An organometallic half-sandwich supramolecular complex {K(18-Crown-6)(η^n-$C_6H_5B(C_6H_5)_3$)} (n = 1-6) exhibiting reversible breaking-symmetry phase transition and switchable dielectric behavior

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Experimental section

Chemicals and Materials

All reagents and chemicals were purchased from commercial sources and used without further purification.

Preparation of {K(18-Crown-6)(η^4-$C_6H_5B(C_6H_5)_3$)} (1)

$KBPh_4$ (358 mg, 1 mmol) and 18-Crown-6 (264 mg, 1 mmol) were mixed in EtOH (25 ml) under stirring at room temperature, and the immediately formed white microcrystals was filtered off, washed with EtOH and then dried in vacuum at ambient temperature to give 610 mg of **1** with 98% yield. Elemental analysis Calcd for $C_{36}H_{44}O_6BK$: C, 69.44%; H, 7.12%; Found: C, 69.40%; H, 7.08%.

The single crystals suitable for X-ray analysis were obtained via diffusion strategy between different solution layers, namely, the more dense EtOH solution of $KBPh_4$ was added carefully to the bottom of a test tube and the less dense EtOH solution of 18-Crown-6 was layered on top of the EtOH solution of $KBPh_4$. The single crystals were gained at ambiet temperature after two weeks.

Physical measurements

Elemental analyses were performed for C and H using an Elementar Vario EL Ⅲ analytical instrument. Powder X-ray diffraction (PXRD) data at room temperature were collected on a Bruker D8 Advance powder diffractometer operating at 40 kV and 40 mA using Cu Kα radiation with λ = 1.5418 Å. The 2θ angles span from 5 to 50° with 0.01° per step. The simulated powder diffraction pattern was obtained from the single crystal X-ray diffraction data of **1** using the 'Mercury 3.8' software. Thermal gravimetric analysis (TGA) was performed using a NETZSCH STA 409 PC/PG thermogravimetric analyzer in nitrogen atmosphere in the temperature range of 303-1073 K (30-800 °C), with a heating rate of 10 K/min. Differential scanning calorimetry (DSC) was performed on a Q2000 V24.9 Build 121 instrumental between

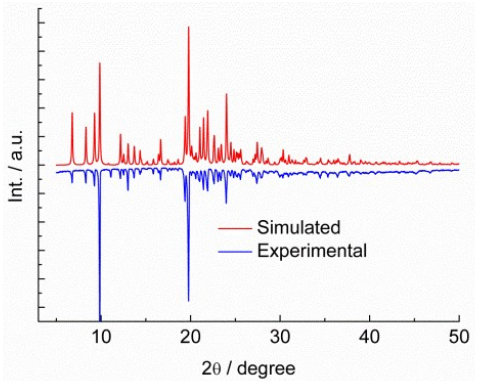
-90 and 180 °C (between 183 and 453 K) with a rate of 20 °C min^{-1}. The temperature and frequency dependent dielectric permittivity measurements were performed using a concept 80 system (Novocontrol, Germany) between -120 and 160 °C (153–433 K), the pellet of the sample was prepared in the form of a disk with a 7 mm diameter and ca. 2.25 mm thickness, and then the disk was sandwiched between two parallel copper electrodes. The ac electrical field frequencies span from 1 to 10^7 Hz.

Single-crystal X-ray Crystallography

Single crystal X-ray diffraction (SCXRD) data were collected for **1** at 173, 293 and 423 K using graphite monochromated Mo/K_α radiation (λ = 0.71073 Å) on a Bruker D8 QUEST Apex III CCD area detector diffractometer. Data reduction and absorption corrections were performed with the SAINT[1] and SADABS[2] software packages, respectively. The structures were solved by the direct method using the SHELXL-2014/7 software package.[3] The non-hydrogen atoms were anisotropically refined using the full-matrix least-squares method on F^2. All the hydrogen atoms were geometrically fixed and placed in ideal positions.

References

1. Bruker, APEX 2, SAINT, XPREP, Bruker AXS Inc., Madison, Wisconsin, USA, **2007**.
2. Bruker, SADABS, Bruker AXS Inc., Madison, Wisconsin, USA, **2001**.
3. G. M. Sheldrick, *Acta Cryst.,* **2015**, C71: 3-8.



