Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Organic Polyanionic High-Spin Molecular Clusters in Solution: Topological-Symmetry Controlled Models for Organic Ferromagnetic Metals with *meta*-Benzoylbenzene Linkers

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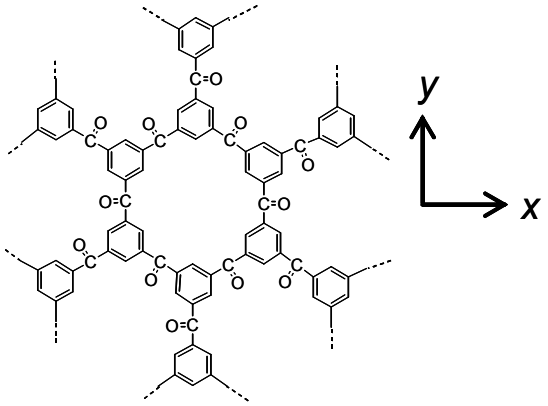
Contents of the Supplementary Information

1. The two-dimensional π-crystal orbital band structure of a two-dimensional system 4 (Fig. S1)



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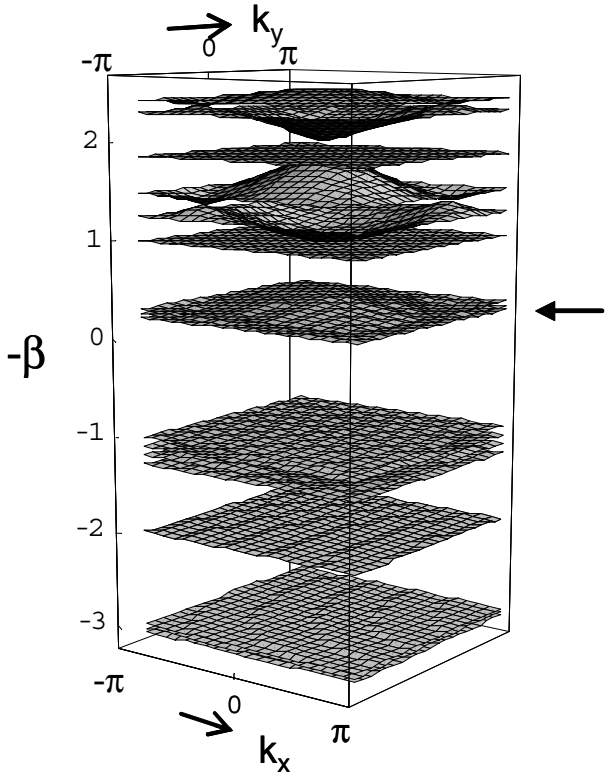


Fig. S1 The two-dimensional π-Crystal Orbital Band structure of a two-dimensional system **4**. The arrow denotes the Lowest Unoccupied Crystal Orbitals (LUCOs), which are pseudo-flat bands. The flat bands originate in the 1,3,5-connectivity of oligoketones, not in the group-theoretical symmetry. The 2D polymeric system **4** incorporates extra electrons into the flat band in a ferromagnetically exchange-coupled manner in the ground state. The next LUCO is closely located above the LUCOs.

2. The optimized molecular structures for *m*-benzoylbenzene in its doublet and triplet states

2.1 The optimized molecular structures for $\mathbf{1}^{-\bullet}K^{+}$ in the spin-doublet state (Fig. S2) and $\mathbf{1}^{2-\bullet}(K^{+})_2$ in the triplet state (Fig. S3) obtained by the DFT quantum chemical calculation (UB3LYP/6-311G*)

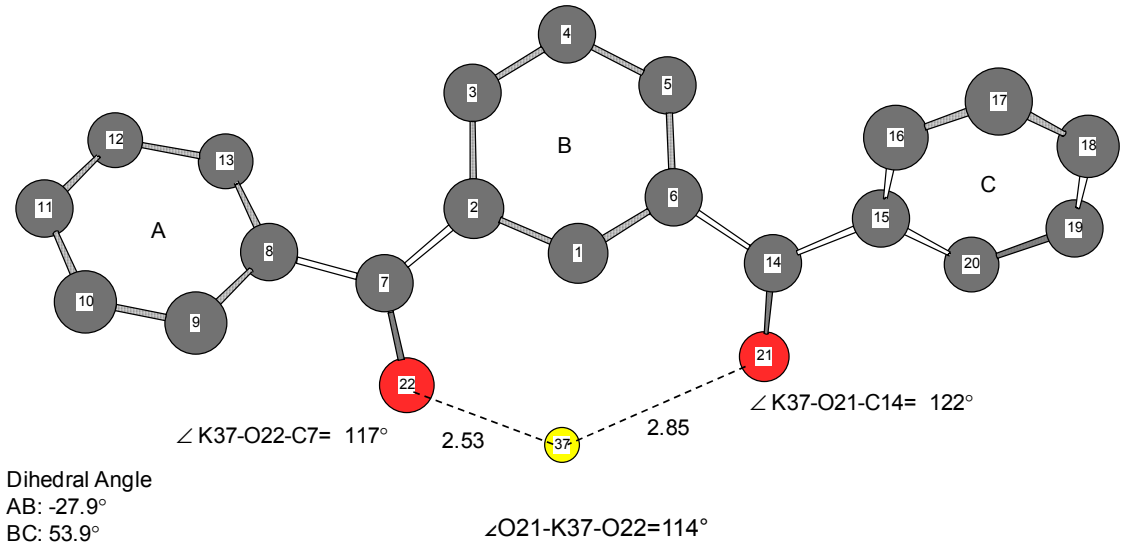


Fig. S2 The optimized molecular structure for $\mathbf{1}^{-\bullet}K^{+}$ in the spin-doublet state obtained by the DFT quantum chemical calculation (UB3LYP/6-311G*).

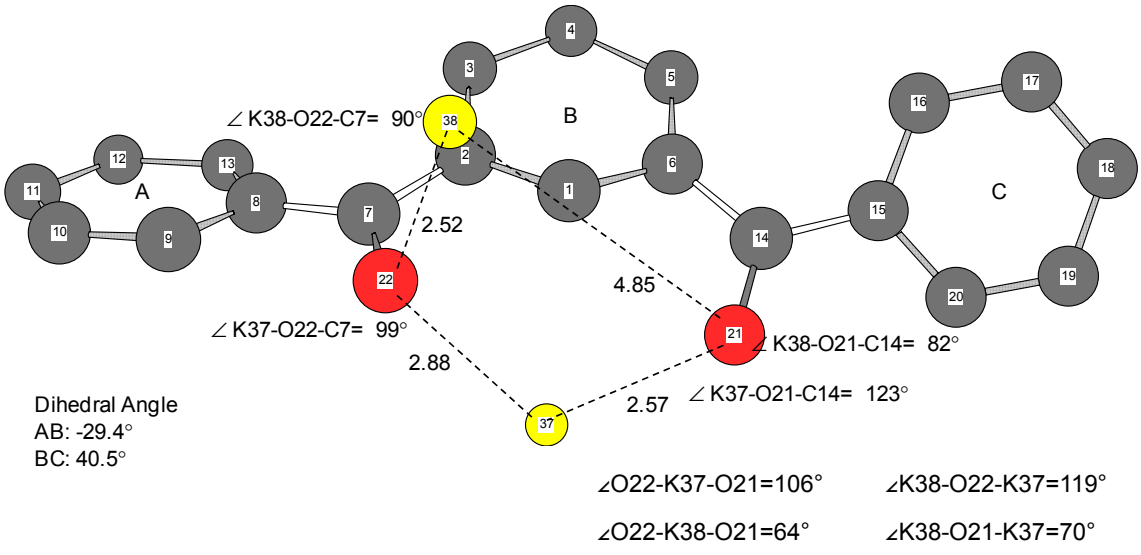


Fig. S3 The optimized structure for $\mathbf{1}^{2-\bullet}(K^{+})_2$ in the triplet state obtained by the DFT quantum chemical calculation (UB3LYP/6-311G*).

3. The optimized molecular structures for *m*-benzoylbenzene-based polyanionic high-spin clusters

3.1 The optimized structure for $1^{-\bullet}(K^{+})_2 1^{-\bullet}$ in the triplet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G) (Fig. S4).

