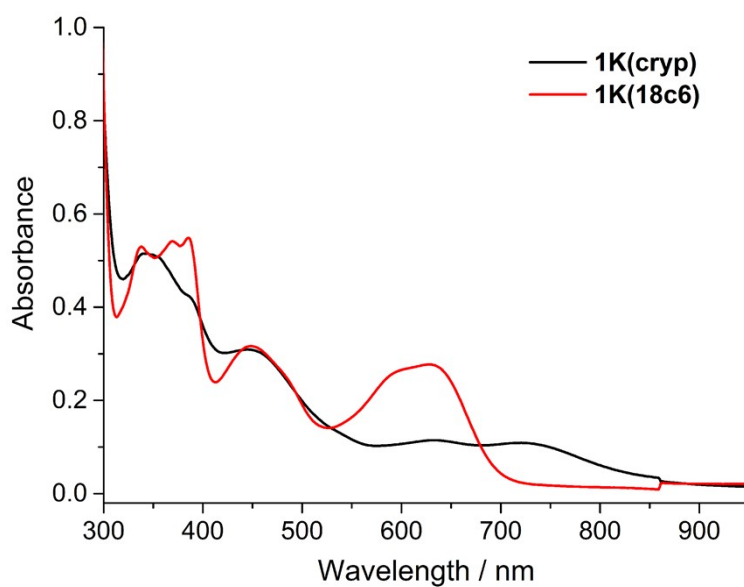


**Fig. S10** EPR spectrum of  $(1K)_{2n}$  in THF solution at room temperature.

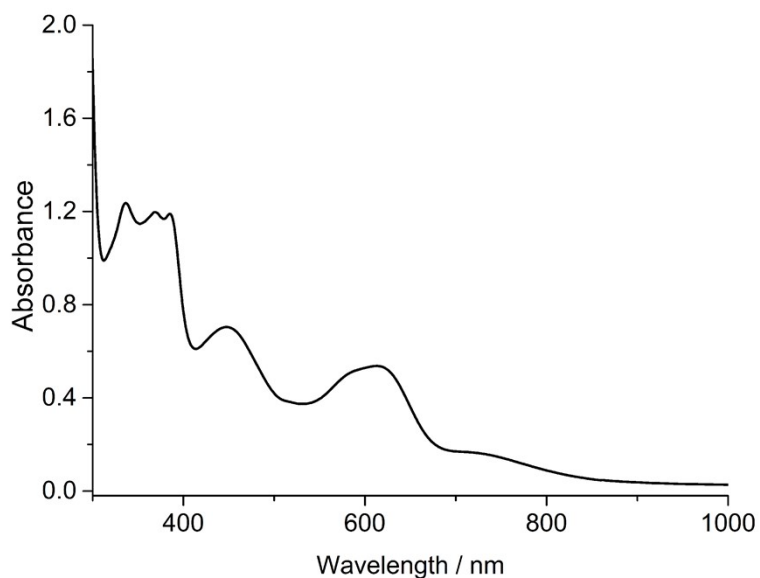


**Fig. S11** SQUID measurement of **(1K)<sub>2n</sub>** in powder.

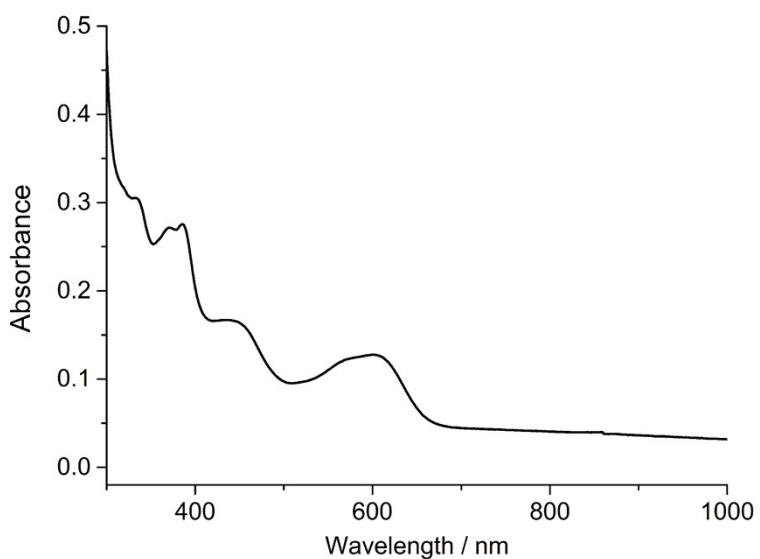
## 6. UV Spectra



**Fig. S12** UV-vis spectra of **1K(cryp)** and **1K(18c6)** in THF solution at room temperature.



**Fig. S13** UV-vis spectra of  $[1\mathbf{K}(15\mathbf{c}5)]_4$  in THF solution at room temperature.



**Fig. S14** UV-vis spectra of  $(1\mathbf{K})_{2n}$  in THF solution at room temperature.

The EPR spectra of  $[1\mathbf{K}(15\mathbf{c}5)]_4$  and  $(1\mathbf{K})_{2n}$  in THF solution at ambient temperature (Fig. S9 and S10) both show monoradical signals ( $g = 2.00491$  G,  $a(^1\text{H}) = 1.44$  G for  $[1\mathbf{K}(15\mathbf{c}5)]_4$ ;  $g = 2.00486$ ,  $a(^1\text{H}) = 1.44$  G for  $(1\mathbf{K})_{2n}$ ), and diradical signals were not observed. Consequently, we believe that both  $[1\mathbf{K}(15\mathbf{c}5)]_4$  and  $(1\mathbf{K})_{2n}$  depolymerize in THF solution at room temperature.

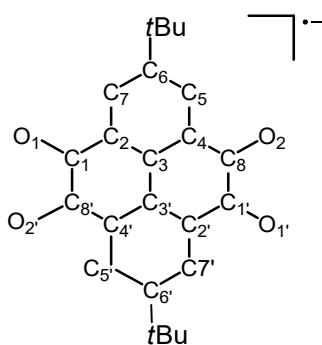
Then, we speculate that PTO moieties of  $(\mathbf{1K})_{2n}$  remain coordinate to  $K^+$  cation in THF solution, just like  $\mathbf{1K}(\mathbf{18c6})$ . So its UV-vis spectrum in THF solution is similar to that of  $\mathbf{1K}(\mathbf{18c6})$ .