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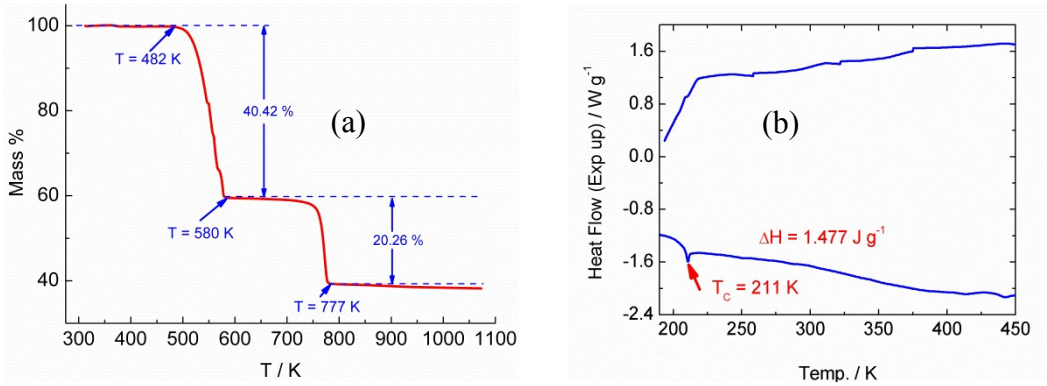

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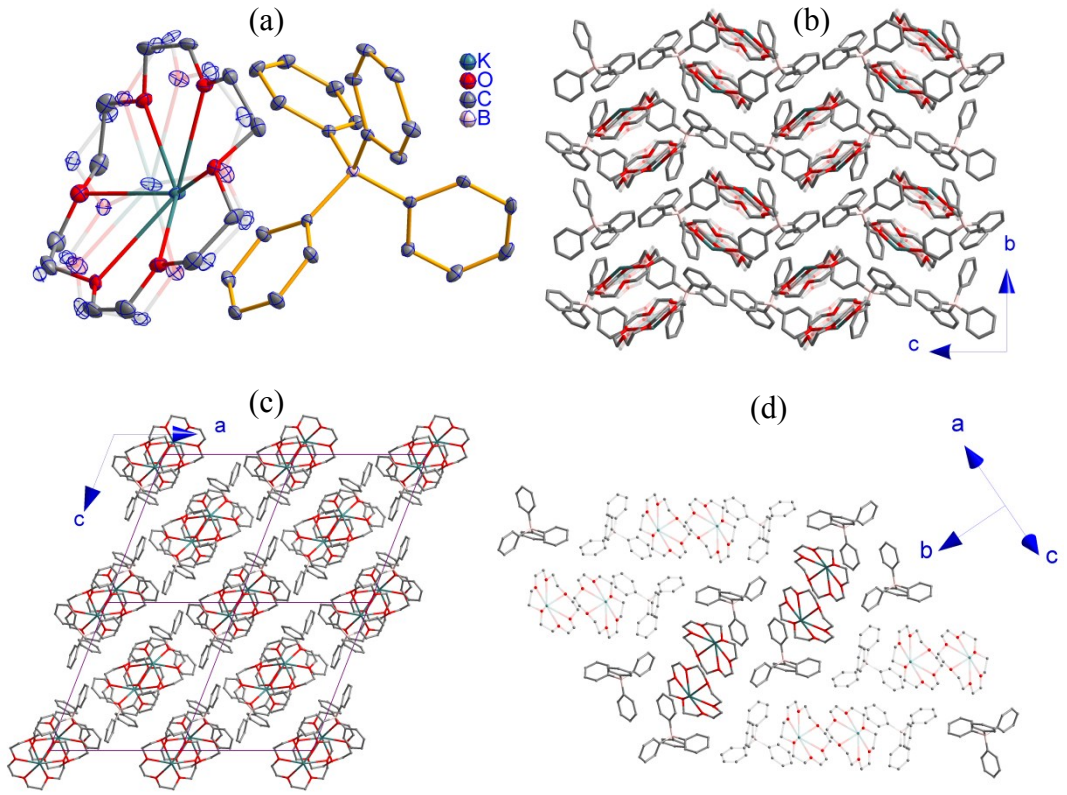

