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Supplementary information for

Structure and Bonding Properties of the Platinum-Mediated Endohedral Tetrametallic Fullerene $La_3Pt@C_{98}$

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1 Supplementary Methods

1.1 Materials

Graphene (Timesnano company), lanthanum (III) chloride (99.5%, Tianjin Guangfu Chemical research institute), platinum (IV) tetrachloride (99%, Energy Chemical company), acetone (99.5%, Concord Tech reagent).

1.2 Experimental Methods

Experiments were performed on a 7.0 T FT ICR MS (Varian IonSpec) employing the commercial MALDI source in positive-ion mode. A 355nm Nd: YAG laser (Orion, New Wave) was used to create ions. Typical laser energy was set to be 85% relative to the maximum energy of 4mJ/pulse. Graphene was dispersed in water/acetone (9:1, vol/vol) at 1mg/ml. Lanthanum (III) chloride and platinum (IV) tetrachloride were dissolved in acetone at 5 mM and 1 mM, respectively. Then the solutions of $LaCl_3$ and $PtCl_4$ were mixed at the ratio of 1:1 (vol/vol). 1μL of graphene solutions was deposited on the stainless steel-plate and dried at room temperature, then 1μL of the mixture of $LaCl_3$/$PtCl_4$ was deposited on it. In the experiments, ions produced by six consecutive laser pulses were accumulated in the hexapole first. After the accumulation, the hexapole exit lens was gated so that ions could be transferred into the quadrupole guide. The DC potential of the trapping plate near the quadrupole was set to be 15 V before the introduction of the ions into the cell. During the period of ion transfer to the cell, the trapping plate was pulsed down to 0 V to allow the ions to enter the ICR cell. The ions were then cooled down by a pulsed nitrogen gas (with pressure in the cell raised to about 10^{-6} Torr) before detection or isolation for tandem MS. Typically, mass spectra were acquired in the *m/z* range of 700–2500.

1.3 Theoretical Methods

All DFT calculations were carried out using the Gaussian 09 program package.[77] In general, given a common +3 oxidation state of M (M = Sc, Y, Ln) in EMF of $M_2@C_{2n}$ and $M_3@C_{2n}$ [53, 78], the fullerene cage is in a valence state of -6. In this research, the valence state of platinum is difficult to be estimated at the first time, thus, all top negatively charged cages of C_{98}^{4-}, C_{98}^{6-}, C_{98}^{7-} and C_{98}^{8-} need to be considered. Therefore, 259 IPR-isomers of C_{98} cages get from CAGE software [79] were first calculated with valences of -4, -6, -7 and -8 at the xTB level [80]. These structures were then

ranked based on their energies, and the top 15 isomers of negatively charged cages C_{98}^{4-}, C_{98}^{6-}, C_{98}^{7-} and C_{98}^{8-} were chosen and optimized at the level of B3LYP/6-31g(d) [81, 82] (**Table. S1-S4)**. It is worth noting that C_{98} empty cages calculated under different valence states (-6, -7, -8) have similar cage stability, so some of their respective top 15 most stable C_{98} cages (C_{98}^{6-}, C_{98}^{7-} and C_{98}^{8-}) are duplicates. Thus, the top five stable IPR isomers of C_{98}^{4-}, the top eight stable IPR isomers of C_{98}^{8-} and the top ten stable IPR isomers of C_{98}^{6-} , C_{98}^{7-} were all selected. Besides, the non-IPR cage of 168785 was also considered in this paper, due to its importance in $Gd_2@C_{98}$ isomers, as shown by *Nagase. et.al*.[31] In total, the nine IPR isomers and one non-IPR isomer are selected here. Then, the La_3Pt metalloclusters were inserted into the optimized cages. For each cage, initial confirmations formed by insertions from more than 8 different directions were tried. All these isomers were optimized at the B3LYP/6-31g(d)/SDD level. The 6-31G(d) basis set is used for C atom, while SDD basis set is used for La and Pt atoms. Results show that for same carbon cage, there are several conformational isomers that are different in their orientations of the La3Pt cluster relative to the cage. The results are shown in **Figures 2, S3** and **S4.** Their electronic energies were calculated with zero-point energy corrections. Two different DFT methods[83] of wB97X-D and TPSSH were applied to these isomers of $La_3Pt@C_{90,}$ and the results are shown in **Table. S4**.

Relative concentrations (W_i) of the i-th isomer at different temperatures were calculated by:[84]

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

where R is the gas constant, T is the absolute temperature, q_i and $\Delta H^o_{0,j}$ are the partition functions and the relative heat of formation at absolute zero temperature of the *i*-th isomer, respectively. And rotational-vibrational partition functions were calculated from the optimized structural and vibrational data obtained at the level of B3LYP/6-31g(d)/SDD without frequency scaling.

A series of wavefunction analyses were used to determine the bonding interactions and electronic properties of the $La_3Pt@C_{98}$ isomers using the Multifwn software.[72] On one hand, the gaussian checkpoint files containing the wavefunction information were imported into Multifwn for ELF analysis, Mayer bonding order calculation, and interaction region indicator (IRI) analysis[85] to verify bonding interactions within these isomers. On the other hand, by combining Multifwn with Visual Molecular Dynamics (VMD)[86], it is feasible to plot the charge distribution maps, spin electron distribution maps, and molecular orbitals of $La_3Pt@C2(231010)\text{-}C_{98}$ and $La_3Pt@C1(231005)\text{-}C_{98}$, which can be used to better demonstrate the interesting electronic properties of EMFs. All of the wavefunction analyses presented above were carried out at the level of of B3LYP /6-31g(d)/SDD. Herein, both spin electron distribution maps and molecular orbital diagrams are drawn in isosurface maps. The isovalue was set at 0.002.

To elucidate the bonding state, the local molecular orbitals (LMOs) were located using the popular

Pipek−Mezey localization method. The obtained LMOs were also verified by the adaptive natural density partitioning (adNDP) method.[73] The selection process is as follows: first, isolate the La_3Pt clusters; second, perform an orbital search in the order 1c-2e, 2c-2e, 3c-2e, 4c-2e; third, select the representative high occupation number of these orbitals (in each step, not all orbitals can be selected, otherwise, there will be no orbitals available for the next step). For a better rendering, the isovalue of all orbits was set at 0.5.

2 Supplementary Figures

Figures. S1–S12

Figure. S1 Comparison of the experimental isotopic distributions of $La_3Pt@C_{112}^+$ and $La_3Pt@C_{114}^+$ ions with their simulated isotopic distributions.

Figure. S2 Laser ablation MS spectrum of the mixture of graphene/$PtCl_4$ in the regions of 800-1500 *m/z* (a), 1500-2200 *m/z* (b) and 2200-2900 *m/z* (c).

Figure. S3 Top and front views of optimized geometric structures of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(230926)$-C_{98} (a), $La_3Pt@C1(230933)$-C_{98} (b), $La_3Pt@C2(230932)$-C_{98} (c), $La_3Pt@C1(230979)$-C_{98} (d), $La_3Pt@C2(230924)$-C_{98} (e), $La_3Pt@C2(230922)$-C_{98} (f).

Figure. S4 Top and front views of optimized geometric structures of conformational isomers: $La_3Pt@C1(231005)$-C_{98}-2 (a), $La_3Pt@C2(230932)$-C_{98}-2 (b), $La_3Pt@C1(230933)$-C_{98}-2 (c).

Figure. S5 Mulliken charge distributions of $La_3Pt@C_{98}$ isomers: $La_3Pt@C2(231010)$-C_{98} (a), $La_3Pt@C1(231005)$-C_{98} (b), $La_3Pt@C1(230926)$-C_{98} (c), $La_3Pt@C1$ (230933)-C_{98} (d), $La_3Pt@C2(230932)$-C_{98} (e), $La_3Pt@C1$ (230979)-C_{98} (f), which were calculated at the level of B3LYP/6-31g(d)/SDD.