While, in the THF solution of  $[\mathbf{1K}(\mathbf{15c5})]_4$ , two K atoms are surrounded by coordinated four 15-crown-5, and there are not enough naked  $K^+$  cations to be coordinated by all the four PTO moieties. Then part of the PTO moieties exist either in the form of  $\mathbf{1}^-$ , or in a coordinated form between  $\mathbf{1}^-$  and  $\mathbf{1K}(\mathbf{18c6})$ . That may be the reason why both  $\mathbf{1K}(\mathbf{cryp})$  and  $[\mathbf{1K}(\mathbf{15c5})]_4$  exhibit absorption bands of 700-800 nm.

## 7. Computation details

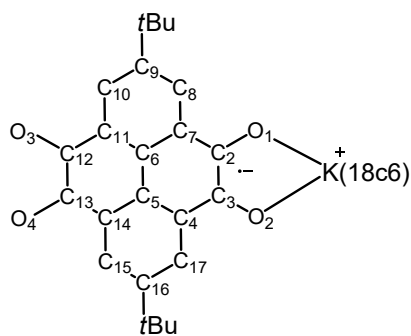
All calculations were performed with the Gaussian 09 program suite.<sup>3,4</sup> The geometry optimizations of  $\mathbf{1K}(\mathbf{cryp})$  and  $\mathbf{1K}(\mathbf{18c6})$  were carried out at the UB3LYP/6-31G\* levels of theory. The obtained stationary points were characterized by frequency calculations. The frontier molecular orbitals and spin densities were calculated at the level of UB3LYP/6-31G\* on the optimized geometries and no imaginary frequency was found, which confirmed the local minimum of the optimized structures. The UV-vis absorption spectra were calculated using the time-dependent DFT (TD-DFT) method at UCAM-B3LYP/6-31+G(d) level on  $\mathbf{1}^-$  and  $\mathbf{1K}(\mathbf{18c6})$ .