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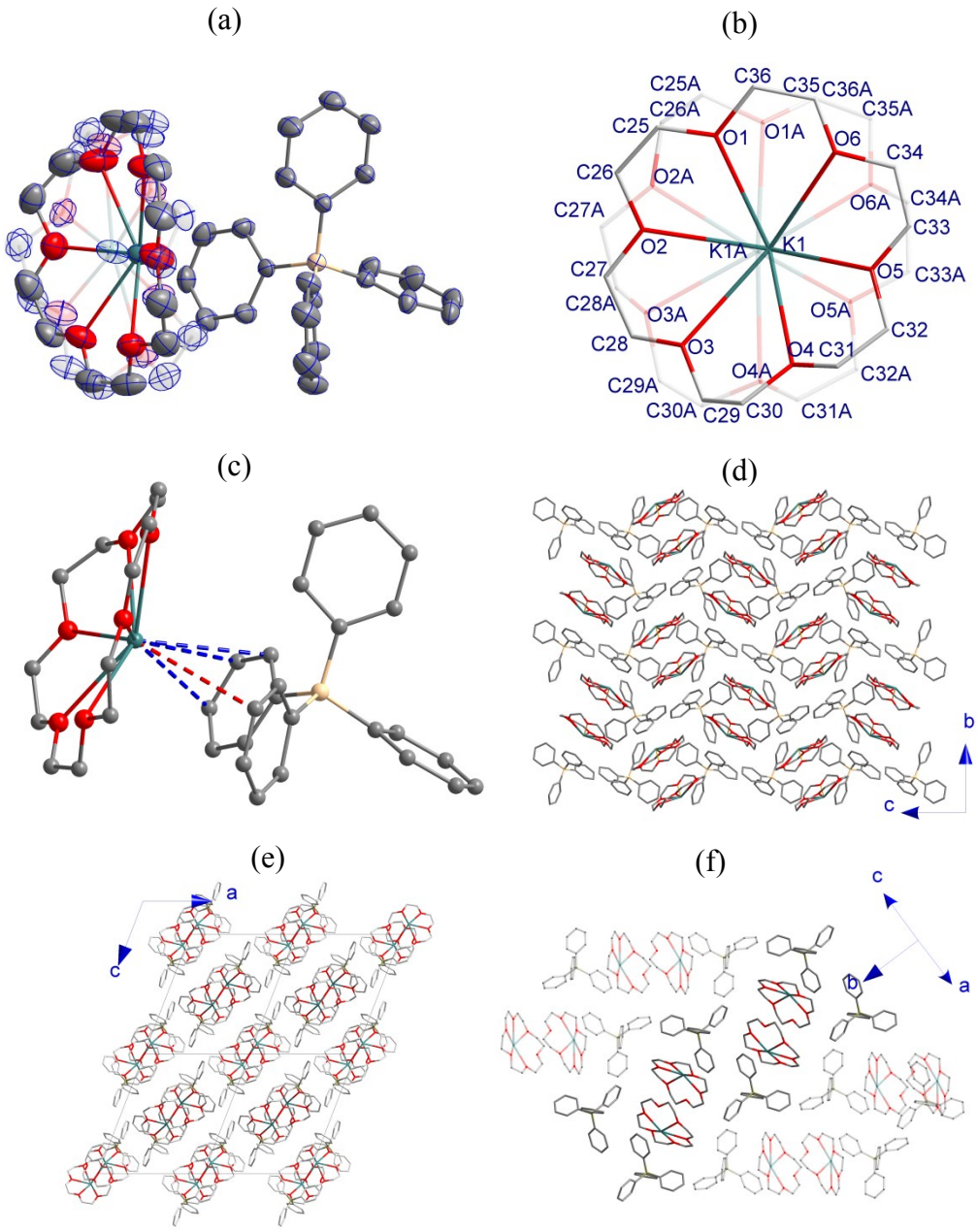

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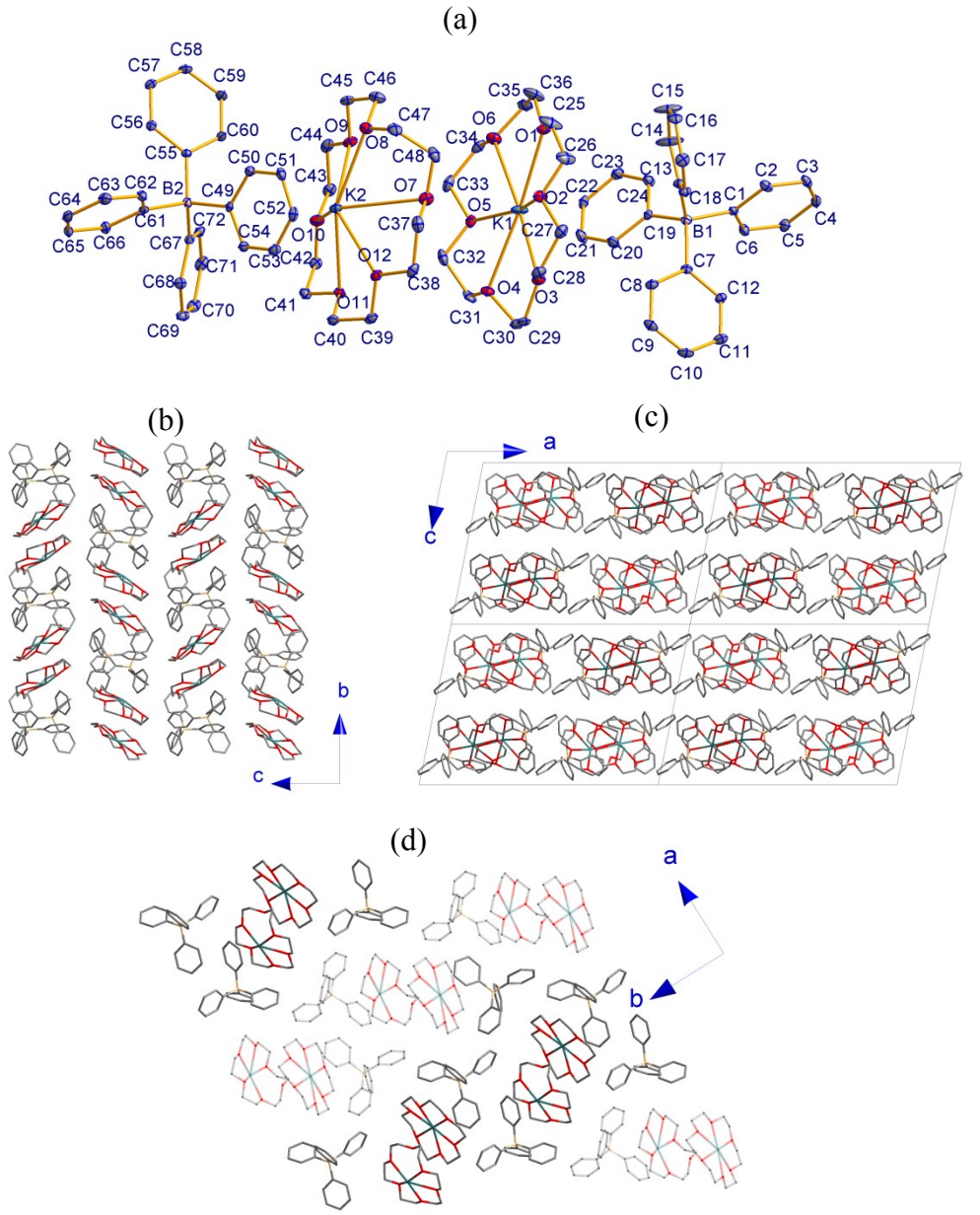

