Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for

Selective Confinement of Potassium, Rubidium, or Caesium Ions in a Non-covalent Hydroxyproline Octamer Cage Stabilized by Cis-hydroxyl Locks

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Supplementary Methods

1. Materials Preparation

The solid samples of cis-4-hydroxy-L-proline and trans-4-hydroxy-L-proline proline were purchased from Sigma. The solid samples of cis-4-hydroxy-D-proline and trans-4-hydroxy-D-proline proline were purchased from Tokyo chemical industry (TCI). The details of these samples are shown in **Table. S1**, and corresponding purities of these samples are better than 98%. For ESI solutions containing only L- or D-hydroxyproline, the samples were prepared in a concentration of 5 mmol/L in 60:38:2 H_2O: MeOH: HAC; for racemic solutions, L- and D- hydroxyproline solutions were mixed just before experiments to form solutions containing each of them in 2.5 mmol/L in the same solvent. For hydroxyproline solutions containing alkali metal ions, alkali metal chlorides (LiCl, NaCl, KCl, RbCl and CsCl) were added to L-, D- or racemic hydroxyproline solutions with the same concentration of 0.5 mmol/L.

2. Experimental Methods

A Varian IonSpec 7.0 T Fourier-transform ion cyclotron resonance (FT ICR) mass spectrometer (Lake Forest, CA, USA) with a Z–Spray electrospray ionization (ESI) source was applied here to perform the experiments. N_2 was used as the cone gas, desolvation gas and collision gas. The ESI source was applied with the probe biased at 3.6 kV and the cone voltage at 20 V. All ions produced by ESI through a syringe with a flow rate of 2 uL/min were injected into an open-ended cylindrical Penning trap via a quadrupole ion guide. All ESI mass spectra reported here were obtained in the positive ion mode. It should be mentioned that the signals of some ions are overlapped and should be separated carefully. Herein all the signals were decomposed according to a simulation method reported previously[31]. The details of the normalization of ion intensities were available in **Equation. S1**(Page S5). The chiral preferences of various amino acid cluster ions were calculated by **Equation. S2** (Page S5).

The precursor ions of $[(C4L(D)P)_8+K]^{1+}$ were further selected by the method of stored waveform inverse Fourier transform (SWIFT). Infrared multiple photon dissociation (IRMPD) spectra were obtained using the same experimental setup described previously [32]. The infrared OPO laser (Firefly-IR, M Squared, UK) was operated in the normal mode, with an output irradiation tunable from 2700 cm^{-1} to 4000 cm^{-1} and a line width of 5 cm^{-1}. The average IR power was 100 mW. The irradiation time (with a typical value of 0.1 s) was controlled using a mechanical shutter (Sigma-Koki, Japan). The spectral intensity at each wavelength was calculated using

Equation. S3(Page S6).

3. Theoretical Methods

To identify the global optimal structure of the complex ion, two search strategies have been adopted: On the one hand, almost 50000 initial configurations of $[(C4LP)_8+K]^{1+}$, including both structures of zwitterionic or non-zwitterionic cis-4-hydroxy-L-proline units, were generated by the Molclus genmer program [33]. On the other hand, hundreds of structures of octamer, also including either zwitterionic or non-zwitterionic units, had been built and adjusted manually. The initial configurations were firstly optimized at a semi-empirical quantum mechanics level of GFN-xTB [34, 35]. These structures were ranked according to their energies, then the 100 lowest energy configurations were selected, optimized, and verified by the DFT method of wB97X-D/6-31G(d) [36-38]. It has been found that these structures are mainly characterized by their salt-bridged conformations. Finally, the three most stable isomers were further selected and optimized at the level of wB97X-D/6-31+G(d)/def2-QZVP [39, 40]. The 6-31+G(d) basis set is used throughout for the atom C, H, O, N, while def2-QZVP basis set is used throughout for the atom K. All theoretical frequencies obtained at the level of wB97XD/6-31+G(d)/def2-QZVP (Scaling factor is taken as 0.938). The electronic energy was calculated at 0 K with zero-point energy corrections and free energies were calculated at 298 K, respectively. The most three optimal structures of the $[(C4LP)_8+K]^{1+}$ complex were identified as C4LP-8-K-1, C4LP-8-K-2 and C4LP-8-K-3, in turn **(Table. S2)**. All DFT calculations were carried out with the Gaussian 09 program[41].

For the global optimal structure of the $[(T4LP)_8+K]^{1+}$ complex, corresponding search strategies are similar to that of $[(C4LP)_8+K]^{1+}$ complex. It was noted that the structures generated by the Molclus genmer program were difficult to optimize successfully, and the energies of all optimized structures were at least 50 kcal/mol higher than C4LP-8-K-1. Herein, the most stable isomer was found in the manually constructed structure, identified as T4LP-8-K-1. The two structures of both C4LP-8-K-1 and T4LP-8-K-1 were calculated at wB97X-D/6-31+G(d)/def2-QZVP and B3LYP-D3/6-31+G(d)/def2-QZVP levels, and were compared for structural information and energetic information, shown in **Table. 1**. The structures of both C4LP-8-K-1 and T4LP-8-K-1 were plotted by Visual Molecular Dynamics (VMD) [42], and the calculation of their cave sizes were performed by Multiwfn software [25]. The binding energies of clusters were calculated by **Equation S4 (Page S6)**.

For structures of $[(C(T)4LP)_8+M]^{1+}$ (M = H, Li, Na, Rb, Cs), potassium atoms centering at both C4LP-8-K-1 and T4LP-8-K-1 were replaced by M atom (M = H, Li, Na, Rb, Cs), and optimized at a lower level of wB97X-D/6-31G(d)/def2-QZVP, respectively. All structures are successfully optimized at the level. The optimized structure of $[(C4LP)_8+M]^{1+}$ (M = H, Li, Na, Rb, Cs) was identified as C4LP-8-M-1 (M = H, Li, Na, Rb, Cs), which has a similar structure to that of C4LP-8-K-1. All structures feature an identical topological hydrogen bonding network. However, there are differences in the distances between metal ions M (M = H, Li, Na, K, Rb, Cs) and O atoms. Similarly, the structure of T4LP-8-M-1, where M can be H, Li, Na, Rb, or Cs, bears resemblance to that of T4LP-8-K-1. The distance between metal ions M (M = H, Li, Na, K, Rb, Cs) and O atoms in these structures plays a crucial role **(Fig. S12)**. Whether it can be less than the sum of effective ionic radii of M^+ and O^{2-} can be a determining factor for the cluster's coordination conditions and its survivability. For instance, and the H^+(Li^+, Na^+) −carbonyl O atom distance is smaller than the sum of the ionic radii of H^+(Li^+, Na^+) and O^{2-}, so structures of $[(C(T)4LP)_8+M]^{1+}$ (M = H, Li, Na) were not found in the **Fig. S3**. Further, it is necessary for these clusters to take some tentative optimized measures at a higher level (wB97X-D/6-31+G(d)/def2-QZVP).

Finally, wavefunction analyses were performed to determine the intra-cluster interactions and to test the stability of clusters. On the one hand, intra-cluster weak interactions were analyzed by Multifwn software using independent gradient model based on Hirshfeld partition (IGMH) analysis [26] **(Fig. 4b)**. On the other hand, the kinetic stabilities of the clusters can be revealed by the color depth of the hydroxyproline units within clusters from the molecular electrostatic potential (MESP) map [27]. MESP mapped on 0.01 au electron density surface for both C4LP-8-K-1 and T4LP-8-K-1 **(Fig. 4c, S13)**. Moreover, the frontier molecular orbitals of C4LP-8-K-1 and T4LP-8-K-1 provide pertinent orbital information that can serve as indicators of their chemical stability **(Fig. S14)**. Herein, molecular orbital diagram all belonged to isosurface maps, and their isovalue was set at 0.02. The wavefunction analyses were visualized using VMD in combination with Mutifwn software. The files containing wavefunction information were calculated at the level of wB97X-D/6-31+G(d)/def2-QZVP.

Supplementary Equation

Equation. S1: Calculation of normalized relative intensities of ions

The normalized relative intensity of each proline cluster ion reported here is calculated according to：

$$I_r = \frac{I_{ai}}{I_{hi}} \times 100 \quad \cdots\cdots(1)$$

, in which I_r is the normalized relative intensity, I_{ai} represents the value of the absolute intensity of the experimentally observed ion, and I_{hi} represents the absolute intensity of the clusters with the highest intensity in a series of experiments of corresponding research. In **Fig. 1**, the highest peak observed in both mass spectra of cis- and trans-4-hydroxyproline solutions is selected as I_{hi} that normalized to has an intensity of I_r =100, and the intensities of other peaks are all calculated with (1) using this peak as the reference. In **Fig. 2a, b**, the absolute intensity of the highest peak of $[(C(T)4LP)_8+M]^{1+}$ (M = H, Li, Na, K, Rb, Cs) observed in all solutions containing different metal ions is selected as I_{hi} (in this case, the most abundant ion is $[(C4LP)_8+Rb]^{1+}$), and other peaks are calculated using it as the reference. In **Fig. 2c, d**, the absolute intensity of the highest peak of $[Hyp_8+K]^{1+}$ observed in all solutions containing different compositions of cis(trans)-4-hydroxy-L-proline and cis(trans)-4-hydroxy-D-proline is selected as I_{hi}, and other peaks are calculated using it as the reference. For both results shown in **Fig. 2**, the experiments were repeated three times under their identical conditions. And the value of I_{hi} was chosen from the first try. Then, we averaged the normalized relative intensities obtained in the three tests, and reported the values in **Fig. 2**, along with the corresponding standard deviations (as the error bar shown in **Fig. 2**).

Equation. S2: Calculation of “chiral preference value”

The “chiral preference value” was calculated here by using:

$$C = \frac{I_L - I_r}{I_L + I_r} \quad (2)$$

In which, C is the chiral preference value, I_L and I_r are the intensities of the corresponding clusters generated from enantiopure (100% L) and racemic (50:50 L:D) cis-4-hydroxyproline solutions. If the cluster has no chiral preference in its formation, it can be generated in both solutions with same intensities and the value of C should be equal to zero. At the same time, the preferences for homochiral or heterochiral clusters are indicated by positive or negative values between 1 and -1, respectively.

Equation. S3: Calculation of the infrared spectral intensity

Typically, these complex ions $[(C4LP)_8+K]^{1+}$ were generated by the ESI method, isolated in the cell of the FT ICR mass spectrometer, and irradiated by a tunable IR laser. Then the spectral intensity of the selected ions at each wavelength can be calculated as:

$$I = -ln(\frac{I_p}{I_p + \sum I_f}) \quad (3)$$

In which, the I_p and I_f represent intensities of precursor and fragment ions observed in the mass spectra, respectively.

Equation. S4: Calculation of the cluster binding energy

The cluster binding energies of structures for both C4LP-8-K-1 and T4LP-8-K-1 can be calculated as:

$$\Delta E_{bind} = E_{cluter} - \sum E_{mono} + E_{BSSE} \quad (4)$$

In which, ΔE_{bind} is defined as the cluster binding energy of C4LP-8-K-1 or T4LP-8-K-1. And $E_{cluster}$ is the energy of C4LP-8-K-1 or T4LP-8-K-1, while E_{mono} is the lowest energy of cis- or trans-hydroxyproline monomer, which was taken from corresponding crystal structures[43]. Besides, E_{BSSE} refers to the correction made to account for the basis set superposition error (BSSE), which is an important correction that takes into consideration the overlap between basis sets and helps to make the calculation of binding energy more accurate [44]. All structures were calculated at wB97X-D/6-

31+G(d)/def2-QZVP and B3LYP-D3/6-31+G(d)/def2-QZVP levels.

Equation. S5: Calculation for the relative concentrations of their contribution to the average theoretical spectrum from each isomer

Relative concentrations (W_i) of the *i*-th isomer at different temperatures were calculated by:

$$W_i = \frac{q_i exp\left(-\frac{\Delta H_{0,i}^{o}}{RT}\right)}{\sum_{j=1}^{n} q_j exp\left(-\frac{\Delta H_{0,j}^{o}}{RT}\right)} \quad \cdots\cdots\cdots\cdots\cdots\cdots(1.1)$$

where R is the gas constant, T is the absolute temperature, q_i and $\Delta H_{0,j}^{o}$ are the partition function and the relative heat of formation at absolute zero temperature of the *i*-th isomer, respectively. Herein, the temperature is taken as 298 K, and rotational-vibrational partition functions were calculated from the optimized structural and vibrational data obtained.

Supplementary Figures

Figures S1 to S13

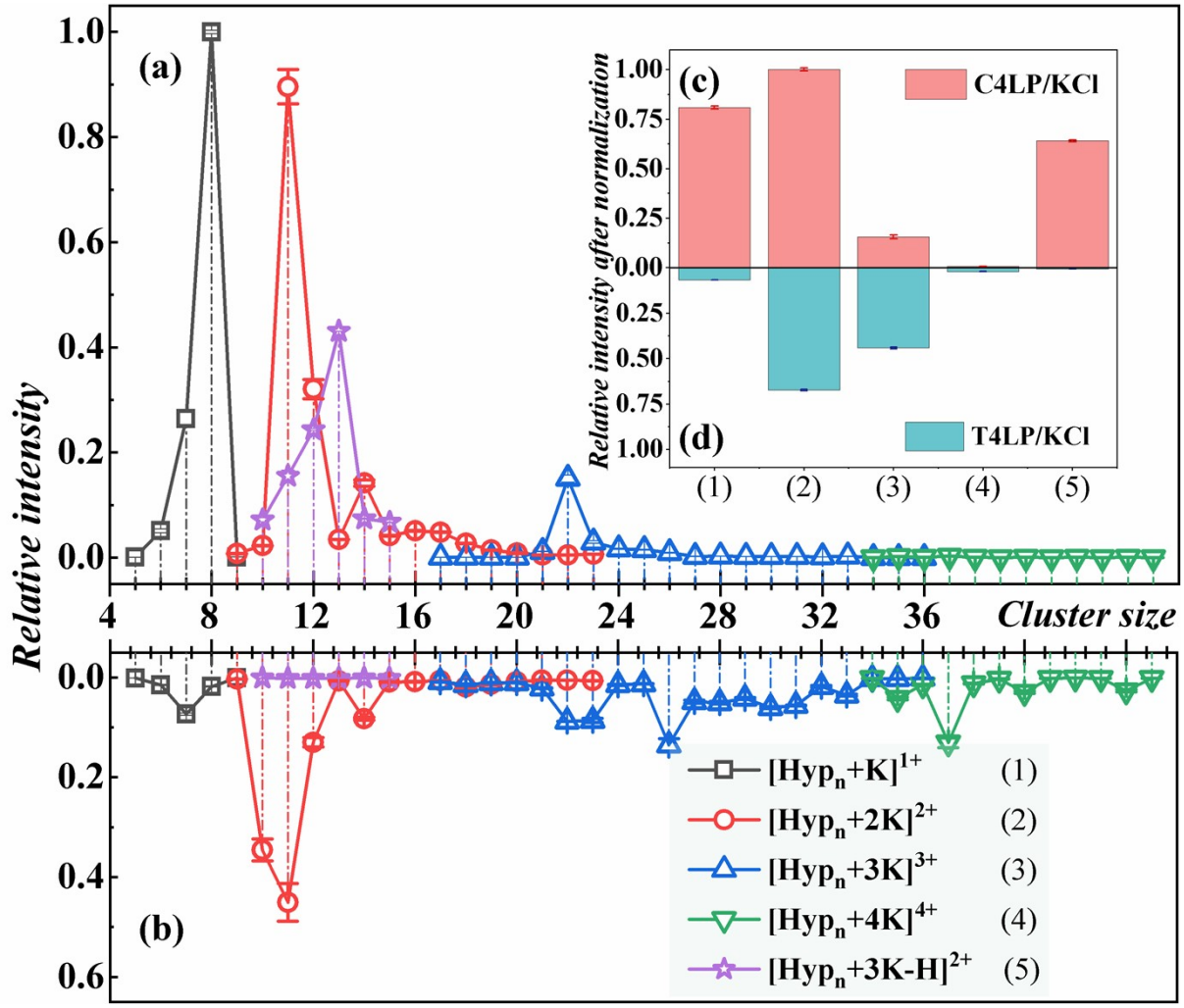


Fig. S1 A comparison between the intensity of potassiated cis-**(a)** and trans-4-hydroxy-L-proline **(b)** clusters versus cluster size for clusters in five types ([Hyp$_n$+K]$^{1+}$, [Hyp$_n$+2K]$^{2+}$, [Hyp$_n$+3K]$^{3+}$, [Hyp$_n$+4K]$^{4+}$, [Hyp$_n$+3K-H]$^{2+}$). The overlapping peaks were decompositioned (see **Fig. S2** for the decomposition process) and normalized with a unified standard to facilitate the comparison. The dashed lines are only for eye guidance.