**Table S2.** Comparison of selected experimental and calculated bond lengths for  $\mathbf{1}^-$  in  $\mathbf{1K}(\mathbf{cryp})$ .



Bond	X-ray	Cal.	Bond	X-ray	Cal.
O1–C1	1.238(3)	1.238	C4–C8	1.470(3)	1.480
O2–C8	1.229(3)	1.238	C3–C3'	1.443(3)	1.429
C1–C8'	1.490(3)	1.521	C4–C5	1.395(3)	1.396
C1–C2	1.469(3)	1.477	C5–C6	1.396(4)	1.405
C2–C3	1.410(3)	1.423	C6–C7	1.384(3)	1.399
C3–C4	1.411(3)	1.425	C2–C7	1.395(3)	1.402

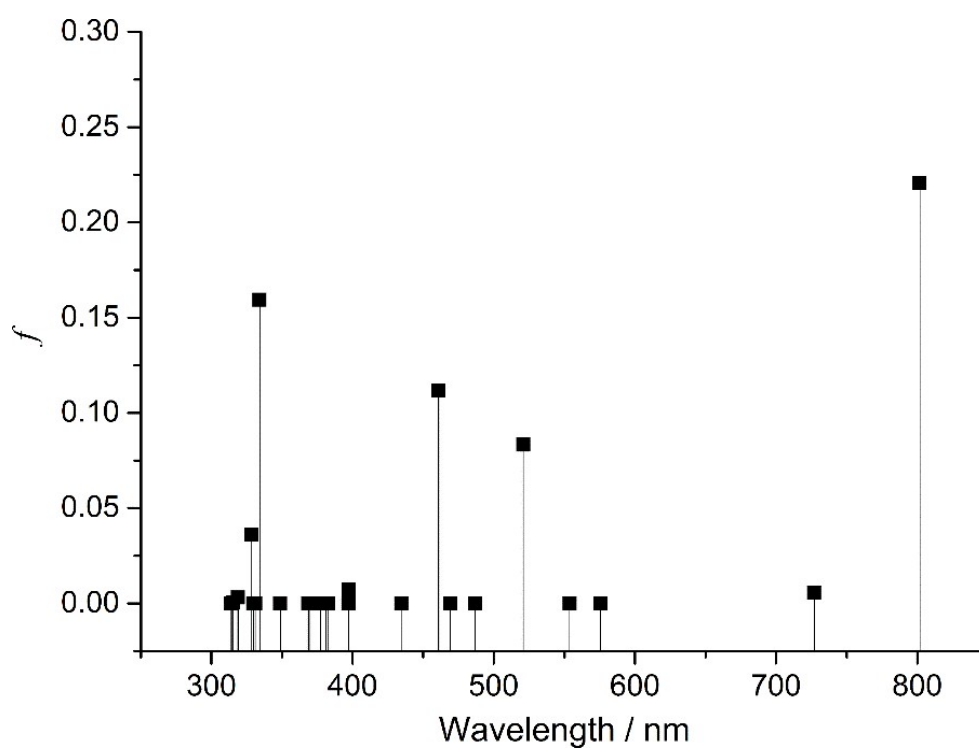
**Table S3.** Comparison of selected experimental and calculated bond lengths for **1K(18c6)**.



Bond	X-ray	Cal.	Bond	X-ray	Cal.
C2–O1	1.253(5)	1.269	C5–C14	1.406(5)	1.414
C3–O2	1.263(5)	1.269	C6–C11	1.408(5)	1.414
C2–C3	1.458(6)	1.468	C11–C12	1.491(6)	1.481
C12–O3	1.202(5)	1.221	C13–C14	1.474(5)	1.481
C13–O4	1.218(5)	1.221	C4–C17	1.410(5)	1.406
C12–C13	1.534(6)	1.553	K1–O1	2.847(3)	2.691
C2–C7	1.478(5)	1.470	K1–O2	2.668(3)	2.691
C3–C4	1.459(5)	1.470	C7–C8	1.409(5)	1.406
C4–C5	1.406(5)	1.417	C8–C9	1.388(6)	1.397
C5–C6	1.455(5)	1.450	C9–C10	1.388(6)	1.403
C6–C7	1.414(5)	1.417	C10–C11	1.386(6)	1.397

