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S = 1/2 Tetracene Monoradical Cation/Anion Ion-Based One-Dimensional Antiferromagnetic Chains

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Content

Experimental Section

All experiments were carried out under inert atmosphere by using standard Schlenk techniques and a glove box. Solvents were dried prior to use. Commercially available chemicals were bought from Energy Chemical or Alfa-Assar and used immediately. *tert*-butyl-substituted hexabenzo[*a,c,f,g,j,l,o,p*]tetracene monoradical (**1**) [S1] and $LiAl(OC(CF_3)_3)_4$[S2] was synthesized according to the reported method. Cyclic voltammetry was carried out in a glove box on a CHI660E electrochemical workstation with $Ag/AgNO_3$ (0.1 M, CH_3CN) as the reference and platinum as the working electrode.The EPR spectra were obtained using a Bruker EMX plus-6/1 variable-temperature X-band apparatus and simulated with the software of WINEPR SimFonia. The magnetic property was measured using a MPMS-XL7 SQUID on a sample prepared in a glove box. UV-Vis spectra were recorded on Lambda 750 spectrometer. The NMR spectra were performed using a Bruker DRX-400 (Germany) at room temperature in ppm downfield from internal Me_4Si. Element analyses were performed on Vario EL III elemental analyser at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. The crystallographic data collection were carried out on a Bruker D8 Venture diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 193(2) K using ω-scan technique. The diffraction data was integrated by using the *SAINT* program, which was also used for the intensity corrections for the Lorentz and polarization effects. Semi-empirical absorption correction was applied using the *SADABS* program. The structure was solved by direct methods and all the non-hydrogen atoms were refined anisotropically on F^2 by the full-matrix least-squares technique using the SHELXL-2018 crystallographic software package. All the hydrogen atoms were generated geometrically and refined isotropically using the riding model.

Synthesis of $\mathbf{1}^{\cdot+}[Al(OC(CF_3)_3)_4]^-$: 1 (0.18 g, 0.3 mmol) and $AgAl(OC(CF_3)_3)_4$ (0.32 g, 0.3 mmol) were placed in a 100 ml Schlenk flask. Then CH_2Cl_2 (40 ml) was added to the mixture under stirring at room temperature. The resultant green solution was kept stirring at 25 °C for 24 h and then filtered to remove the gray precipitate (Ag metal). The filtration was concentered to afford green crystals of $\mathbf{1}^{\cdot+}[Al(OC(CF_3)_3)_4]^-\cdot CH_2Cl_2$ that were suitable for X-ray crystallography. Isolated yield: 216 mg, 43.2% (crystals). The crystals were pumped off to remoe solvent free CH_2Cl_2 to perform element analyses. Elemental analysis calcd for $C_{64}H_{38}AlF_{36}O_4$ (%) C 48.59; H 2.42; found: C 48.63; H 2.38.

Synthesis of [K(18-c-6)]·$\mathbf{1}^{\cdot-}$**: 1** (0.18 g, 0.3 mmol), K (12 mg, 0.3 mmol) and 18-crown-6 (0.08 g, 0.3 mmol) were placed in a 100 ml Schlenk flask. Then THF (40 ml) was added to the mixture under stirring at room temperature. The resultant blue solution was kept stirring at 25 °C for 24 h and filtered. The filtration was concentered to afford blue crystals of [K(18-c-6)]·$\mathbf{1}^{\cdot-}\cdot(THF)_2$ that were suitable for X-ray crystallography. Isolated

yield: 102 mg, 31.9% (crystals). The crystals were pumped off to remove solvent free THF to perform element analyses. Elemental analysis calcd for $C_{60}H_{62}KO_6$ (%) C 78.48; H 6.81; found: C 78.39; H 6.85.

Table S1. Crystal Data and Structure Refinement for $\mathbf{1}^{\cdot+}[Al(OC(CF_3)_3)_4]^-\cdot CH_2Cl_2$ and $[K(18\text{-c-}6)]\cdot\mathbf{1}^{\cdot-}\cdot(THF)_2$.

	$\mathbf{1}^{\cdot+}[Al(OC(CF_3)_3)_4]^-\cdot CH_2Cl_2$	$[K(18\text{-c-}6)]\cdot\mathbf{1}^{\cdot-}\cdot(THF)_2$
Formula	$C_{65}H_{40}AlCl_2F_{36}O_4$	$C_{68}H_{78}KO_8$
M/g mol^{-1}	1666.85	1062.40
Crystal system	Triclinic	Monoclinic
Space group	*P* -1	*P* 21/c
a, Å	11.206(2)	14.6441(10)
b, Å	14.384(3)	16.7198(11)
c, Å	22.981(4)	11.8214(9)
α, deg	72.206(6)	
β, deg	78.785(6)	91.187(3)
γ, deg	70.084(7)	
V, Å^3	3299.0(11)	2893.8(4)
Z	2	2
Temperature, K	193(2)	193(2)
*R*1 (*I*>2σ(*I*))	0.0709	0.0606
*wR*2 (all data)	0.2185	0.1804

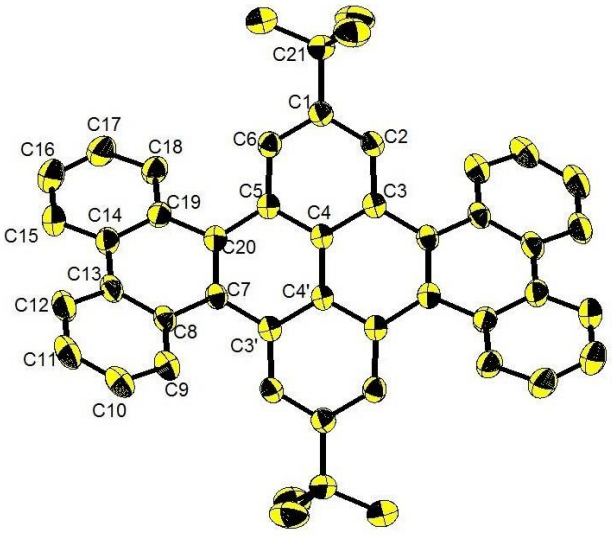


Fig. S1 Stick and Thermal ellipsoid (50%) drawing of $\mathbf{1}^{\bullet-}$ in ([K(18-c-6)] $\bullet\mathbf{1}^{\bullet-}\bullet(THF)_2$. Yellow C. Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (deg): C1–C2 1.390(3), C2-C3 1.411(3), C3-C4 1.426(3), C4-C5 1.424(3), C5-C6 1.416(3), C1-C6 1.385(3), C5-C20 1.433(3), C20-C7 1.413(3), C7-C3' 1.443(3), C4-C4' 1.432(5), C19-C20 1.461(3), C19-C14 1.413(4), C18-C19 1.410(4), C17-C18 1.383(4), C16-C17 1.377(5), C15-C16 1.375(5), C14-C15 1.407(4), C13-C14 1.450(4), C8-C13 1.416(4), C8-C9 1.409(4), C9-C10 1.375(4), C10-C11 1.379(4), C11-C12 1.370(4), C12-C13 1.406(4), C7-C8 1.459(3), C5-C20-C7 119.6(2), C20-C7-C3' 118.9(2), C3'-C4'-C4 120.1(3), C4'-C4-C5 120.2(3), C4-C5-C20 118.8(2), C19-C20-C7 117.4(2), C20-C7-C8 117.6(2), C7-C8-C13 119.6(2), C8-C13-C14 119.0(2), C13-C14-C19 118.8(2), C14-C19-C20 119.7(2).

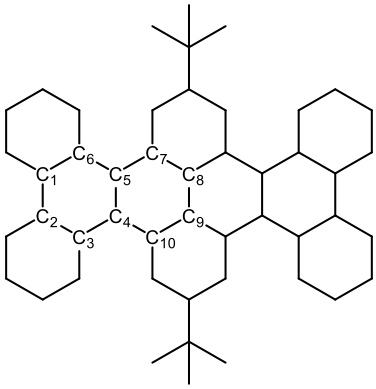


Table S2. Structure parameters of **1**, $\mathbf{1}^{\bullet+}$ and $\mathbf{1}^{\bullet-}$.