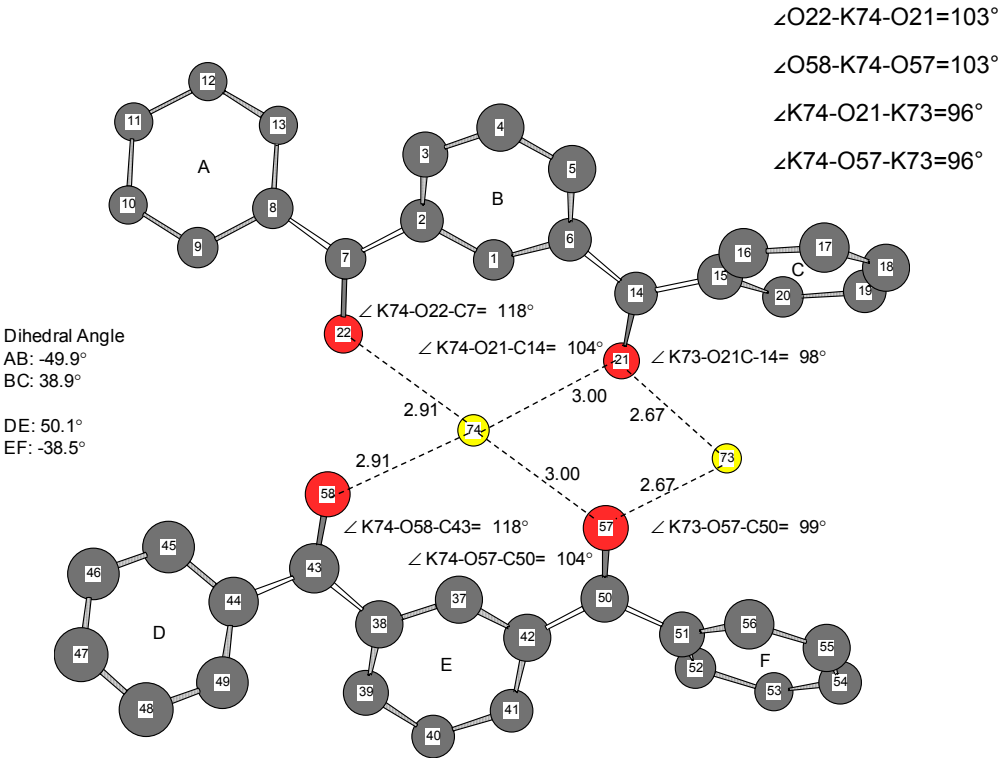


Fig. S4 The optimized structure for $1^{-\bullet}(K^{+})_2 1^{-\bullet}$ in the triplet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G).

3.2 The optimized structure for $1^{2-\bullet}(K^{+})_3 1^{-\bullet}$ in the quartet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G) (Fig. S5).

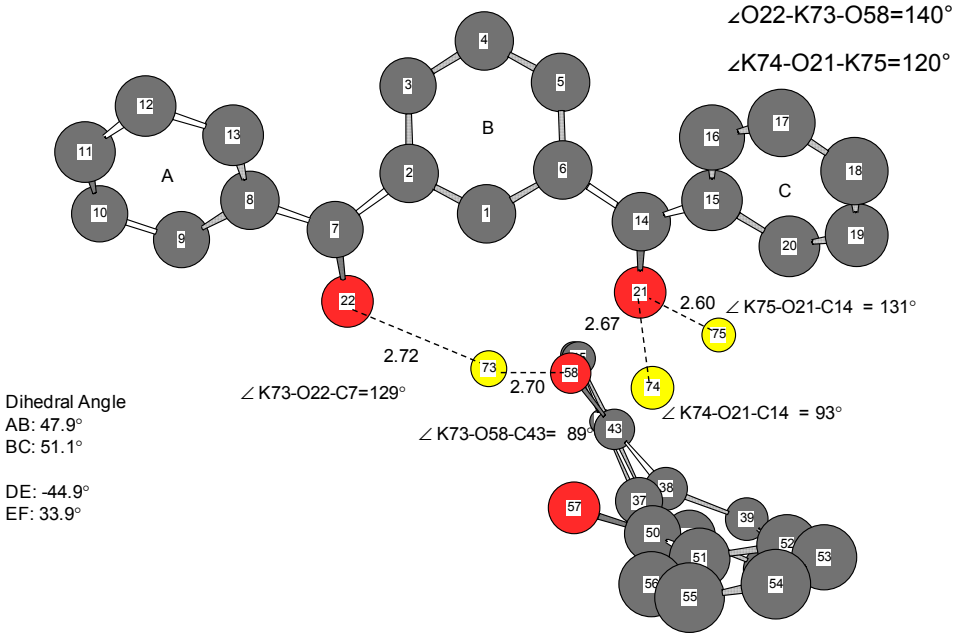


Fig. S5 The optimized structure for $\mathbf{1}^{2-\bullet}(K^{+})_3\mathbf{1}^{-\bullet}$ in the quartet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G).

3.3 The optimized structure for $\mathbf{1}^{2-\bullet}(K^{+})_4\mathbf{1}^{2-\bullet}$ in the quintet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G) (Fig. S6).

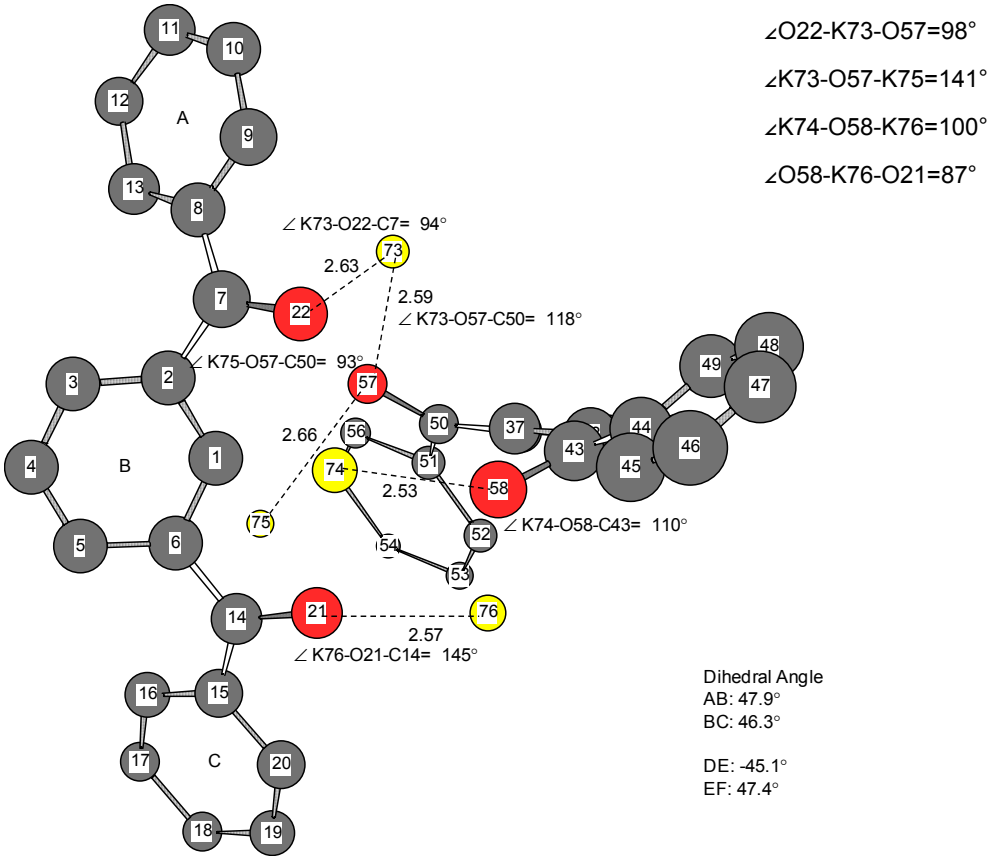
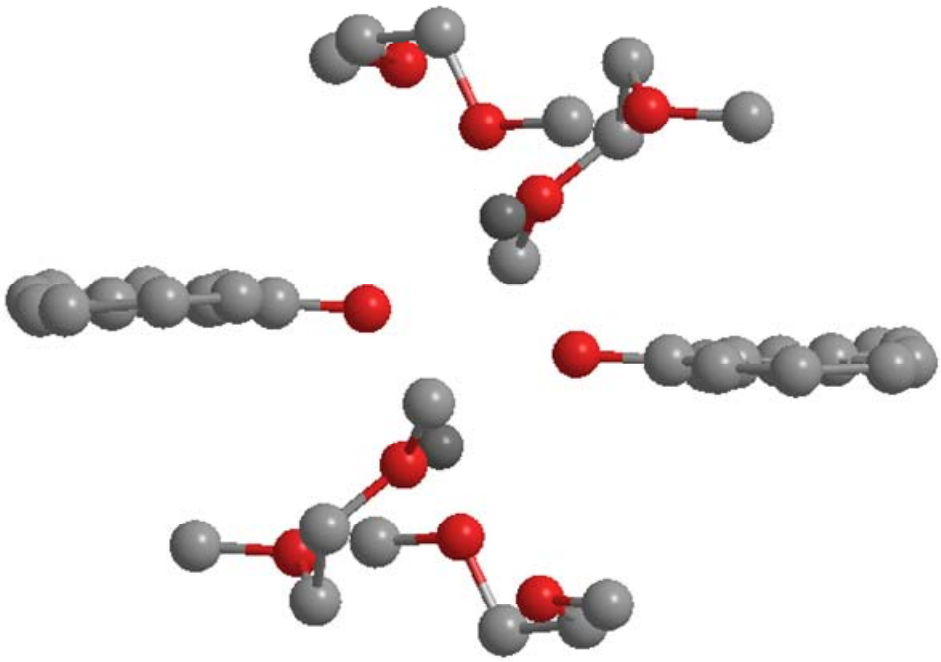


Fig. S6 The optimized structure for $\mathbf{1}^{2-\bullet}(K^{+})_4\mathbf{1}^{2-\bullet}$ in the quintet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G).