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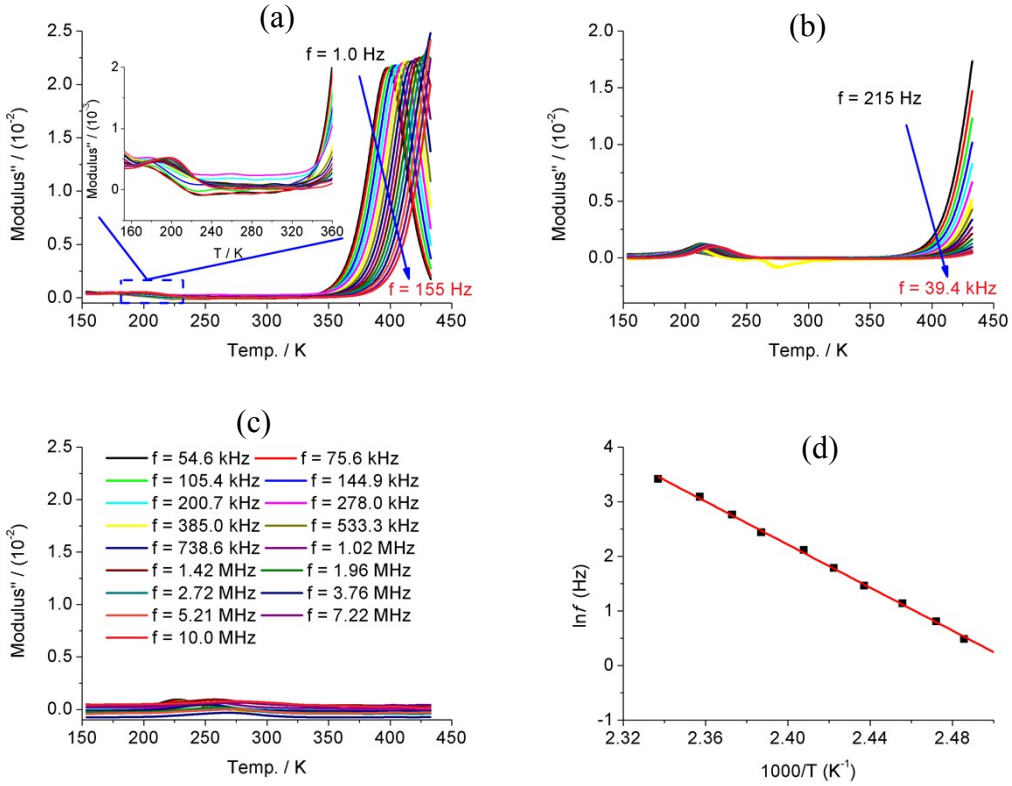

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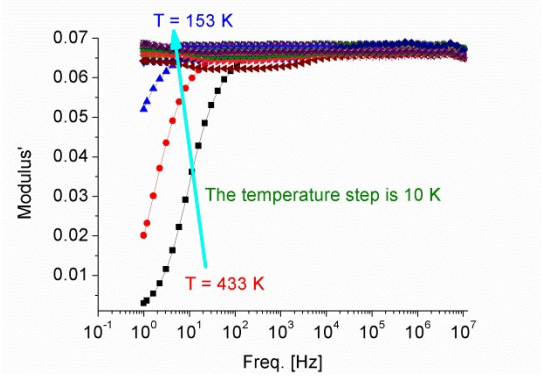

Figure S7: Plots of Modulus' vs. frequency of **1** at the selected temperatures in 153-433 K (the temperature step is 10 K).