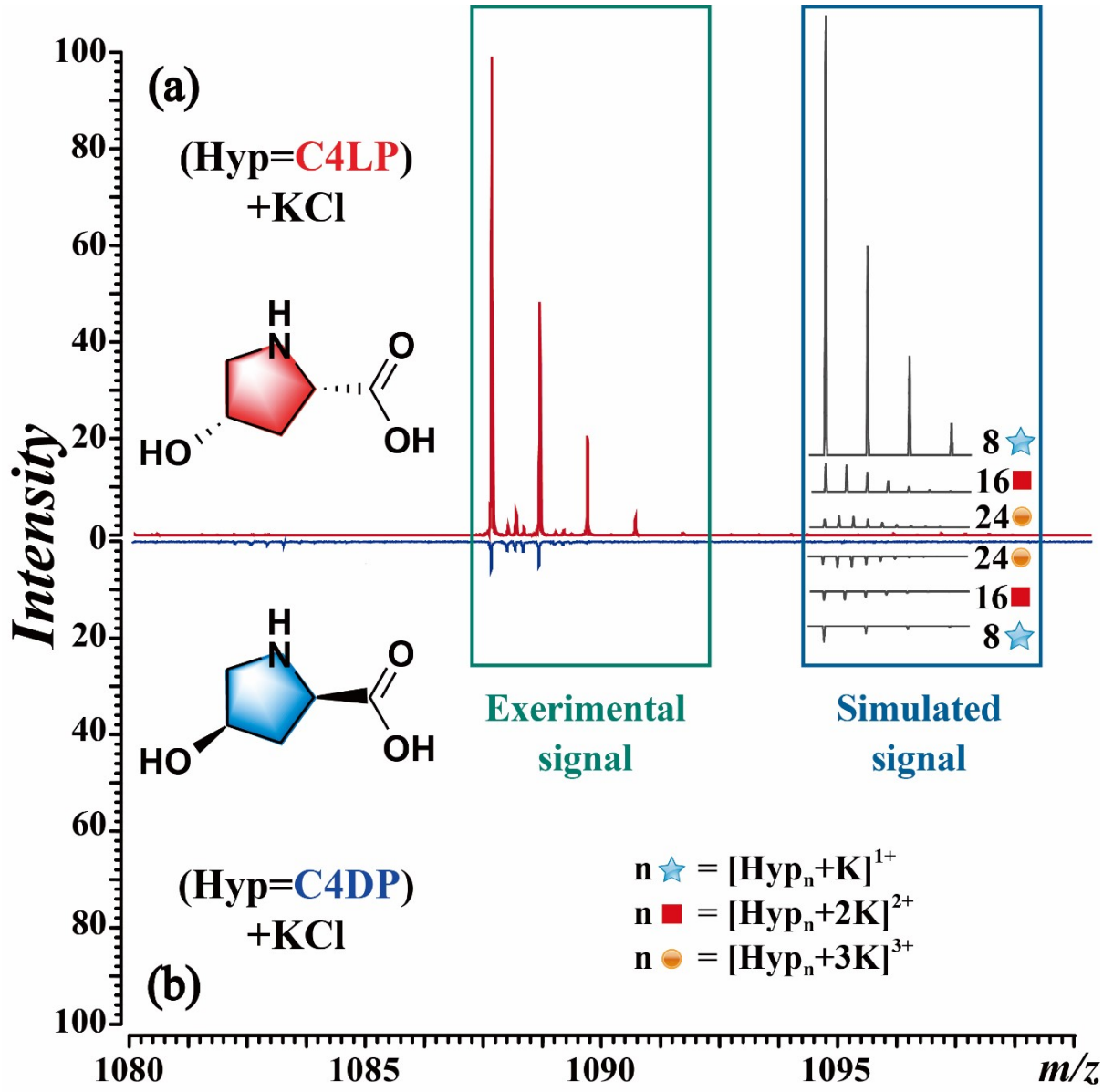


Fig. S2 The isotopic comparison of experimental and simulated signals. The ESI mass spectra generated from 5 mM/L cis-4-hydroxy-L-proline **(**C4LP, red above, **a)** and cis-4-hydroxy-D-proline **(**T4LP, blue below, **b)** solutions with 0.5 mM/L KCl ranging from *m/z* = 1080 to *m/z* = 1100. The experimental peak intensities are normalized with a unified standard to facilitate the comparison. In the Figure, the cluster ions at *m/z* = 1087 can be decomposed into $[(Hyp)_8+K]^{1+}$, $[(Hyp)_{16}+2K]^{2+}$, and $[(Hyp)_{24}+3K]^{3+}$ (Hyp = C4LP, T4LP). Other overlapping cluster ions in **Fig. 1** also were decomposed with this method, which had been previously reported by us[14].

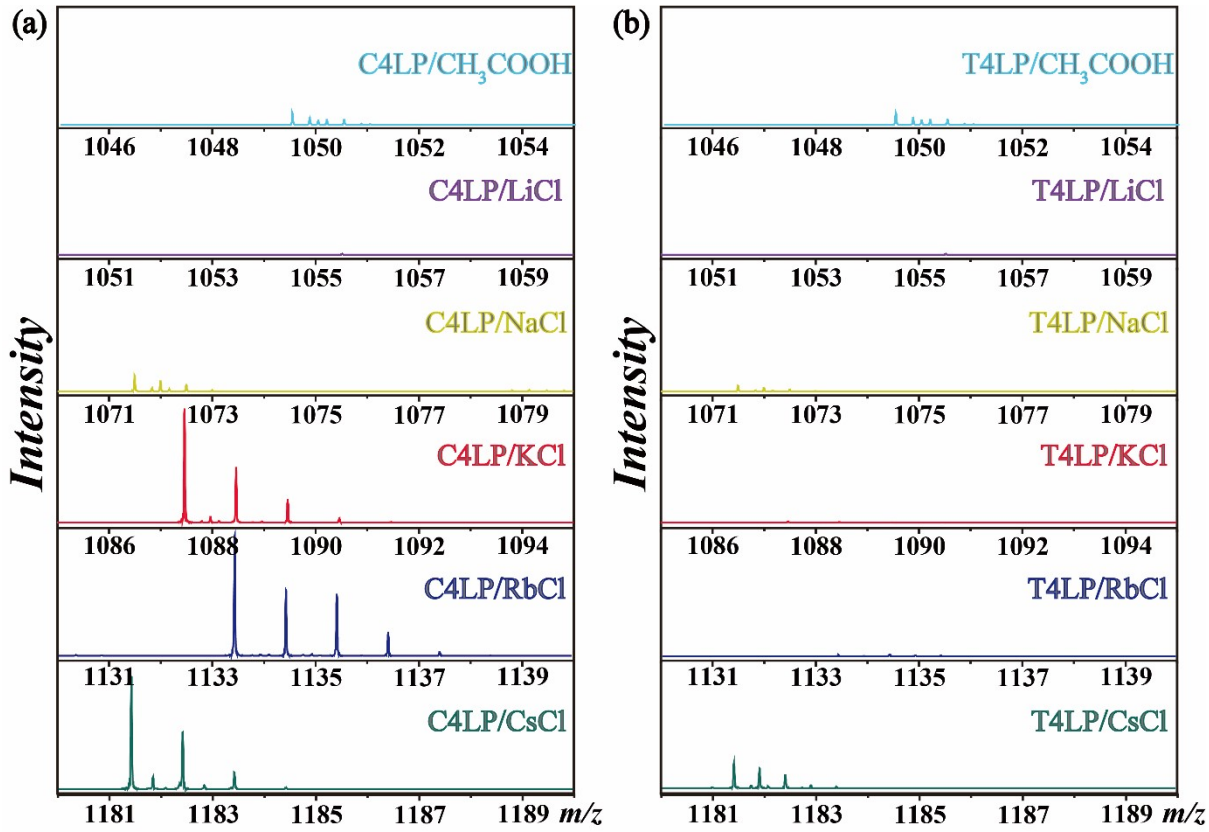


Fig. S3 Mass spectra of cis- **(a)** and trans- **(b)** 4-hydroxy-L-proline samples after adding CH_3COOH or various alkali metal ions in corresponding *m/z* ranges. The ESI mass spectra shown here were generated from solutions of 5 mM/L cis-4-hydroxy-L-proline **(**C4LP, left, **a)** and trans-4-hydroxy-L-proline **(**T4LP, right, **b)** containing 0.5mM/L CH_3COOH, LiCl, NaCl, KCl, RbCl and CsCl, in turn. For weak signals observed in either C4LP/NaCl or T4LP/CsCl, the most contributions are coming from the doubly charged species of $[Hyp_{16}+2M]^{2+}$ (Hyp=C4LP, M=Na; Hyp=T4LP, M=Cs). For the strong signals observed in C4LP/MCl (M = K, Rb, Cs), the contributions from the singly charged species of $[(C4LP)_8+M]^{1+}$ (M = K, Rb, Cs) are all larger than 95%.

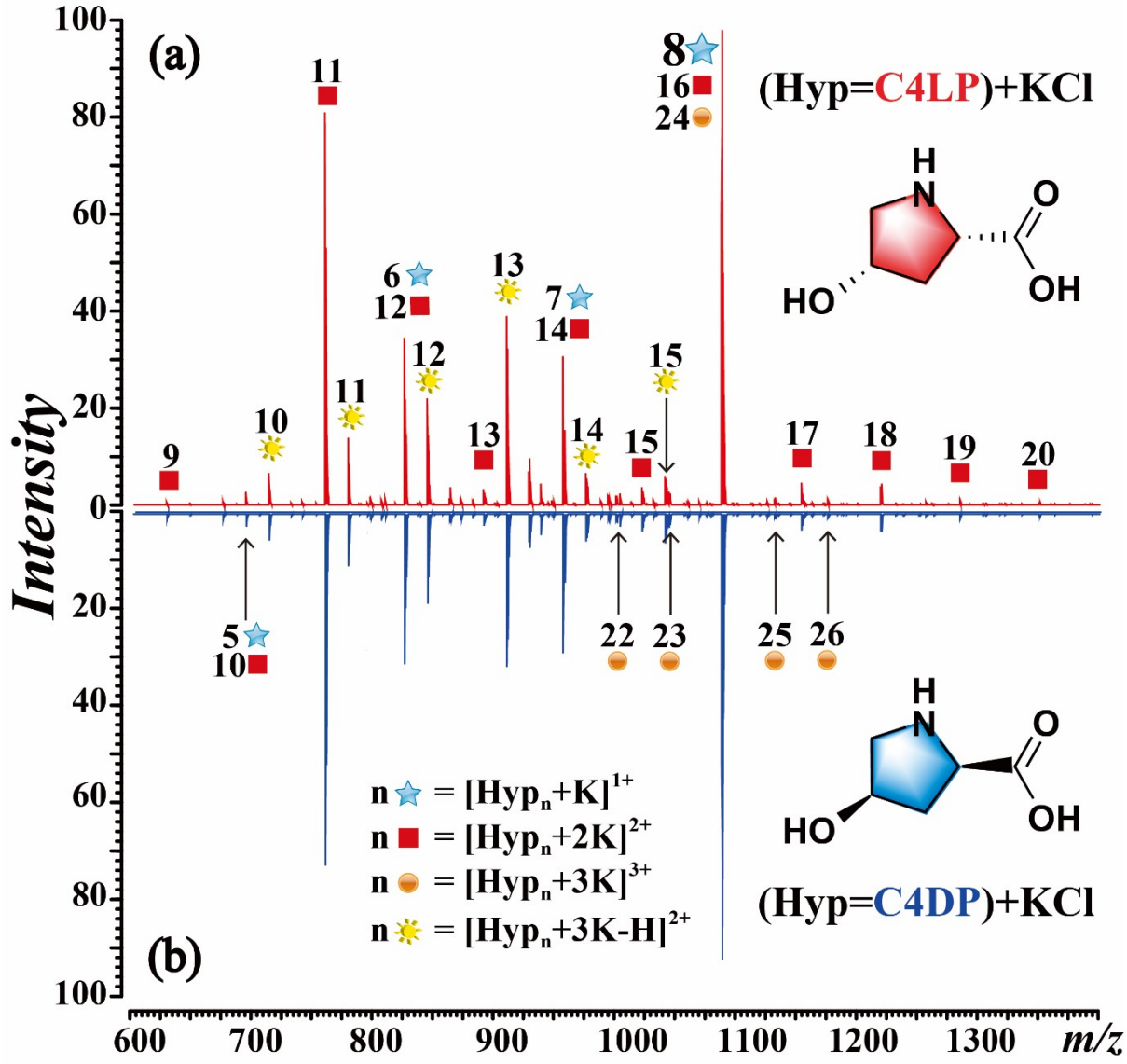


Fig. S4 A comparison of ESI mass spectra generated from 5 mM/L cis-4-hydroxy-L-proline **(**red above, **a**) and cis-4-hydroxy-D-proline **(**blue below, **b**) solutions with 0.5 mM/L KCl at the region of *m/z* ~ 600-1400. There are five types of clusters ($[Hyp_n+K]^{1+}$, $[Hyp_n+2K]^{2+}$, $[Hyp_n+3K]^{3+}$, $[Hyp_n+3K-H]^{2+}$), and the results show consistent spectra for the two samples. The experimental peak intensities are normalized to facilitate the comparison.