Figure. S6 Electron localization function analysis of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(231005)$-C_{98} (a), $La_3Pt@C1(230926)$-C_{98} (b), $La_3Pt@C1(230933)$-C_{98} (c) in the La_1-La_2-La_3 (left) and La_1-Pt-La_2 (right) planes.

Figure. S7 Color-coded map of intra-cluster interactions described by the interaction

region indicator of $La_3Pt@C_{98}$ isomers: Color-coded map of intra-cluster interactions described by the interaction region indicator of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(231005)\text{-}C_{98}$ (a,b) and $La_3Pt@C1(231005)\text{-}C_{98}$ (c,d), from full (a, c,) and half section views (b, d). The standard coloring method applied was shown in the right of the figure.

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Figure. S8 Adaptive natural density partitioning (adNDP) analysis results of $La_3Pt@C1(231005)\text{-}C_{98}$.

Figure. S9 Electron spin density distributions of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(230926)\text{-}C_{98}$ (a), $La_3Pt@C1(230933)\text{-}C_{98}$ (b), $La_3Pt@C2(230932)\text{-}C_{98}$ (c), $La_3Pt@C1(230979)\text{-}C_{98}$ (d), which were calculated at the level of B3LYP/6-31g(d)/SDD.

Figure. S10 Main frontier molecular orbitals of $La_3Pt@C1(231005)\text{-}C_{98}$, calculated at the B3LYP/6-31g(d)/SDD level.

Figure. S11 The comparison of molecular orbitals of $La_3Pt@C2(231010)\text{-}C_{98}$ with those of empty C_{98}.

Figure. S12 Simulated IR spectra of $La_3Pt@C2(231010)\text{-}C_{98}$ (a), $La_3Pt@C1(231005)\text{-}C_{98}$ (b), $La_3Pt@C1(230926)\text{-}C_{98}$ (c) and $La_3Pt@C1(230933)\text{-}C_{98}$ (d), which were calculated at the B3LYP/6-31g(d)/SDD level.

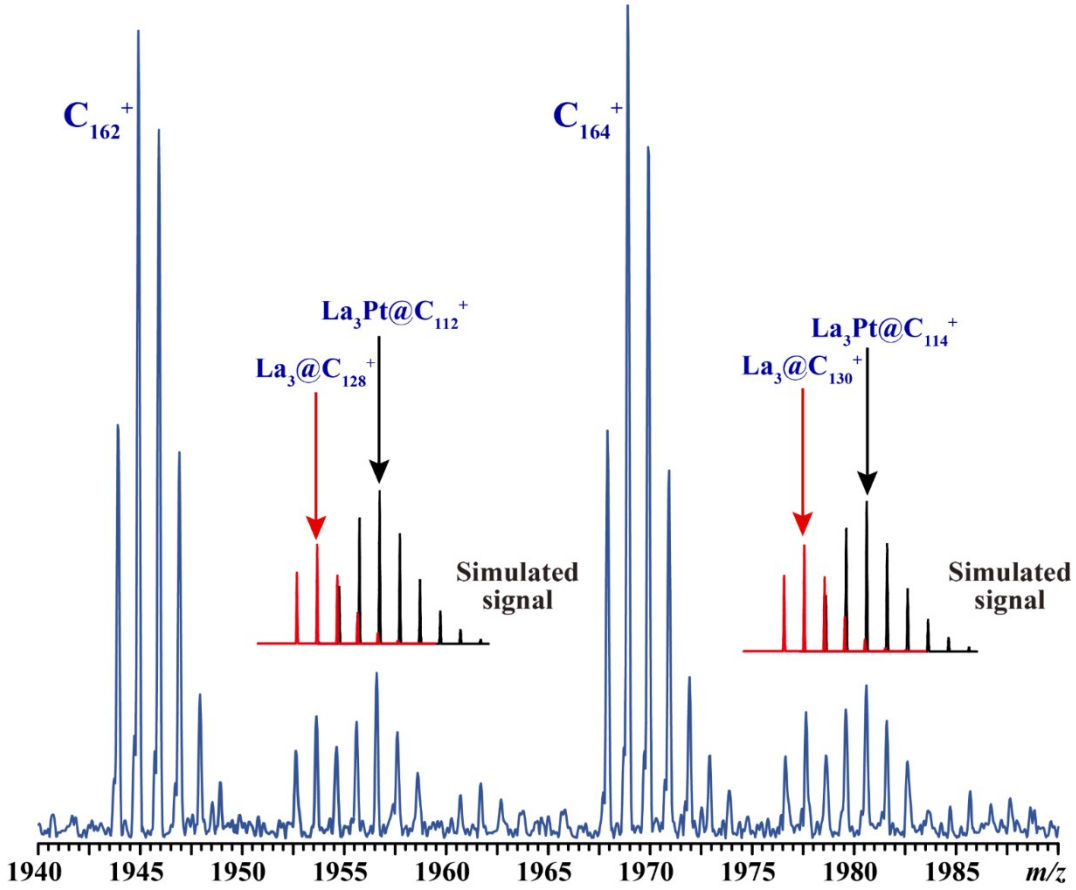

Figure. S1 Comparison of the experimental isotopic distributions of $La_3Pt@C_{112}^+$ and $La_3Pt@C_{114}^+$ ions with their simulated isotopic distributions.