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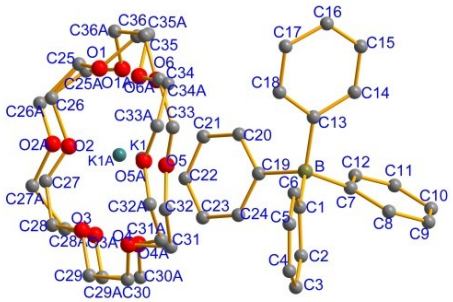
Table S1: Crystallographic data and refinement parameters in **1**

Temp. [K]	173 K	293 K	423 K
Formula	$C_{36}H_{44}BKO_6$	$C_{36}H_{44}BKO_6$	$C_{36}H_{44}BKO_6$
Formula weight	622.62	622.62	622.62
CCDC no.	1863436	1849020	1863437
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$
a (Å)	26.2242(9)	14.5831(5)	14.6855(10)
b (Å)	14.1111(5)	14.0002(6)	14.1873(12)
c (Å)	18.0007(7)	17.5535(8)	17.7565(15)
α (°)	90	90	90
β (°)	101.2680(10)	111.2770(10)	111.078(2)
γ (°)	90	90	90
V(Å^3) / Z	6532.8(4) /4	3339.5(2) /4	3452.0(5) /4
ρ (g·cm^{-3})	1.266	1.238	1.198
F(000)	2656	1328	1328
Abs. coeff. (mm^{-1})	0.207	0.203	0.196
θ Ranges of data collection (°)	2.308-27.453	2.490-24.979	2.458-20.412
Index range	$-31 \le h \le 26$ $-16 \le k \le 16$ $-19 \le l \le 21$	$-15 \le h \le 17$ $-14 \le k \le 16$ $-20 \le l \le 20$	$-17 \le h \le 15$ $-14 \le k \le 16$ $-21 \le l \le 20$
R_{int}	0.0487	0.0404	0.0510
Independent reflections /restraints/parameters	11510/0/793	5858/895/571	6034/784/558
Refine method	Full-matrix least-squares on F^2		
Goodness-of-fit on F^2	1.150	1.029	1.014
R_1, wR_2 [I>2σ(I)]	$R_1 = 0.0679$ $wR_2 = 0.1544$	$R_1 = 0.0526$ $wR_2 = 0.1379$	$R_1 = 0.0698$ $wR_2 = 0.1807$
R_1, wR_2 [all data]	$R_1 = 0.0882$ $wR_2 = 0.1632$	$R_1 = 0.0884$ $wR_2 = 0.1644$	$R_1 = 0.1501$ $wR_2 = 0.2259$
Residual (e·Å^{-3})	0.969/-0.556	0.248/-0.221	0.226/-0.182

$R_1 = \Sigma(||F_o|-|F_c||)/\Sigma|F_o|$, $wR_2 = \Sigma w(|F_o|^2-|F_c|^2)^2/\Sigma w\,(|F_o|^2)^2]^{1/2}$

Table S2: The K-O and K-C bond lengths in **1** at 293 and 423 K in HTP



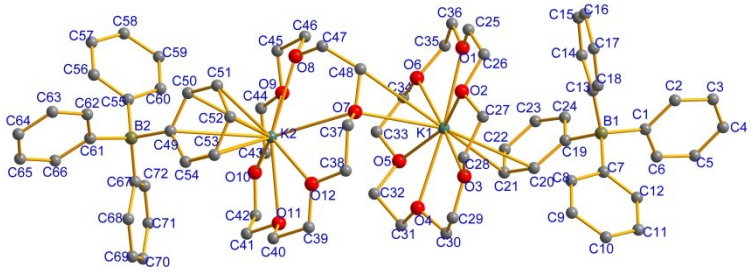
Bond	T = 293 K	T = 423 K
K1-O1	2.914(6)	2.799(5)
K1-O2	2.918 (5)	2.812(5)
K1-O3	2.823(15)	2.846(5)
K1-O4	2.920(9)	2.922(5)
K1-O5	2.785(6)	2.829(5)
K1-O6	2.787 (10)	2.873(5)
K1A-O1A	2.820(9)	2.809(18)
K1A-O2A	2.649(14)	2.790(18)
K1A-O3A	2.77(2)	2.853(18)
K1A-O4A	2.797(18)	2.849(18)
K1A-O5A	2.717(11)	2.58(3)
K1A-O6A	2.704(16)	2.869(18)
K1-C19	3.580(4)	3.650(5)
K1-C20	3.385(4)	3.447(5)
K1-C21	3.315(4)	3.352(5)
K1-C22	3.407(4)	3.441(5)
K1-C23	3.523(4)	3.568(5)
K1-C24	3.581(4)	3.634(5)

Note: The K-C distances yellow marked fall into the range less than 3.5 Å, indicating the existence of K...π interactions.