	$\mathbf{1}_{\text{x-ray}}$	$\mathbf{1}_{\text{cal}}$	$\mathbf{1}^{\bullet+}{}_{\text{x-ray}}$	$\mathbf{1}^{\bullet+}{}_{\text{cal}}$	$\mathbf{1}^{\bullet-}{}_{\text{x-ray}}$	$\mathbf{1}^{\bullet-}{}_{\text{cal}}$
C1-C2	1.452	1.457	1.455	1.463	1.450	1.462
C2-C3	1.417	1.415	1.427	1.416	1.416	1.418
C3-C4	1.465	1.463	1.457	1.455	1.459	1.463
C4-C5	1.394	1.386	1.403	1.410	1.413	1.413
C5-C6	1.466	1.464	1.463	1.457	1.461	1.460
C1-C6	1.417	1.415	1.415	1.416	1.413	1.419
C5-C7	1.455	1.462	1.446	1.441	1.433	1.441
C7-C8	1.418	1.416	1.418	1.416	1.424	1.429
C8-C9	1.428	1.429	1.414	1.417	1.432	1.431
C9-C10	1.420	1.418	1.420	1.417	1.426	1.427
C10-C4	1.459	1.462	1.451	1.443	1.443	1.437

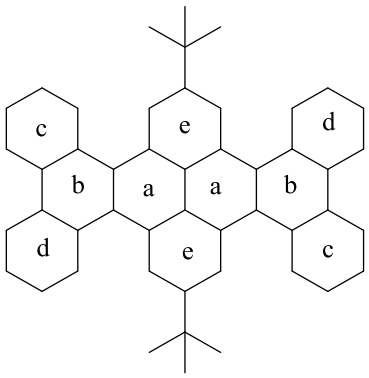


Table S3. The HOMA index in **1**, $\mathbf{1}^{\bullet+}$ and $\mathbf{1}^{\bullet-}$.

	$\mathbf{1}_{\text{x-ray}}$	$\mathbf{1}_{\text{cal}}$	$\mathbf{1}^{\cdot+}{}_{\text{x-ray}}$	$\mathbf{1}^{\cdot+}{}_{\text{cal}}$	$\mathbf{1}^{\cdot-}$	$\mathbf{1}^{\cdot-}{}_{\text{cal}}$
a	0.441	0.385	0.567	0.627	0.552	0.537
b	0.237	0.240	0.256	0.270	0.300	0.195
c	0.905	0.911	0.902	0.922	0.922	0.908
d	0.893	0.911	0.916	0.924	0.909	0.902
e	0.903	0.909	0.860	0.869	0.825	0.791

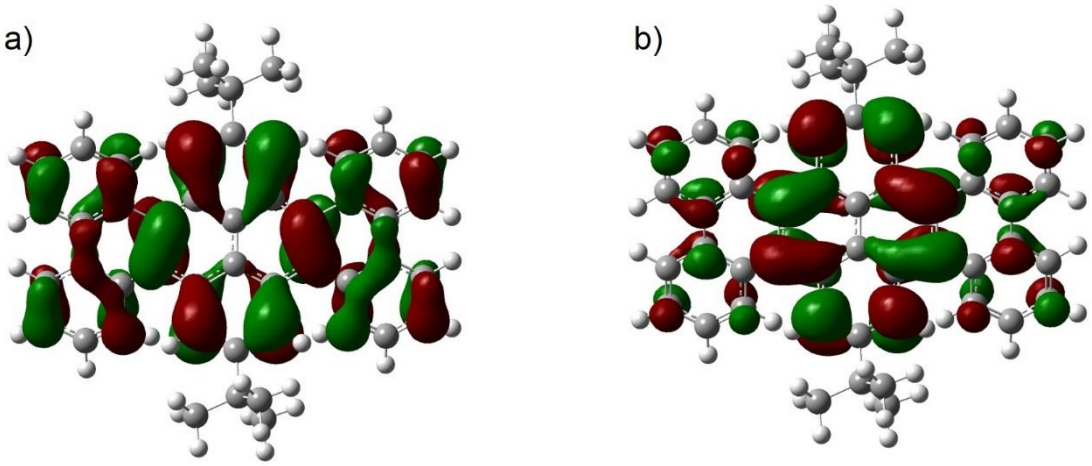


Fig. S2 The SOMO of $\mathbf{1}^{\cdot+}$ a) and LUMO of $\mathbf{1}^{\cdot+}$ b) calculated at the (U)m062x/6-31G(d) level.

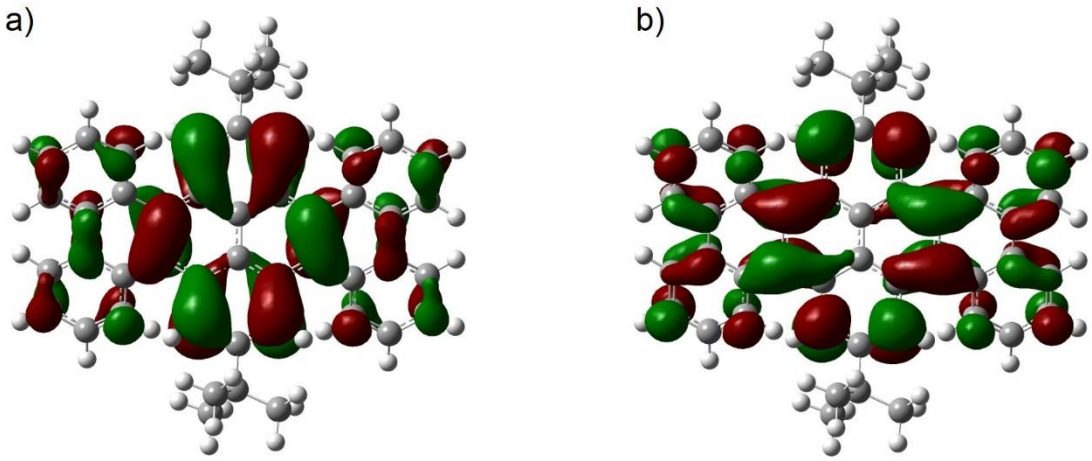


Fig. S3 The SOMO of $\mathbf{1}^{\cdot-}$ a) and LUMO of $\mathbf{1}^{\cdot-}$ b) calculated at the (U)m062x/6-31G(d) level.

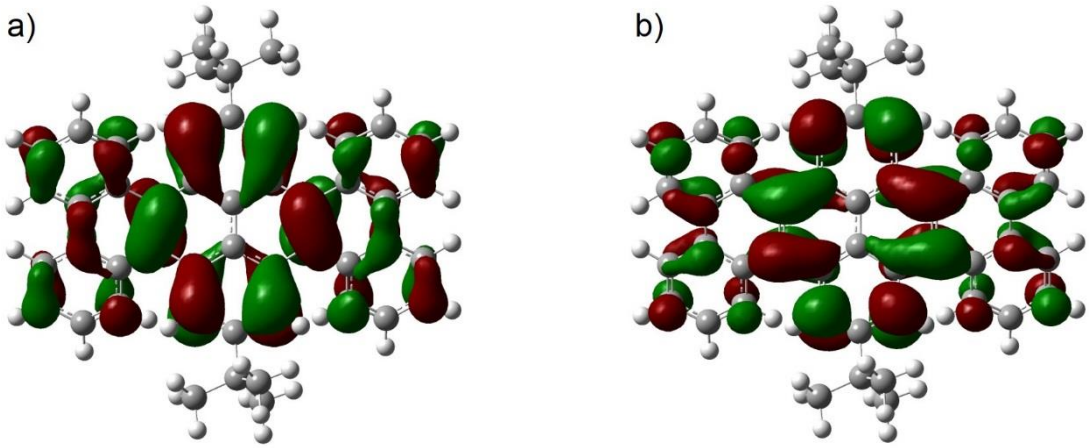


Fig. S4 The HOMO (isoval = 0.02) a) and LUMO of **1** b) calculated at the (U)m062x/6-31G(d) level.