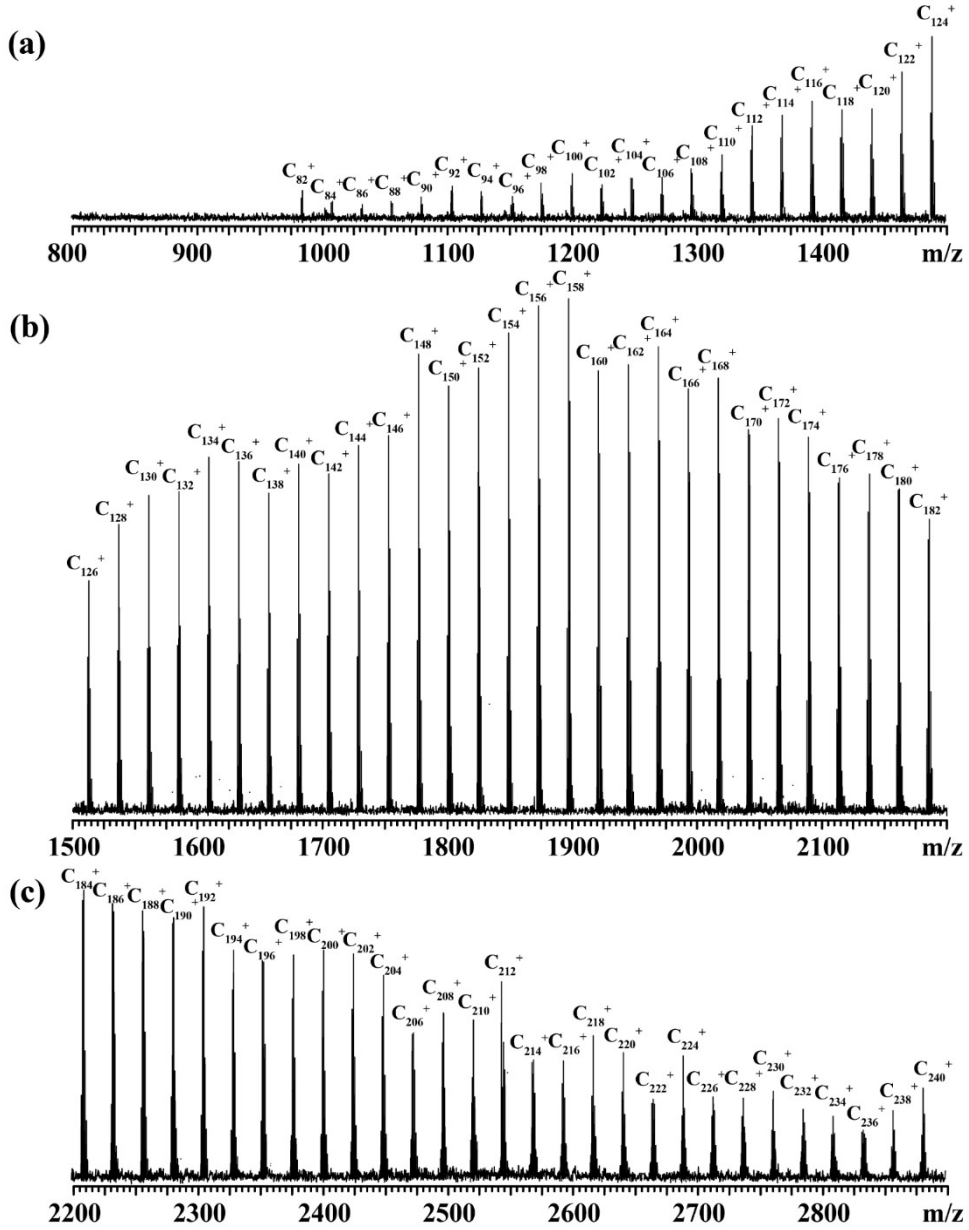

Figure. S2 Laser ablation MS spectrum of the mixture of graphene/$PtCl_4$ in the regions of 800-1500 *m/z* (a), 1500-2200 *m/z* (b) and 2200-2900 *m/z* (c).

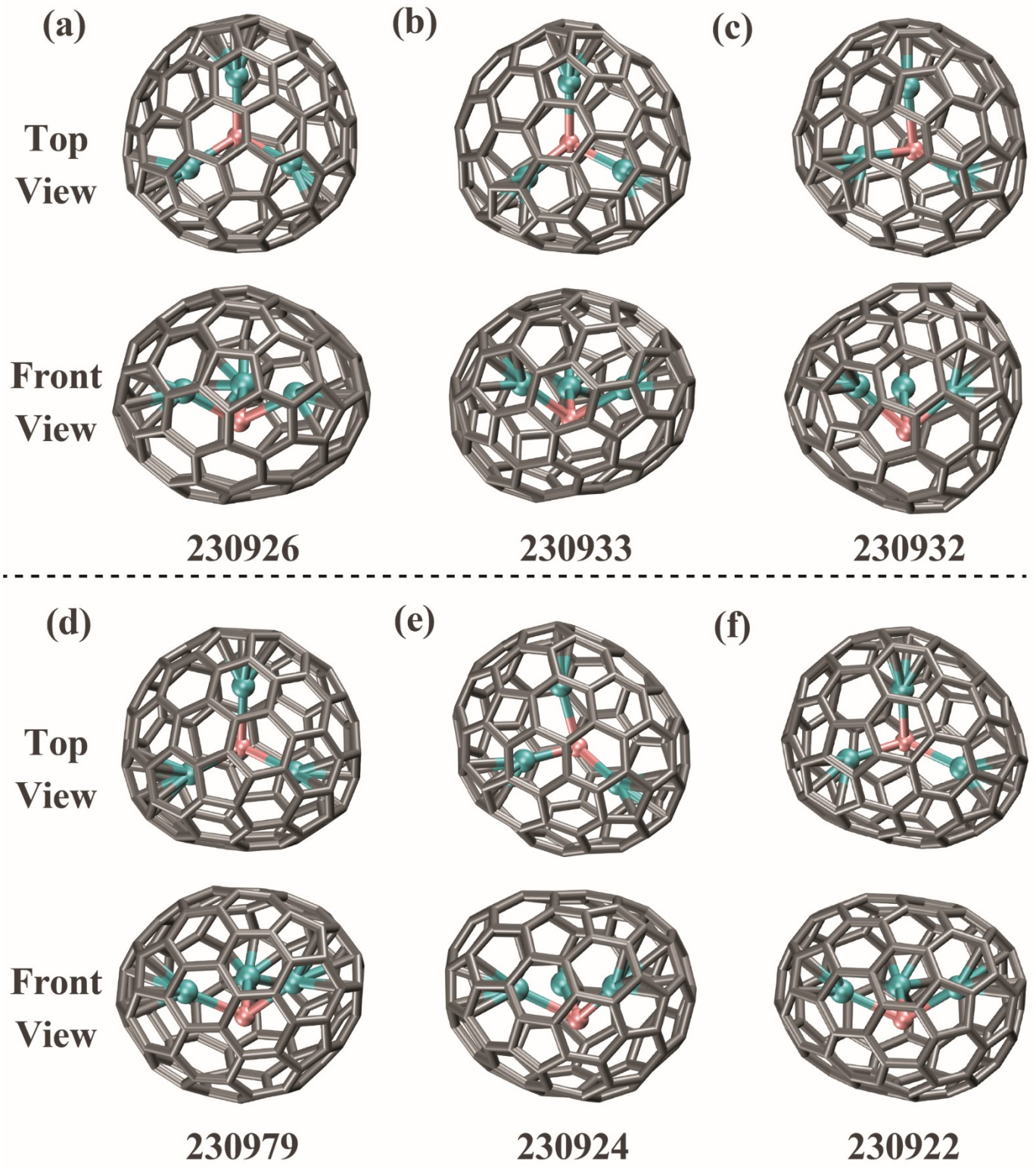

Figure. S3 Top and front views of optimized geometric structures of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(230926)\text{-}C_{98}$ (a), $La_3Pt@C1(230933)\text{-}C_{98}$ (b), $La_3Pt@C2(230932)\text{-}C_{98}$ (c), $La_3Pt@C1(230979)\text{-}C_{98}$ (d), $La_3Pt@C2(230924)\text{-}C_{98}$ (e), $La_3Pt@C2(230922)\text{-}C_{98}$ (f).