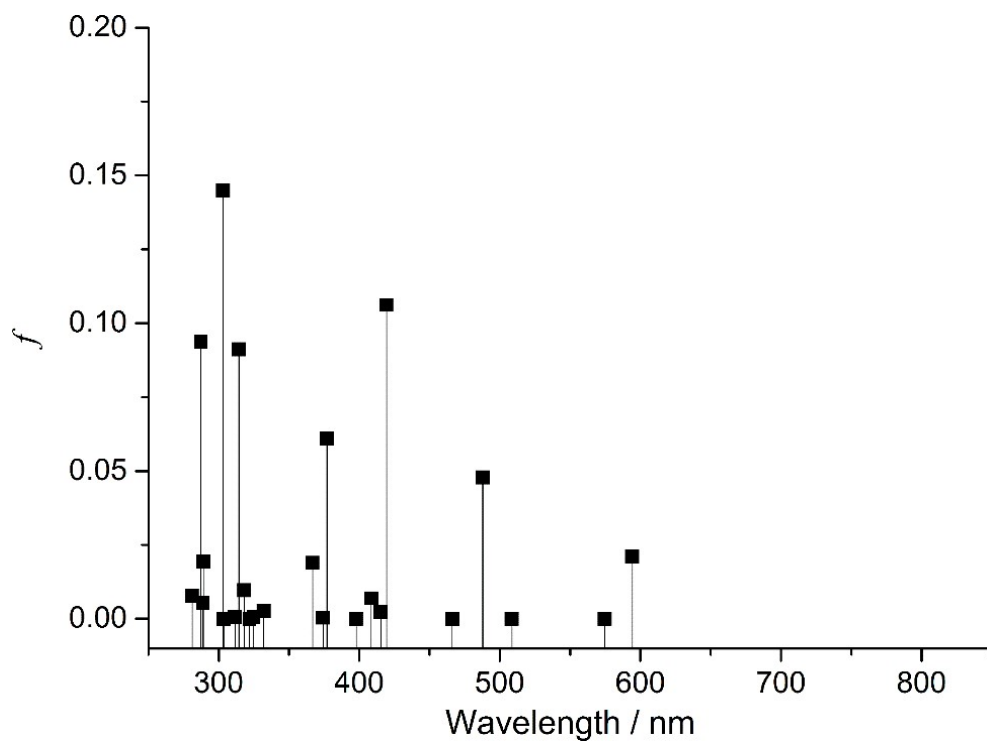
**Table S4.** Calculated excited wavelengths ( $\lambda$ ) and oscillator strengths ( $f$ ) of selected transitions of **1<sup>-</sup>** (in **1K(cryp)**) and **1K(18c6)**.

Compound	Excited state	Wavelength/nm	$f$	Transition nature	
<b>1<sup>-</sup></b>	S <sub>1</sub>	801.9	0.2205	HOMO( $\alpha$ )→LUMO+1( $\alpha$ )	97%
	S <sub>2</sub>	727.0	0.0054	HOMO-1( $\alpha$ )→LUMO( $\alpha$ )	74%
				HOMO( $\beta$ )→LUMO( $\beta$ )	16%
<b>1K(18c6)</b>	S <sub>1</sub>	594.2	0.0211	HOMO-1( $\alpha$ )→LUMO( $\alpha$ )	27%
				HOMO( $\alpha$ )→LUMO+1( $\alpha$ )	15%
				HOMO-2( $\beta$ )→LUMO( $\beta$ )	12%
				HOMO( $\beta$ )→LUMO( $\beta$ )	22%
	S <sub>2</sub>	487.8	0.0478	HOMO( $\alpha$ )→LUMO+1( $\alpha$ )	64%