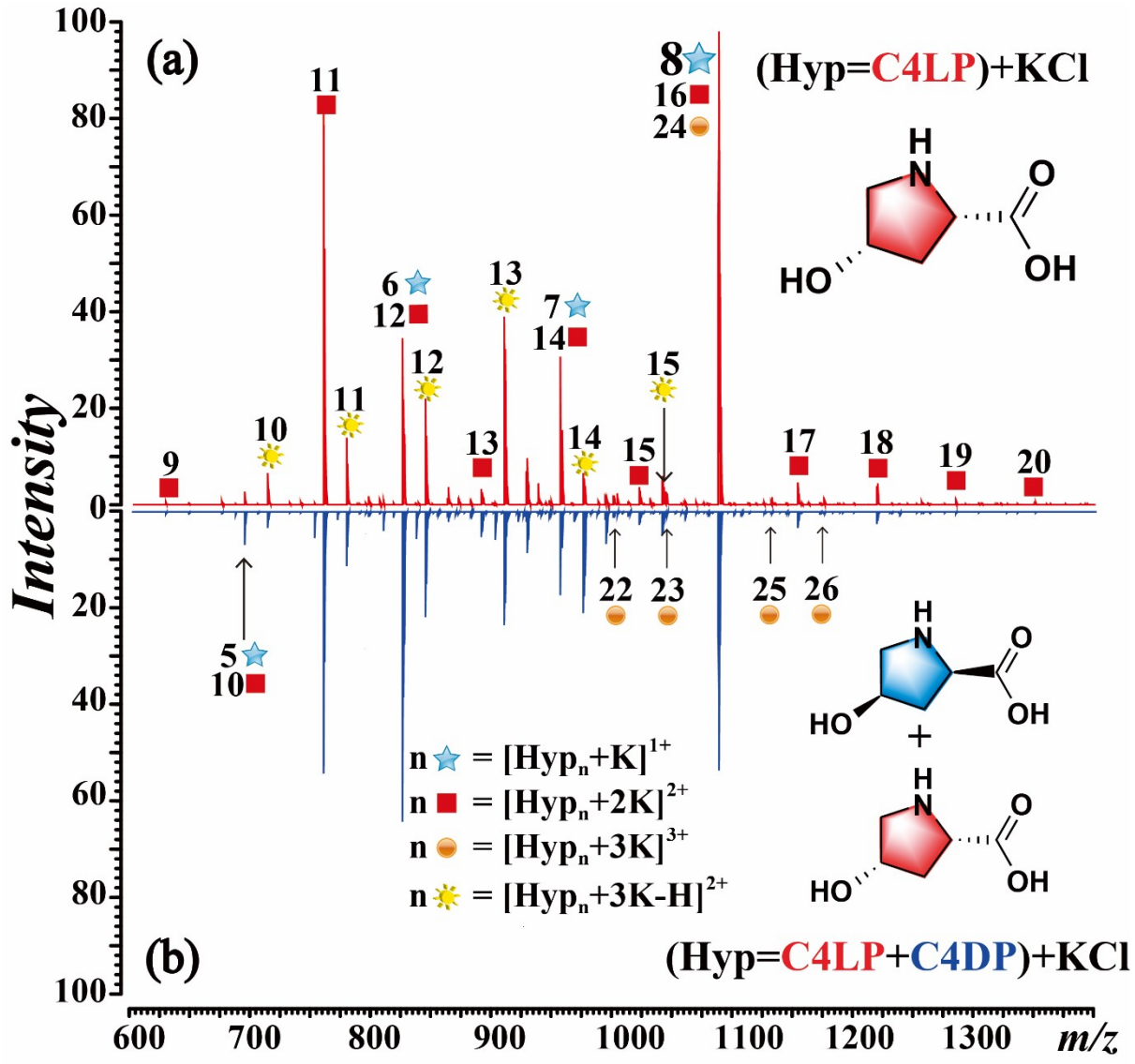


Fig. S5 A comparison of ESI mass spectra generated from 5mM/L enantiopure **(**100% L, red above, **a)** and racemic **(**50:50 L:D, blue below, **b)** cis-4-hydroxyproline solutions with 0.5mM/L KCl at the region of *m/z* ~ 600-1400. There are five types of cluster ions ($[Hyp_n+K]^{1+}$, $[Hyp_n+2K]^{2+}$, $[Hyp_n+3K]^{3+}$, $[Hyp_n+3K-H]^{2+}$), and their intensities vary considerably generated from enantiopure and racemic solutions, respectively. The experimental peak intensities are normalized to facilitate the comparison.

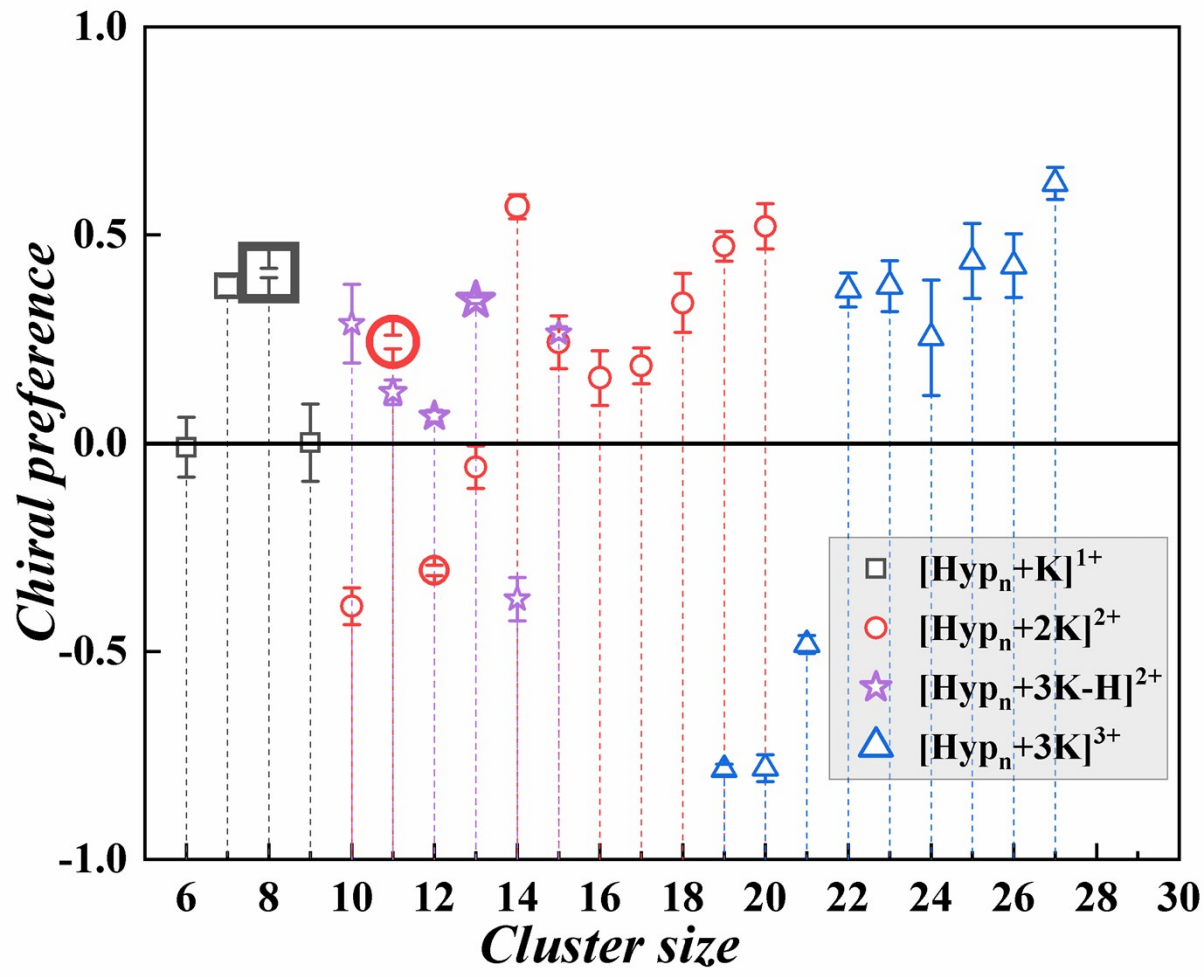


Fig. S6 A summary of the intensity and chiral preference of various clusters observed in **Fig. S5**. The chiral preference was calculated according to **Equation. S1**. Positive and negative values indicate preferences for homochirality and heterochirality, respectively. The error bars represent the standard deviations obtained by collecting data sets in triplicate. The size of each point is positive correlation with the abundance of the cluster in the mass spectra. The dashed lines are only for guidance.

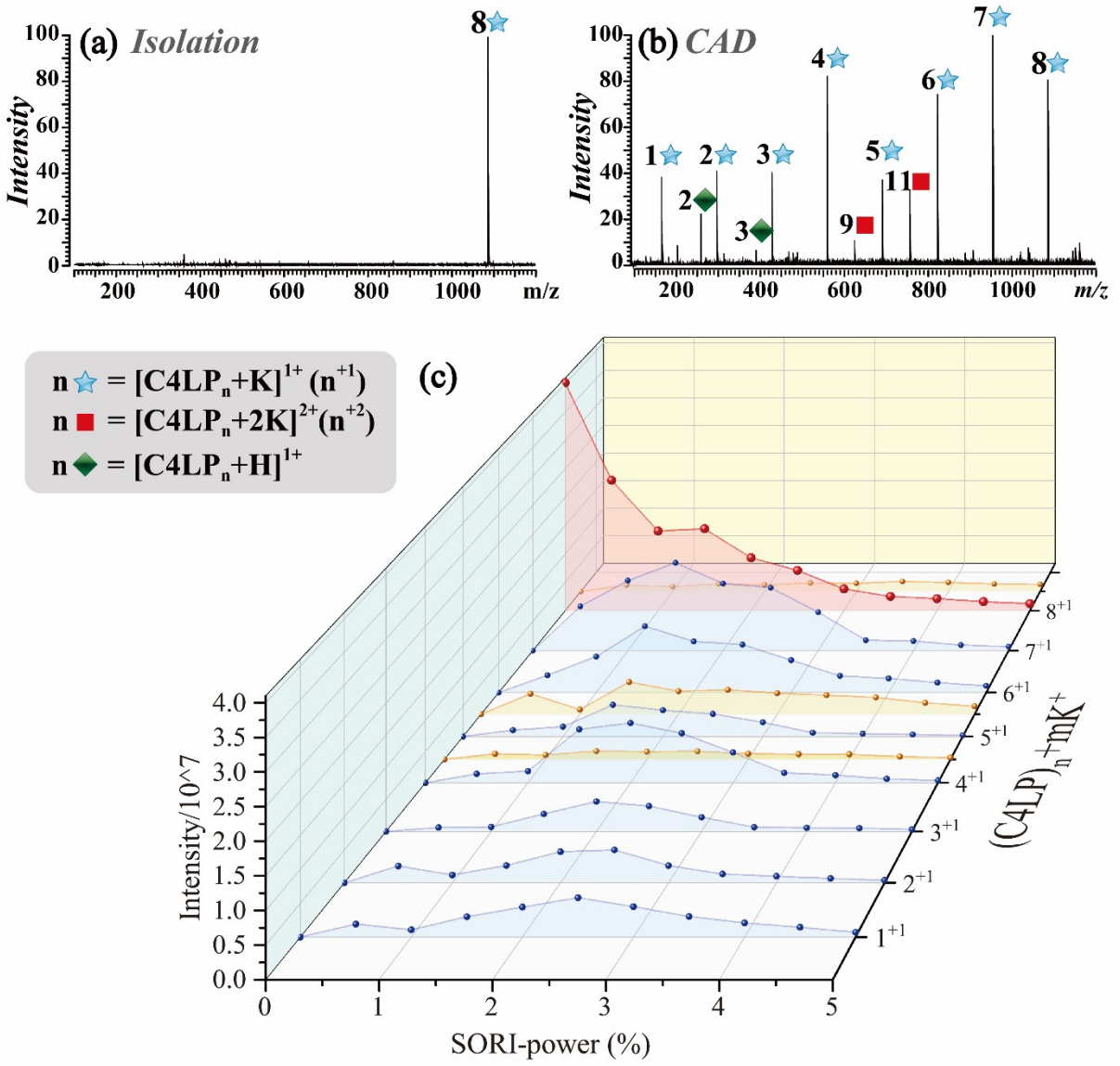


Fig. S7 Details about CID experiment of $[(C4LP)_8+K]^{1+}$: **(a)** The mass spectrum of $[(C4LP)_8+K]^{1+}$ after the isolation in the cell of the FT ICR mass spectrometer, **(b)** the typical CID mass spectrum showing its product ions, obtaining with a SORI-power of 3% and the collision gas of nitrogen; **(c)** Intensities of different CID fragment ions versus collision voltages from 0% to 5%(SORI-power (%), step size = 0.5%) applied in the experiments.

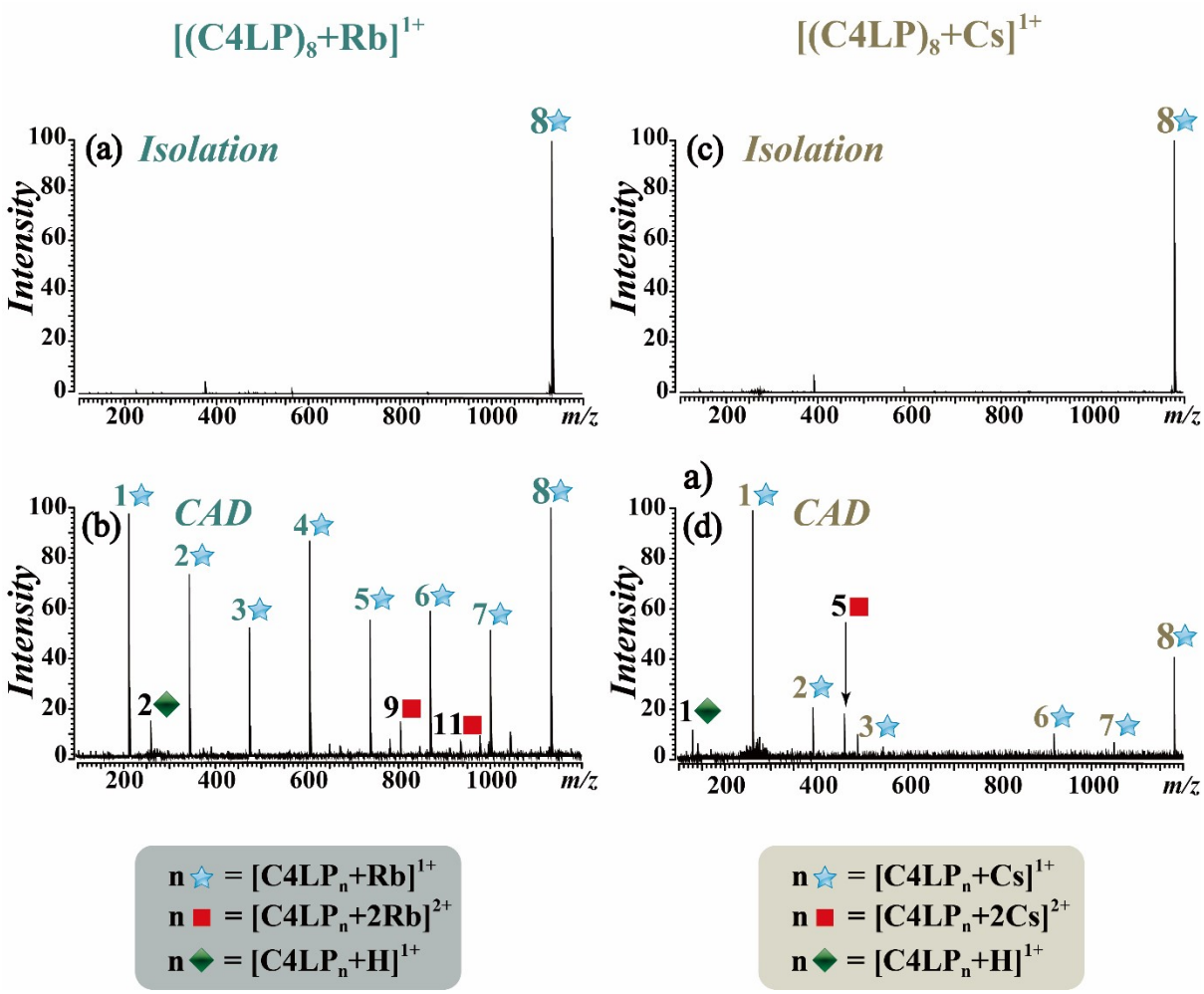


Fig. S8 Details about CID experiment of $[(C4LP)_8+Rb]^{1+}$ and $[(C4LP)_8+Cs]^{1+}$: The mass spectrum of $[(C4LP)_8+Rb]^{1+}$ **(a)** and $[(C4LP)_8+Cs]^{1+}$ **(c)** after the isolation in the cell of the FT ICR mass spectrometer; The typical CID mass spectrum of $[(C4LP)_8+Rb]^{1+}$ **(b)** and $[(C4LP)_8+Cs]^{1+}$ **(d)** showing its product ions, obtaining with a SORI-power of 3% and the collision gas of nitrogen.