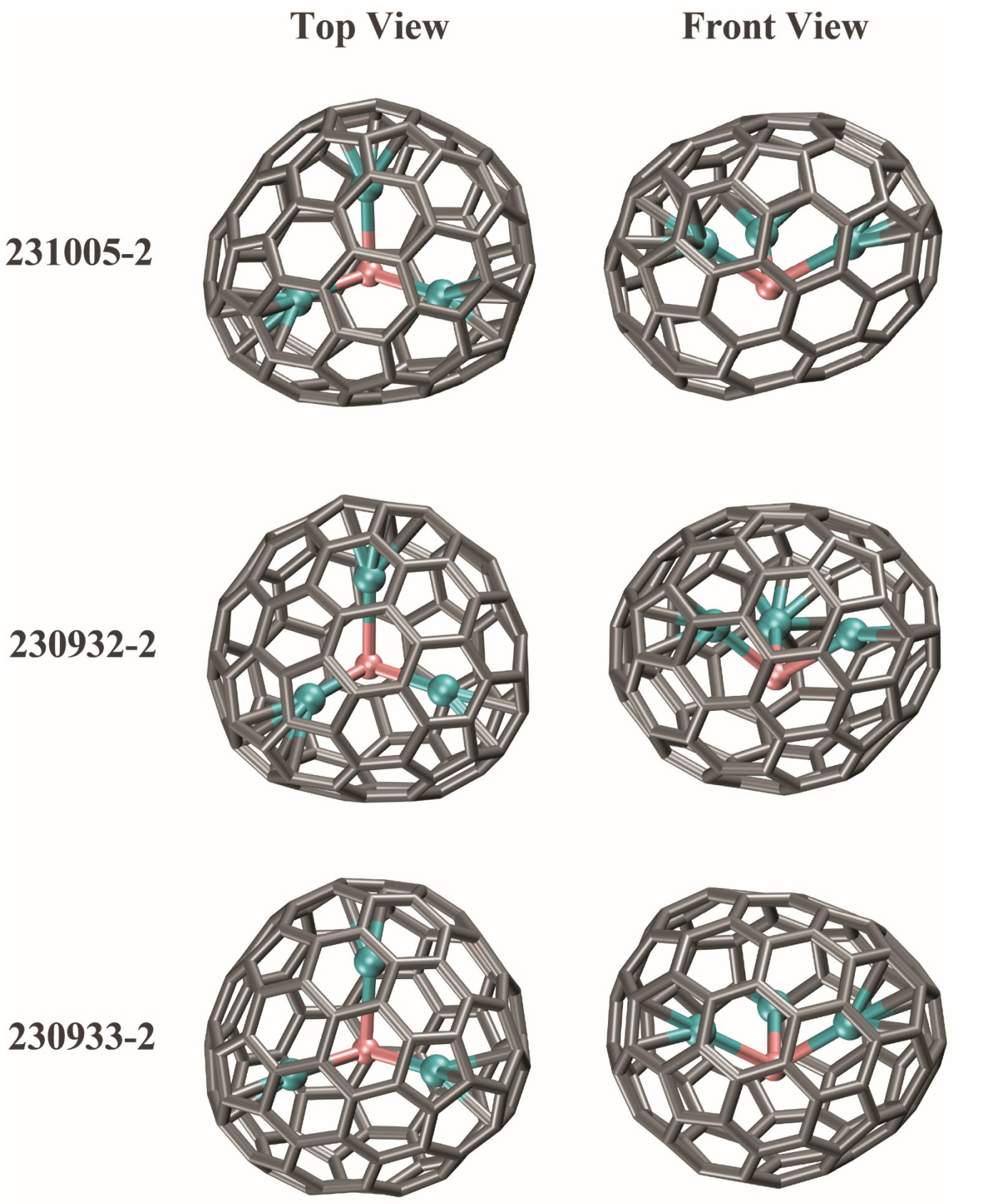

Figure. S4 Top and front views of optimized geometric structures of conformational isomers: $La_3Pt@C1(231005)$-C_{98}-2 (a), $La_3Pt@C2(230932)$-C_{98}-2 (b), $La_3Pt@C1(230933)$-C_{98}-2 (c).

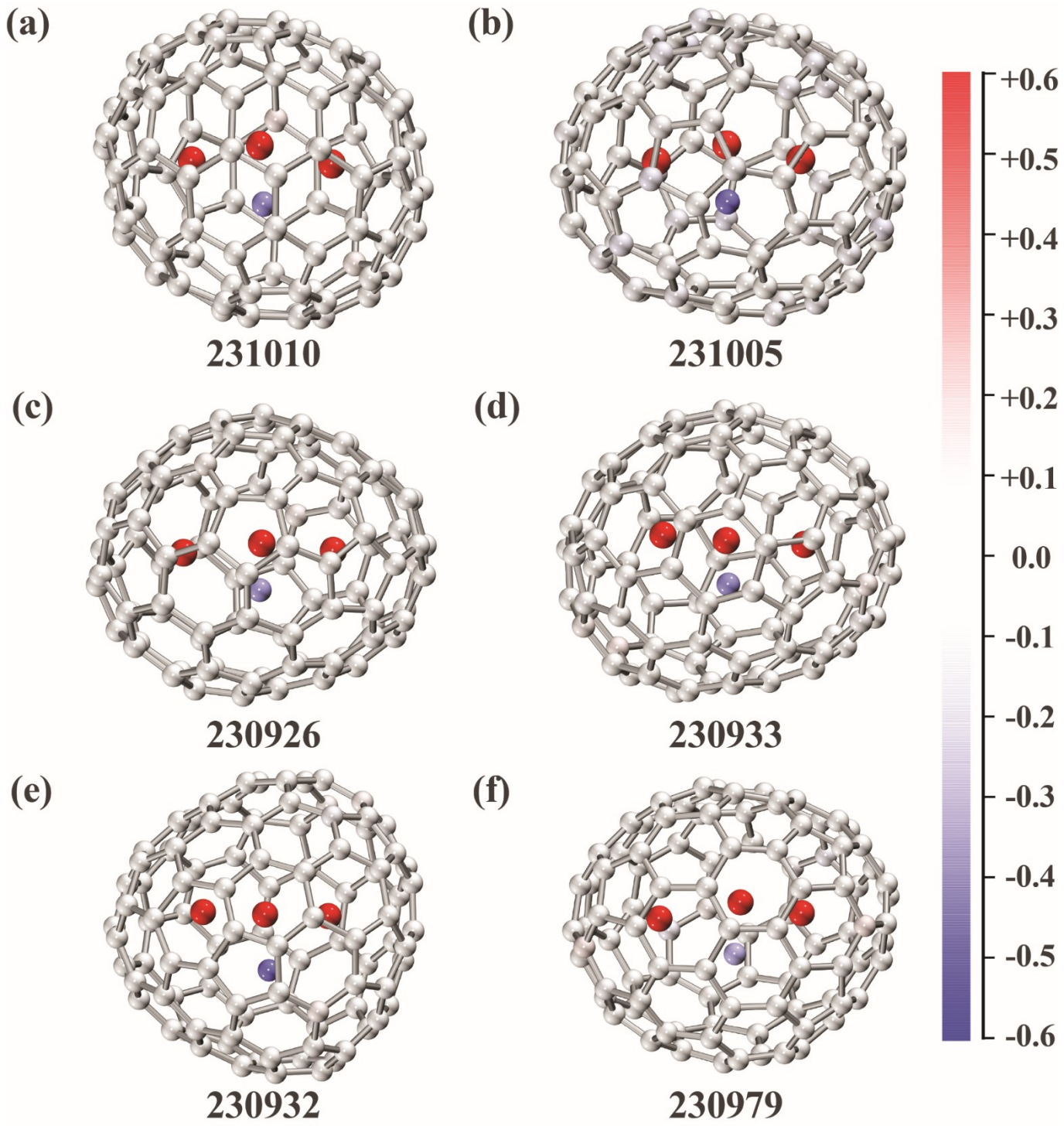

Figure. S5 Mulliken charge distributions of $La_3Pt@C_{98}$ isomers: $La_3Pt@C2(231010)\text{-}C_{98}$ (a), $La_3Pt@C1(231005)\text{-}C_{98}$ (b), $La_3Pt@C1(230926)\text{-}C_{98}$ (c), $La_3Pt@C1(230933)\text{-}C_{98}$ (d), $La_3Pt@C2(230932)\text{-}C_{98}$ (e), $La_3Pt@C1(230979)\text{-}C_{98}$ (f), which were calculated at the level of B3LYP/6-31g(d)/SDD.