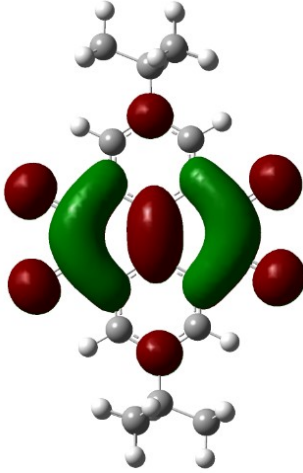
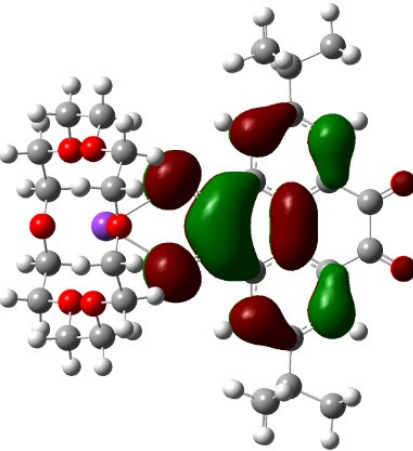
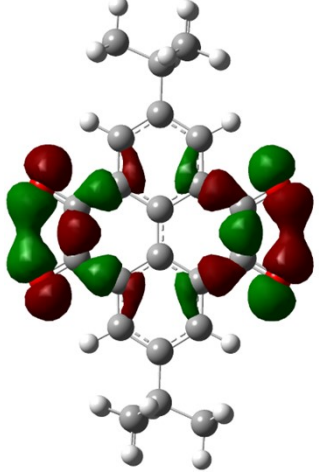
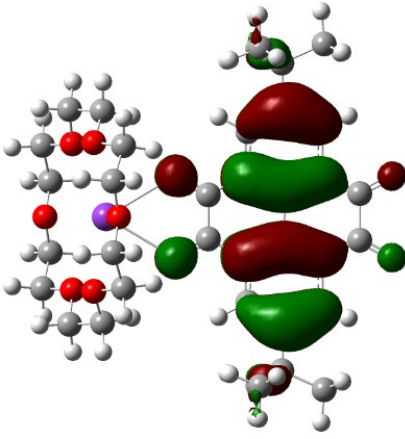
**Fig. S15** Calculated UV/vis absorption spectra of  $1^-$ .