DFIX constraints were used in structure refinement at 293 K with 3.7 Å for K1-C31and C30-K1; 3.65 Å for K1A-C30a, C31a-K1A, C33a-K1A, K1A-C35a, K1-C30, C26a-K1A, C27a-K1A, K1A-C25a, C36a-K1A.

DFIX constraints were used in structure refinement at 423 K with 3.65Å for C36A-K1A, K1A-C34A, C32A-K1A, K1A-C31A, K1A-C25A, C27A-K1A, K1A-C33A, K1A-C29A, C30A-K1A, C28A-K1A and C26A-K1A; 2.86 Å O6A-K1A, K1A-O1A, K1A-O2A, K1A-O3A and O4A-K1A.

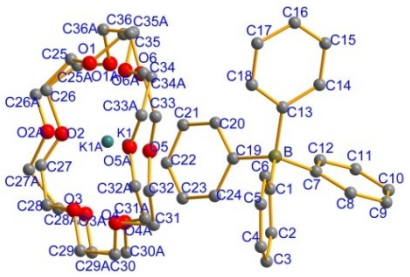
Table S3: The K-O and K-C bond lengths in **1** at 173 K in LTP



Bond	Length (Å)	Bond	Length (Å)
K1-O1	2.715(2)	K1-C19	4.283(4)
K1-O2	2.787(2)	K1-C20	3.520(4)
K1-O3	2.751(2)	K1-C21	3.397(4)
K1-O4	2.770(2)	K1-C22	4.067 (4)
K1-O5	2.805(2)	K1-C23	4.719(4)
K1-O6	2.789(3)	K1-C24	4.801(4)
K1-O7	3.145(3)	K1-C48	3.493(4)
K2-O7	3.146(3)	K2-C49	3.475(3)
K2-O8	2.780(3)	K2-C50	3.332(3)
K2-O9	2.830(3)	K2-C51	3.307(4)
K2-O10	2.759(2)	K2-C52	3.391(3)
K2-O11	2.865(2)	K2-C53	3.452(4)
K2-O12	2.767(2)	K2-C54	3.474(4)

Note: The K-C distances yellow marked fall into the range less than 3.5 Å, indicating the existence of K...π interactions.

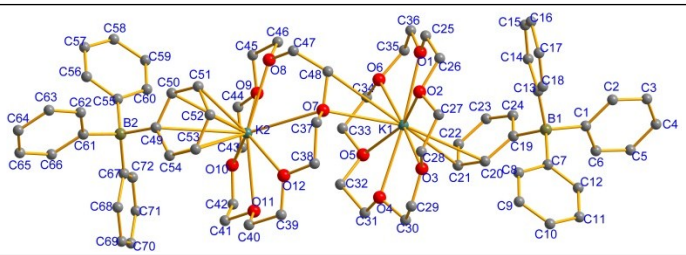
Table S4: The C-C, C=C, C-O and C-B bond lengths in **1** at 293 and 423 K in HTP



293 K		423 K	
Bond	Length (Å)	Bond	Length (Å)
C1=C2	1.409(3)	C1=C2	1.393(5)
C2=C3	1.382(4)	C2-C3	1.398(6)
C3=C4	1.374(4)	C3-C4	1.354(6)
C4=C5	1.365(4)	C4=C5	1.354(6)
C5=C6	1.378(4)	C5=C6	1.386(5)
C6=C1	1.394(3)	C6=C1	1.394(5)
C7=C8	1.396(3)	C7=C8	1.379(5)
C8=C9	1.394(4)	C8=C9	1.384(6)
C9=C10	1.363(4)	C9=C10	1.357(7)
C10=C11	1.360(4)	C10=C11	1.347(11)
C11=C12	1.383(4)	C11=C12	1.383(6)
C12=C7	1.391(3)	C12=C7	1.385(5)
C13=C14	1.395(3)	C13=C14	1.386(5)
C14=C15	1.388(3)	C14=C15	1.373(6)
C15=C16	1.359(4)	C15=C16	1.356(6)
C16=C17	1.375(4)	C16=C17	1.365(7)
C17=C18	1.390(3)	C17=C18	1.377(6)
C18=C13	1.397(3)	C18=C13	1.395(5)
C19=C20	1.386(3)	C19=C20	1.378(5)
C20=C21	1.390(4)	C20=C21	1.393(6)
C21=C22	1.362(4)	C21=C22	1.326(6)
C22=C23	1.353(4)	C22=C23	1.344(6)
C23=C24	1.388(4)	C23=C24	1.376(5)
C24=C19	1.382(3)	C24=C19	1.380(5)
C25-C26	1.26(2)	C25-C26	1.401(10)
C25A-C26A	1.62(2)	C25A-C26A	1.44(2)
C27-C28	1.33(2)	C27-C28	1.435(12)
C27A-C28A	1.55(3)	C27A-C28A	1.53(2)
C29-C30	1.46(2)	C29-C30	1.298(11)
C29A-C30A	1.38(3)	C29A-C30A	1.087(13)
C31-C32	1.471(15)	C31-C32	1.377(11)