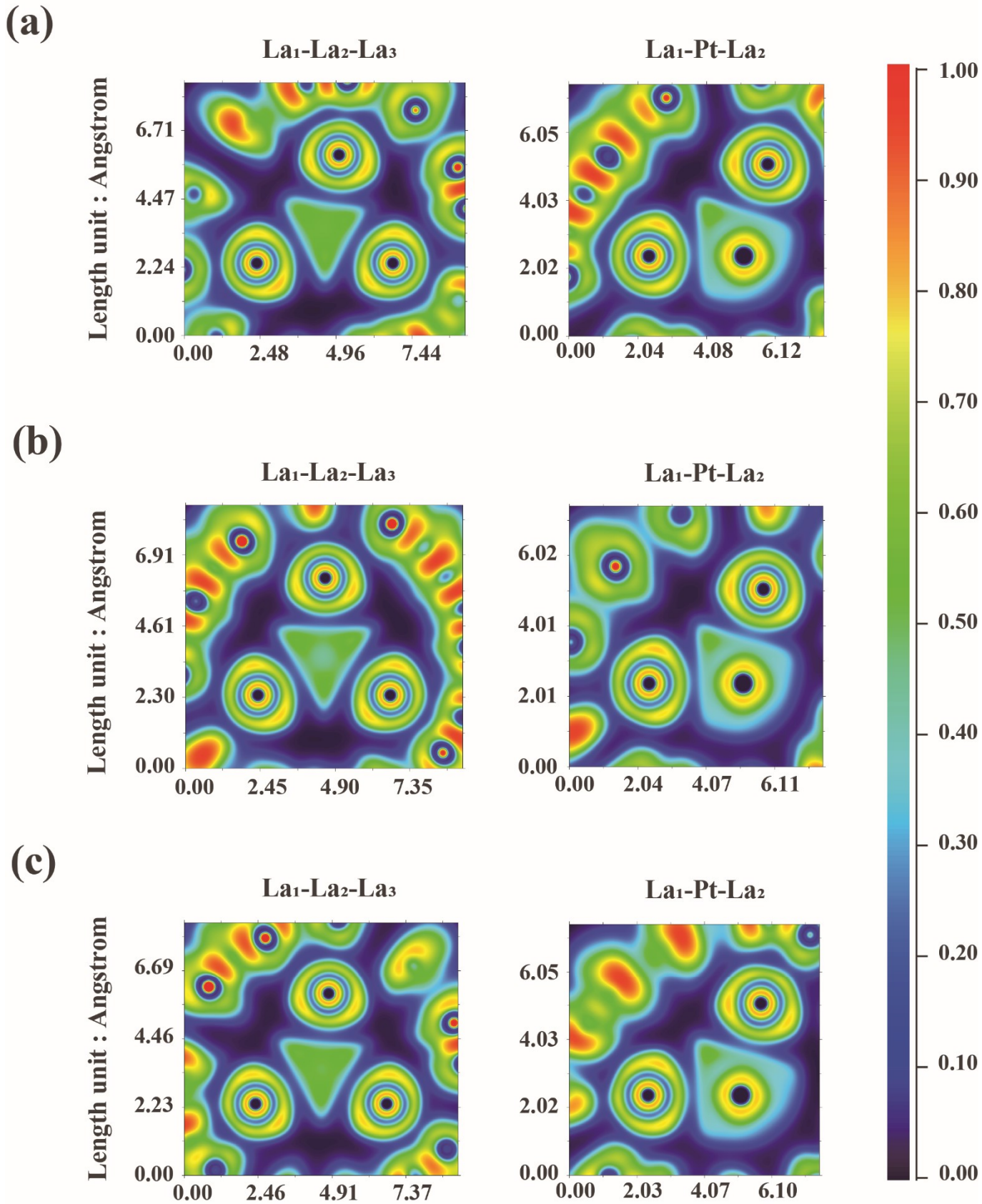

Figure. S6 Electron localization function (ELF) analysis of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(231005)$-C_{98} (a), $La_3Pt@C1(230926)$-C_{98} (b), $La_3Pt@C1(230933)$-C_{98} (c) in the La_1-La_2-La_3 (left) and La_1-Pt-La_2 (right) planes.

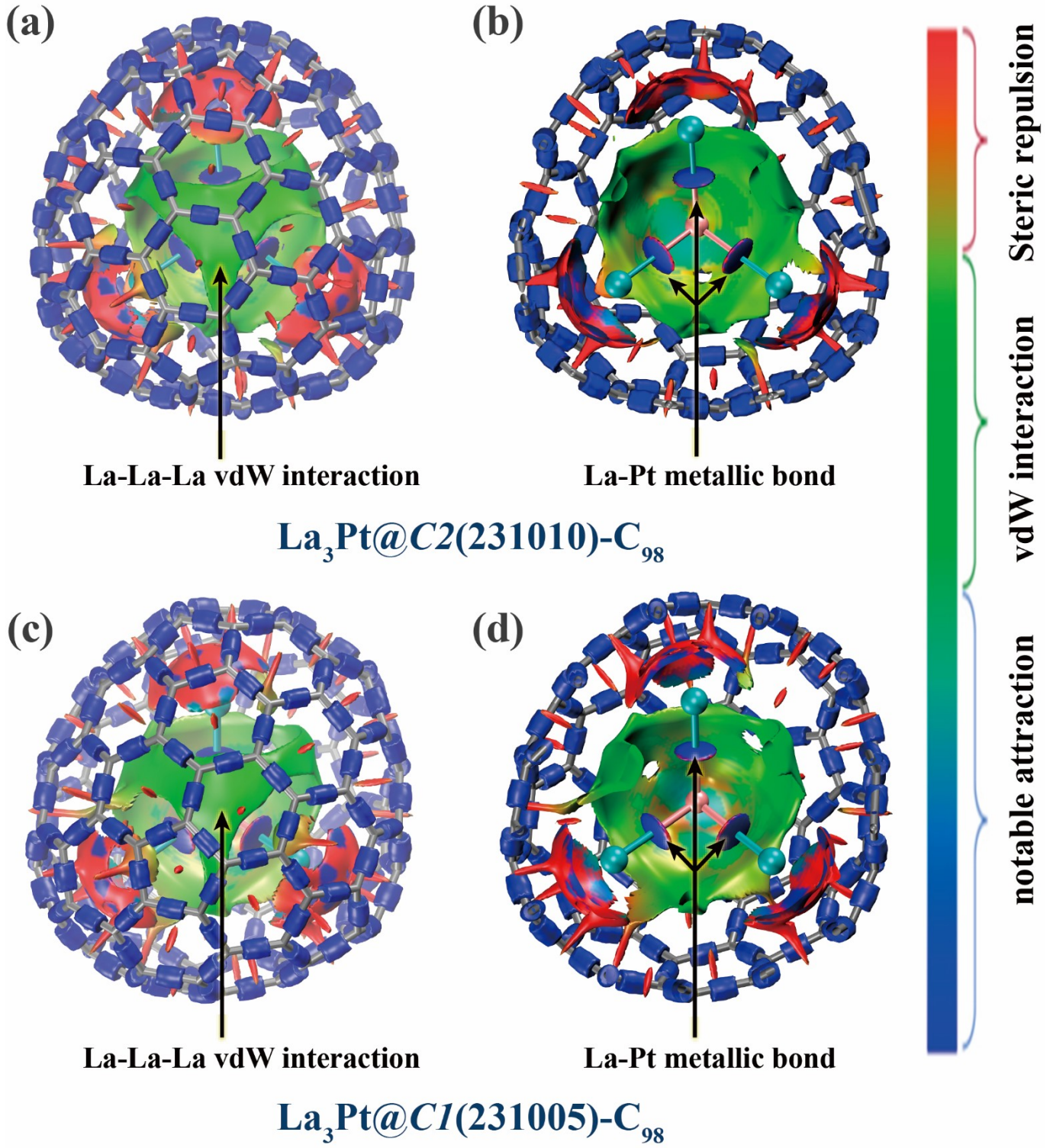

Figure. S7 Color-coded map of intra-cluster interactions described by the interaction region indicator of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(231005)$-C_{98} (a,b) and $La_3Pt@C1(231005)$-C_{98} (c,d), from full (a, c,) and half section views (b, d). The standard coloring method applied was shown in the right of the figure.