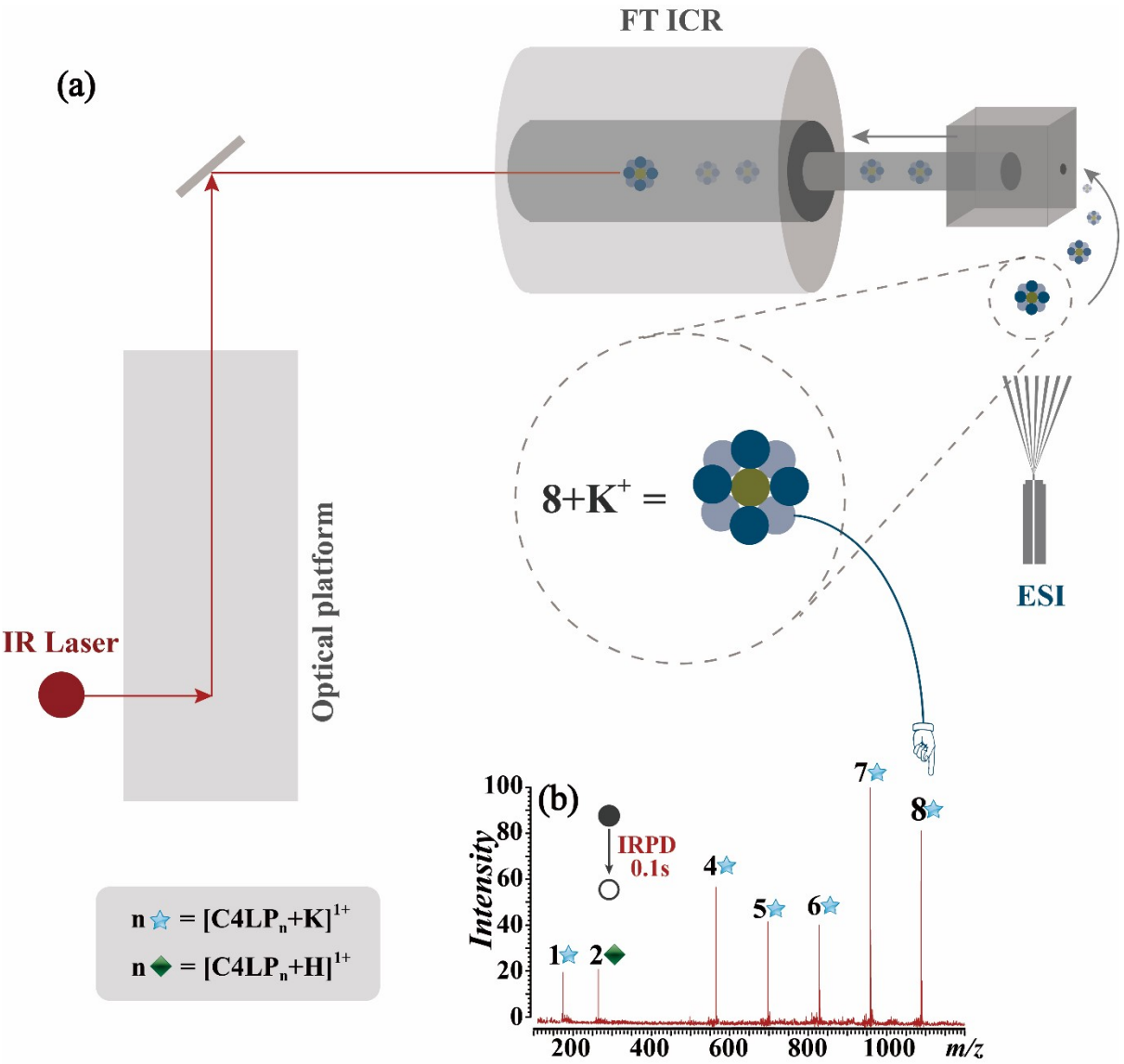


Fig. S9 Details about IRPD experiment of $[(C4LP)_8+K]^{1+}$: **(a)** Schematic diagram of the principle of infrared photodissociation experiment setup. **(b)** A infrared laser at 3080 cm^{-1} can dissociate the parent cluster ions $[(C4LP)_8+K]^{1+}$ into fragmental ions. By adjusting the tunable IR wavelength, the IRPD spectral intensity of the selected ion at each wavelength can be calculated as **Equation. S3**, and plotted in **Fig. 3a**.

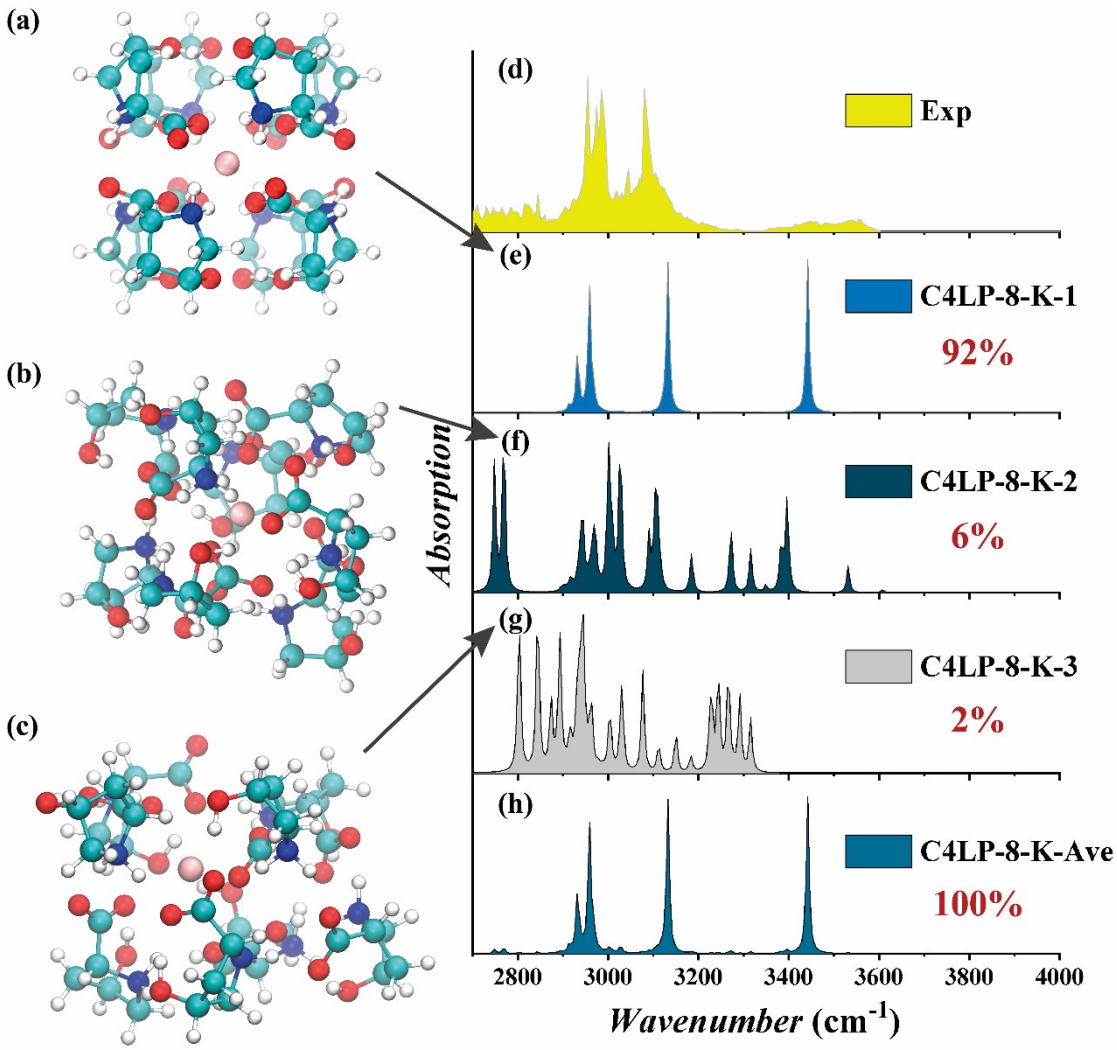


Fig. S10 Configurations **(a-c)** and experimental **(d)**, theoretical **(e-g)** and average theoretical **(h)** IR spectra of the three most stable isomers of $[(C4LP)_8+K]^{1+}$. The configurations of **(a)** C4LP-8-K-1, **(b)** C4LP-8-K-2 and **(c)** C4LP-8-K-3 and their theoretical IR spectra of: **(e)** C4LP-8-K-1, **(f)** C4LP-8-K-2 and **(g)** C4LP-8-K-3 in the region of 2700-4000 cm^{-1}. The average theoretical spectra **(h)** of the three most stable isomers by their contributions to compare with the experimental spectra. The calculation of their respective contributions (highlighted with red numbers) was shown in **Equation. S5**. Hence, the broadening of the experimental spectrum compared with the theoretical spectrum may be suggested to be the contribution of other isomers with similar structures but less structural symmetry. The calculations were performed at the wB97X-D/6-31+G(d)/def2-QZVP level.

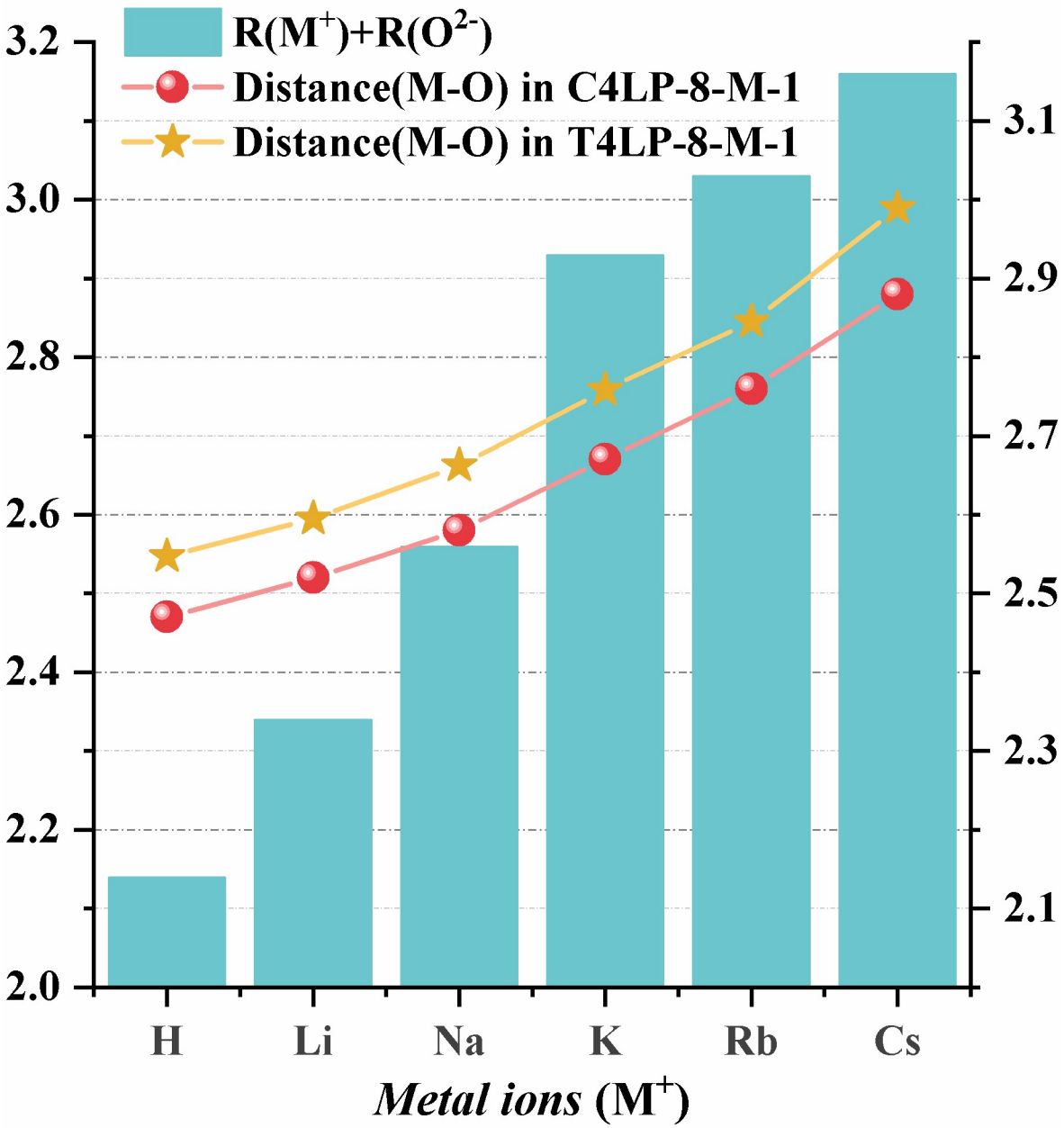


Fig. S11 Sums of effective ionic radii of M^+ and O^{2-} (cyan bars) and M^+–O^{2-} distances in C4LP-8-M-1 (red balls) and T4LP-8-M-1 (orange stars). To economize computing power, the calculations were performed at a lower level (wB97X-D/6-31G(d)/def2-QZVP). Besides, the distance(M-O) in C(T)4LP-8-K-1 (M = K, Rb, Cs) at the higher level (wB97X-D/6-31+G(d)/def2-QZVP) is slightly larger than at the lower level, while the structures of C(T)4LP-8-H (Li, Na)-1 failed to optimize at the higher level.