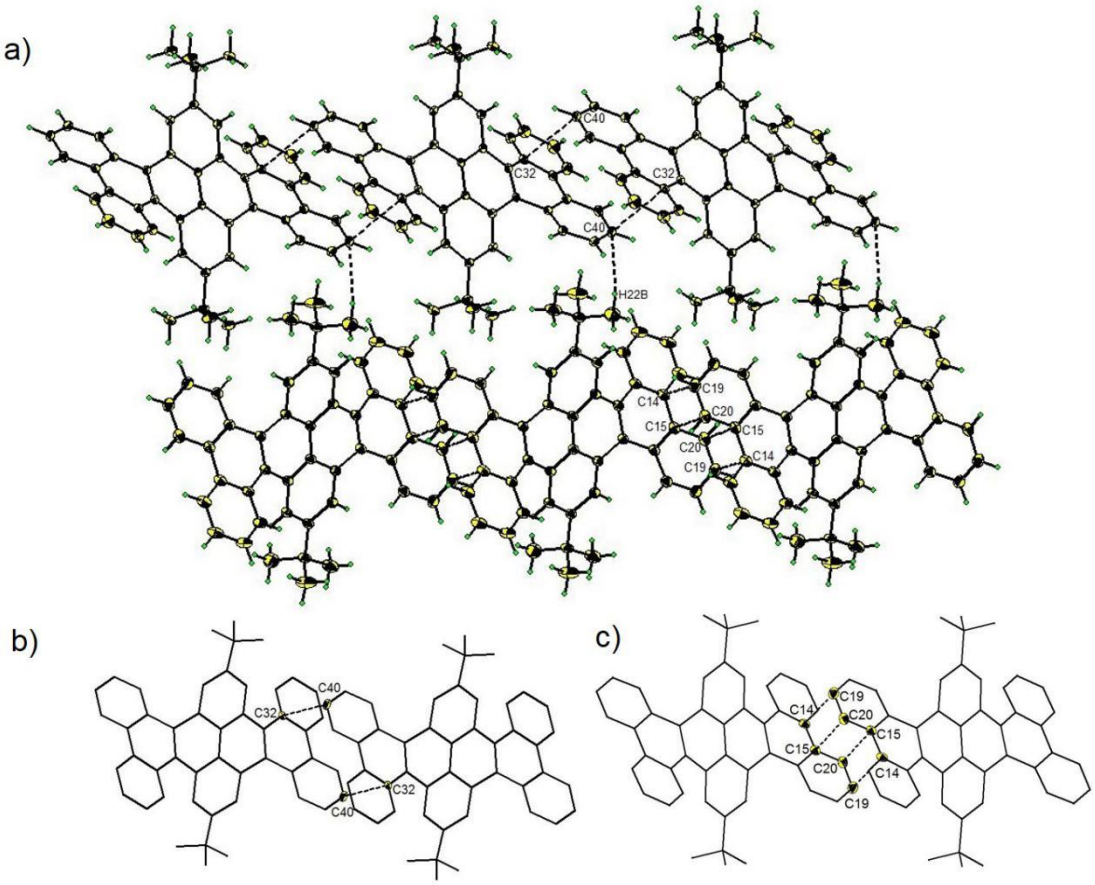


Fig. S5 a) Depiction of the polymer structure $(\mathbf{1}^{\cdot+})_n$. b), c) Two types of side-views of intermolecular C···C π interactions Selected bond distances (Å): C32…C40 3.400(3), C14…C19 3.554(5), C15…C20 3.555(4), C40…H22B 2.849(2).

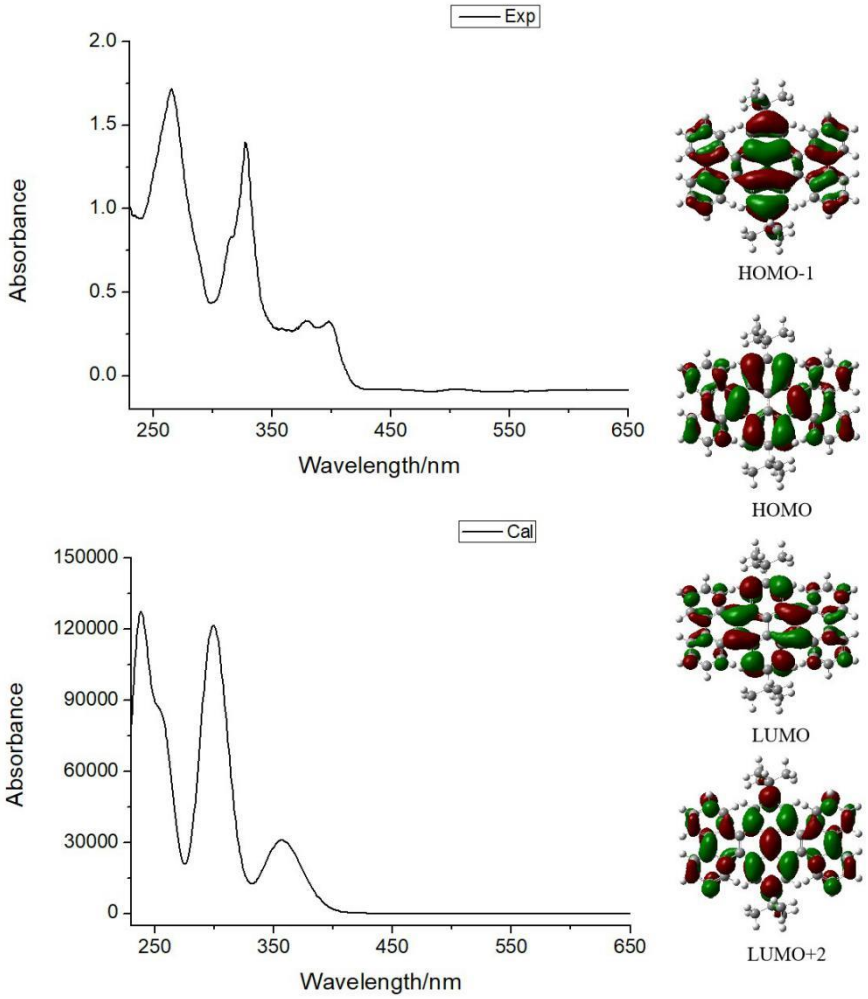


Fig. S6 Absorption spectrum of 1.0 x 10^{-4} M **1** in CH_2Cl_2 at 25 ºC (top) and calculated absorption spectrum of **1** (bottom), together with related molecular orbitals.