C31A-C32A	1.41(2)	C31A-C32A	1.47(2)
C33-C34	1.50(2)	C33-C34	1.419(10)
C33A-C34A	1.40(3)	C33A-C34A	1.52(2)
C35-C36	1.532(18)	C35-C36	1.376(10)
C35A-C36A	1.41(2)	C35A-C36A	1.485(14)
C25-O1	1.301(14)	C25-O1	1.284(8)
C25A-O1A	1.507(16)	C25A-O1A	1.452(19)
C26-O2	1.470(18)	C26-O2	1.372(8)
C26A-O2A	1.325(19)	C26A-O2A	1.438(19)
C27-O2	1.224(13)	C27-O2	1.331(9)
C27A-O2A	1.469(18)	C27A-O2A	1.48(2)
C28-O3	1.33(2)	C28-O3	1.272(9)
C28A-O3A	1.41(3)	C28A-O3A	1.44(2)
C29-O3	1.388(19)	C29-O3	1.364(11)
C29A-O3A	1.36(3)	C29A-O3A	1.522(17)
C30-O4	1.380(11)	C30-O4	1.396(9)
C30A-O4A	1.331(16)	C30A-O4A	1.546(18)
C31-O4	1.457(16)	C31-O4	1.266(11)
C31A-O4A	1.43(3)	C31A-O4A	1.48(2)
C32-O5	1.410(13)	C32-O5	1.382(9)
C32A-O5A	1.359(19)	C32A-O5A	1.48(2)
C33-O5	1.292(12)	C33-O5	1.287(9)
C33A-O5A	1.278(16)	C33A-O5A	1.46(2)
C34-O6	1.32(2)	C34-O6	1.361(8)
C34A-O6A	1.53(3)	C34A-O6A	1.46(2)
C35-O6	1.369(17)	C35-O6	1.339(8)
C35A-O6A	1.49(2)	C35A-O6A	1.435(14)
C36-O1	1.442(13)	C36-O1	1.411(8)
C36A-O1A	1.414(15)	C36A-O1A	1.424(14)
B1-C1	1.648(3)	B1-C1	1.645(5)
B1-C7	1.650(3)	B1-C7	1.656(5)
B1-C13	1.649(3)	B1-C13	1.642(5)
B1-C19	1.662(3)	B1-C19	1.655(5)

Table S5: The C-C, C=C, C-O and C-B bond lengths in **1** at 173 K in LTP



Bond	Length (Å)	Bond	Length (Å)
C1=C2	1.402(5)	C37-C38	1.493 (6)
C2=C3	1.380(5)	C39-C40	1.481(5)
C3=C4	1.374(6)	C41-C42	1.485(5)
C4=C5	1.374(5)	C43-C44	1.475(5)
C5=C6	1.390(5)	C45-C46	1.491(6)
C6=C1	1.396(5)	C47-C48	1.465 (6)
C7=C8	1.401(5)	C49=C50	1.392(5)
C8=C9	1.388(5)	C50=C51	1.392(5)
C9=C10	1.385(5)	C51=C52	1.389(5)
C10=C11	1.374(6)	C52=C53	1.368(5)
C11=C12	1.397(5)	C53=C54	1.383(5)
C12=C7	1.398(5)	C54=C49	1.405(4)
C13=C14	1.387(5)	C55=C56	1.397(4)
C14=C15	1.391(6)	C56=C57	1.399(5)
C15=C16	1.370 (6)	C57=C58	1.373(5)
C16=C17	1.362(5)	C58=C59	1.389(5)
C17=C18	1.385(5)	C59=C60	1.388(5)
C18=C13	1.380(5)	C60=C55	1.397(5)
C19=C20	1.384(5)	C61=C62	1.395(5)
C20=C21	1.389(5)	C62=C63	1.387(5)
C21=C22	1.367(5)	C63=C64	1.382(5)
C22=C23	1.375(5)	C64=C65	1.380(5)
C23=C24	1.380(5)	C65=C66	1.383(5)
C24=C19	1.408(5)	C66=C61	1.402(5)
C25-C26	1.403(6)	C67=C68	1.416(5)
C27-C28	1.481(5)	C68=C69	1.390(5)
C29-C30	1.485(5)	C69=C70	1.387(5)
C31-C32	1.494(6)	C70=C71	1.372(6)
C33-C34	1.480(6)	C71=C72	1.387(5)
C35-C36	1.422(6)	C72=C67	1.392(5)
C25-O1	1.370(5)	C37-O7	1.420(5)
C26-O2	1.437(5)	C38-O12	1.418(4)
C27-O2	1.408(4)	C39-O12	1.428(4)