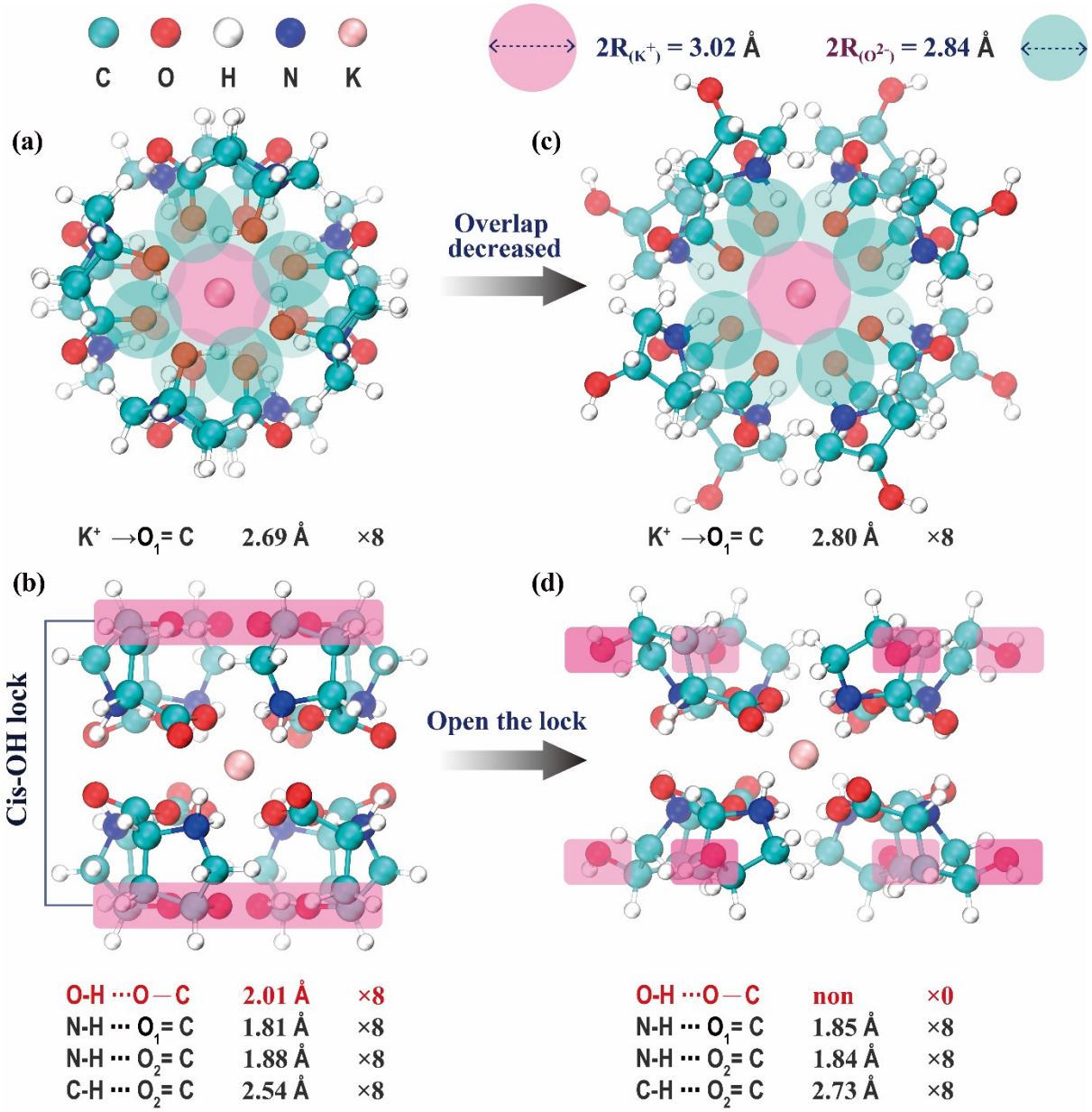


Fig. S12 Top **(a, c)** and **(b, d)** side views of the calculated configurations of C4LP-8-K-1 **(a, b)** and T4LP-8-K-1 **(c, d)**. The calculations were performed at the wB97X-D/6-31G(d)/def2-QZVP level. The effective ionic size of K^+ and oxygen anion are indicated by the larger pink and cyan circles, respectively. The central eight O atoms are arranged in two layers, indicated by cyan and light cyan shading. The H-bonds and K-O coordinated bonds are identified and the lengths are shown in Å.

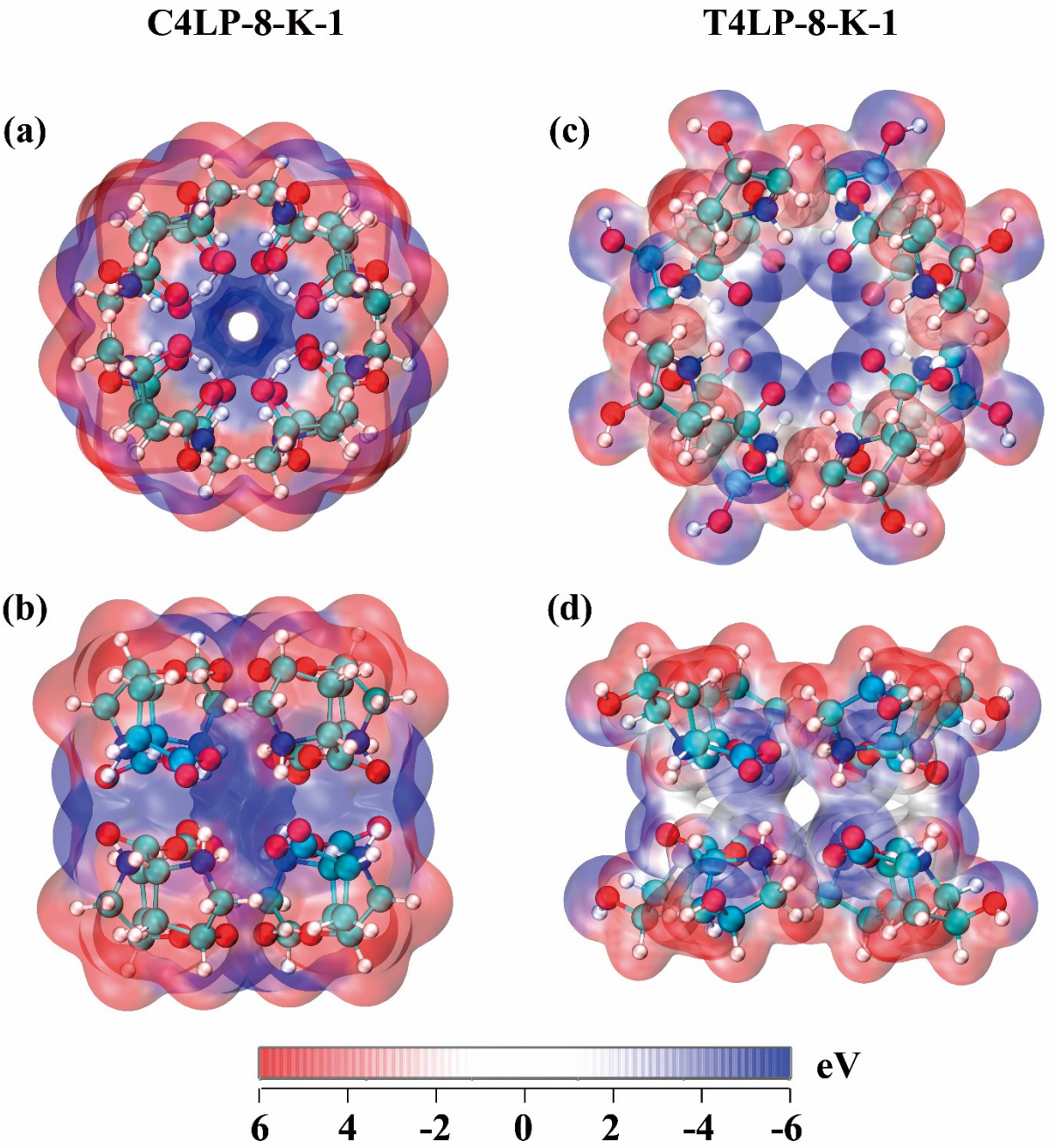


Fig. S13 Top **(a, c)** and **(b, d)** side views of molecular electrostatic potential (MESP) of the octamer C4LP-8-K-1 **(a, b)** and T4LP-8-K-1 **(c, d).** The MESP mapped on 0.01 au electron density surface for various molecular systems. Blue regions indicate electron-rich negative MESP, while the red region corresponds to electron-deficient positive MESP. The calculations were performed at the wB97X-D/6-31+G(d)/def2-QZVP level.

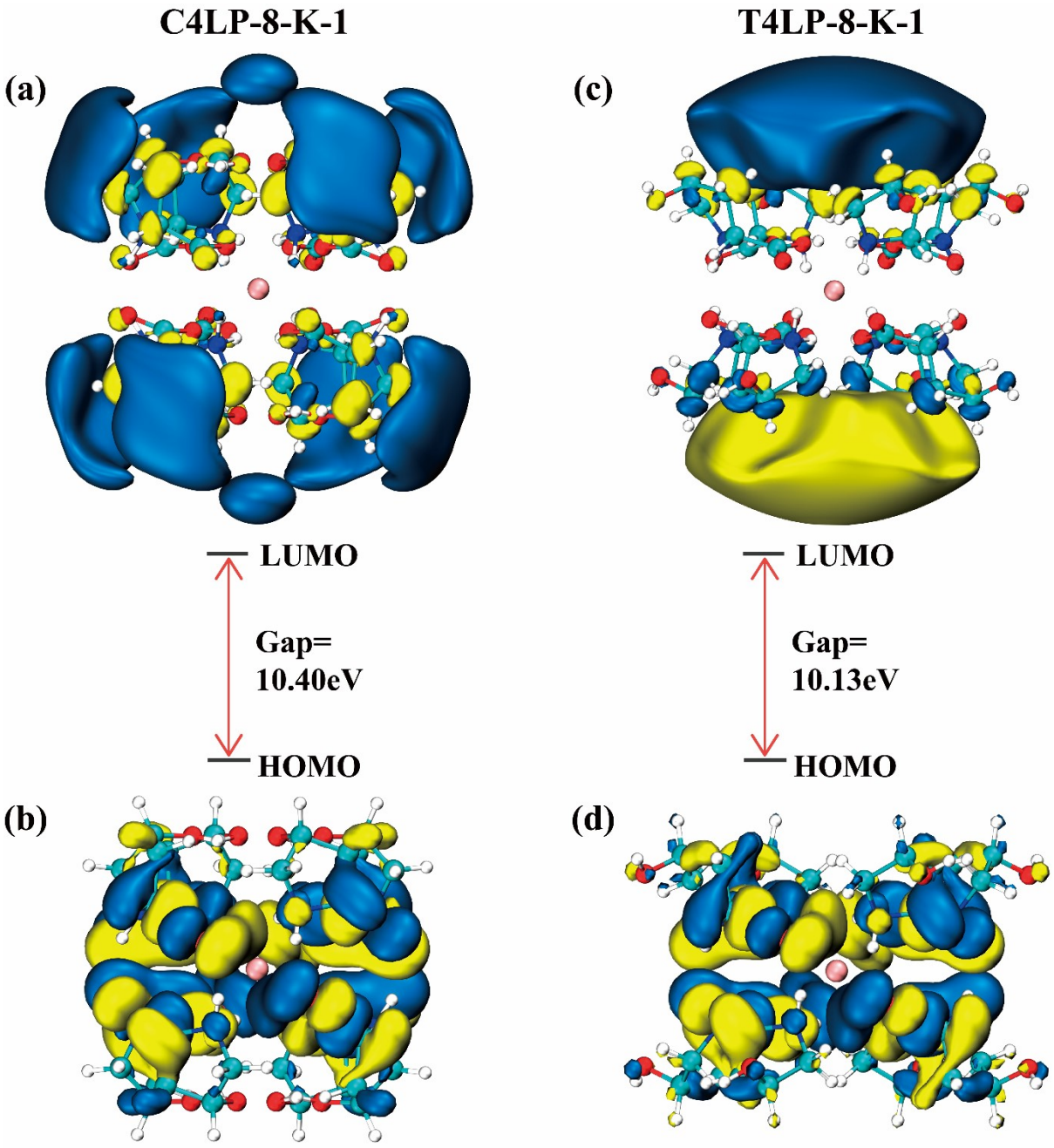
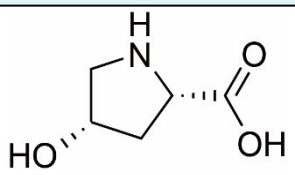
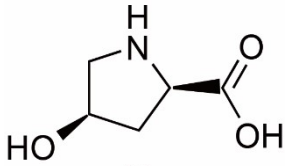
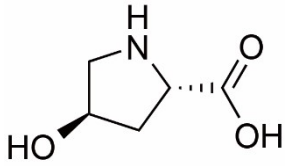
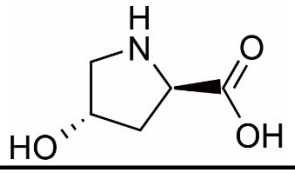


Fig. S14 The HOMO **(**below, **b, d)** and LUMO **(**above, **a, c)** orbitals of the octamer C4LP-8-K-1 **(a, b)** and T4LP-8-K-1 **(c, d)**. The HOMO-LUMO energy gaps of C4LP-8-1 and C4LP-8-1 reach 10.40 eV and 10.13 eV, respectively, which are calculated at the wB97X-D/6-31+G(d)/def2-QZVP level. The blue and yellow isosurfaces represent wave functions of opposite phases.

Supplementary Tables

Tables S1 to S2

Table S1 Names, abbreviations and compound structures of the hydroxyproline (Hyp) molecules used in the experiment *

Name	Abbreviation	Compound structure
Cis-4-OH-L-Proline	C4LP	
Cis-4-OH-D-Proline	C4DP	
Trans-4-OH-L-Proline	T4LP	
Trans-4-OH-D-Proline	T4DP	

* Note: The abbreviation C4L(D)P (T4L(D)P) mentioned in **Fig. 2** refers to solutions containing different ratios of cis-4-OH-L-Proline (trans-4-OH-L-Proline) to cis-4-OH-D-Proline (trans-4-OH-D-Proline); Abbreviation “C4P” mentioned in manuscript generally refers to cis-4- OH- Proline with no chiral isomeric distinction, which is used to test the chiral preference of cis-4- OH- Proline.

Table S2 Relative energies, enthalpies and Gibbs free energies (both in *kcal/mol*) of the three isomers of $[(C4LP)_8+K]^{1+}$ at the level of wB97X-D/6-31+G(d)/def2-QZVP together with coordination number of K^+ and H-bond number in these isomers.

Isomers§	wB97X-D/6-31+G(d)/def2-QZVP				
	ΔE* (kcal/mol)	ΔH† (kcal/mol)	ΔG† (kcal/mol)	Coordination number of K^+ ‡	H-bond number #
C4LP-8-K-1	0.00	0.00	0.00	8	24
C4LP-8-K-2	5.57	5.03	4.45	6	19
C4LP-8-K-3	18.91	17.16	15.83	6	17

§ Structures of the three isomers with the lowest energies are shown in **Fig. S10**.

* Those energies were calculated after zero-point correction at 0 K;

† Relative enthalpies ΔH and relative Gibbs free energies ΔG were calculated after zero-point correction at 298 K.

‡ Number of carboxyl atoms ligated around each potassium ion. (The coordination is determined by the comparison of whether the distance between K and the O atom is less than the sum of the effective ionic radii of the two.)

Number of hydrogen bonds in the isomers. (All three isomers are made up of proline in the zwitterionic forms.)