4. The clustering structure of the dimer, [Fluorenone$^{-\bullet}$ {Na^{+}(dimethoxyethan)$_2$}]$_2$ (Fig. S7), and the comparison of the lengths, Na-O, Na-Na, and O-O and angles, O-Na-O, and Na-O-Na between the X-ray single-crystal analysis and the structural optimization (Fig. S7).

(a)



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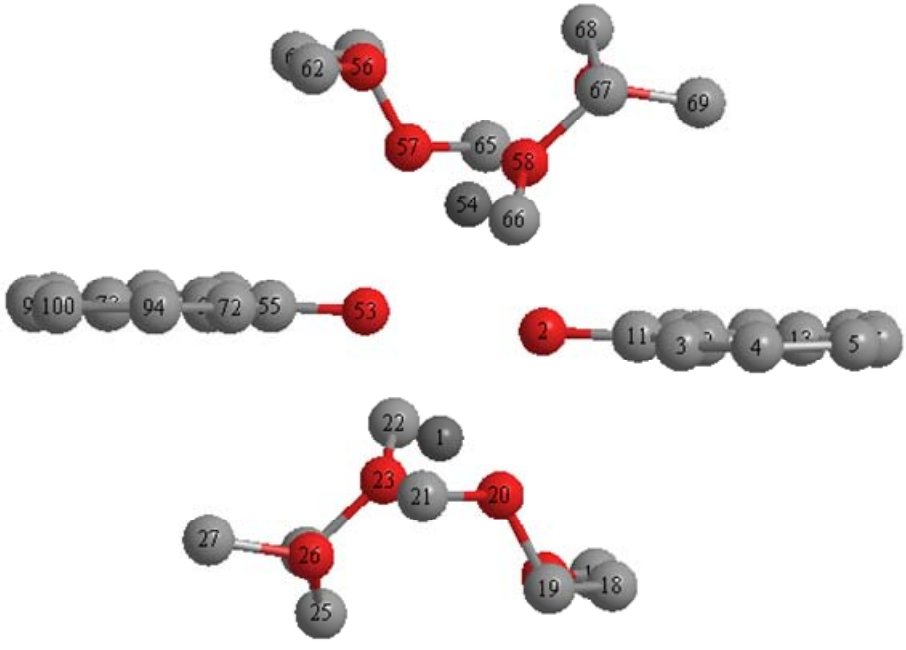

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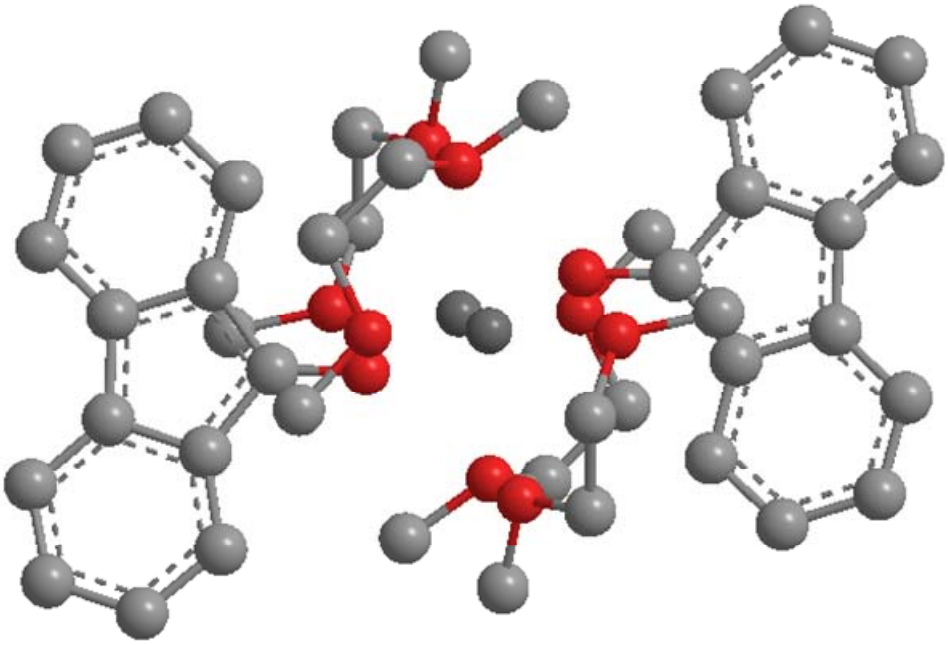
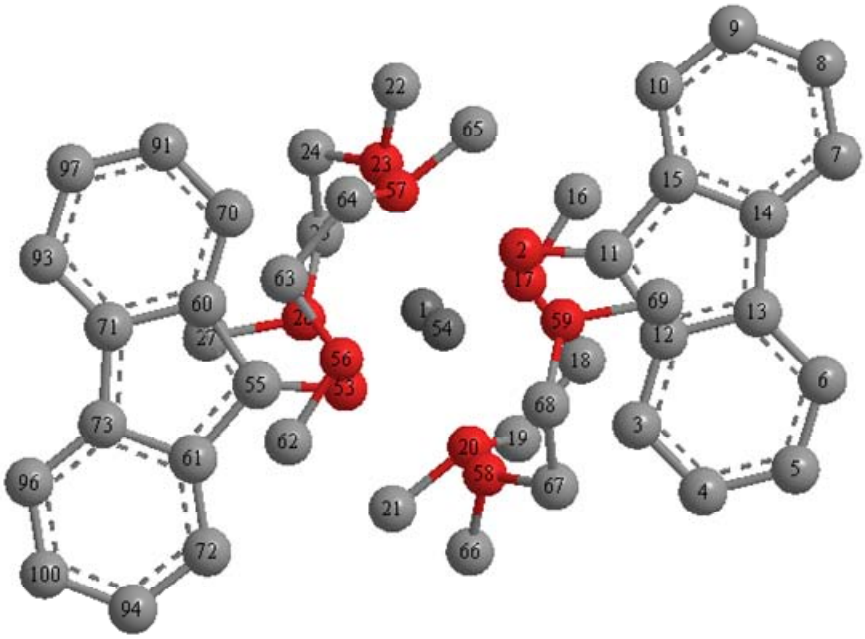


(d)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(e)

	X-ray Analysis	Optimization
Length/Å		
Na1-O53	**2.398**	**2.344**
Na1-O2	**2.282**	**2.325**
Na54-O53	**2.283**	**2.324**
Na54-O2	**2.398**	**2.344**
Na1-Na54	**3.350**	**3.270**
O53-O2	**3.270**	**3.333**
Angle/Degrees		
O53-Na1-O2	**88.6**	**91.1**
O53-Na54-O2	**88.6**	**91.1**
Na1-O53-Na54	**91.4**	**88.9**
Na1-O2-Na54	**91.4**	**88.9**

Fig. S7 The clustering structure of the dimer, [Fluorenone$^{-\bullet}$ {Na^{+}(dimethoxyethan)$_2$}]$_2$. **a**, **c**: The structures of the dimeric cluster, [Fluorenone$^{-\bullet}$ {Na^{+}(dimethoxyethan)$_2$}]$_2$ determined by X-ray analysis. **b**, **d**: The optimized structures for [Fluorenone$^{-\bullet}$ {Na^{+}(dme)$_2$}]$_2$ in the triplet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G). **e**: The comparison of the lengths, Na-O, Na-Na, and O-O and angles, O-Na-O, and Na-O-Na between the X-ray single-crystal analysis and the structural optimization.

5. Mulliken atomic charges for [Fluorenone$^{-\bullet}$ {Na^{+}(dimethoxyethan)$_2$}]$_2$ (Tables S1 and S2)

Table S1 Mulliken atomic charges for [Fluorenone$^{-\bullet}$ {Na^{+}(dimethoxyethan)$_2$}]$_2$
Note that atomic charges with hydrogens are non-vanishing and summed into the attached carbon atoms.

1Na	.156597	31H	.000000	61C	-.031762	91C	-.041327
2O	-.600824	32H	.000000	62C	.312250	92H	.000000
3C	-.024160	33H	.000000	63C	.300060	93C	-.066469
4C	-.041288	34H	.000000	64C	.283897	94C	-.021034
5C	-.027989	35H	.000000	65C	.297786	95H	.000000
6C	-.066458	36H	.000000	66C	.291617	96C	-.061849
7C	-.061845	37H	.000000	67C	.273595	97C	-.028005
8C	-.021376	38H	.000000	68C	.272017	98H	.000000
9C	-.021030	39H	.000000	69C	.307736	99H	.000000
10C	-.061624	40H	.000000	70C	-.024047	100C	-.021379
11C	.319763	41H	.000000	71C	.007416	101H	.000000
12C	-.042658	42H	.000000	72C	-.061615	102H	.000000
13C	.007414	43H	.000000	73C	.009115	103H	.000000
14C	.009118	44H	.000000	74H	.000000	104H	.000000
15C	-.031774	45H	.000000	75H	.000000	105H	.000000
16C	.312336	46H	.000000	76H	.000000	106H	.000000
17O	-.457486	47H	.000000	77H	.000000	107H	.000000
18C	.300058	48H	.000000	78H	.000000	108H	.000000
19C	.283903	49H	.000000	79H	.000000	109H	.000000
20O	-.458500	50H	.000000	80H	.000000	110H	.000000
21C	.297792	51H	.000000	81H	.000000		
22C	.291609	52H	.000000	82H	.000000		
23O	-.467870	53O	-.600851	83H	.000000		
24C	.273573	54Na	.156432	84H	.000000		
25C	.271950	55C	.319771	85H	.000000		
26O	-.446884	56O	-.457479	86H	.000000		
27C	.307745	57O	-.458508	87H	.000000		
28H	.000000	58O	-.467853	88H	.000000		
29H	.000000	59O	-.446884	89H	.000000		
30H	.000000	60C	-.042725	90H	.000000		