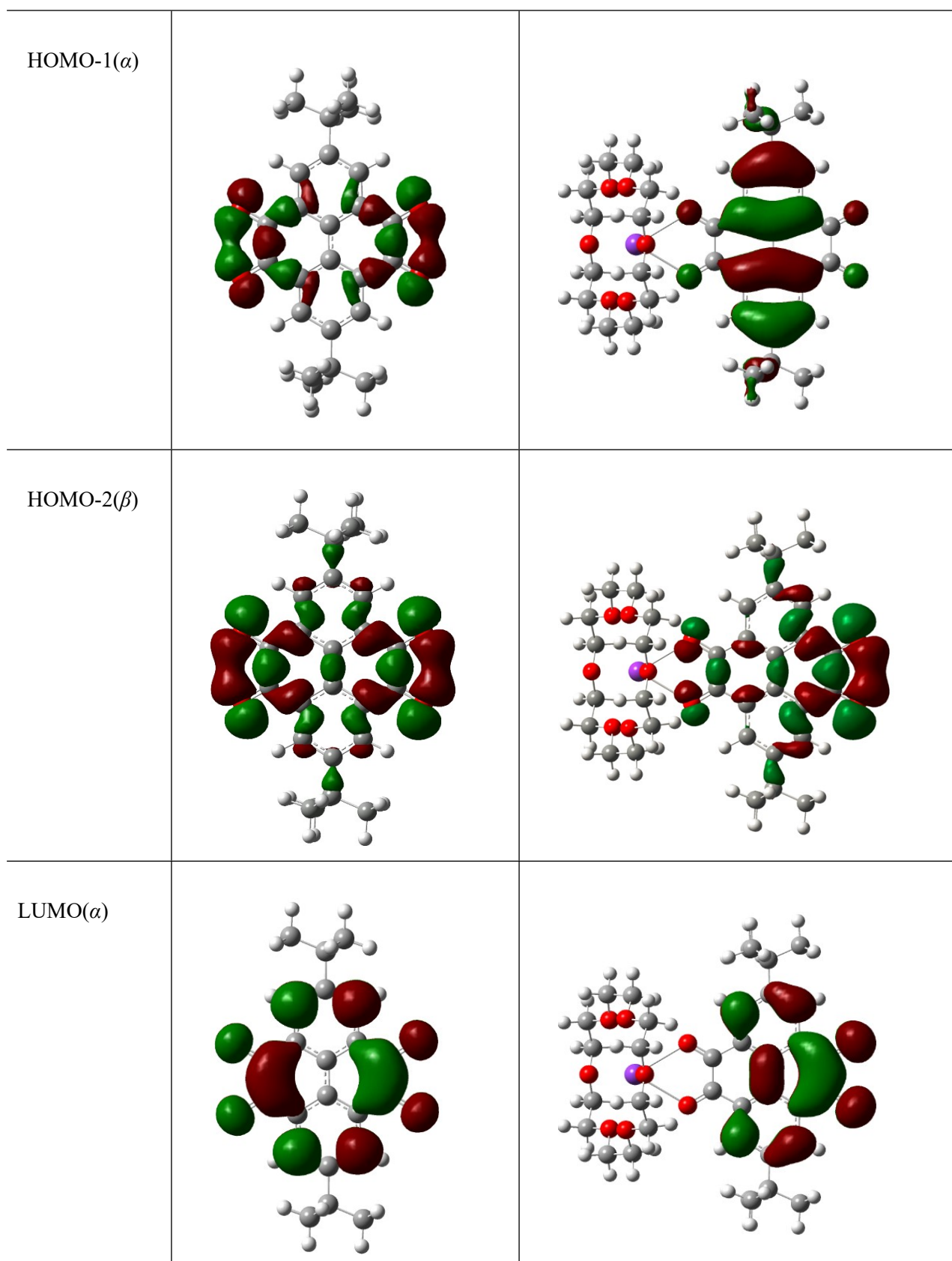




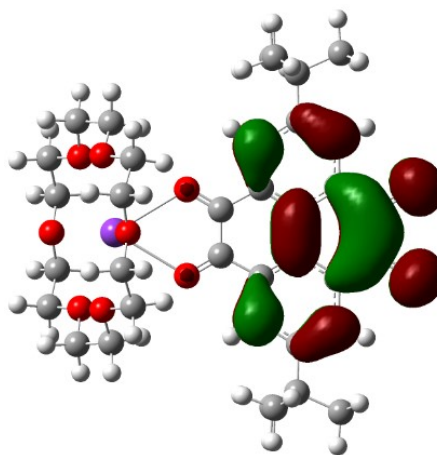
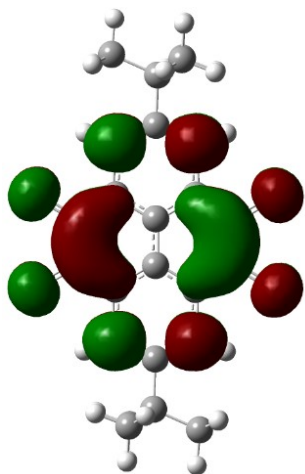
**Fig. S16** Calculated UV/vis absorption spectra of **1K(18c6)**.

**Table S5.** Main frontier molecular orbitals related to UV/vis absorption transitions of **1<sup>-</sup>** and **1K(18c6)**.

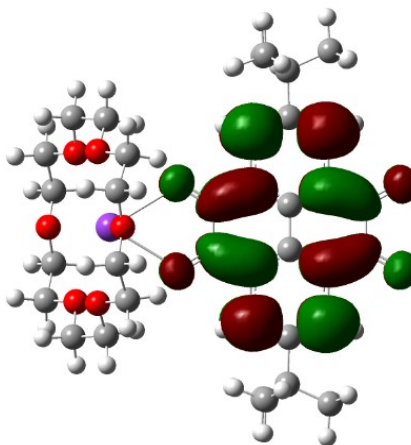
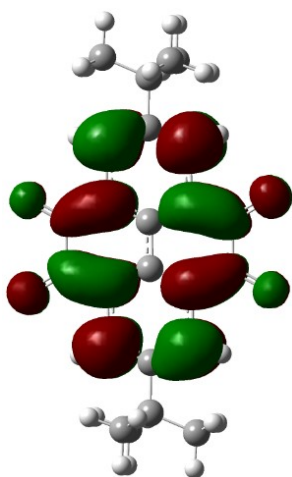
	<b>1<sup>-</sup></b>	<b>1K(18c6)</b>
HOMO( $\alpha$ )		
HOMO( $\beta$ )		