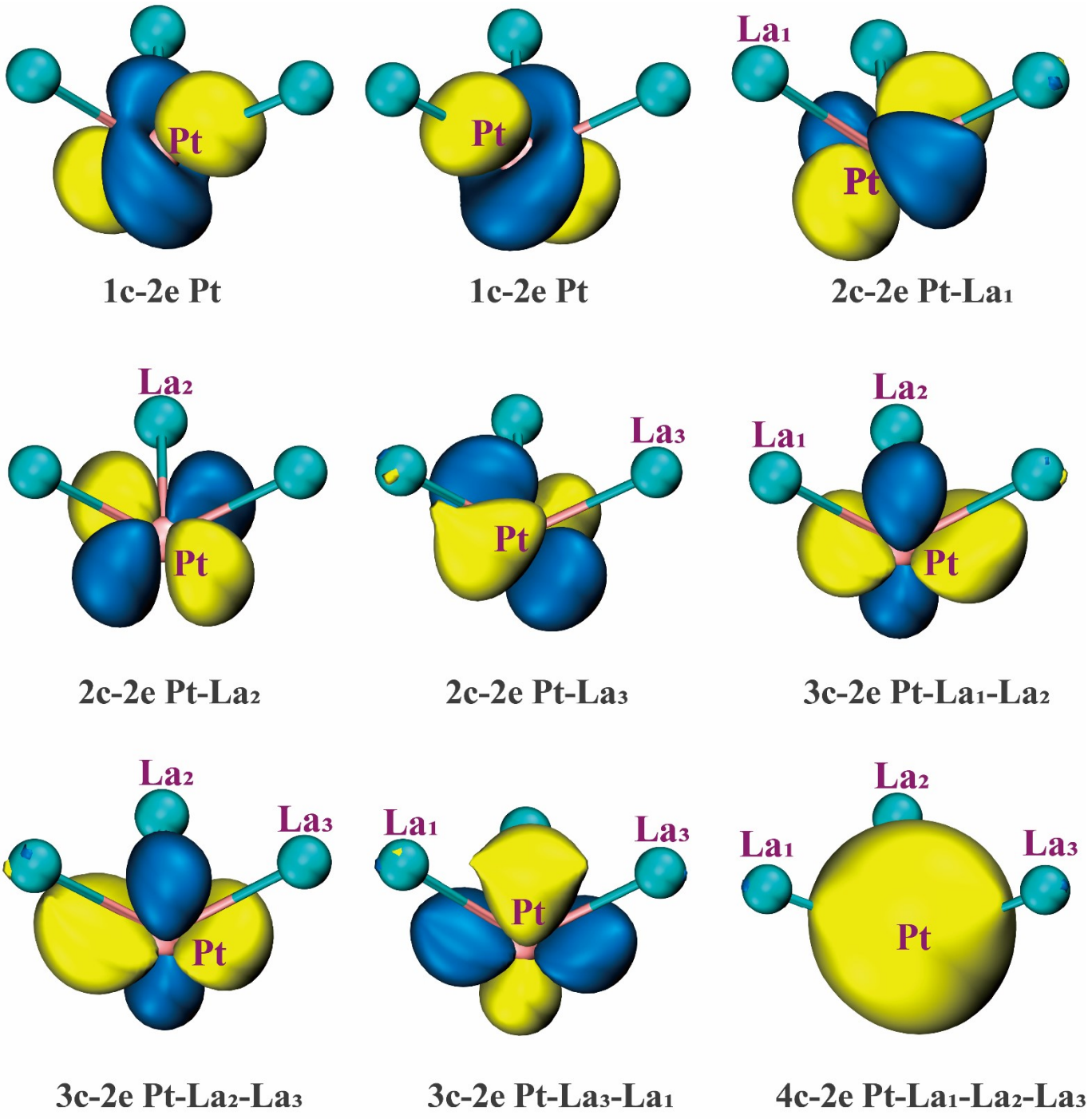

Figure. S8 Adaptive natural density partitioning (adNDP) analysis results of $La_3Pt@C1(231005)\text{-}C_{98}$. To make the picture clearer, the outer fullerene cage has been removed purposely.

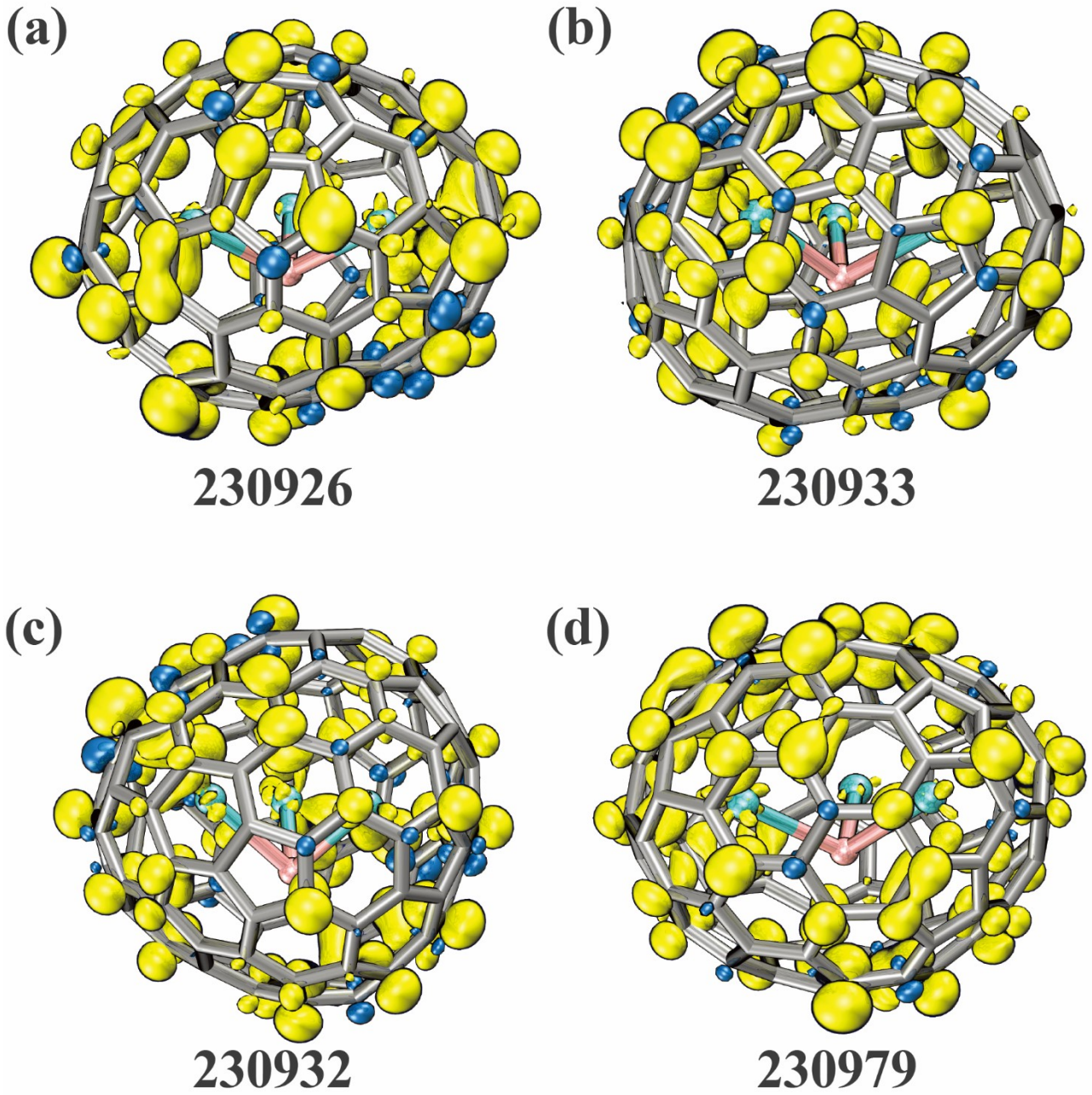

Figure. S9 Electron spin density distributions of $La_3Pt@C_{98}$ isomers: $La_3Pt@C1(230926)\text{-}C_{98}$ (a), $La_3Pt@C1(230933)\text{-}C_{98}$ (b), $La_3Pt@C2(230932)\text{-}C_{98}$ (c), $La_3Pt@C1(230979)\text{-}C_{98}$ (d), which were calculated at the level of B3LYP/6-31g(d)/SDD.