Table S2 Mulliken atomic spin densities for [Fluorenone$^{-\bullet}${Na^{+}(dimethoxyethan)$_2$}]$_2$

1Na	-.002399	31H	.002086	61C	-.026853	91C	-.035931
2O	.239565	32H	.002109	62C	.003019	92H	-.004706
3C	.094146	33H	-.007048	63C	.000212	93C	-.064346
4C	-.035943	34H	.001021	64C	.000105	94C	-.040127
5C	.143915	35H	-.005068	65C	.000306	95H	-.005068
6C	-.064352	36H	-.000151	66C	.000232	96C	-.064549
7C	-.064545	37H	.000169	67C	.000414	97C	.143911
8C	.142852	38H	.001039	68C	-.000033	98H	.000857
9C	-.040123	39H	.000033	69C	.001633	99H	.002086
10C	.102752	40H	-.000671	70C	.094144	100C	.142861
11C	.307343	41H	.000007	71C	.120613	101H	.001021
12C	-.024503	42H	-.000012	72C	.102762	102H	.002109
13C	.120609	43H	-.000078	73C	.118429	103H	-.007134
14C	.118419	44H	-.000378	74H	-.000150	104H	-.007049
15C	-.026842	45H	-.000027	75H	.000168	105H	-.000173
16C	.003025	46H	.000253	76H	.001036	106H	.000820
17O	.000220	47H	-.000019	77H	.000033	107H	-.000204
18C	.000213	48H	-.000688	78H	-.000672	108H	-.000205
19C	.000105	49H	.000178	79H	.000007	109H	.000822
20O	.000304	50H	.000006	80H	-.000012	110H	-.000173
21C	.000306	51H	-.000017	81H	-.000078		
22C	.000231	52H	-.000005	82H	-.000378		
23O	.000232	53O	.239557	83H	-.000027		
24C	.000414	54Na	-.002391	84H	.000255		
25C	-.000032	55C	.307371	85H	-.000019		
26O	.000247	56O	.000221	86H	-.000688		
27C	.001633	57O	.000304	87H	.000177		
28H	-.004706	58O	.000230	88H	.000006		
29H	.000857	59O	.000248	89H	-.000017		
30H	-.007134	60C	-.024529	90H	-.000005		

6. The Calculation of D_i of the intramolecular interaction in terms of point-dipole approximation

Dipolar spin-spin interaction between electron spins, $\mathbf{S}_1$ and $\mathbf{S}_2$ is given by

$$W_{SS} = (\frac{\mu_0}{4\pi})(g\beta)^2 \{\frac{S_1 \bullet S_2}{r_{12}^3} - \frac{3(S_1 \bullet r_{12})(S_2 \bullet r_{12})}{r_{12}^5}\}, \qquad \text{(S1)}$$

$\mathbf{r}_{12}$ is the distance vector from an electron i to j, μ_0 is the permeability of free space, and β is Bohr magneton. The D tensor corresponding to the dipolar interaction can be calculated in terms of a wave function Ψ_T,

$$\mathbf{D} = \int \psi_T^* W_{SS} \psi_T dv_1 dv_2 . \qquad \text{(S2)}$$

The calculation of the **D** tensor for the intramolecular triplet state was made by the point-dipole approximation with the optimized molecular structure and the coefficients of $2p_{x,y,z}$ of the LUMOs and next LUMOs with α spins. We assume that each $2p_{x,y,z}$ orbital is approximated in terms of a pair of points separated by 0.68 Å from the position of the carbon atom along the x, y, z directions. The MOs were calculated by the DFT method (USVWN/sto-3g). The D and E values are calculated to be -0.00427 cm^{-1} and 0.00108cm^{-1}, respectively. The sign of the D value is negative. The principal direction for D_z is close to along the long-axis of the molecule.

6.1 The Calculation of the $\mathbf{D}_{12}$ tensors for the doublet, quartet, and quintet clusters in terms of point-dipole approximation

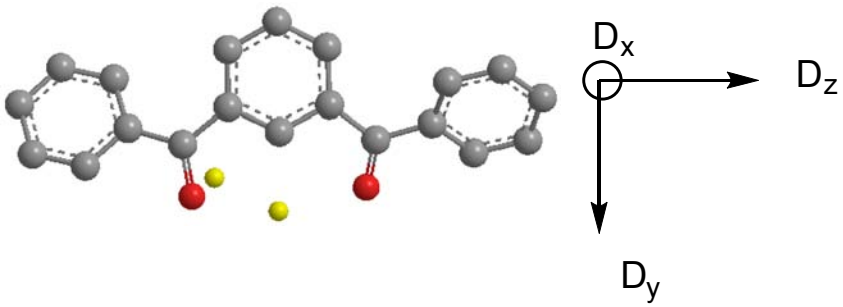


Fig. S8. The orientation of the principal axes of the $\mathbf{D}_1$ tensor for the intramolecular triplet state of *m*-benzoylbenzene dianion.

The $\mathbf{D}_{12}$ tensors for the quartet and quintet states of the molecular clusters were estimated by a semi-empirical method with both the observed D value for the triplet cluster and the theoretical D value obtained by the point-dipole approximation approach, in which the optimized molecular structure and the calculated α spin density distribution are employed. The spin density distributions were calculated by the DFT method (UB3LYP/6-31G*//UB3LYP/3-21G). The calculated D_{12}^{c} was obtained by the following equation,

$$D_{12}^{c} = \sum_{i,j} \rho_i W_{ss} \rho_j \qquad \text{(S3)}$$

where ρ_i denotes the spin density on the i_{th} atom in one dibenzoylbenzene moiety and ρ_j the spin density on the j_{th} atom in the other dibenzoylbenzene moiety. The calculated results for the high-spin clusters are in the following:

$D_{12}^{c}(\text{triplet cluster}) = -0.0041\,\text{cm}^{-1}$,
$D_{12}^{c}(\text{quartet cluster}) = -0.0064\,\text{cm}^{-1}$,
$D_{12}^{c}(\text{quintet cluster}) = -0.0070\,\text{cm}^{-1}$.

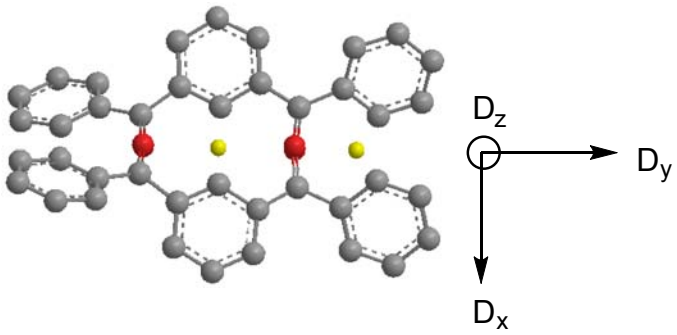


Fig. S9 The principal axes of the **D** tensor for the intermolecular dianionic triplet state.

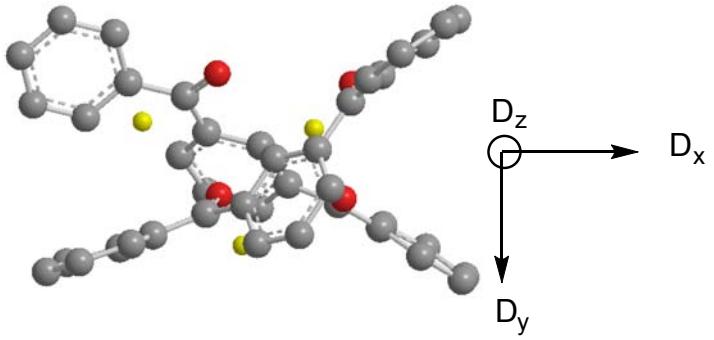


Fig. S10 The principal axes of the $\mathbf{D}_{12}$ tensor for the tetraanionic quartet state.
The direction of D_z is along the direction connected between the dibenzoylbenzene molecules.

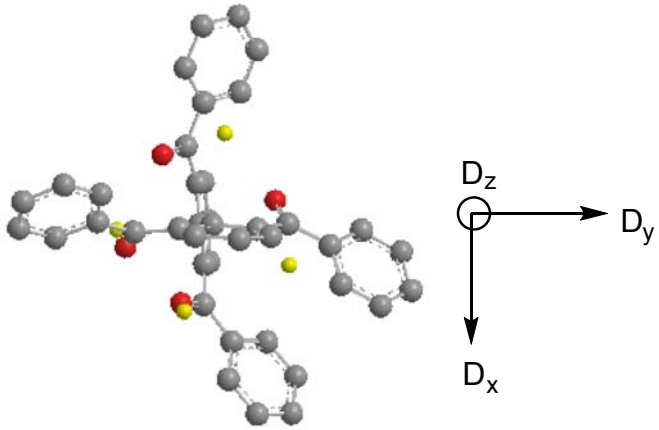


Fig. S11 The principal axes of the $\mathbf{D}_{12}$ tensor for the tetraanionic quintet state.
The direction of D_z is along the direction connected between the dibenzoylbenzene molecules.