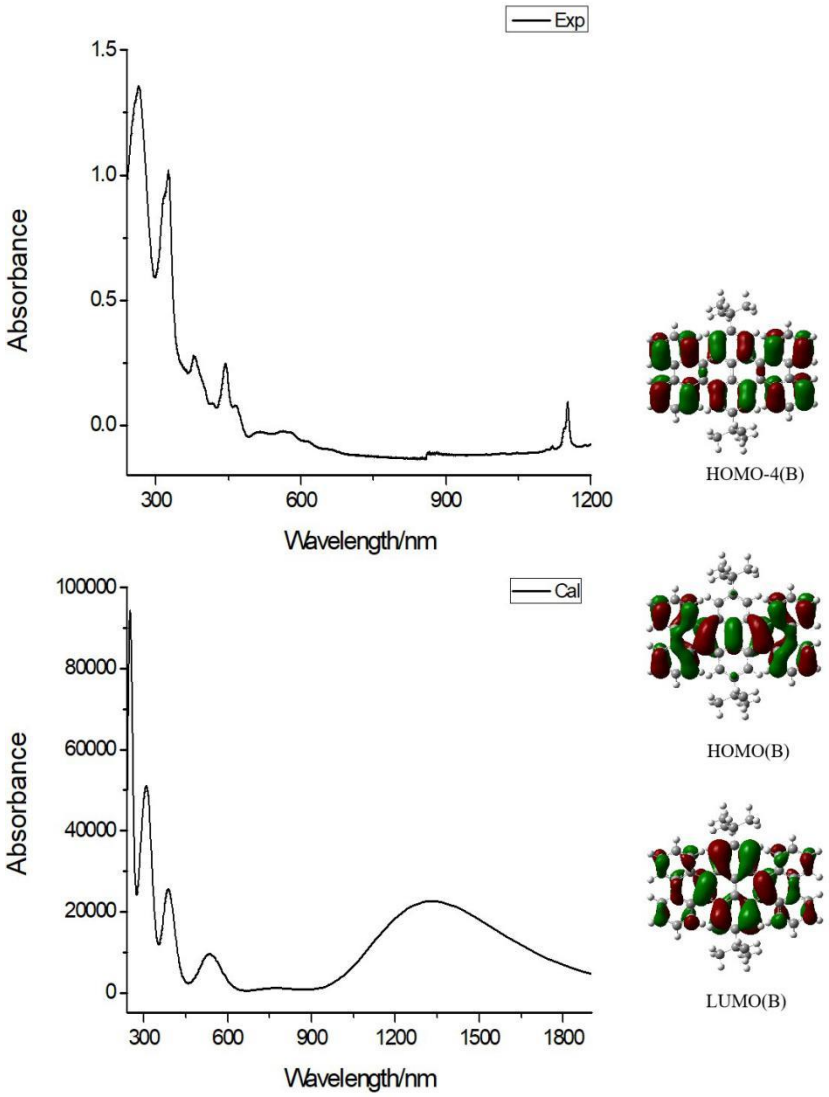


Fig. S7 Absorption spectrum of 1.0 x 10^{-4} M $\mathbf{1}^{\cdot+}[Al(OC(CF_3)_3)_4]^-$ in CH_2Cl_2 at 25 °C (top) and calculated absorption spectrum of $\mathbf{1}^{\cdot+}$ (bottom), together with related molecular orbitals.

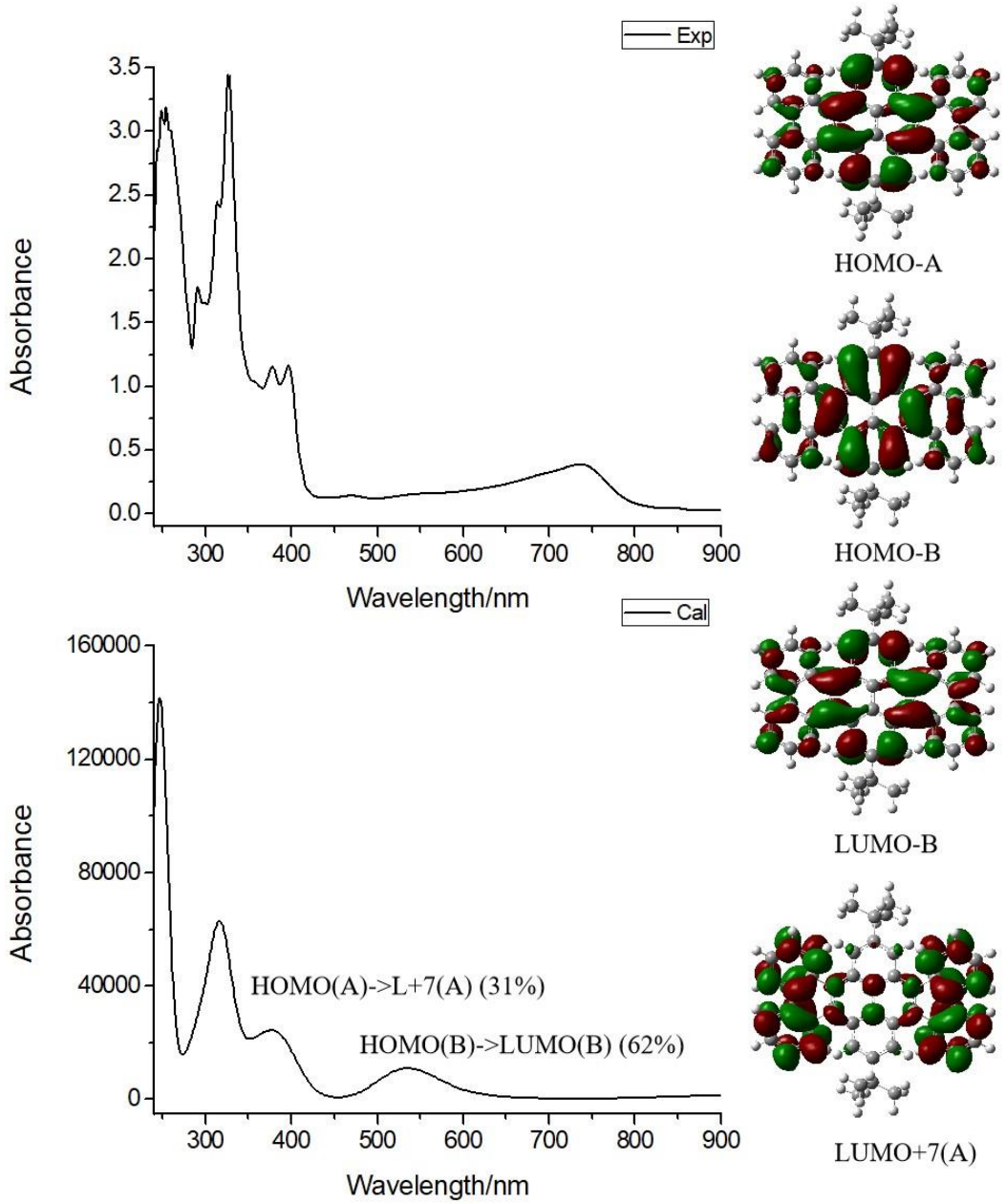


Fig. S8 Absorption spectrum of 1.0 x 10^{-4} M [K(18-c-6)]·**1**$^{\cdot-}$ in THF at 25 °C (top) and calculated absorption spectrum of **1**$^{\cdot-}$ (bottom), together with related molecular orbitals.

SQUID Magnetic Studies:

The electronic coupling interaction between the radicals $\mathbf{1}^{\cdot+}\cdot[Al(OC(CF_3)_3)_4]^-$ and $[K(18\text{-c-}6)]\cdot\mathbf{1}^{\cdot-}$ were evaluated by careful fitting of the fitted with the SQUID data (X_mT-T) with 1-D antiferromagnetic spin-1/2 chain model.[S3]

$$\hat{H} = -2J\sum_{i=1}^{n/2}(\hat{S}_{2i}\hat{S}_{2i-1} + \alpha\hat{S}_{2i}\hat{S}_{2i+1})$$

where J is the exchange integral between a spin and its right neighbor and αJ is the exchange integral between a spin and its left neighbor. When $\alpha = 0$, the model reduces to the dimer model. When $\alpha = 1$, the model reduces to the regular linear-chain model.

1. The $\chi_M T$ vs. T data of $\mathbf{1}^{\cdot+}\cdot[Al(OC(CF_3)_3)_4]^-$ was fitted with a coefficient of determination R^2 = 98.0 %. The parameters are fitted with g = 2.002, α = 1 and J = 2.2511 cm^{-1} = -6.44 cal/mol.

2. The $\chi_M T$ vs. T data of $[K(18\text{-c-}6)]\cdot\mathbf{1}^{\cdot-}$ was fitted with a coefficient of determination R^2 = 98.1 %. The parameters are fitted with g = 2.001, α = 1 and J = 0.07671 cm^{-1} = –0.22 cal/mol.

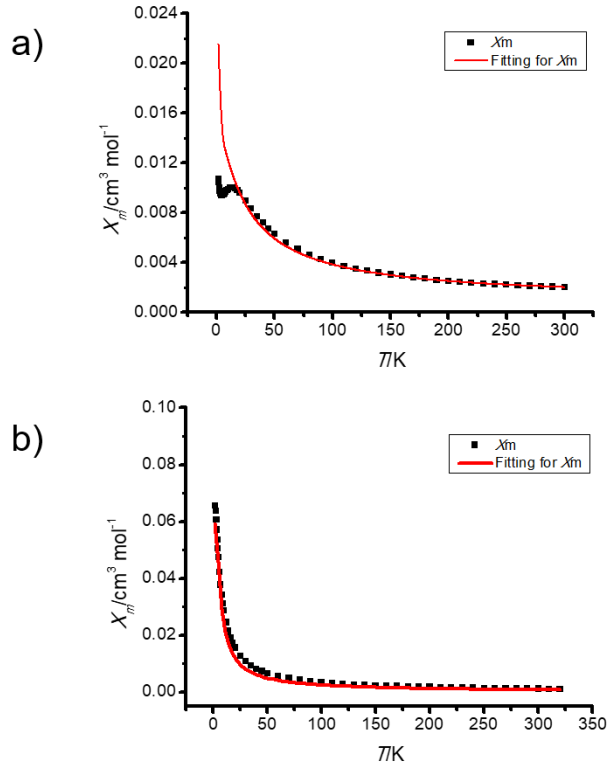


Fig. S9 The temperature-dependence of magnetic susceptibility χ_M–T plots for the crystallite sample of a) $\mathbf{1}^{\cdot+}$·$[Al(OC(CF_3)_3)_4]^-$ and b) [K(18-c-6)]·$\mathbf{1}^{\cdot-}$ in 2–300 K under 1000 Oe DC field and the fitting result (red curves).