Supplementary Notes

Note. S1 Coordinates of the calculated molecules.

a. XYZ Coordinates of C4LP-8-K-1 (Calculated at the wB97X-D/6-31+g(d)/def2-QZVP level.)

atom	X	Y	Z
K	0.00000000	0.00000000	0.00000000
N	1.63800800	3.37946600	1.76937600
H	1.43733200	2.36751300	1.57850900
H	2.09499800	3.70987500	0.89895000
C	2.43371100	3.43899000	3.01818900
C	0.37087100	4.13082800	2.02664500
H	3.23808800	2.70925100	2.97977100
H	2.85796300	4.44125100	3.12481800
C	1.35496000	3.18144900	4.06876500
C	0.22856100	4.10123500	3.57216500
H	0.48975900	5.14183500	1.63814900
C	-0.80185400	3.42329500	1.33159700
H	1.69645000	3.45651700	5.07237800
H	-0.74972500	3.73999300	3.89894200
H	0.36150300	5.10396300	3.98653500
O	-1.71138100	4.14257000	0.86343800
O	-0.74638800	2.17083300	1.36902800
N	3.37946600	-1.63800800	1.76937600
H	2.36751300	-1.43733200	1.57850900
H	3.70987500	-2.09499800	0.89895000
C	3.43899000	-2.43371100	3.01818900
C	4.13082800	-0.37087100	2.02664500
H	2.70925100	-3.23808800	2.97977100
H	4.44125100	-2.85796300	3.12481800
C	3.18144900	-1.35496000	4.06876500
C	4.10123500	-0.22856100	3.57216500
H	5.14183500	-0.48975900	1.63814900
C	3.42329500	0.80185400	1.33159700
H	3.45651700	-1.69645000	5.07237800
H	3.73999300	0.74972500	3.89894200
H	5.10396300	-0.36150300	3.98653500
O	4.14257000	1.71138100	0.86343800
O	2.17083300	0.74638800	1.36902800
N	-3.37946600	1.63800800	1.76937600
H	-2.36751300	1.43733200	1.57850900

H	-3.70987500	2.09499800	0.89895000
C	-3.43899000	2.43371100	3.01818900
C	-4.13082800	0.37087100	2.02664500
H	-2.70925100	3.23808800	2.97977100
H	-4.44125100	2.85796300	3.12481800
C	-3.18144900	1.35496000	4.06876500
C	-4.10123500	0.22856100	3.57216500
H	-5.14183500	0.48975900	1.63814900
C	-3.42329500	-0.80185400	1.33159700
H	-3.45651700	1.69645000	5.07237800
H	-3.73999300	-0.74972500	3.89894200
H	-5.10396300	0.36150300	3.98653500
O	-4.14257000	-1.71138100	0.86343800
O	-2.17083300	-0.74638800	1.36902800
N	-1.63800800	-3.37946600	1.76937600
H	-1.43733200	-2.36751300	1.57850900
H	-2.09499800	-3.70987500	0.89895000
C	-2.43371100	-3.43899000	3.01818900
C	-0.37087100	-4.13082800	2.02664500
H	-3.23808800	-2.70925100	2.97977100
H	-2.85796300	-4.44125100	3.12481800
C	-1.35496000	-3.18144900	4.06876500
C	-0.22856100	-4.10123500	3.57216500
H	-0.48975900	-5.14183500	1.63814900
C	0.80185400	-3.42329500	1.33159700
H	-1.69645000	-3.45651700	5.07237800
H	0.74972500	-3.73999300	3.89894200
H	-0.36150300	-5.10396300	3.98653500
O	1.71138100	-4.14257000	0.86343800
O	0.74638800	-2.17083300	1.36902800
N	1.63800800	-3.37946600	-1.76937600
H	1.43733200	-2.36751300	-1.57850900
H	2.09499800	-3.70987500	-0.89895000
C	2.43371100	-3.43899000	-3.01818900
C	0.37087100	-4.13082800	-2.02664500
H	3.23808800	-2.70925100	-2.97977100
H	2.85796300	-4.44125100	-3.12481800
C	1.35496000	-3.18144900	-4.06876500
C	0.22856100	-4.10123500	-3.57216500
H	0.48975900	-5.14183500	-1.63814900
C	-0.80185400	-3.42329500	-1.33159700
H	1.69645000	-3.45651700	-5.07237800
H	-0.74972500	-3.73999300	-3.89894200
H	0.36150300	-5.10396300	-3.98653500

O	-1.71138100	-4.14257000	-0.86343800
O	-0.74638800	-2.17083300	-1.36902800
N	3.37946600	1.63800800	-1.76937600
H	2.36751300	1.43733200	-1.57850900
H	3.70987500	2.09499800	-0.89895000
C	3.43899000	2.43371100	-3.01818900
C	4.13082800	0.37087100	-2.02664500
H	2.70925100	3.23808800	-2.97977100
H	4.44125100	2.85796300	-3.12481800
C	3.18144900	1.35496000	-4.06876500
C	4.10123500	0.22856100	-3.57216500
H	5.14183500	0.48975900	-1.63814900
C	3.42329500	-0.80185400	-1.33159700
H	3.45651700	1.69645000	-5.07237800
H	3.73999300	-0.74972500	-3.89894200
H	5.10396300	0.36150300	-3.98653500
O	4.14257000	-1.71138100	-0.86343800
O	2.17083300	-0.74638800	-1.36902800
N	-3.37946600	-1.63800800	-1.76937600
H	-2.36751300	-1.43733200	-1.57850900
H	-3.70987500	-2.09499800	-0.89895000
C	-3.43899000	-2.43371100	-3.01818900
C	-4.13082800	-0.37087100	-2.02664500
H	-2.70925100	-3.23808800	-2.97977100
H	-4.44125100	-2.85796300	-3.12481800
C	-3.18144900	-1.35496000	-4.06876500
C	-4.10123500	-0.22856100	-3.57216500
H	-5.14183500	-0.48975900	-1.63814900
C	-3.42329500	0.80185400	-1.33159700
H	-3.45651700	-1.69645000	-5.07237800
H	-3.73999300	0.74972500	-3.89894200
H	-5.10396300	-0.36150300	-3.98653500
O	-4.14257000	1.71138100	-0.86343800
O	-2.17083300	0.74638800	-1.36902800
N	-1.63800800	3.37946600	-1.76937600
H	-1.43733200	2.36751300	-1.57850900
H	-2.09499800	3.70987500	-0.89895000
C	-2.43371100	3.43899000	-3.01818900
C	-0.37087100	4.13082800	-2.02664500
H	-3.23808800	2.70925100	-2.97977100
H	-2.85796300	4.44125100	-3.12481800
C	-1.35496000	3.18144900	-4.06876500
C	-0.22856100	4.10123500	-3.57216500
H	-0.48975900	5.14183500	-1.63814900

C	0.80185400	3.42329500	-1.33159700
H	-1.69645000	3.45651700	-5.07237800
H	0.74972500	3.73999300	-3.89894200
H	-0.36150300	5.10396300	-3.98653500
O	1.71138100	4.14257000	-0.86343800
O	0.74638800	2.17083300	-1.36902800
O	-1.81101700	-1.00076100	-4.04990100
H	-1.69647800	-0.04106800	-3.91285100
O	1.00076100	-1.81101700	-4.04990100
H	0.04106800	-1.69647800	-3.91285100
O	1.81101700	1.00076100	-4.04990100
H	1.69647800	0.04106800	-3.91285100
O	-1.00076100	1.81101700	-4.04990100
H	-0.04106800	1.69647800	-3.91285100
O	-1.81101700	1.00076100	4.04990100
H	-1.69647800	0.04106800	3.91285100
O	1.00076100	1.81101700	4.04990100
H	0.04106800	1.69647800	3.91285100
O	1.81101700	-1.00076100	4.04990100
H	1.69647800	-0.04106800	3.91285100
O	-1.00076100	-1.81101700	4.04990100
H	-0.04106800	-1.69647800	3.91285100

b. XYZ Coordinates of C4LP-8-K-2 (Calculated at the wB97X-D/6-31+g(d)/def2-QZVP level.)

atom	X	Y	Z
K	1.59680400	-1.04600800	-0.49757600
N	6.13505300	-2.07006500	-0.03616500
H	5.55713900	-1.22785700	0.19889700
H	6.98042400	-2.02576000	0.53167400
C	6.42152200	-2.07446100	-1.50452300
C	5.27593300	-3.27072100	0.28224600
H	6.65150300	-1.05934700	-1.82723100
H	7.26582600	-2.74152500	-1.69622800
C	5.12834300	-2.65998800	-2.06823500
C	4.86684100	-3.82052400	-1.10125400
H	5.86380000	-3.98886800	0.85589100
C	4.07428300	-2.79697500	1.13154100
H	5.27182900	-3.00512000	-3.09829200
H	3.81988500	-4.12854600	-1.10787000
H	5.47980400	-4.68670900	-1.37185400
O	3.95177700	-1.56328100	1.29760000
O	3.33249100	-3.72082700	1.53588200

N	4.05875400	-1.74325400	-2.00976300
H	4.38829100	-0.84154200	-1.79353800
H	-3.78956200	-2.14111300	0.75200300
C	-3.45138700	-1.34231600	0.18324800
C	-3.02102000	-2.84646000	0.69636300
H	-5.03204000	-2.68099800	0.11467900
H	-4.11197100	-1.73104300	2.16655600
C	-4.99002200	-2.51191300	-0.96147500
C	-5.08060900	-3.75464600	0.31702200
H	-6.14538300	-1.91644400	0.82643100
C	-5.64435700	-1.90750200	2.27836300
H	-3.56404500	-2.38971400	2.83693600
H	-3.65436100	-0.27663400	2.37809200
H	-7.10678800	-2.42287900	0.71925700
O	-6.11754700	-1.11541000	2.86390100
O	-5.86954600	-2.86440700	2.75903100
N	-4.07321200	0.55710200	1.50615700
H	-2.92541000	0.00153500	3.34375800
H	-6.29844100	-0.61648400	0.30177500
C	-5.58507700	-0.06598800	0.68132200
C	-2.35056000	2.70773400	1.92339300
H	-2.57694600	3.39495900	1.18837000
H	-2.96777600	1.88611700	1.76294700
C	-2.56263100	3.24326700	3.30531800
C	-0.90137800	2.35748600	1.74619700
H	-3.25318900	4.08627600	3.27565800
C	-2.96985600	2.42866500	3.90683600
H	-1.16949700	3.62740600	3.77381000
H	-0.30192100	2.53985100	3.14029700
H	-0.81217500	1.32206000	1.41005500
O	-0.33020700	3.24447000	0.62261900
O	-1.10733600	3.64001100	4.86837200
N	0.75929500	2.78663300	3.10523800
H	-0.40065300	1.60803500	3.70455600
H	-1.15788900	3.85071400	-0.10351900
C	0.91582700	3.24340600	0.48260500
C	-0.90286500	4.91170900	3.23267400
H	-0.01270700	5.18929400	3.48069700
H	-1.23730200	-2.53891800	-2.69978400
C	-1.81809900	-1.97306900	-2.04769500
C	-0.48524900	-1.87190100	-3.02305600
H	-2.09650400	-3.03804700	-3.81243600
C	-0.60437800	-3.72915800	-2.00922200
H	-2.92501800	-2.34634100	-3.96504500

H	-1.48889700	-3.09807600	-4.71982100
H	-2.53544500	-4.41668300	-3.31872500
O	-1.23520900	-4.95005300	-2.70041300
O	0.47254400	-3.66355500	-2.17398400
N	-0.89762600	-3.59122300	-0.49460000
H	-2.89153500	-5.03923900	-4.14396600
H	-1.42146200	-5.76731900	-2.00021000
C	-0.57224100	-5.31760900	-3.49028400
C	-2.03369400	-3.99428200	-0.11124200
H	-0.02353200	-3.03965300	0.19852500
H	-3.57463500	-4.30555200	-2.37413200
C	-3.16603300	-4.28307800	-1.48208900
C	1.07278600	2.20693600	-2.26432400
H	0.19031500	1.83899600	-1.85361300
C	1.78663400	2.09949200	-1.52191200
H	0.90144700	3.63504400	-2.68031200
H	1.48018800	1.39805700	-3.48427300
H	0.15949400	4.10795500	-2.03508000
O	1.86241900	4.14142900	-2.55495900
O	0.52251400	3.52014300	-4.15244600
N	1.47670900	2.42175600	-4.63105400
H	2.46626100	0.98325400	-3.27816900
H	0.47199100	0.23457900	-3.65291600
C	0.66032600	4.46663000	-4.67991100
C	1.16221500	1.97890200	-5.57875600
H	2.47783700	2.84330400	-4.76460200
H	-0.60801200	0.47129600	-4.24499100
C	0.81133900	-0.86026600	-3.13576400
C	-0.83684600	3.12543300	-4.30354500
H	-0.85032800	2.14310100	-4.45421200
C	-2.63071500	2.87117500	-2.19070600
H	-2.08476000	3.00669000	-1.31103700
H	-1.98862300	3.13607100	-2.96502900
H	-3.84802600	3.73023400	-2.12897900
O	-3.08441800	1.44366500	-2.33509600
O	-3.61038100	4.65813500	-1.60701900
N	-4.18580600	3.94135000	-3.14669300
H	-4.83197900	2.84193600	-1.38138800
H	-4.59295800	1.47304700	-2.02379400
C	-2.90125800	1.14486600	-3.37127100
C	-2.22286700	0.49142800	-1.49041500
H	-5.86561700	3.18640100	-1.49517600
H	-4.89352800	0.63757300	-1.38765200
C	-5.17571100	1.39920600	-2.94712800

C	-2.71622300	-0.65559300	-1.31753100
H	-1.10232300	0.88842000	-1.10569600
C	-4.43737600	2.87819500	-0.02304900
H	-4.66783000	2.04879600	0.42508400
H	3.21499300	2.24447600	1.69047500
H	2.42569500	2.16557800	1.02302000
O	2.95394100	1.58989500	2.49063800
O	3.33582000	3.66407700	2.11021800
N	4.48879100	1.87532800	0.99999100
H	2.34275100	4.08630900	2.26153900
H	3.90933200	3.70927300	3.04021200
C	4.10798900	4.28645000	0.95227600
C	5.19322000	3.22836100	0.71390800
H	5.06945700	1.24113400	1.67174800
H	4.20253700	1.08707300	-0.27844000
C	4.53770900	5.25560200	1.22796600
C	5.58638500	3.28274100	-0.30296300
H	6.02460600	3.37787300	1.41031300
C	3.04095900	1.13193900	-0.74828500
H	5.16879800	0.45349600	-0.76976100
H	3.31065900	4.43913900	-0.20509200
H	2.37536100	4.22755400	-0.01506100
O	1.12718100	-2.71943400	2.76767000
O	0.50261200	-2.32940800	2.04419600
O	1.94958300	-3.14514500	2.26250300
H	0.36469000	-3.69861300	3.58018800
O	1.57351200	-1.64830100	3.70313900
H	-0.23276200	-4.33473000	2.92634200
O	1.07197200	-4.29827500	4.15982100
H	-0.47573800	-2.77713500	4.45678200
O	0.51331900	-1.65874200	4.83418200
H	2.55649600	-1.93786300	4.07916700
O	1.71073800	-0.29937100	2.98913800
H	-0.87402100	-3.29261200	5.33887600
O	0.00451300	-0.69452200	4.92740400
H	0.98607000	-1.86920500	5.79710500
O	1.09067300	-0.14456600	1.91399600
H	2.42235600	0.54794100	3.59151800
O	-1.52070500	-2.32940400	3.62400900
H	-1.84758400	-1.43414500	3.84293700

c. XYZ Coordinates of C4LP-8-K-3 (Calculated at the wB97X-D/6-31+g(d)/def2-QZVP level.)