Table S3. The D_{12}-values for the triplet, quartet, and quintet clusters calculated by Equation S3 in terms of the optimized molecular structures and the calculated spin density distributions.

	Calculated		
	$S = 1$	$S = 3/2$	$S = 2$
D_{12} / cm^{-1}	-0.0041	-0.0064	-0.0070

The $\mathbf{D}_{12}$ tensors for the quartet and quintet clusters were estimated by the following equations which include $\mathbf{D}_{12}$ derived from the observed D value of the dianionic triplet cluster and the calculated D_{12}^{c}-values.

$$\mathsf{D}_{12}(\text{quartet cluster}) = \mathsf{D}_{12}(\text{triplet cluster}) \times \frac{\mathsf{D}_{12}^{c}(\text{quartet cluster})}{\mathsf{D}_{12}^{c}(\text{triplet cluster})}$$

$$\mathsf{D}_{12}(\text{quintet cluster}) = \mathsf{D}_{12}(\text{triplet cluster}) \times \frac{\mathsf{D}_{12}^{c}(\text{quintet cluster})}{\mathsf{D}_{12}^{c}(\text{triplet cluster})}. \qquad \text{(S4)}$$

The results are as follows:

D_{12}(quartet) = -0.0281 cm^{-1},
D_{12}(quintet) = -0.0307 cm^{-1}.

Table S4. The D_{12}-values for the high-spin clusters estimated by Equations S4.

	Calculated		
	$S = 1$	$S = 3/2$	$S = 2$
D_{12} / cm^{-1}	-0.018	-0.0281	-0.0307

6.2 The *D* and *E* values for the quartet and quintet molecular clusters

The **D** tensor for the quartet cluster is calculated by using $\mathbf{D_1}$ and $\mathbf{D_{12}}$ (quartet cluster). The *D* and *E value*s are -0.0135 cm^{-1} and 0.00097 cm^{-1}, respectively.

The **D** tensor for the quintet cluster is calculated by Equation 12 with $\mathbf{D_1}$ and $\mathbf{D_{12}}$ (quintet cluster). The *D* and *E* values are -0.0096 cm^{-1} and 0.0 cm^{-1}, respectively.

Table S5. The calculated *D* and *E* values for the quartet and quintet clusters compared with the observed values.

	Observed	Calculated
$S = 3/2$		
D / cm^{-1}	0.0066	-0.0135
E / cm^{-1}	<0.0002	0.00097
$S = 2$		
D / cm^{-1}	0.00585	-0.0096
E / cm^{-1}	<0.0002	0.0

7. The charge density and spin density for $1^{-\bullet}K^{+}$ in the doublet state, $1^{2(-\bullet)}K_2$ in the triplet ground state, $1^{-\bullet}(K^{+})_2 1^{-\bullet}$ in the triplet state, $1^{2(-\bullet)}(K^{+})_3 1^{(-\bullet)}$ in the quartet state, $1^{2(-\bullet)}(K^{+})_4 1^{2(-\bullet)}$ in the quintet state, as calculated by the DFT quantum chemical calculations (UB3LYP/6-31G*//UB3LYP/3-21G)

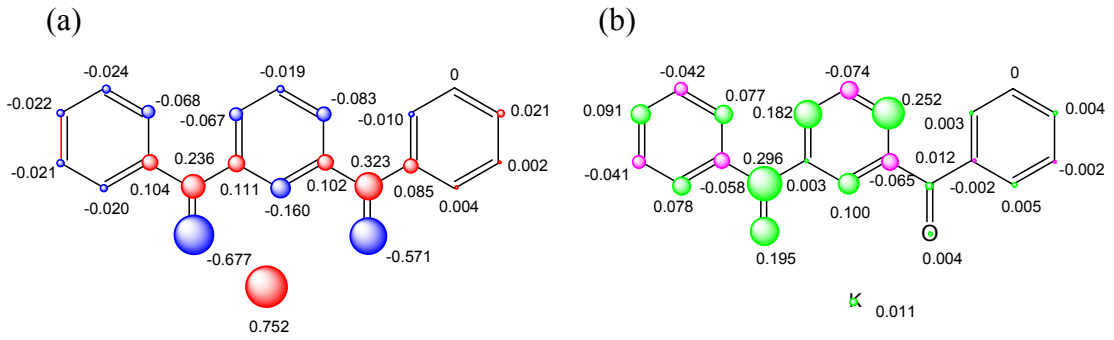


Fig. S12 (a) The charge density and (b) the spin density for $\mathbf{1}^{-\bullet}K^{+}$ in the doublet state, as calculated by the DFT quantum chemical calculations (UB3LYP/6-31G*//UB3LYP/3-21G). The red and blue colors indicate positive and negative charge densities, respectively. The green and purple colors indicate α and β spin densities, respectively.

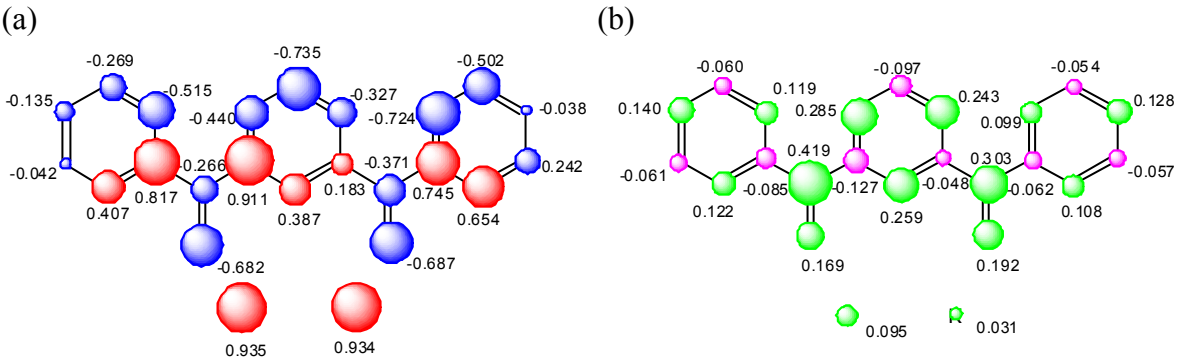


Fig. S13 (a) The charge density and (b) the spin density for $\mathbf{1}^{2(-\bullet)}K_2$ in the triplet ground state, as calculated by the DFT quantum chemical calculations (UB3LYP/6-31G*//UB3LYP/3-21G). The red and blue colors indicate positive and negative charge densities, respectively. The green and purple colors indicate α and β spin densities, respectively.

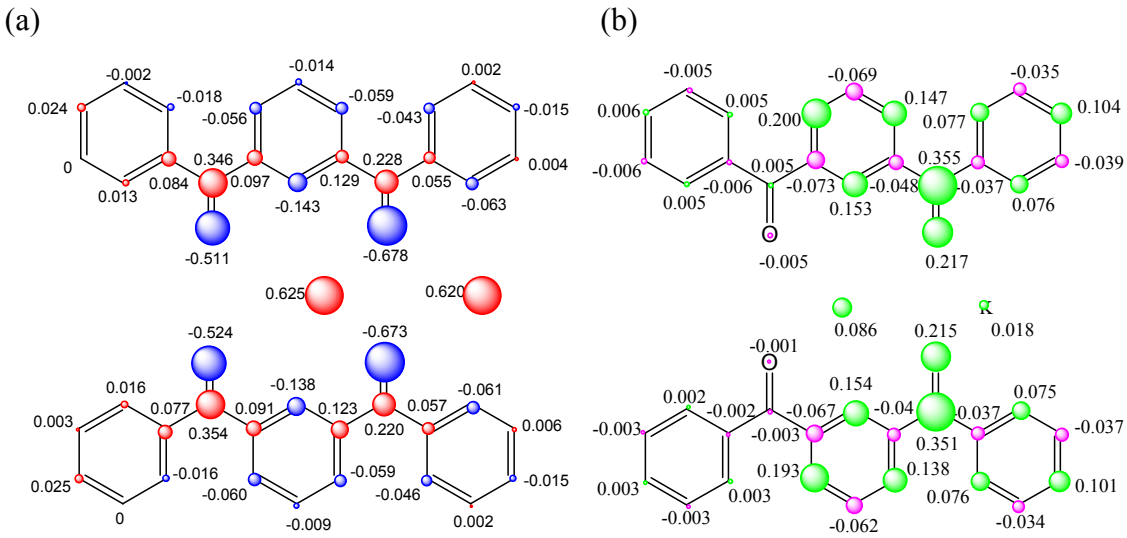


Fig. S14 (a) The charge density and (b) the spin density for $\mathbf{1}^{-\bullet}(K^{+})_2\mathbf{1}^{-\bullet}$ in the triplet state calculated by DFT method (UB3LYP/6-31G*//UB3LYP/3-21G). The red and blue colors indicate positive and negative charge densities, respectively. The green and purple colors indicate α and β spin densities, respectively.