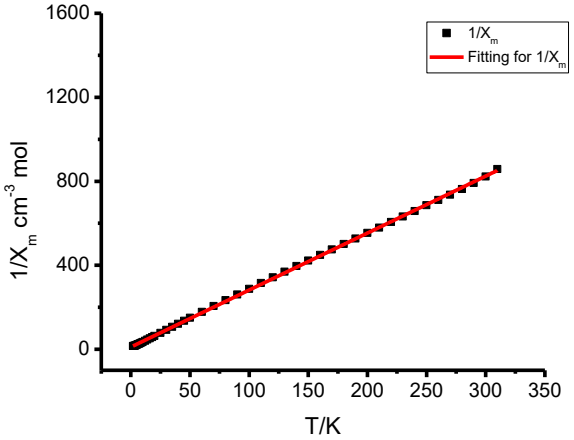
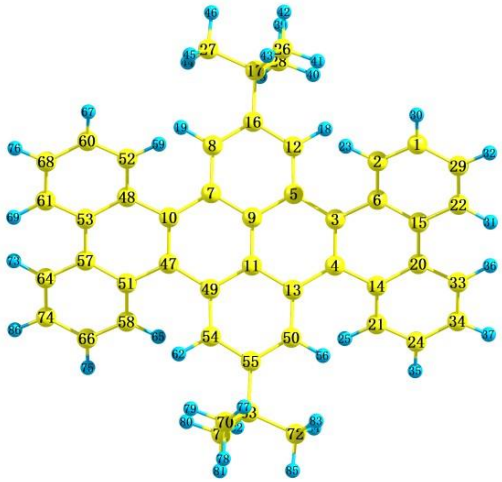


Fig. S10 χ_M^{-1}–*T* plots of [K(18-c-6)]·**1**$^{\cdot-}$ and the fitting results (red line) using Curie–Weiss law.

Computational details:

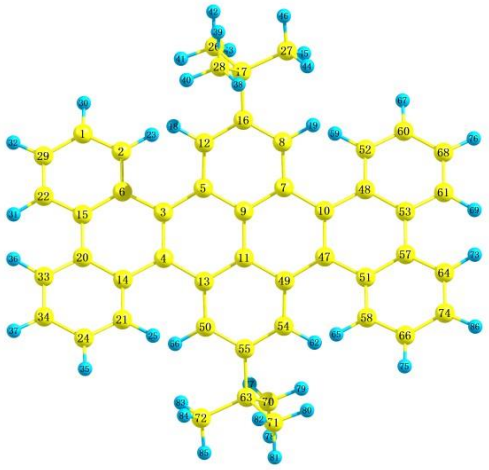
All calculations were performed with the Gaussian 09 program suite.[S3] The geometry optimizations were carried out at the Um062x/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The UV-vis absorption spectra were calculated using time-dependent DFT (TD-DFT) method at the level of (U)cam-b3lyp/6-31G(d) and polarized continuum model (PCM) was adopted to consider solvent effects.

Mulliken spin densities for the optimized geometry of **1**$^{\bullet+}$ (Um062x/6-31G(d) level).



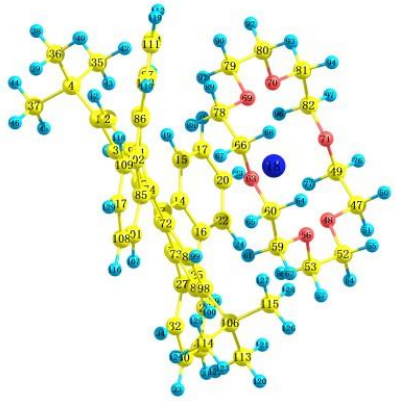
1	C	-0.016241	31	H	0.000097	61	C	-0.002303
2	C	0.041119	32	H	-0.001723	62	H	-0.010120
3	C	0.102227	33	C	-0.002302	63	C	0.003384
4	C	0.082244	34	C	0.029468	64	C	-0.005981
5	C	-0.041973	35	H	0.000401	65	H	-0.003374
6	C	-0.022013	36	H	-0.000044	66	C	-0.016241
7	C	-0.022762	37	H	-0.001408	67	H	0.000401
8	C	0.173431	38	H	-0.000040	68	C	0.029468
9	C	0.001078	39	H	-0.000126	69	H	-0.000044
10	C	0.082243	40	H	0.000124	70	C	-0.001100
11	C	0.001079	41	H	0.000170	71	C	-0.001024
12	C	0.208522	42	H	-0.000056	72	C	0.000205
13	C	-0.022762	43	H	-0.000037	73	H	0.000097
14	C	-0.018788	44	H	-0.000038	74	C	0.036349
15	C	0.021039	45	H	-0.000032	75	H	0.000535
16	C	-0.077146	46	H	-0.000060	76	H	-0.001408
17	C	0.003384	47	C	0.102228	77	H	-0.000040
18	H	-0.010120	48	C	-0.018788	78	H	-0.000126
19	H	-0.008357	49	C	-0.041973	79	H	0.000124
20	C	0.014390	50	C	0.173431	80	H	0.000170
21	C	0.035624	51	C	-0.022013	81	H	-0.000056
22	C	-0.005982	52	C	0.035624	82	H	-0.000037
23	H	-0.003374	53	C	0.014390	83	H	-0.000038
24	C	-0.012690	54	C	0.208522	84	H	-0.000032
25	H	-0.002971	55	C	-0.077146	85	H	-0.000060
26	C	-0.001024	56	H	-0.008357	86	H	-0.001723
27	C	0.000205	57	C	0.021039			
28	C	-0.001100	58	C	0.041118			
29	C	0.036348	59	H	-0.002971			
30	H	0.000535	60	C	-0.012690			

Mulliken spin densities for the optimized geometry of **1**$^{\bullet-}$ (Um062x/6-31G(d) level).



1	C	-0.013860	31	H	0.000242	61	C	-0.002392
2	C	0.030035	32	H	-0.001627	62	H	-0.009067
3	C	0.113256	33	C	-0.002392	63	C	0.003007
4	C	0.094226	34	C	0.022766	64	C	-0.006870
5	C	-0.029613	35	H	0.000496	65	H	-0.000662
6	C	-0.020584	36	H	0.000075	66	C	-0.013860
7	C	-0.008470	37	H	-0.001188	67	H	0.000496
8	C	0.155430	38	H	-0.000142	68	C	0.022766
9	C	-0.006865	39	H	-0.000218	69	H	0.000075
10	C	0.094229	40	H	0.000237	70	C	0.000342
11	C	-0.006865	41	H	0.000220	71	C	-0.000057
12	C	0.186273	42	H	-0.000111	72	C	0.000337
13	C	-0.008469	43	H	-0.000151	73	H	0.000242
14	C	-0.017185	44	H	0.000241	74	C	0.031546
15	C	0.020942	45	H	0.000303	75	H	0.000653
16	C	-0.059816	46	H	-0.000134	76	H	-0.001188
17	C	0.003007	47	C	0.113256	77	H	-0.000142
18	H	-0.009067	48	C	-0.017185	78	H	-0.000218
19	H	-0.007309	49	C	-0.029613	79	H	0.000237
20	C	0.012378	50	C	0.155430	80	H	0.000220
21	C	0.024496	51	C	-0.020584	81	H	-0.000111
22	C	-0.006871	52	C	0.024495	82	H	-0.000151
23	H	-0.000662	53	C	0.012378	83	H	0.000241
24	C	-0.010201	54	C	0.186274	84	H	0.000303
25	H	-0.000981	55	C	-0.059816	85	H	-0.000134
26	C	-0.000057	56	H	-0.007309	86	H	-0.001627
27	C	0.000337	57	C	0.020942			
28	C	0.000343	58	C	0.030035			
29	C	0.031546	59	H	-0.000982			
30	H	0.000653	60	C	-0.010200			

Mulliken spin densities for the optimized geometry of [K(18-c-6)]·**1**$^{\bullet-}$ (Um062x/6-31G(d) level).