C28-O3	1.422(4)	C40-O11	1.415(4)
C29-O3	1.416(4)	C41-O11	1.423(4)
C30-O4	1.412(4)	C42-O10	1.424(4)
C31-O4	1.429(4)	C43-O10	1.408(4)
C32-O5	1.430(4)	C44-O9	1.416(4)
C33-O5	1.424(4)	C45-O9	1.410(4)
C34-O6	1.404(4)	C46-O8	1.407(5)
C35-O6	1.424(4)	C47-O8	1.438(5)
C36-O1	1.391(5)	C48-O7	1.425(5)
B1-C1	1.651(5)	B2-C49	1.656(5)
B1-C7	1.652(5)	B2-C55	1.648(5)
B1-C13	1.647(5)	B2-C61	1.656(5)
B1-C19	1.653(5)	B2-C67	1.648(5)

Table S6: The equivalent displacement parameters (U_{eq}) in **1** at 293 and 423 K

Non-hydrogen atom	U_{eq} (423 K) in HTP	U_{eq} (293 K) in ITP	U_{eq}(423K)/U_{eq} (293K)
B	0.0605(10)	0.0385(6)	1.571
K1	0.0897(5)	0.0540(4)	1.661
K1A	0.136(5)	0.073(4)	1.863
O1	0.1540(18)	0.0757(15)	2.034
O1A	0.153(6)	0.071(2)	2.154
O2	0.1473(17)	0.0608(13)	2.422
O2A	0.149(6)	0.105(3)	1.419
O3	0.186(2)	0.071(2)	2.619
O3A	0.160(6)	0.073(3)	2.191
O4	0.1459(17)	0.0542(14)	2.691
O4A	0.146(6)	0.102(4)	1.431
O5	0.1416(18)	0.0683(14)	2.073
O5A	0.145(6)	0.084(2)	1.726
O6	0.1337(15)	0.0710(19)	1.883
O6A	0.147(6)	0.070(3)	2.100
C1	0.0649(9)	0.0421(6)	1.541
C2	0.0901(12)	0.0580(7)	1.553
C3	0.1092(15)	0.0722(9)	1.512
C4	0.1074(14)	0.0718(9)	1.495
C5	0.0986(13)	0.0669(8)	1.473
C6	0.0779(10)	0.0526(6)	1.480
C7	0.0630(9)	0.0526(6)	1.197
C8	0.1149(16)	0.0537(7)	2.139
C9	0.0899(12)	0.0684(8)	1.314

C10	0.1159(17)	0.0725(9)	1.598
C11	0.1060(15)	0.0709(8)	1.495
C12	0.0871(12)	0.0546(7)	1.595
C13	0.0675(9)	0.0403(5)	1.674
C14	0.0879(12)	0.0474(6)	1.854
C15	0.1126(15)	0.0613(7)	1.836
C16	0.1189(17)	0.0647(8)	1.837
C17	0.1192(17)	0.0646(8)	1.845
C18	0.0973(13)	0.0548(7)	1.775
C19	0.0605(8)	0.0375(5)	1.613
C20	0.0925(12)	0.0592(7)	1.562
C21	0.1088(15)	0.0705(8)	1.543
C22	0.0955(13)	0.0605(7)	1.578
C23	0.1119(15)	0.0717(9)	1.560
C24	0.1002(14)	0.0629(8)	1.593
C25	0.152(3)	0.101(3)	1.504
C25A	0.159(6)	0.076(3)	2.092
C26	0.133(2)	0.094(3)	1.414
C26A	0.147(6)	0.072(3)	2.041
C27	0.144(3)	0.094(3)	1.531
C27A	0.154(7)	0.084(3)	1.833
C28	0.188(4)	0.097(4)	1.938
C28A	0.162(7)	0.079(3)	2.050
C29	0.173(3)	0.076(3)	2.276
C29A	0.173(3)	0.081(4)	2.135
C30	0.147(2)	0.079(3)	1.860
C30A	0.147(2)	0.086(4)	1.709
C31	0.167(4)	0.075(2)	2.226
C31A	0.167(7)	0.091(4)	1.835
C32	0.152(3)	0.071(2)	2.140
C32A	0.161(7)	0.083(4)	1.939
C33	0.145(3)	0.081(3)	1.790
C33A	0.165(7)	0.078(3)	2.115
C34	0.147(3)	0.080(3)	1.837
C34A	0.161(8)	0.074(4)	2.175
C35	0.149(3)	0.079(3)	1.88608
C35A	0.168(7)	0.076(4)	2.21053
C36	0.154(3)	0.090(2)	1.71111
C36A	0.174(8)	0.078(3)	2.2307