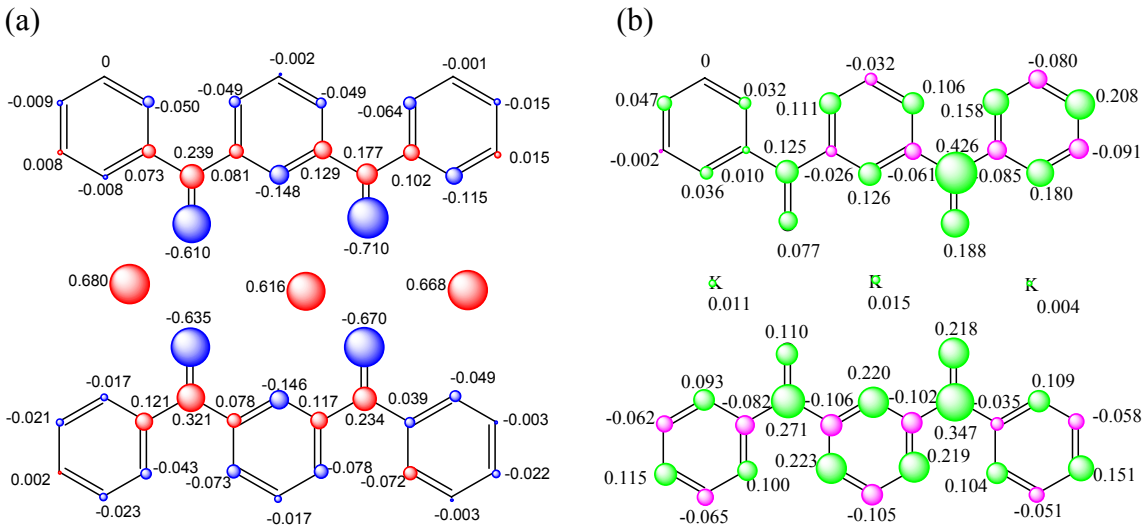


Fig. S15 (a) The charge density and (b) the spin density for $\mathbf{1}^{2(-\bullet)}(K^{+})_3\mathbf{1}^{(-\bullet)}$ in the quartet state calculated by DFT method (UB3LYP/6-31G*//UB3LYP/3-21G). The red and blue colors indicate positive and negative charge densities, respectively. The green and purple colors indicate α and β spin densities, respectively.

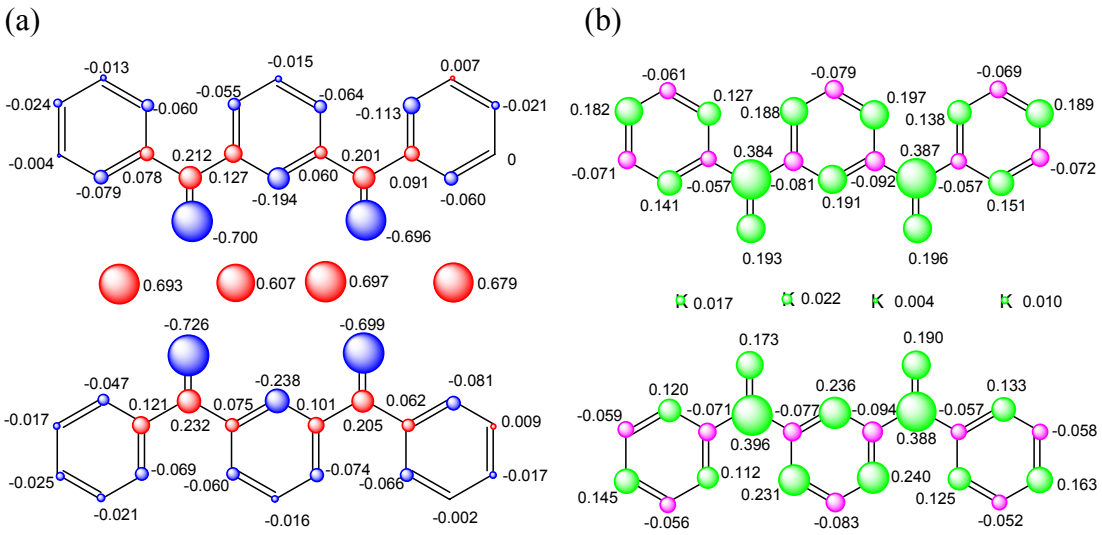


Fig. S16 (a) The charge density and (b) the spin density for $\mathbf{1}^{2(-\bullet)}(K^+)_4\mathbf{1}^{2(-\bullet)}$ in the quintet state calculated by DFT method (UB3LYP/6-31G*//UB3LYP/3-21G). The red and blue colors indicate positive and negative charge densities, respectively. The green and purple colors indicate α and β spin densities, respectively.

8. The charge density distribution and the spin density distribution for $\mathbf{1}^{2(-\bullet)}(K^+)_2$ in the triplet state calculated by DFT method (UB3LYP/6-311++G** //UB3LYP/6-311G*)

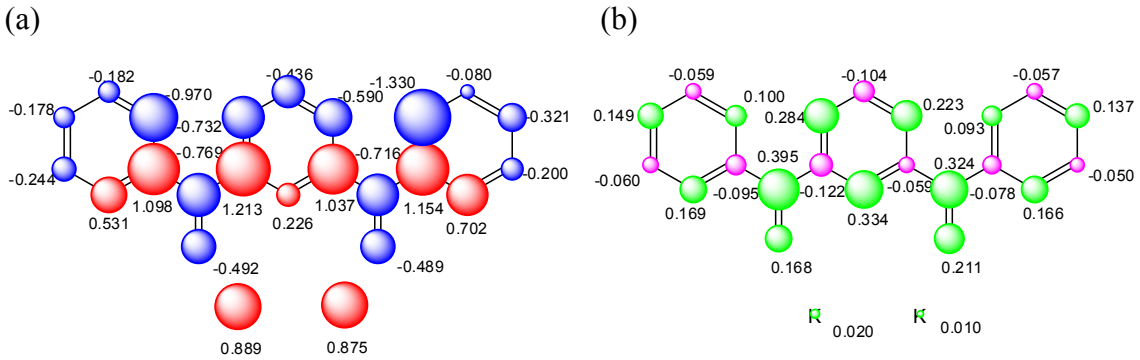
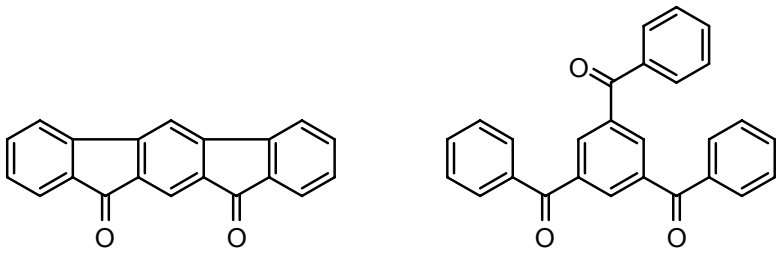


Fig. S17 (a) The charge density distribution and (b) the spin density distribution for $\mathbf{1}^{2(-\bullet)}(K^+)_2$ in the triplet state calculated by DFT method (UB3LYP/6-311++G** //UB3LYP/6-311G*). The red and blue colors indicate positive and negative charge densities, respectively. The green and purple colors indicate α and β spin densities, respectively.

9. The molecular structures of fluorenone-based diketone **5** and 1,3,5- tribenzoyl benzene **6**



5 **6**

Fig. S18 Fluorenone-based diketone **5** and 1,3,5- tribenzoyl benzene **6**.

10. Atomic coordinates of the optimized structures for $1^{-\bullet}K^{+}$ and the molecular high0spin clusters obtained by the DFT quantum chemical calculations

10.1 Atomic coordinates of the optimized structure for $1^{-\bullet}K^{+}$ in the spin-doublet state obtained by the DFT quantum chemical calculation (UB3LYP/6-311G*)

C	-0.075918	0.114960	0.353161
C	1.186456	-0.486313	0.087203
C	1.113522	-1.820805	-0.411820
C	-0.093305	-2.381678	-0.796573
C	-1.306499	-1.675389	-0.700716
C	-1.286301	-0.409487	-0.095001
C	2.349591	0.351865	0.295442
C	3.751554	-0.120821	0.208791
C	4.699506	0.491208	1.054107
C	6.039203	0.130323	1.018765
C	6.488289	-0.837424	0.117389
C	5.574419	-1.425389	-0.754527
C	4.227522	-1.073490	-0.712728
C	-2.456416	0.510081	-0.061593
C	-3.844345	-0.006149	0.099460
C	-4.116809	-1.221494	0.743878
C	-5.432590	-1.641830	0.921737
C	-6.485981	-0.861119	0.451641
C	-6.224002	0.353532	-0.186113
C	-4.914267	0.782437	-0.350285
O	-2.268145	1.727548	-0.184042
O	2.156578	1.587694	0.617307
H	-0.090072	1.001626	0.970704
H	2.011125	-2.418881	-0.501766
H	-0.097934	-3.387290	-1.206973
H	-2.218534	-2.087836	-1.114847
H	4.350853	1.256275	1.737602