1	C	-0.018691	34	H	-0.002223	67	H	-0.000915	100	H	-0.006518
2	C	0.061322	35	C	0.000141	68	H	0.000026	101	C	0.009792
3	C	0.096438	36	C	0.000171	69	O	-0.000332	102	C	0.008144
4	C	0.001837	37	C	0.000532	70	O	-0.000443	103	C	0.001346
5	C	-0.036637	38	H	-0.000087	71	O	-0.000738	104	C	-0.000044
6	H	-0.004952	39	H	0.000131	72	C	-0.035049	105	H	0.000302
7	C	-0.011647	40	H	0.000282	73	C	-0.024166	106	C	0.002993
8	C	0.158755	41	H	-0.000345	74	C	0.044004	107	H	-0.000293
9	C	0.025332	42	H	0.000055	75	C	-0.000568	108	C	-0.004764
10	C	0.032703	43	H	-0.000032	76	H	0.000039	109	C	-0.003781
11	C	0.003638	44	H	-0.000245	77	H	0.000423	110	H	-0.000042
12	H	-0.002897	45	H	0.000013	78	C	-0.000513	111	C	0.000117
13	C	0.193021	46	H	-0.000039	79	C	0.000344	112	H	0.000014
14	C	-0.006449	47	C	-0.000055	80	C	-0.000142	113	C	0.000019
15	C	0.082674	48	O	-0.000620	81	C	-0.000150	114	C	-0.000277
16	C	0.059375	49	C	0.000740	82	C	0.000826	115	C	-0.000113
17	C	-0.039609	50	H	-0.000039	83	C	0.190105	116	H	0.000258
18	K	0.010985	51	H	-0.000006	84	C	0.153219	117	C	0.008365
19	H	-0.003173	52	C	-0.000170	85	C	-0.008623	118	H	0.000156
20	C	0.113601	53	C	0.000572	86	C	-0.001531	119	H	-0.000006
21	H	0.001272	54	H	-0.000017	87	C	0.001285	120	H	-0.000123
22	C	-0.020536	55	H	-0.000055	88	H	0.000620	121	H	0.000559
23	H	-0.006216	56	O	-0.000450	89	H	-0.000005	122	H	0.000160
24	H	0.000351	57	H	0.000084	90	H	-0.000026	123	H	-0.000128
25	C	0.011679	58	H	-0.000591	91	H	0.000798	124	H	-0.000117
26	C	0.003010	59	C	0.005172	92	H	-0.000004	125	H	0.000287
27	C	-0.028396	60	C	0.000806	93	H	-0.000032	126	H	-0.000292
28	C	0.030080	61	H	-0.001567	94	H	-0.000031	127	H	0.000194
29	H	-0.000103	62	H	0.000378	95	H	-0.000002	128	H	0.000096
30	C	-0.010042	63	O	-0.000421	96	H	0.000329	129	H	-0.000383
31	H	-0.001629	64	H	-0.000061	97	H	0.000035			
32	C	0.038401	65	H	-0.000619	98	C	-0.062041			
33	H	0.000450	66	C	0.001406	99	H	-0.009455			

Coordinates for optimized geometries.

1

C	-4.95717600	3.02932100	1.68633900
C	-3.77601100	2.49077300	1.21849900
C	-2.49153600	0.64524400	0.09805400
C	-2.46963400	-0.72597300	-0.09989400
C	-1.24999800	1.40267000	-0.05075000
C	-3.75079800	1.27467800	0.49718800
C	1.20328600	1.44233100	-0.04527700
C	1.15224500	2.81408500	-0.33674800
C	-0.01049200	0.71354600	-0.02984200
C	2.46963300	0.72596300	0.09987400
C	0.01049100	-0.71355700	0.02982700
C	-1.23983600	2.77002400	-0.34408500
C	-1.20328700	-1.44234200	0.04526600
C	-3.71215800	-1.39290800	-0.49260000
C	-4.96852600	0.57346600	0.33341800
C	-0.05358200	3.48279000	-0.52814500
C	-0.12294400	4.96161200	-0.91855700
H	-2.18597200	3.27731500	-0.49420200
H	2.08372100	3.34443000	-0.47949100
C	-4.95000800	-0.72945700	-0.31950700
C	-3.70565300	-2.60750900	-1.21651200
C	-6.16104500	1.14117600	0.82099100
H	-2.84350500	2.98522000	1.46217800
C	-4.87284400	-3.18037600	-1.67877300
H	-2.76022500	-3.07342100	-1.46586500
C	-0.92488000	5.72977000	0.14609900
C	1.26686000	5.59730400	-1.02499100
C	-0.82518800	5.09610200	-2.27995700
C	-6.16648200	2.35836400	1.46984500
H	-4.93943900	3.95699900	2.24983500
H	-7.09331400	0.59647300	0.72225600
H	-7.09816400	2.77058400	1.84437400
C	-6.12772700	-1.33220600	-0.80053800
C	-6.10058500	-2.54718100	-1.45282400
H	-4.83088100	-4.10611100	-2.24418800
H	-7.07541600	-0.81643100	-0.69376300
H	-7.02180200	-2.98651000	-1.82241300
H	-0.27301500	4.55664300	-3.05622600
H	-0.88666800	6.15110600	-2.57057500
H	-1.84280900	4.69488900	-2.24843400
H	-1.95346400	5.36200100	0.22219900
H	-0.96905700	6.79434600	-0.10981900

H	-0.45554400	5.63135700	1.13072300
H	1.87308000	5.11623600	-1.79968400
H	1.81165400	5.53980000	-0.07592700
H	1.16577000	6.65491800	-1.28948000
C	2.49153600	-0.64525500	-0.09807200
C	3.71215400	1.39290300	0.49257200
C	1.24999800	-1.40268100	0.05074100
C	-1.15224500	-2.81409100	0.33676300
C	3.75080200	-1.27468700	-0.49720400
C	3.70564300	2.60751800	1.21646100
C	4.95000600	0.72945400	0.31948900
C	1.23983600	-2.77003100	0.34409700
C	0.05358300	-3.48279300	0.52817200
H	-2.08371900	-3.34443400	0.47952300
C	4.96852900	-0.57347200	-0.33343000
C	3.77602000	-2.49077700	-1.21852300
H	2.76021200	3.07343500	1.46579500
C	4.87283100	3.18039300	1.67871900
C	6.12772200	1.33221100	0.80051700
H	2.18597100	-3.27731900	0.49422700
C	0.12294500	-4.96160600	0.91861300
C	6.16105000	-1.14117900	-0.82100000
H	2.84351600	-2.98522300	-1.46221200
C	4.95718700	-3.02932200	-1.68636100
H	4.83086400	4.10613700	2.24411800
C	6.10057300	2.54719500	1.45278700
H	7.07541200	0.81643800	0.69375100
C	0.82517500	-5.09606800	2.28002300
C	0.92489400	-5.72978200	-0.14601900
C	-1.26685800	-5.59730100	1.02504500
H	7.09331800	-0.59647400	-0.72226200
C	6.16649200	-2.35836500	-1.46985800
H	4.93945300	-3.95699600	-2.24986300
H	7.02178900	2.98653200	1.82237300
H	0.27299300	-4.55659500	3.05627600
H	0.88665500	-6.15106600	2.57066200
H	1.84279600	-4.69485200	2.24850300
H	1.95347800	-5.36201000	-0.22211600
H	0.96907300	-6.79435300	0.10991900
H	0.45556900	-5.63138900	-1.13065100
H	-1.87308800	-5.11621900	1.79972200
H	-1.81164200	-5.53981800	0.07597300
H	-1.16576800	-6.65491000	1.28955600
H	7.09817500	-2.77058200	-1.84438600