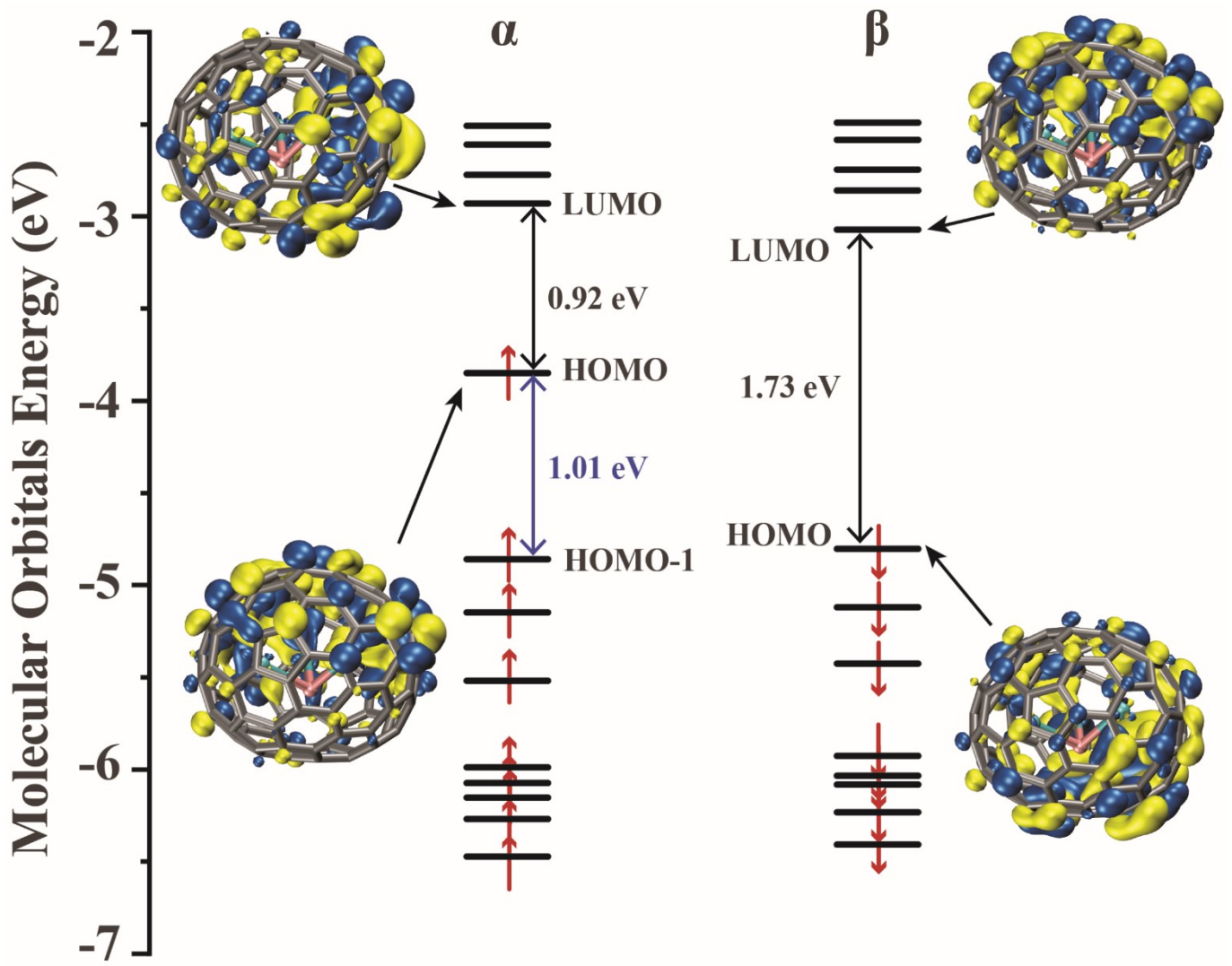

Figure. S10 Main frontier molecular orbitals of $La_3Pt@C1(231005)\text{-}C_{98}$, calculated at the B3LYP/6-31g(d)/SDD level.

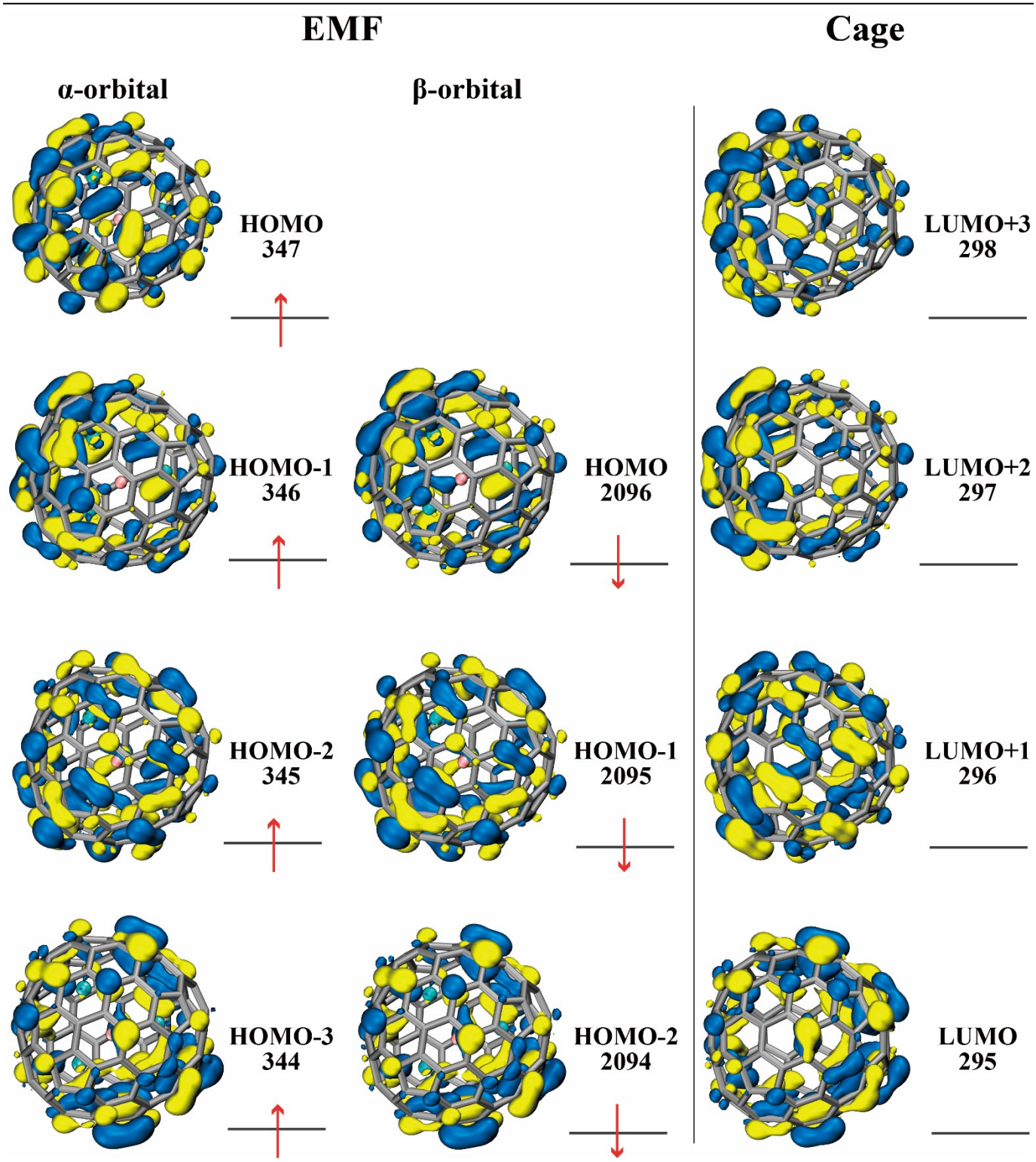

Figure. S11 The comparison of molecular orbitals of $La_3Pt@C2(231010)$-C_{98} with those of empty C_{98}.