LUMO( $\beta$ )



LUMO+1( $\alpha$ )



## Coordinates of the studied molecules

1<sup>-</sup>

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.417970	3.591586	-0.000302
2	8	0	-1.343085	-3.621486	-0.000296
3	6	0	-0.786248	2.527280	-0.000037
4	6	0	-1.456423	1.208032	0.000028
5	6	0	-2.851911	1.164300	0.000166
6	1	0	-3.358766	2.125627	0.000004
7	6	0	-3.573358	-0.041045	0.000308
8	6	0	-2.831352	-1.227457	0.000120
9	1	0	-3.311628	-2.199801	-0.000021
10	6	0	-1.429888	-1.239061	-0.000007
11	6	0	-0.714353	-0.008902	0.000006
12	6	0	-0.734839	-2.542672	-0.000172
13	6	0	-5.112966	-0.014170	0.000076
14	6	0	-5.722351	-1.429002	0.000484
15	1	0	-5.422782	-2.000599	0.886008
16	1	0	-5.423597	-2.000761	-0.885234
17	1	0	-6.817322	-1.360545	0.000978
18	6	0	-5.617503	0.726445	-1.260904
19	1	0	-5.285051	0.214321	-2.171353
20	1	0	-5.243254	1.754557	-1.302356
21	1	0	-6.715121	0.766929	-1.273441
22	6	0	-5.618098	0.727529	1.260196
23	1	0	-6.715511	0.773148	1.269221
24	1	0	-5.239100	1.753781	1.303975
25	1	0	-5.290972	0.212944	2.171196
26	8	0	1.417968	-3.591584	0.000258
27	8	0	1.343083	3.621490	0.000331
28	6	0	0.786246	-2.527278	0.000265
29	6	0	1.456422	-1.208030	0.000053
30	6	0	2.851910	-1.164299	-0.000087
31	1	0	3.358765	-2.125626	0.000166
32	6	0	3.573358	0.041045	-0.000314
33	6	0	2.831353	1.227458	-0.000210
34	1	0	3.311631	2.199802	-0.000141
35	6	0	1.429890	1.239064	-0.000099
36	6	0	0.714354	0.008906	-0.000023
37	6	0	0.734840	2.542675	-0.000083
38	6	0	5.112967	0.014168	-0.000064
39	6	0	5.722355	1.428997	-0.000558
40	1	0	5.422784	2.000543	-0.886114
41	1	0	5.423607	2.000810	0.885128
42	1	0	6.817325	1.360537	-0.001054
43	6	0	5.617489	-0.726367	1.260969
44	1	0	5.285025	-0.214186	2.171381
45	1	0	5.243242	-1.754477	1.302481
46	1	0	6.715107	-0.766848	1.273520
47	6	0	5.618109	-0.727615	-1.260131
48	1	0	6.715522	-0.773248	-1.269137
49	1	0	5.239099	-1.753866	-1.303852
50	1	0	5.291003	-0.213083	-2.171168