atom	X	Y	Z
K	0.84703300	0.81529900	0.06303500
N	1.94750300	-1.18417500	3.71870200
H	1.42898200	-0.74603400	2.93778400
H	1.83316300	-2.21221200	3.58684200
C	1.40247300	-0.60411200	4.98776600
C	3.41963500	-0.80552500	3.62122700
H	0.32514900	-0.47775400	4.88528500
H	1.63804000	-1.27925300	5.81549900
C	2.18276900	0.71497900	5.08268900
C	3.61033600	0.25276400	4.73693400
H	4.01338200	-1.70601700	3.77432600
C	3.66785100	-0.22106500	2.21613200
H	2.11430700	1.14918200	6.08298200
H	4.23744700	1.08540000	4.40978700
H	4.08174900	-0.20025100	5.61504500
O	2.75496700	0.57265200	1.81863400
O	4.71051600	-0.55305100	1.62735600
N	1.67485600	1.68152100	4.17658300
H	1.97913500	1.46193200	3.26331600
H	-0.50851100	-3.35492400	0.99399300
C	-0.21680400	-2.37312500	0.86278800
C	-1.51910000	-3.38792100	0.71388500
H	-0.44924300	-3.78272700	2.43266900
H	0.32091300	-4.32182200	0.16527800
C	-0.48375300	-2.89700800	3.06444800
C	-1.32847000	-4.40550100	2.61981900
H	0.84104900	-4.59101700	2.53699300
C	0.84974400	-5.34558700	1.19819000
H	-0.34794000	-4.77306400	-0.56576200
H	1.47269500	-3.59464500	-0.56654800
H	0.82922700	-5.26554800	3.39640100
O	1.84312100	-5.72183000	0.94209900
O	0.16806600	-6.20026000	1.25987800
N	2.28320800	-2.94230100	0.16544600
H	1.54276300	-3.75487400	-1.80492200
H	1.97830500	-3.73939200	2.69294900
C	2.22764000	-3.39843400	1.78532800
C	-2.07923700	3.18221700	-1.39030100
H	-2.21287100	2.68373100	-0.50016400
H	-1.04879300	3.13888000	-1.58744000
C	-2.50687600	4.61613600	-1.22366500
C	-2.95886200	2.52622600	-2.43078300
H	-2.34714000	4.91637200	-0.18819800

C	-1.88758900	5.22083600	-1.89140700
H	-3.97882700	4.59456800	-1.63467100
H	-3.95225500	3.64176200	-2.84360500
H	-2.33590700	2.16853700	-3.24577100
O	-3.68454600	1.33931000	-1.78182400
O	-4.33905600	5.59185300	-1.89493200
N	-4.94273400	3.24765100	-3.08406200
H	-3.57177500	4.17038700	-3.72385400
H	-3.93141300	1.45161500	-0.53161600
C	-4.05025500	0.39928100	-2.52446000
C	-4.81608000	4.12707600	-0.57970200
H	-4.65080000	3.16673200	-0.46521000
H	4.35211800	-1.42142800	-0.94136900
C	4.59116000	-0.83195300	-0.11370000
C	3.55696800	-2.01809000	-0.61980600
H	5.55015400	-2.25505800	-1.31159500
C	3.95881100	-0.58759700	-2.15689400
H	6.16657400	-2.40971300	-0.42555500
H	5.18787000	-3.21177900	-1.69946300
H	6.24182900	-1.41978900	-2.39514900
O	5.03943300	-0.90824700	-3.20807800
O	2.96949400	-0.90648100	-2.47660900
N	3.90761200	0.89411700	-1.74071900
H	6.91239700	-2.04182700	-2.99530300
H	5.30198600	-0.03402400	-3.80816300
C	4.66814300	-1.68866200	-3.88009300
C	4.98202600	1.48924700	-1.48840800
H	2.74267400	1.40129600	-1.66629500
H	7.02017200	-0.38419700	-1.83359600
C	6.43730800	0.38922100	-1.64736000
C	-0.91704300	-2.85964300	-3.08173500
H	-0.21575300	-2.96685200	-2.32232200
C	-1.75841200	-3.35714500	-2.73998000
H	-0.32574400	-3.35504300	-4.36251500
H	-1.14631300	-1.37216700	-3.20893700
H	0.19847600	-4.29510100	-4.18361700
O	-1.13246700	-3.50352000	-5.08528300
O	0.58741500	-2.19346200	-4.77021000
N	-0.26662900	-0.95374900	-4.41625200
H	-2.20690400	-1.18747600	-3.38847200
H	-0.73473700	-0.69839200	-1.88750800
C	0.81184500	-2.22664500	-5.84018600
C	0.37052600	-0.10049800	-4.17550300
H	-0.90049900	-0.67701900	-5.26521300

H	-0.10452700	-1.42219700	-1.06327700
C	-1.01869300	0.51485900	-1.77380700
C	1.83248900	-2.20839900	-4.08871000
H	1.79388700	-2.73637100	-3.26037100
C	-3.64737200	1.01249000	2.21019900
H	-3.48211300	0.90986300	1.18424700
H	-4.49798900	0.47323900	2.40145700
H	-3.73026300	2.47369800	2.56072500
O	-2.46995200	0.41139000	2.96735600
O	-4.16367800	3.02965400	1.72928800
N	-4.34575200	2.58596200	3.45612200
H	-2.27471300	2.83106100	2.84977000
H	-1.77121500	1.61043800	3.63294700
C	-2.88188000	-0.28178700	3.70582500
C	-1.65131900	-0.43225300	1.96514200
H	-2.20376900	3.76128900	3.42489600
H	-0.68338300	1.51900600	3.60255400
C	-2.07201900	1.69875100	4.68355800
C	-2.26999300	-0.82309800	0.95188400
H	-0.45243900	-0.68169800	2.28044600
C	-1.60671500	2.95948500	1.59873400
H	-0.67859600	3.25097900	1.75469400
H	-4.67379300	-1.35258100	-0.61179900
H	-3.84878000	-1.15928200	-0.01000500
O	-4.49032800	-0.80194600	-1.50191900
O	-5.90007200	-0.85116500	0.08121500
N	-4.86899400	-2.85236300	-0.77853500
H	-5.71577000	0.14916700	0.46475700
H	-6.71350400	-0.80756000	-0.64950200
C	-6.11309900	-1.94771500	1.11982200
C	-5.97921500	-3.20671300	0.24600400
H	-5.16553500	-3.03362100	-1.81191300
H	-3.52055900	-3.53189300	-0.47376400
C	-7.07999900	-1.87670600	1.62382800
C	-5.72369600	-4.09022300	0.83363600
H	-6.92702900	-3.39642200	-0.26721100
C	-3.21452900	-3.57123000	0.75850700
H	-2.82328400	-3.93862700	-1.42984500
H	-5.08973200	-1.85058000	2.11636500
H	-4.33933700	-2.43332900	1.84607600
O	3.29416900	3.78719600	-0.70101900
O	2.91605600	2.87446600	-1.14465600
O	4.21254000	3.88360000	-1.14123300
H	3.45148200	3.57117300	0.78799700

O	2.39248700	4.98815500	-0.94228000
H	3.47535200	2.50120200	0.99828000
O	4.38744700	4.03506400	1.10926400
H	2.24507600	4.29498200	1.39315700
O	2.12199500	5.53151500	0.48333500
H	2.91105000	5.70519100	-1.57777100
O	1.06995500	4.56127300	-1.63001100
H	2.41602300	4.54893300	2.44085800
O	1.14452700	6.01432800	0.56063900
H	2.88560600	6.26756100	0.75865600
O	0.57295100	3.45285300	-1.18764700
H	0.56741400	5.31709000	-2.45998500
O	1.07005800	3.47882200	1.34819600
H	0.81724800	3.42660300	0.37601800

d. XYZ Coordinates of T4LP-8-K-1 (Calculated at the wB97X-D/6-31+g(d)/def2-QZVP level.)

atom	X	Y	Z
K	0.00000000	0.00000000	0.00000000
N	-1.26472100	3.64594900	1.68553900
H	-0.66341700	2.79166500	1.65740500
H	-1.12669500	4.09443900	0.76293300
C	-0.84196500	4.51672600	2.83116800
C	-2.71299300	3.30091000	1.84154100
H	-0.14353200	3.94272300	3.44264300
H	-0.34554600	5.40934300	2.45563600
C	-2.12720100	4.82742800	3.59012100
C	-2.99086900	3.59084300	3.31830700
H	-3.28067700	3.98235900	1.20700600
C	-2.99635400	1.84821600	1.43755300
H	-1.92974000	4.97758600	4.65870200
H	-2.64968800	2.75461000	3.94192700
H	-4.05458200	3.75569900	3.50711600
O	-4.15260900	1.60545000	1.01672100
O	-2.05625300	1.02823700	1.59175000
N	3.64594900	1.26472100	1.68553900
H	2.79166500	0.66341700	1.65740500
H	4.09443900	1.12669500	0.76293300
C	4.51672600	0.84196500	2.83116800
C	3.30091000	2.71299300	1.84154100
H	3.94272300	0.14353200	3.44264300
H	5.40934300	0.34554600	2.45563600
C	4.82742800	2.12720100	3.59012100

C	3.59084300	2.99086900	3.31830700
H	3.98235900	3.28067700	1.20700600
C	1.84821600	2.99635400	1.43755300
H	4.97758600	1.92974000	4.65870200
H	2.75461000	2.64968800	3.94192700
H	3.75569900	4.05458200	3.50711600
O	1.60545000	4.15260900	1.01672100
O	1.02823700	2.05625300	1.59175000
N	-3.64594900	-1.26472100	1.68553900
H	-2.79166500	-0.66341700	1.65740500
H	-4.09443900	-1.12669500	0.76293300
C	-4.51672600	-0.84196500	2.83116800
C	-3.30091000	-2.71299300	1.84154100
H	-3.94272300	-0.14353200	3.44264300
H	-5.40934300	-0.34554600	2.45563600
C	-4.82742800	-2.12720100	3.59012100
C	-3.59084300	-2.99086900	3.31830700
H	-3.98235900	-3.28067700	1.20700600
C	-1.84821600	-2.99635400	1.43755300
H	-4.97758600	-1.92974000	4.65870200
H	-2.75461000	-2.64968800	3.94192700
H	-3.75569900	-4.05458200	3.50711600
O	-1.60545000	-4.15260900	1.01672100
O	-1.02823700	-2.05625300	1.59175000
N	1.26472100	-3.64594900	1.68553900
H	0.66341700	-2.79166500	1.65740500
H	1.12669500	-4.09443900	0.76293300
C	0.84196500	-4.51672600	2.83116800
C	2.71299300	-3.30091000	1.84154100
H	0.14353200	-3.94272300	3.44264300
H	0.34554600	-5.40934300	2.45563600
C	2.12720100	-4.82742800	3.59012100
C	2.99086900	-3.59084300	3.31830700
H	3.28067700	-3.98235900	1.20700600
C	2.99635400	-1.84821600	1.43755300
H	1.92974000	-4.97758600	4.65870200
H	2.64968800	-2.75461000	3.94192700
H	4.05458200	-3.75569900	3.50711600
O	4.15260900	-1.60545000	1.01672100
O	2.05625300	-1.02823700	1.59175000
N	3.64594900	-1.26472100	-1.68553900
H	2.79166500	-0.66341700	-1.65740500
H	4.09443900	-1.12669500	-0.76293300
C	4.51672600	-0.84196500	-2.83116800

C	3.30091000	-2.71299300	-1.84154100
H	3.94272300	-0.14353200	-3.44264300
H	5.40934300	-0.34554600	-2.45563600
C	4.82742800	-2.12720100	-3.59012100
C	3.59084300	-2.99086900	-3.31830700
H	3.98235900	-3.28067700	-1.20700600
C	1.84821600	-2.99635400	-1.43755300
H	4.97758600	-1.92974000	-4.65870200
H	2.75461000	-2.64968800	-3.94192700
H	3.75569900	-4.05458200	-3.50711600
O	1.60545000	-4.15260900	-1.01672100
O	1.02823700	-2.05625300	-1.59175000
N	1.26472100	3.64594900	-1.68553900
H	0.66341700	2.79166500	-1.65740500
H	1.12669500	4.09443900	-0.76293300
C	0.84196500	4.51672600	-2.83116800
C	2.71299300	3.30091000	-1.84154100
H	0.14353200	3.94272300	-3.44264300
H	0.34554600	5.40934300	-2.45563600
C	2.12720100	4.82742800	-3.59012100
C	2.99086900	3.59084300	-3.31830700
H	3.28067700	3.98235900	-1.20700600
C	2.99635400	1.84821600	-1.43755300
H	1.92974000	4.97758600	-4.65870200
H	2.64968800	2.75461000	-3.94192700
H	4.05458200	3.75569900	-3.50711600
O	4.15260900	1.60545000	-1.01672100
O	2.05625300	1.02823700	-1.59175000
N	-1.26472100	-3.64594900	-1.68553900
H	-0.66341700	-2.79166500	-1.65740500
H	-1.12669500	-4.09443900	-0.76293300
C	-0.84196500	-4.51672600	-2.83116800
C	-2.71299300	-3.30091000	-1.84154100
H	-0.14353200	-3.94272300	-3.44264300
H	-0.34554600	-5.40934300	-2.45563600
C	-2.12720100	-4.82742800	-3.59012100
C	-2.99086900	-3.59084300	-3.31830700
H	-3.28067700	-3.98235900	-1.20700600
C	-2.99635400	-1.84821600	-1.43755300
H	-1.92974000	-4.97758600	-4.65870200
H	-2.64968800	-2.75461000	-3.94192700
H	-4.05458200	-3.75569900	-3.50711600
O	-4.15260900	-1.60545000	-1.01672100
O	-2.05625300	-1.02823700	-1.59175000

N	-3.64594900	1.26472100	-1.68553900
H	-2.79166500	0.66341700	-1.65740500
H	-4.09443900	1.12669500	-0.76293300
C	-4.51672600	0.84196500	-2.83116800
C	-3.30091000	2.71299300	-1.84154100
H	-3.94272300	0.14353200	-3.44264300
H	-5.40934300	0.34554600	-2.45563600
C	-4.82742800	2.12720100	-3.59012100
C	-3.59084300	2.99086900	-3.31830700
H	-3.98235900	3.28067700	-1.20700600
C	-1.84821600	2.99635400	-1.43755300
H	-4.97758600	1.92974000	-4.65870200
H	-2.75461000	2.64968800	-3.94192700
H	-3.75569900	4.05458200	-3.50711600
O	-1.60545000	4.15260900	-1.01672100
O	-1.02823700	2.05625300	-1.59175000
O	-2.67201000	-5.99805400	-3.00904900
H	-3.48781700	-6.23900200	-3.46535000
O	5.99805400	-2.67201000	-3.00904900
H	6.23900200	-3.48781700	-3.46535000
O	2.67201000	5.99805400	-3.00904900
H	3.48781700	6.23900200	-3.46535000
O	-5.99805400	2.67201000	-3.00904900
H	-6.23900200	3.48781700	-3.46535000
O	-2.67201000	5.99805400	3.00904900
H	-3.48781700	6.23900200	3.46535000
O	-5.99805400	-2.67201000	3.00904900
H	-6.23900200	-3.48781700	3.46535000
O	2.67201000	-5.99805400	3.00904900
H	3.48781700	-6.23900200	3.46535000
O	5.99805400	2.67201000	3.00904900
H	6.23900200	3.48781700	3.46535000

e. XYZ Coordinates of C4LP-8-Na-1 (Calculated at the wB97X-D/6-31g(d)/def2-QZVP level.)

atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	3.52442000	1.19497700	1.76704600
H	2.66769100	0.61521200	1.57147400
H	4.08267600	1.10167800	0.89931100
C	4.13399200	0.69292700	3.02041600
C	3.14045400	2.61664400	2.01051100
H	4.20374500	-0.39118700	2.98963900

H	5.13666100	1.11700600	3.12501200
C	3.18159200	1.27249700	4.06377600
C	3.02752200	2.71397200	3.55580400
H	3.92454600	3.25970200	1.61216000
C	1.80424300	2.91566000	1.31703100
H	3.61307300	1.23424600	5.06966100
H	2.08233100	3.15185700	3.88514200
H	3.83220500	3.33545400	3.95724800
O	1.64551100	4.07508500	0.87268200
O	0.97827200	1.97181000	1.33184800
N	1.19497700	-3.52442000	1.76704600
H	0.61521200	-2.66769100	1.57147400
H	1.10167800	-4.08267600	0.89931100
C	0.69292700	-4.13399200	3.02041600
C	2.61664400	-3.14045400	2.01051100
H	-0.39118700	-4.20374500	2.98963900
H	1.11700600	-5.13666100	3.12501200
C	1.27249700	-3.18159200	4.06377600
C	2.71397200	-3.02752200	3.55580400
H	3.25970200	-3.92454600	1.61216000
C	2.91566000	-1.80424300	1.31703100
H	1.23424600	-3.61307300	5.06966100
H	3.15185700	-2.08233100	3.88514200
H	3.33545400	-3.83220500	3.95724800
O	4.07508500	-1.64551100	0.87268200
O	1.97181000	-0.97827200	1.33184800
N	-1.19497700	3.52442000	1.76704600
H	-0.61521200	2.66769100	1.57147400
H	-1.10167800	4.08267600	0.89931100
C	-0.69292700	4.13399200	3.02041600
C	-2.61664400	3.14045400	2.01051100
H	0.39118700	4.20374500	2.98963900
H	-1.11700600	5.13666100	3.12501200
C	-1.27249700	3.18159200	4.06377600
C	-2.71397200	3.02752200	3.55580400
H	-3.25970200	3.92454600	1.61216000
C	-2.91566000	1.80424300	1.31703100
H	-1.23424600	3.61307300	5.06966100
H	-3.15185700	2.08233100	3.88514200
H	-3.33545400	3.83220500	3.95724800
O	-4.07508500	1.64551100	0.87268200
O	-1.97181000	0.97827200	1.33184800
N	-3.52442000	-1.19497700	1.76704600
H	-2.66769100	-0.61521200	1.57147400

H	-4.08267600	-1.10167800	0.89931100
C	-4.13399200	-0.69292700	3.02041600
C	-3.14045400	-2.61664400	2.01051100
H	-4.20374500	0.39118700	2.98963900
H	-5.13666100	-1.11700600	3.12501200
C	-3.18159200	-1.27249700	4.06377600
C	-3.02752200	-2.71397200	3.55580400
H	-3.92454600	-3.25970200	1.61216000
C	-1.80424300	-2.91566000	1.31703100
H	-3.61307300	-1.23424600	5.06966100
H	-2.08233100	-3.15185700	3.88514200
H	-3.83220500	-3.33545400	3.95724800
O	-1.64551100	-4.07508500	0.87268200
O	-0.97827200	-1.97181000	1.33184800
N	-1.19497700	-3.52442000	-1.76704600
H	-0.61521200	-2.66769100	-1.57147400
H	-1.10167800	-4.08267600	-0.89931100
C	-0.69292700	-4.13399200	-3.02041600
C	-2.61664400	-3.14045400	-2.01051100
H	0.39118700	-4.20374500	-2.98963900
H	-1.11700600	-5.13666100	-3.12501200
C	-1.27249700	-3.18159200	-4.06377600
C	-2.71397200	-3.02752200	-3.55580400
H	-3.25970200	-3.92454600	-1.61216000
C	-2.91566000	-1.80424300	-1.31703100
H	-1.23424600	-3.61307300	-5.06966100
H	-3.15185700	-2.08233100	-3.88514200
H	-3.33545400	-3.83220500	-3.95724800
O	-4.07508500	-1.64551100	-0.87268200
O	-1.97181000	-0.97827200	-1.33184800
N	3.52442000	-1.19497700	-1.76704600
H	2.66769100	-0.61521200	-1.57147400
H	4.08267600	-1.10167800	-0.89931100
C	4.13399200	-0.69292700	-3.02041600
C	3.14045400	-2.61664400	-2.01051100
H	4.20374500	0.39118700	-2.98963900
H	5.13666100	-1.11700600	-3.12501200
C	3.18159200	-1.27249700	-4.06377600
C	3.02752200	-2.71397200	-3.55580400
H	3.92454600	-3.25970200	-1.61216000
C	1.80424300	-2.91566000	-1.31703100
H	3.61307300	-1.23424600	-5.06966100
H	2.08233100	-3.15185700	-3.88514200
H	3.83220500	-3.33545400	-3.95724800

O	1.64551100	-4.07508500	-0.87268200
O	0.97827200	-1.97181000	-1.33184800
N	-3.52442000	1.19497700	-1.76704600
H	-2.66769100	0.61521200	-1.57147400
H	-4.08267600	1.10167800	-0.89931100
C	-4.13399200	0.69292700	-3.02041600
C	-3.14045400	2.61664400	-2.01051100
H	-4.20374500	-0.39118700	-2.98963900
H	-5.13666100	1.11700600	-3.12501200
C	-3.18159200	1.27249700	-4.06377600
C	-3.02752200	2.71397200	-3.55580400
H	-3.92454600	3.25970200	-1.61216000
C	-1.80424300	2.91566000	-1.31703100
H	-3.61307300	1.23424600	-5.06966100
H	-2.08233100	3.15185700	-3.88514200
H	-3.83220500	3.33545400	-3.95724800
O	-1.64551100	4.07508500	-0.87268200
O	-0.97827200	1.97181000	-1.33184800
N	1.19497700	3.52442000	-1.76704600
H	0.61521200	2.66769100	-1.57147400
H	1.10167800	4.08267600	-0.89931100
C	0.69292700	4.13399200	-3.02041600
C	2.61664400	3.14045400	-2.01051100
H	-0.39118700	4.20374500	-2.98963900
H	1.11700600	5.13666100	-3.12501200
C	1.27249700	3.18159200	-4.06377600
C	2.71397200	3.02752200	-3.55580400
H	3.25970200	3.92454600	-1.61216000
C	2.91566000	1.80424300	-1.31703100
H	1.23424600	3.61307300	-5.06966100
H	3.15185700	2.08233100	-3.88514200
H	3.33545400	3.83220500	-3.95724800
O	4.07508500	1.64551100	-0.87268200
O	1.97181000	0.97827200	-1.33184800
O	-1.96579100	0.54944600	-4.03927700
H	-1.20556900	1.14690400	-3.90057400
O	-0.54944600	-1.96579100	-4.03927700
H	-1.14690400	-1.20556900	-3.90057400
O	1.96579100	-0.54944600	-4.03927700
H	1.20556900	-1.14690400	-3.90057400
O	0.54944600	1.96579100	-4.03927700
H	1.14690400	1.20556900	-3.90057400
O	-0.54944600	1.96579100	4.03927700
H	-1.14690400	1.20556900	3.90057400

O	1.96579100	0.54944600	4.03927700
H	1.20556900	1.14690400	3.90057400
O	0.54944600	-1.96579100	4.03927700
H	1.14690400	-1.20556900	3.90057400
O	-1.96579100	-0.54944600	4.03927700
H	-1.20556900	-1.14690400	3.90057400

f. XYZ Coordinates of T4LP-8-Na-1 (Calculated at the wB97X-D/6-31g(d)/def2-QZVP level.)

atom	X	Y	Z
Na	0.00000000	0.00000000	0.00000000
N	-1.20603000	3.60002400	1.67727500
H	-0.61613900	2.73429600	1.62655000
H	-1.05627700	4.06135800	0.76271400
C	-0.78168700	4.43626900	2.84529800
C	-2.65484200	3.26308400	1.81466100
H	-0.11228300	3.83048900	3.45837900
H	-0.25458400	5.32141700	2.49698500
C	-2.07490100	4.76231600	3.58305400
C	-2.94272600	3.53224400	3.29330500
H	-3.21354800	3.95428300	1.18457700
C	-2.92948500	1.81434900	1.39336900
H	-1.89430900	4.91014800	4.65587100
H	-2.60738200	2.68487000	3.90427700
H	-4.00679200	3.69643500	3.47966800
O	-4.09209900	1.56984700	0.99660800
O	-1.97528400	1.00619200	1.52253100
N	3.60002400	1.20603000	1.67727500
H	2.73429600	0.61613900	1.62655000
H	4.06135800	1.05627700	0.76271400
C	4.43626900	0.78168700	2.84529800
C	3.26308400	2.65484200	1.81466100
H	3.83048900	0.11228300	3.45837900
H	5.32141700	0.25458400	2.49698500
C	4.76231600	2.07490100	3.58305400
C	3.53224400	2.94272600	3.29330500
H	3.95428300	3.21354800	1.18457700
C	1.81434900	2.92948500	1.39336900
H	4.91014800	1.89430900	4.65587100
H	2.68487000	2.60738200	3.90427700
H	3.69643500	4.00679200	3.47966800
O	1.56984700	4.09209900	0.99660800
O	1.00619200	1.97528400	1.52253100

N	-3.60002400	-1.20603000	1.67727500
H	-2.73429600	-0.61613900	1.62655000
H	-4.06135800	-1.05627700	0.76271400
C	-4.43626900	-0.78168700	2.84529800
C	-3.26308400	-2.65484200	1.81466100
H	-3.83048900	-0.11228300	3.45837900
H	-5.32141700	-0.25458400	2.49698500
C	-4.76231600	-2.07490100	3.58305400
C	-3.53224400	-2.94272600	3.29330500
H	-3.95428300	-3.21354800	1.18457700
C	-1.81434900	-2.92948500	1.39336900
H	-4.91014800	-1.89430900	4.65587100
H	-2.68487000	-2.60738200	3.90427700
H	-3.69643500	-4.00679200	3.47966800
O	-1.56984700	-4.09209900	0.99660800
O	-1.00619200	-1.97528400	1.52253100
N	1.20603000	-3.60002400	1.67727500
H	0.61613900	-2.73429600	1.62655000
H	1.05627700	-4.06135800	0.76271400
C	0.78168700	-4.43626900	2.84529800
C	2.65484200	-3.26308400	1.81466100
H	0.11228300	-3.83048900	3.45837900
H	0.25458400	-5.32141700	2.49698500
C	2.07490100	-4.76231600	3.58305400
C	2.94272600	-3.53224400	3.29330500
H	3.21354800	-3.95428300	1.18457700
C	2.92948500	-1.81434900	1.39336900
H	1.89430900	-4.91014800	4.65587100
H	2.60738200	-2.68487000	3.90427700
H	4.00679200	-3.69643500	3.47966800
O	4.09209900	-1.56984700	0.99660800
O	1.97528400	-1.00619200	1.52253100
N	3.60002400	-1.20603000	-1.67727500
H	2.73429600	-0.61613900	-1.62655000
H	4.06135800	-1.05627700	-0.76271400
C	4.43626900	-0.78168700	-2.84529800
C	3.26308400	-2.65484200	-1.81466100
H	3.83048900	-0.11228300	-3.45837900
H	5.32141700	-0.25458400	-2.49698500
C	4.76231600	-2.07490100	-3.58305400
C	3.53224400	-2.94272600	-3.29330500
H	3.95428300	-3.21354800	-1.18457700
C	1.81434900	-2.92948500	-1.39336900
H	4.91014800	-1.89430900	-4.65587100

H	2.68487000	-2.60738200	-3.90427700
H	3.69643500	-4.00679200	-3.47966800
O	1.56984700	-4.09209900	-0.99660800
O	1.00619200	-1.97528400	-1.52253100
N	1.20603000	3.60002400	-1.67727500
H	0.61613900	2.73429600	-1.62655000
H	1.05627700	4.06135800	-0.76271400
C	0.78168700	4.43626900	-2.84529800
C	2.65484200	3.26308400	-1.81466100
H	0.11228300	3.83048900	-3.45837900
H	0.25458400	5.32141700	-2.49698500
C	2.07490100	4.76231600	-3.58305400
C	2.94272600	3.53224400	-3.29330500
H	3.21354800	3.95428300	-1.18457700
C	2.92948500	1.81434900	-1.39336900
H	1.89430900	4.91014800	-4.65587100
H	2.60738200	2.68487000	-3.90427700
H	4.00679200	3.69643500	-3.47966800
O	4.09209900	1.56984700	-0.99660800
O	1.97528400	1.00619200	-1.52253100
N	-1.20603000	-3.60002400	-1.67727500
H	-0.61613900	-2.73429600	-1.62655000
H	-1.05627700	-4.06135800	-0.76271400
C	-0.78168700	-4.43626900	-2.84529800
C	-2.65484200	-3.26308400	-1.81466100
H	-0.11228300	-3.83048900	-3.45837900
H	-0.25458400	-5.32141700	-2.49698500
C	-2.07490100	-4.76231600	-3.58305400
C	-2.94272600	-3.53224400	-3.29330500
H	-3.21354800	-3.95428300	-1.18457700
C	-2.92948500	-1.81434900	-1.39336900
H	-1.89430900	-4.91014800	-4.65587100
H	-2.60738200	-2.68487000	-3.90427700
H	-4.00679200	-3.69643500	-3.47966800
O	-4.09209900	-1.56984700	-0.99660800
O	-1.97528400	-1.00619200	-1.52253100
N	-3.60002400	1.20603000	-1.67727500
H	-2.73429600	0.61613900	-1.62655000
H	-4.06135800	1.05627700	-0.76271400
C	-4.43626900	0.78168700	-2.84529800
C	-3.26308400	2.65484200	-1.81466100
H	-3.83048900	0.11228300	-3.45837900
H	-5.32141700	0.25458400	-2.49698500
C	-4.76231600	2.07490100	-3.58305400

C	-3.53224400	2.94272600	-3.29330500
H	-3.95428300	3.21354800	-1.18457700
C	-1.81434900	2.92948500	-1.39336900
H	-4.91014800	1.89430900	-4.65587100
H	-2.68487000	2.60738200	-3.90427700
H	-3.69643500	4.00679200	-3.47966800
O	-1.56984700	4.09209900	-0.99660800
O	-1.00619200	1.97528400	-1.52253100
O	-2.59746400	-5.92849700	-2.98294100
H	-3.44682600	-6.13403900	-3.39208800
O	5.92849700	-2.59746400	-2.98294100
H	6.13403900	-3.44682600	-3.39208800
O	2.59746400	5.92849700	-2.98294100
H	3.44682600	6.13403900	-3.39208800
O	-5.92849700	2.59746400	-2.98294100
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O	-2.59746400	5.92849700	2.98294100
H	-3.44682600	6.13403900	3.39208800
O	-5.92849700	-2.59746400	2.98294100
H	-6.13403900	-3.44682600	3.39208800
O	2.59746400	-5.92849700	2.98294100
H	3.44682600	-6.13403900	3.39208800
O	5.92849700	2.59746400	2.98294100
H	6.13403900	3.44682600	3.39208800

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