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C	-4.91838100	3.03788300	1.69462100
C	-3.73579600	2.49089300	1.23622300
C	-2.47331900	0.65652800	0.09757900
C	-2.45184600	-0.73858800	-0.10420100
C	-1.24645800	1.39697200	-0.06905500
C	-3.72240600	1.27645000	0.51358500
C	1.20296200	1.43720600	-0.06369100
C	1.14980900	2.82330500	-0.35509000
C	-0.00955400	0.70652800	-0.05109400
C	2.45184500	0.73856800	0.10416300
C	0.00955500	-0.70654900	0.05106300
C	-1.23512200	2.77543200	-0.36463300
C	-1.20296300	-1.43722600	0.06367100
C	-3.68763000	-1.39554800	-0.50966300
C	-4.93997200	0.57348800	0.34108300
C	-0.05090500	3.50015500	-0.53574200
C	-0.12287500	4.97915900	-0.92024700
H	-2.18401200	3.27171300	-0.53781400
H	2.08448500	3.34532000	-0.51451900
C	-4.92342700	-0.72890500	-0.32500200
C	-3.67289700	-2.60751200	-1.23484300
C	-6.12687800	1.14557600	0.82207100
H	-2.79947100	2.97050300	1.49866600
C	-4.84332700	-3.18641700	-1.68614800
H	-2.72553000	-3.06064800	-1.50384500
C	-0.94259800	5.73237600	0.14201700
C	1.26816800	5.61513000	-1.00282600
C	-0.80959600	5.11287700	-2.29000800
C	-6.12480600	2.36799900	1.47091100
H	-4.90293100	3.96349100	2.26011100
H	-7.06469200	0.61246900	0.71858200
H	-7.05630700	2.78266400	1.84190200
C	-6.09783300	-1.33325000	-0.79732600
C	-6.06664700	-2.55276300	-1.45045400
H	-4.80618100	-4.11018500	-2.25367300
H	-7.04944500	-0.82737100	-0.68354200
H	-6.98903900	-2.99308200	-1.81459100
H	-0.24757200	4.58130400	-3.06434200
H	-0.86961500	6.16848500	-2.57412800
H	-1.82892400	4.71395100	-2.27410100
H	-1.97206900	5.36287900	0.20182700
H	-0.98948300	6.79651600	-0.11006400
H	-0.48537000	5.63514500	1.13229600

H	1.88296300	5.15059600	-1.78111200
H	1.80278600	5.54799600	-0.04832700
H	1.16816700	6.67540200	-1.25206200
C	2.47332000	-0.65654800	-0.09761500
C	3.68762500	1.39553700	0.50961600
C	1.24645900	-1.39699200	0.06903600
C	-1.14980800	-2.82331600	0.35511800
C	3.72241200	-1.27646400	-0.51362600
C	3.67288200	2.60752000	1.23476100
C	4.92342300	0.72889500	0.32497000
C	1.23512300	-2.77544200	0.36466100
C	0.05090500	-3.50015800	0.53579400
H	-2.08448200	-3.34532400	0.51457600
C	4.93997600	-0.57349900	-0.34111100
C	3.73581000	-2.49089200	-1.23628900
H	2.72551000	3.06066400	1.50373300
C	4.84330700	3.18643700	1.68606400
C	6.09782500	1.33325200	0.79729200
H	2.18401100	-3.27171700	0.53787000
C	0.12287500	-4.97914700	0.92035900
C	6.12688700	-1.14557900	-0.82209700
H	2.79949000	-2.97049600	-1.49875800
C	4.91840000	-3.03787300	-1.69468600
H	4.80615500	4.11022000	2.25356400
C	6.06662900	2.55277800	1.45039600
H	7.04944000	0.82737600	0.68352000
C	0.80957500	-5.11280900	2.29013600
C	0.94261700	-5.73240200	-0.14186300
C	-1.26816800	-5.61511900	1.00294100
H	7.06469800	-0.61246900	-0.71859900
C	6.12482300	-2.36799300	-1.47095400
H	4.90295500	-3.96347100	-2.26019400
H	6.98901900	2.99310700	1.81453000
H	0.24753800	-4.58120800	3.06444000
H	0.86959300	-6.16840600	2.57429700
H	1.82890200	-4.71388000	2.27422900
H	1.97208700	-5.36290200	-0.20167100
H	0.98950300	-6.79653200	0.11025900
H	0.48540500	-5.63521100	-1.13215300
H	-1.88297600	-5.15055600	1.78119800
H	-1.80277000	-5.54802600	0.04843000
H	-1.16816600	-6.67538100	1.25222000
H	7.05632700	-2.78265000	-1.84194600

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C	-4.94817900	-3.06030400	-1.66365800
C	-3.76868500	-2.52652600	-1.18255900
C	-2.47596500	-0.67397300	-0.07006500
C	-2.45886600	0.73041900	0.08690500
C	-1.25026700	-1.41490600	0.08858500
C	-3.73148500	-1.29802600	-0.47811700
C	1.22017300	-1.44166700	0.06965800
C	1.17127300	-2.83490100	0.34388800
C	-0.00646000	-0.71315200	0.05449700
C	2.45886700	-0.73042900	-0.08693300
C	0.00646200	0.71314000	-0.05451500
C	-1.22740900	-2.80003200	0.36339600
C	-1.22017100	1.44165500	-0.06967600
C	-3.70626100	1.38247200	0.48438500
C	-4.95590500	-0.59452800	-0.33747500
C	-0.03120400	-3.50182300	0.52127500
C	-0.09049500	-4.98606600	0.89923000
H	-2.16819300	-3.30738500	0.54263300
H	2.10523600	-3.35442400	0.50577100
C	-4.94453200	0.71073600	0.32052400
C	-3.72099800	2.60494400	1.19781700
C	-6.14234600	-1.15352300	-0.84156900
H	-2.83738800	-3.03759300	-1.39516600
C	-4.89360200	3.16816700	1.66304100
H	-2.77964200	3.08944600	1.42740000
C	-0.91895800	-5.74655500	-0.14987500
C	1.29871500	-5.62904300	0.96349200
C	-0.75619500	-5.13829700	2.27666100
C	-6.15603300	-2.37874900	-1.48157100
H	-4.92605900	-3.99871900	-2.21138200
H	-7.06893500	-0.59393600	-0.76173500
H	-7.08672800	-2.78557200	-1.86631300
C	-6.12388800	1.29793800	0.80959600
C	-6.11514700	2.51946100	1.45660200
H	-4.85621500	4.10257200	2.21660700
H	-7.06346600	0.76353800	0.71212700
H	-7.04100900	2.94796900	1.82943300
H	-0.18148700	-4.60326400	3.03997900
H	-0.81111400	-6.19680700	2.56176300
H	-1.77146800	-4.73090200	2.27431600
H	-1.94652800	-5.37292200	-0.19929800
H	-0.95819700	-6.81563800	0.09471300
H	-0.47184900	-5.63495800	-1.14364100