1K(18c6)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.477164	0.734047	-0.114152
2	6	0	0.477211	-0.733917	-0.114145
3	6	0	1.770139	-1.432321	-0.162342
4	6	0	2.997910	-0.724979	-0.199833
5	6	0	2.997865	0.725267	-0.199866
6	6	0	1.770048	1.432529	-0.162383
7	6	0	1.791450	2.838573	-0.173366
8	1	0	0.824374	3.330118	-0.149509
9	6	0	2.973308	3.582620	-0.217357
10	6	0	4.179050	2.865483	-0.248443
11	1	0	5.138782	3.367049	-0.282092
12	6	0	4.199678	1.468709	-0.240587
13	6	0	5.509132	0.776974	-0.277618
14	6	0	5.509188	-0.776515	-0.277418
15	6	0	4.199774	-1.468341	-0.240466
16	6	0	4.179246	-2.865115	-0.248270
17	1	0	5.139017	-3.366614	-0.281806
18	6	0	2.973552	-3.582333	-0.217237
19	6	0	1.791642	-2.838365	-0.173294
20	1	0	0.824605	-3.329988	-0.149442
21	6	0	2.918165	5.121596	-0.231813
22	6	0	2.210798	5.623171	1.049301
23	1	0	2.757988	5.310754	1.946122
24	1	0	1.190158	5.233727	1.127754
25	1	0	2.152984	6.718892	1.051038
26	6	0	2.125024	5.595789	-1.472557
27	1	0	2.064779	6.691176	-1.492784
28	1	0	1.102419	5.203493	-1.475128
29	1	0	2.611377	5.265321	-2.397416
30	6	0	4.320884	5.756067	-0.285803
31	1	0	4.231229	6.848426	-0.295692
32	1	0	4.867976	5.460104	-1.187849
33	1	0	4.927403	5.481318	0.584461
34	6	0	2.918501	-5.121320	-0.231745
35	6	0	4.321269	-5.755727	-0.285244
36	1	0	4.231666	-6.848091	-0.295150
37	1	0	4.927477	-5.480926	0.585224
38	1	0	4.868667	-5.459768	-1.187105
39	6	0	2.125836	-5.595481	-1.472811
40	1	0	1.103282	-5.203059	-1.475809
41	1	0	2.065487	-6.690866	-1.493041
42	1	0	2.612612	-5.265084	-2.397472
43	6	0	2.210694	-5.623015	1.049068
44	1	0	1.189965	-5.233727	1.127131
45	1	0	2.757479	-5.310548	1.946118
46	1	0	2.153027	-6.718740	1.050748
47	6	0	-3.043779	3.526649	0.772535
48	1	0	-2.070122	3.355915	0.293760
49	1	0	-3.018821	4.494485	1.301162
50	6	0	-4.137516	3.575988	-0.273109
51	1	0	-5.123941	3.609152	0.216285
52	1	0	-4.021709	4.492980	-0.873786
53	6	0	-5.033527	2.383509	-2.113046
54	1	0	-5.004577	3.296225	-2.731103
55	1	0	-6.036677	2.308188	-1.663263
56	6	0	-4.776238	1.184378	-3.001440
57	1	0	-5.482162	1.205040	-3.847939

58	1	0	-3.753450	1.234691	-3.407277
59	6	0	-4.776506	-1.183184	-3.002128
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61	1	0	-3.753909	-1.233221	-3.408463
62	6	0	-5.033362	-2.382804	-2.114256
63	1	0	-6.036578	-2.308131	-1.664505
64	1	0	-5.003978	-3.295225	-2.732732
65	6	0	-4.136777	-3.576048	-0.275143
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67	1	0	-5.123187	-3.610121	0.214201
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69	1	0	-1.350969	-2.229448	2.260039
70	1	0	-2.330980	-3.290196	3.319989
71	6	0	-2.678730	-1.192063	3.597894
72	1	0	-3.715587	-1.272302	3.962758
73	1	0	-2.006589	-1.200216	4.471681
74	6	0	-2.678602	1.190044	3.598404
75	1	0	-2.006307	1.197840	4.472078
76	1	0	-3.715394	1.270135	3.963482
77	6	0	-2.343252	2.370496	2.709933
78	1	0	-2.330872	3.288282	3.321331
79	1	0	-1.351079	2.227991	2.260729
80	6	0	-3.043081	-3.526990	0.770554
81	1	0	-3.017713	-4.495236	1.298424
82	1	0	-2.069481	-3.355464	0.291952
83	19	0	-2.916346	-0.000134	0.057302
84	8	0	-0.612324	1.384070	-0.072583
85	8	0	-0.612244	-1.383999	-0.072597
86	8	0	6.578269	1.364931	-0.308419
87	8	0	6.578371	-1.364406	-0.307856
88	8	0	-3.327472	2.475025	1.687673
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90	8	0	-4.950466	0.000385	-2.239262
91	8	0	-4.039528	-2.430633	-1.108826
92	8	0	-3.327255	-2.476204	1.686500
93	8	0	-2.503016	-0.000859	2.852319

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