H	6.741791	0.607641	1.696162
H	7.536704	-1.117256	0.086234
H	5.913004	-2.154460	-1.485302
H	3.556399	-1.506393	-1.444090
H	-3.300260	-1.823181	1.124130
H	-5.634647	-2.577840	1.432111
H	-7.510422	-1.193425	0.586547
H	-7.044239	0.964509	-0.548986
H	-4.694743	1.730503	-0.827241
K	0.326934	2.818209	-0.613880

10.2 Atomic coordinates of the optimized structure for $1^{2-\bullet}(K^{+})_2$ in the triplet state obtained by the DFT quantum chemical calculation (UB3LYP/6-311G*)

C	0.181073	0.008300	0.286863
C	-1.073942	0.633613	0.091712
C	-1.024704	2.035695	-0.161037
C	0.217519	2.664904	-0.318426
C	1.428177	1.977133	-0.287594
C	1.438942	0.580131	-0.012371
C	-2.244382	-0.246808	0.161349
C	-3.615844	0.131103	-0.198000
C	-4.676280	-0.676599	0.281822
C	-6.000461	-0.396208	-0.024324
C	-6.326526	0.688191	-0.841874
C	-5.295539	1.471968	-1.362683
C	-3.967754	1.201714	-1.053667
C	2.523081	-0.378279	-0.191957
C	3.943530	-0.012649	-0.147400
C	4.442708	1.152803	0.475569
C	5.805225	1.425304	0.508418
C	6.721766	0.544485	-0.069336
C	6.249269	-0.627093	-0.666555
C	4.890372	-0.905342	-0.698365
O	2.202861	-1.616333	-0.409655
O	-2.045930	-1.474144	0.603003
H	0.201418	-1.023568	0.597774
H	-1.926665	2.628875	-0.219314
H	0.231265	3.732053	-0.526302
H	2.340899	2.499333	-0.546051
H	-4.422587	-1.538987	0.886695
H	-6.787870	-1.032070	0.371376
H	-7.361735	0.906225	-1.084235
H	-5.527411	2.296008	-2.031557
H	-3.194274	1.795633	-1.521642
H	3.758774	1.832225	0.970824
H	6.157898	2.327447	1.001144
H	7.785297	0.761013	-0.043666
H	6.951217	-1.329201	-1.108862
H	4.520042	-1.819084	-1.147443
K	-0.089524	-2.339640	-1.324743
K	-1.262008	-0.552271	2.810091

10.3 Atomic coordinates of the optimized structure for $1^{-\bullet}(K^{+})_2 1^{-\bullet}$ in the triplet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G)

C	0.303191	-2.943909	-0.422439
C	1.561481	-3.381919	-0.018953
C	1.670639	-4.299217	1.045478
C	0.489926	-4.789634	1.627849
C	-0.762463	-4.331993	1.236713
C	-0.891582	-3.324042	0.235976
C	2.722719	-2.697624	-0.655360
C	4.007281	-3.420727	-0.858905
C	5.154909	-2.651442	-1.109455
C	6.379941	-3.267963	-1.339524
C	6.467513	-4.664794	-1.343437
C	5.325238	-5.438040	-1.122917
C	4.097342	-4.821034	-0.880642
C	-2.096115	-2.636425	-0.178032
C	-3.435289	-3.002372	0.326015
C	-3.738676	-3.212952	1.692696
C	-5.056545	-3.389340	2.116939
C	-6.114639	-3.359153	1.201024
C	-5.835062	-3.148611	-0.157599
C	-4.522764	-2.964411	-0.586448
8	-2.014485	-1.654941	-1.065145
8	2.609040	-1.499693	-1.014652
H	0.210066	-2.331169	-1.308761
H	2.639900	-4.604607	1.417459
H	0.558268	-5.534218	2.414018
H	-1.648388	-4.752036	1.694903
H	5.055445	-1.572980	-1.118928
H	7.264294	-2.668523	-1.521379
H	7.420725	-5.147537	-1.526201
H	5.389463	-6.519536	-1.146512
H	3.205653	-5.415688	-0.729570
H	-2.941005	-3.190357	2.425335
H	-5.261485	-3.535518	3.172322
H	-7.135296	-3.501123	1.536052
H	-6.643885	-3.144475	-0.881578
H	-4.300724	-2.809753	-1.637577
C	0.211830	2.924677	0.404048
C	1.449938	3.432589	0.020656
C	1.517007	4.419680	-0.983118
C	0.314987	4.903475	-1.525379
C	-0.916898	4.377412	-1.155586
C	-1.001628	3.304876	-0.219718
C	2.641535	2.752919	0.602813
C	3.897600	3.511784	0.850129
C	5.076671	2.774400	1.044884
C	6.277100	3.423210	1.312673
C	6.308471	4.819011	1.411055
C	5.134881	5.558475	1.246488
C	3.931581	4.909913	0.966150
C	-2.178857	2.552810	0.161016

C	-3.534771	2.902438	-0.307054
C	-3.861039	3.198842	-1.652611
C	-5.188767	3.359768	-2.051037
C	-6.234851	3.228810	-1.130237
C	-5.932799	2.932307	0.207368
C	-4.610337	2.763255	0.610084
O	-2.054195	1.524333	0.988038
O	2.578042	1.529879	0.879690
H	0.147023	2.252548	1.249368
H	2.471699	4.783293	-1.340214
H	0.349928	5.698742	-2.262568
H	-1.821092	4.794400	-1.579502
H	5.020762	1.694594	0.982121
H	7.185827	2.849161	1.451154
H	7.242523	5.326405	1.623514
H	5.155532	6.637616	1.343074
H	3.015995	5.476994	0.857831
H	-3.071766	3.257289	-2.392334
H	-5.410510	3.573967	-3.091327
H	-7.263391	3.359650	-1.445056
H	-6.732516	2.849503	0.936745
H	-4.370803	2.544200	1.645871
K	-3.918762	-0.072051	-0.059947
K	0.294991	-0.001516	-0.087493

10.4 Atomic coordinates of the optimized structure for $1^{2-\bullet}(K^{+})_3 1^{-\bullet}$ in the quartet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G)

C	2.340607	-1.797773	-0.218769
C	3.697013	-1.533276	-0.381569
C	4.304851	-1.839485	-1.590545
C	3.535105	-2.380455	-2.616393
C	2.166682	-2.538297	-2.477208
C	1.527930	-2.215405	-1.271537
C	4.359190	-0.726936	0.730278
C	5.758275	-1.057966	1.212597
C	6.466998	-0.091429	1.923702
C	7.739460	-0.364105	2.396271
C	8.309023	-1.609580	2.168849
C	7.604470	-2.580404	1.471102
C	6.333422	-2.306578	0.992887
C	0.044271	-2.103874	-1.090149
C	-0.877845	-3.207908	-1.477941
C	-0.425843	-4.522045	-1.686120
C	-1.304150	-5.540642	-1.993899
C	-2.670288	-5.295934	-2.095536
C	-3.140892	-4.011058	-1.898810
C	-2.258322	-2.979296	-1.601283
O	-0.408052	-1.051926	-0.373043
O	3.729324	0.218321	1.213893
H	1.895442	-1.651802	0.755648
H	5.355255	-1.633526	-1.749024
H	4.006509	-2.622470	-3.561311

H	1.580993	-2.883453	-3.319732
H	6.009311	0.874841	2.099607
H	8.287621	0.392221	2.943420
H	9.303971	-1.825256	2.539248
H	8.046508	-3.553677	1.300666
H	5.783498	-3.068728	0.455955
H	0.629108	-4.739197	-1.593339
H	-0.926166	-6.544419	-2.146810
H	-3.353823	-6.100564	-2.330237
H	-4.199547	-3.798610	-1.989018
H	-2.646304	-1.973144	-1.512215
C	-1.968420	2.155875	0.689176
C	-1.708754	3.280174	-0.103912
C	-2.804241	4.074270	-0.463123
C	-4.077319	3.726038	-0.036024
C	-4.316756	2.575558	0.695117
C	-3.256568	1.731863	1.068697
C	-0.313604	3.445293	-0.658897
C	0.346528	4.766443	-0.745080
C	1.495616	4.909630	-1.538666
C	2.167715	6.112936	-1.620987
C	1.719213	7.218338	-0.912174
C	0.590604	7.095430	-0.115953
C	-0.084345	5.892044	-0.028054
C	-3.352166	0.460147	1.817328
C	-4.482474	-0.462579	1.738549
C	-5.488717	-0.435062	0.736699
C	-6.467790	-1.396747	0.668150
C	-6.509000	-2.459667	1.569291
C	-5.543318	-2.522027	2.555035
C	-4.554627	-1.552593	2.647776
O	-2.257693	0.061575	2.474352
O	0.246158	2.377175	-1.252812
H	-1.140798	1.564495	1.052583
H	-2.661922	4.947789	-1.082485
H	-4.914668	4.358968	-0.306578
H	-5.326090	2.342727	0.998547
H	1.844638	4.049233	-2.092939
H	3.049479	6.195065	-2.244614
H	2.243990	8.161361	-0.977154
H	0.235058	7.949019	0.448029
H	-0.953609	5.816634	0.609578
H	-5.479273	0.352752	0.000287
H	-7.214831	-1.335125	-0.114838
H	-7.281639	-3.210720	1.500422
H	-5.563895	-3.326878	3.280993
H	-3.862759	-1.577033	3.477654
K	1.317645	0.799045	0.262141
K	-2.037751	-2.041542	1.246099
K	-1.523744	0.743594	-1.702700