H	1.92172900	-5.16241100	1.73332900
H	1.82302000	-5.54459900	0.00513700
H	1.20216400	-6.69366100	1.20648900
C	2.47596400	0.67396100	0.07005400
C	3.70626400	-1.38246900	-0.48443600
C	1.25026700	1.41489600	-0.08859100
C	-1.17127300	2.83489400	-0.34387600
C	3.73148000	1.29800900	0.47812400
C	3.72100800	-2.60490900	-1.19792200
C	4.94453300	-0.71073300	-0.32055300
C	1.22740900	2.80002600	-0.36338300
C	0.03120300	3.50182000	-0.52125000
H	-2.10523900	3.35442000	-0.50574000
C	4.95590100	0.59451500	0.33747700
C	3.76867500	2.52649700	1.18258800
H	2.77965700	-3.08940100	-1.42754100
C	4.89361600	-3.16811100	-1.66316400
C	6.12389300	-1.29791400	-0.80964000
H	2.16819200	3.30738200	-0.54260900
C	0.09049600	4.98607100	-0.89917400
C	6.14233800	1.15350200	0.84158800
H	2.83737600	3.03755900	1.39519800
C	4.94816600	3.06026700	1.66370500
H	4.85623300	-4.10249300	-2.21676900
C	6.11515900	-2.51941300	-1.45669000
H	7.06346900	-0.76351300	-0.71215200
C	0.75619100	5.13833100	-2.27660400
C	0.91896300	5.74653600	0.14994500
C	-1.29871300	5.62905200	-0.96341700
H	7.06892900	0.59391800	0.76174800
C	6.15602100	2.37871500	1.48161300
H	4.92604100	3.99867200	2.21144500
H	7.04102400	-2.94790500	-1.82953500
H	0.18148000	4.60331500	-3.03993100
H	0.81111000	6.19684700	-2.56168300
H	1.77146400	4.73093500	-2.27427000
H	1.94653300	5.37290000	0.19935600
H	0.95820300	6.81562400	-0.09462000
H	0.47185700	5.63491700	1.14371000
H	-1.92173200	5.16243800	-1.73326300
H	-1.82301600	5.54458900	-0.00506200
H	-1.20216100	6.69367500	-1.20639200
H	7.08671300	2.78553300	1.86636800

[K(18-c-6)]·**1**$^{\bullet-}$

C	1.34859500	-2.99958200	2.27193400
C	2.41786800	-2.66117800	1.46238700
C	0.32478100	-2.05569900	2.45701500
C	1.22327100	-4.37099600	2.93869800
C	0.37495500	-0.77702900	1.89424200
H	-0.51907900	-2.30612000	3.09096200
C	1.57661800	-0.38305400	1.22845300
C	-0.73608600	0.15525000	1.92991200
C	2.54168300	-1.36617300	0.89796700
C	1.76698400	0.98271700	0.84617100
C	3.68058100	-0.98782900	0.08483000
H	3.22885000	-3.36221400	1.32037800
C	-0.44135400	1.54920600	1.80529300
C	-2.10702000	-0.27138800	1.89284100
C	-2.51917500	-1.61676100	1.63165300
C	-3.15902600	0.70732900	1.95094300
C	-3.84402700	-1.96910200	1.45368900
K	-3.16673700	-0.48595200	-1.17871800
H	-1.76805500	-2.38866400	1.52988900
C	-4.85250800	-0.99634900	1.48736000
H	-4.08935800	-3.00673600	1.23929100
C	-4.48616800	0.32701200	1.71921900
H	-5.89756500	-1.26512500	1.36788200
H	-5.25938900	1.09015800	1.71522500
C	-2.81248600	2.08056100	2.33665400
C	-3.78163200	2.97971000	2.81246600
C	-1.45529300	2.48628600	2.28156600
C	-3.44493500	4.25570700	3.23384600
H	-4.81452000	2.65695800	2.89576500
C	-2.10233100	4.64051600	3.23672100
H	-4.21298000	4.92896200	3.60198100
C	-1.13058600	3.76474300	2.78533100
H	-1.81204200	5.61417200	3.62071200
H	-0.08646100	4.04877600	2.85506200
C	-0.04996000	-5.06164500	2.41924000
C	2.41805800	-5.27885100	2.63051600
C	1.12573500	-4.19960600	4.46298600
H	2.28040300	-6.24834800	3.12102200
H	3.35481300	-4.84640600	2.99665400
H	2.52206900	-5.45828200	1.55438300
H	-0.15882400	-6.05589400	2.86834200
H	-0.00054600	-5.18016100	1.32998500
H	-0.94941800	-4.48428500	2.65984300

H	1.02285000	-5.17672400	4.94937700
H	0.26384500	-3.58808400	4.74551100
H	2.02579000	-3.71323100	4.85245300
C	-6.45729100	0.98859200	-2.12229000
O	-5.23249000	1.37988700	-1.55070800
C	-6.82681800	-0.36541100	-1.57362400
H	-6.36970900	0.93925900	-3.21852700
H	-7.24945000	1.71081700	-1.87067300
C	-4.86352600	2.69182400	-1.92333400
C	-3.51855200	2.99983100	-1.32030200
H	-5.60970700	3.41262900	-1.55661900
H	-4.80813900	2.77176200	-3.01947000
O	-2.55522000	2.15732000	-1.91722000
H	-3.27139000	4.05596700	-1.50875100
H	-3.54549500	2.84372900	-0.22998900
C	-1.25635200	2.47037200	-1.43391500
C	-0.25118000	1.50720800	-2.00806800
H	-1.24918200	2.39916400	-0.34099300
H	-0.98541200	3.49785900	-1.72335800
O	-0.53663800	0.21272400	-1.51674500
H	-0.30611200	1.51035300	-3.10905100
H	0.75872400	1.81879600	-1.70222700
C	0.42753500	-0.73297600	-1.92773800
H	1.43045400	-0.43766200	-1.58462500
H	0.43825200	-0.80241100	-3.02748100
O	-1.19742800	-2.46432200	-1.84820400
O	-3.87435500	-3.23259400	-1.60793300
O	-5.84230400	-1.29336100	-1.97457100
C	2.96653900	1.36473000	0.19026600
C	0.77290400	1.96442000	1.17463200
C	3.99379900	0.36420300	-0.04754200
C	4.47817300	-1.95865900	-0.67293900
H	-7.81248800	-0.66290900	-1.96361100
H	-6.88226100	-0.31868800	-0.47656300
C	0.06947900	-2.07197600	-1.33815100
C	-1.56993700	-3.73830600	-1.38263700
C	-2.86864400	-4.12376700	-2.04237200
C	-5.13290800	-3.54575200	-2.15516600
C	-6.15615000	-2.60705600	-1.56900700
C	3.07702900	2.67643100	-0.31575400
C	0.98566300	3.28652300	0.69353500
C	5.38085100	0.72054400	-0.35948700
C	5.72589800	-1.57256400	-1.21927300
C	3.96015400	-3.21989500	-1.04795300

H	0.03027500	-2.01630400	-0.24236200
H	0.83579800	-2.80785600	-1.62663100
H	-0.79884800	-4.48307700	-1.63550600
H	-1.69320600	-3.72962400	-0.28871800
H	-3.13243800	-5.15650700	-1.76790700
H	-2.76147500	-4.06962400	-3.13619500
H	-5.11180400	-3.44023600	-3.25064100
H	-5.41014600	-4.58338600	-1.91277700
H	-6.14503300	-2.68041100	-0.47166000
H	-7.15749600	-2.88943800	-1.92939800
C	2.08808200	3.63235100	-0.07574300
H	3.91795100	2.92542300	-0.95069500
H	0.20784400	4.02054800	0.84452800
C	5.93787700	1.95608200	0.04371600
C	6.25357300	-0.24909400	-0.90605100
C	6.41997800	-2.46204200	-2.05936600
C	4.66016000	-4.07974200	-1.87163000
H	2.97142200	-3.50822700	-0.71255500
C	2.23765100	5.02347300	-0.70097500
H	5.31577100	2.66976700	0.56998600
C	7.27167700	2.25005200	-0.15687300
C	7.60904400	0.07242800	-1.10508800
H	7.36052300	-2.15177900	-2.50163800
C	5.91073300	-3.70552000	-2.37428100
H	4.22413100	-5.03593900	-2.14573600
C	1.11662600	5.97887100	-0.27937100
C	3.57882800	5.64026600	-0.26945800
C	2.20897100	4.89213700	-2.23303000
H	7.66747500	3.20316700	0.18076700
C	8.11485900	1.30840500	-0.75749800
H	8.28483800	-0.67867900	-1.49935100
H	6.46340700	-4.37075000	-3.03049400
H	1.28596100	6.96520700	-0.72437900
H	0.13610200	5.62437700	-0.61637600
H	1.07872800	6.09908200	0.80874100
H	3.69824300	6.63790600	-0.70815000
H	3.62477600	5.73563800	0.82060900
H	4.42826000	5.02906600	-0.59067600
H	2.32204400	5.87508600	-2.70553100
H	3.01370700	4.24515700	-2.59480500
H	1.25631000	4.46146800	-2.56493800
H	9.16630700	1.52971400	-0.91262000

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