10.5 Atomic coordinates of the optimized structure for $1^{2-\bullet}(K^{+})_4 1^{2-\bullet}$ in the quintet state obtained by the DFT quantum chemical calculation (UB3LYP/3-21G)

C	1.188174	1.451536	-1.556073
C	1.131157	2.847668	-1.380442
C	2.152904	3.616579	-1.992917
C	3.135694	2.982704	-2.758568
C	3.151648	1.593886	-2.948056
C	2.161531	0.791455	-2.326458
C	-0.062107	3.362366	-0.700022
C	-0.040587	4.536115	0.154855
C	-1.287342	5.063111	0.605261
C	-1.340748	6.113816	1.515480
C	-0.162692	6.680875	2.021652
C	1.073734	6.174408	1.592366
C	1.141016	5.125245	0.682956
C	2.009312	-0.673719	-2.440475
C	3.155864	-1.565544	-2.432157
C	4.499309	-1.163287	-2.152432
C	5.517315	-2.101759	-2.002558
C	5.261566	-3.473649	-2.132846
C	3.954048	-3.890740	-2.424200
C	2.927712	-2.967331	-2.561873
O	0.783166	-1.174970	-2.326429
O	-1.178043	2.640139	-0.780436
H	0.481042	0.851628	-0.999069
H	2.135770	4.697148	-1.917708
H	3.884210	3.588793	-3.259758
H	3.879019	1.145705	-3.614169
H	-2.193130	4.648389	0.176414
H	-2.304466	6.510280	1.821357
H	-0.205254	7.502556	2.726856
H	1.992626	6.600949	1.981994
H	2.105468	4.726654	0.391693
H	4.734648	-0.108405	-2.061984
H	6.525826	-1.760293	-1.789545
H	6.061312	-4.196193	-2.023776
H	3.744745	-4.948577	-2.551408
H	1.928304	-3.292022	-2.824826
C	-1.558814	-1.030763	1.137538
C	-2.850116	-1.572377	0.893129
C	-3.343632	-2.517009	1.841070
C	-2.566126	-2.884788	2.938984
C	-1.284234	-2.362406	3.146621
C	-0.748068	-1.420169	2.227631
C	-3.478241	-1.294884	-0.396391
C	-4.920787	-1.388341	-0.606403
C	-5.394550	-1.482994	-1.938550
C	-6.753964	-1.544925	-2.219292
C	-7.695687	-1.498351	-1.183277
C	-7.248524	-1.376552	0.137952
C	-5.887823	-1.317762	0.426565
C	0.559915	-0.776408	2.384965
C	1.686412	-1.439801	3.028806
C	1.835614	-2.850281	3.148302
C	3.010994	-3.410635	3.636673
C	4.089203	-2.602797	4.029089

C	3.963435	-1.209599	3.927983
C	2.794801	-0.636847	3.436185
O	0.756546	0.427602	1.849860
O	-2.689827	-1.001550	-1.426433
H	-1.158180	-0.329769	0.412095
H	-4.306646	-2.984270	1.679130
H	-2.963841	-3.604255	3.648872
H	-0.715567	-2.642002	4.024546
H	-4.657797	-1.515425	-2.731519
H	-7.088366	-1.631071	-3.248370
H	-8.756272	-1.545136	-1.401288
H	-7.968868	-1.312747	0.946849
H	-5.563232	-1.181487	1.451013
H	1.023687	-3.495201	2.832873
H	3.096282	-4.490374	3.707391
H	4.999354	-3.048068	4.412880
H	4.778191	-0.569758	4.254137
H	2.681587	0.441185	3.387832
K	-1.221729	2.103172	1.791241
K	-1.419632	0.785515	-2.688930
K	2.848747	-0.355251	0.406470
K	-0.744705	-2.770503	-1.010437

10.6 Atomic coordinates of the optimized structure of the dimeric cluster for [Fluorenone$^{-\bullet}$ {Na^{+}(dimethoxyethan)$_2$}]$_2$ calculated by UB3LYP/3-21G

Na	-0.14575806	-1.60830379	0.25451523
O	1.50755692	-0.25549775	-0.66209173
C	2.58084798	0.19007227	2.25483227
C	3.30852485	0.42336926	3.42311835
C	4.71727705	0.48276424	3.40034628
C	5.42019701	0.28522524	2.20591521
C	6.39320993	-0.29949975	-0.93472177
C	6.49284601	-0.56664574	-2.30434871
C	5.33477306	-0.74555469	-3.08511066
C	4.06613874	-0.65472472	-2.51423979
C	2.76778293	-0.22459073	-0.29347277
C	3.27517390	0.01146727	1.05115533
C	4.70913315	0.04397427	1.03070033
C	5.13294172	-0.20650972	-0.34760576
C	3.94658089	-0.37843275	-1.14317274
C	2.45317483	-3.61276460	-0.34873176
O	1.40076196	-3.43992662	0.66549522
C	1.94378388	-3.28966069	2.02083135
C	0.74415594	-3.14999056	2.94011140
O	0.04547095	-1.91978574	2.56139827
C	-1.28002608	-1.82363582	3.18956637
C	0.24178395	-2.09390163	-3.05667162
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C	-1.23825812	-3.71682072	-1.93128169
C	-1.40945113	-4.28699160	-0.52384174
O	-1.92836308	-3.27922559	0.41242924
C	-3.38674212	-3.10373569	0.30193123

H	1.50397193	0.07714027	2.27747035
H	2.78756595	0.54672527	4.36782312
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H	7.29087782	-0.16980273	-0.33878377
H	7.46921778	-0.64227372	-2.76932168
H	5.43544912	-0.96058470	-4.14356089
H	3.18005395	-0.80514973	-3.12163568
H	1.91733396	-3.58233166	-1.29488468
H	2.96610403	-4.57383871	-0.21493076
H	3.17209387	-2.78987861	-0.31163475
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H	2.56789684	-2.39280176	2.07424331
H	1.07079995	-3.10559273	3.98772526
H	0.07439994	-4.00830889	2.79841137
H	-1.19218612	-1.66960180	4.27254725
H	-1.74745011	-0.96897274	2.70693231
H	-1.86194110	-2.72636962	2.97477126
H	-0.57296908	-1.69857478	-3.67293477
H	0.79528695	-2.85591769	-3.62312269
H	0.90496993	-1.29281473	-2.73158169
H	-2.17580914	-3.32019377	-2.33798671
H	-0.85807508	-4.50428343	-2.59841466
H	-0.42416504	-4.53158855	-0.12505077
H	-2.06170797	-5.17084169	-0.53997278
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O	-0.04618206	1.91979420	-2.56120181
O	0.25456497	2.64353442	1.79566228
O	1.92856395	3.27920723	-0.41255075
C	-3.27501512	-0.01182173	-1.05101371
C	-3.94657016	0.37906227	1.14309835
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C	-0.74574608	3.14933825	-2.94041777
C	1.27919090	1.82406425	-3.18965864
C	-0.24114905	2.09406543	3.05681920
C	1.23888397	3.71683335	1.93121934
C	1.41010094	4.28710127	0.52383322
C	3.38695884	3.10357428	-0.30258477
C	-2.58059216	-0.19111173	-2.25453472
C	-4.70897388	-0.04432773	-1.03063571
C	-4.06621504	0.65589827	2.51405025
C	-5.13287592	0.20677628	0.34752825
H	-1.91640413	3.58379340	1.29506135
H	-2.96594501	4.57467127	0.21522924
H	-3.17160296	2.79073238	0.31282625
H	-2.53210402	4.17344046	-2.30498171
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H	-1.07312310	3.10390925	-3.98775673
H	-0.07633106	4.00812626	-2.79992771
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H	1.74713898	0.96980029	-2.70682478
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H	0.57423896	1.69813025	3.67183423
H	-0.79392910	2.85568333	3.62450027
H	-0.90473706	1.29328823	2.73178840
H	2.17617583	3.31899428	2.33734131
H	0.85991794	4.50452328	2.59877038
H	0.42484796	4.53207731	0.12518224
H	2.06265092	5.17072916	0.53993726
C	-3.30818415	-0.42506373	-3.42273664
H	-1.50371408	-0.07828073	-2.27711082
C	-5.41995430	-0.28623775	-2.20576859
C	-5.33488512	0.74691427	3.08480740
H	-3.18016696	0.80660528	3.12143326
C	-6.39318228	0.29996327	0.93453324
C	-4.71694231	-0.48444375	-3.40003276
H	-2.78716302	-0.54895669	-4.36733675
H	-6.50478411	-0.31638774	-2.20109081
C	-6.49290609	0.56765831	2.30404639
H	-5.43563223	0.96236432	4.14316511
H	-7.29081106	0.16998927	0.33859724
H	-5.26017904	-0.66935474	-4.32005215
H	-7.46930790	0.64344031	2.76893139
H	-3.68065596	-2.73889375	-0.68554276
H	-3.89638400	-4.05132866	0.52178723
H	-3.65797901	-2.35013175	1.03940833
H	3.65786791	2.34996033	-1.04016471
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H	3.68119287	2.73868632	0.68478322