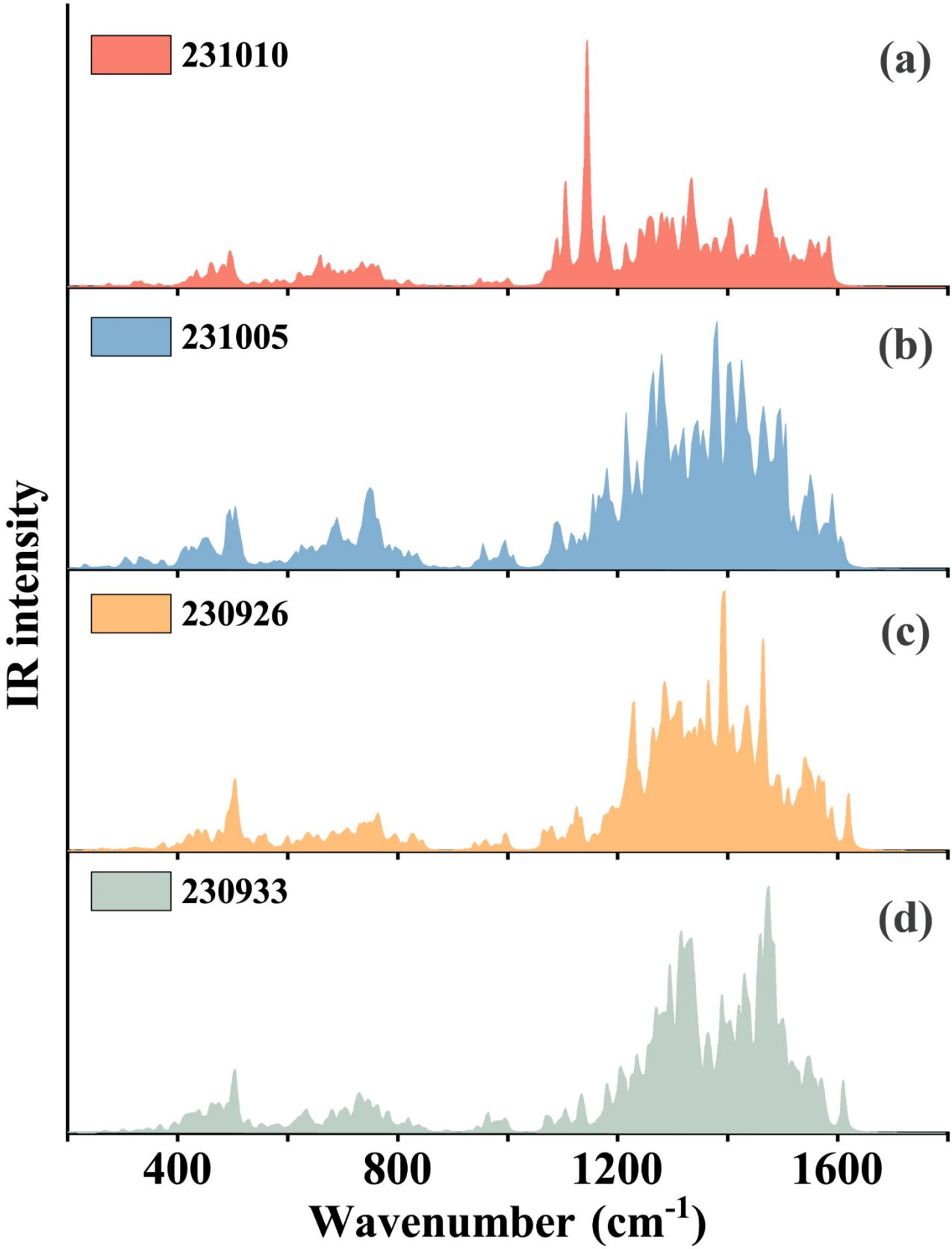

Figure. S12 Simulated IR spectra of $La_3Pt@C2(231010)-C_{98}$ (a), $La_3Pt@C1(231005)-C_{98}$ (b), $La_3Pt@C1(230926)-C_{98}$ (c) and $La_3Pt@C1(230933)-C_{98}$ (d), which were calculated at the B3LYP/6-31g(d)/SDD level.

3 Supplementary Tables

Tables. S1–S15

Table. S1 Relative energies of the top 15 isomers of C_{98}^{4-} before and after encapsulating La_3Pt clusters.

Table. S2 Relative energies of the top 15 isomers of C_{98}^{6-} before and after encapsulating La_3Pt clusters.

Table. S3 Relative energies of the top 15 isomers of C_{98}^{7-} before and after encapsulating La_3Pt clusters.

Table. S4 Relative energies of the top 15 isomers of C_{98}^{8-} before and after encapsulating La_3Pt clusters.

Table. S5 Relative energies and corresponding ranks of $La_3Pt@C_{98}$ isomers based on three different methods.

Table. S6 Relative energies and corresponding ranks, together with HOMO-LUMO gaps of $La_3Pt@C_{98}$ and $La_3Pt@C_{98}^{+}$ isomers at the B3LYP/6-31g(d)/SDD level.

Table. S7 Comparison of La-C and Pt-C bond lengths (in Å) in $La_3Pt@C_{98}$ isomers.

Table. S8 Comparison of La-La, La-Pt and La-C bond lengths (in Å) in the cages of $La_3N@C_{88,92,96}$ and $La_3Pt@C_{98}$. *

Table. S9 Relative energies and HOMO−LUMO gaps of conformational isomers of $La_3Pt@C_{98}$ at the B3LYP/6-31g(d)/SDD level.

Table. S10 La-La and La-Pt bond lengths (in Å), La-Pt-La bond angles (in degree) of the metal cluster La_3Pt in these conformational isomers of $La_3Pt@C_{98}$ at the

B3LYP/6-31g(d)/SDD level.

Table. S11 La-C, Pt-C bond lengths (in Å), and the coordinated environment of three La atoms in the cages of these conformational isomers of $La_3Pt@C_{98}$ at the B3LYP/6-31g(d)/SDD level.

Table. S12 Mulliken charge distributions of the top 10 $La_3Pt@C_{98}$ isomers

Table. S13 Hirshfeld charge distributions of the top 10 $La_3Pt@C_{98}$ isomers

Table. S14 Voronoi deformation density (VDD) charge distributions of the top 10 $La_3Pt@C_{98}$ isomers

Table. S15 Total Mayer Bond Orders between La (Pt) and C atoms coordinated to them in $La_3Pt@C_{98}$ isomers.

Table. S1 Relative energies of the top 15 isomers of C_{98}^{4-} before and after encapsulating La_3Pt clusters.

Spiral ID	IPR code	Symmetry	Empty cage [a]	EMF [b]
230979	221	C_1	0.00	5.58
230933	175	C_1	0.32	3.72
230926	168	C_1	0.82	3.09
230925	167	C_{2v}	1.13	12.61
230924	166	C_2	1.49	7.36
230927	169	C_1	3.23	----
230941	183	C_1	3.32	----
230839	81	C_{2v}	3.44	----
230938	180	C_2	4.97	----
230931	173	C_1	5.43	----
230889	131	C_1	6.54	----
230932	174	C_2	6.63	5.57
230969	211	C_2	6.83	----
231005	247	C_1	7.19	1.21
230947	189	C_2	7.33	----

a. Empty carbon cages C_{98}^{4-} were optimized with the method of B3LYP/6-31g(d). The top five fullerenes were selected for the next-step optimization. Due to the complexity of computation, the calculation for some less important EMFs with higher-energy empty cages was not performed here.

b. Optimized with the method of 6-31g(d)/SDD.

Table. S2 Relative energies of the top 15 isomers of C_{98}^{6-} before and after encapsulating La_3Pt clusters.

Spiral ID	IPR code	Symmetry	Empty cage [a]	EMF [b]
230924	166	C_2	0.00	7.36
231005	247	C_1	3.71	1.21
231010	252	C_2	7.42	0.00
230933	175	C_1	10.74	3.72
230926	168	C_1	11.16	3.09
230932	174	C_1	11.27	5.57
230979	221	C_2	11.62	5.58
231004	246	C_2	12.42	8.67
230925	167	C_{2v}	12.61	12.61
230919	161	C_1	12.91	17.68
231006	248	C_2	13.17	----
230947	189	C_2	13.87	----
231017	259	C_2	15.00	----
230973	215	C_2	15.12	----
230944	186	C_1	15.17	----

a. Empty carbon cages C_{98}^{6-} were optimized with the method of B3LYP/6-31g(d). The top ten fullerenes were selected for the next-step optimization. Due to the complexity of computation, the calculation for some less important EMFs with higher-energy empty cages was not performed here.

b. Optimized with the method of 6-31g(d)/SDD.

Table. S3 Relative energies of the top 15 isomers of C_{98}^{7-} before and after encapsulating La_3Pt clusters.

Spiral ID	IPR code	Symmetry	Empty cage [a]	EMF [b]
230924	166	C_2	0.00	7.36
231005	247	C_1	4.69	1.21
230925	167	C_{2v}	6.09	12.61
230979	221	C_2	6.48	5.58
230926	168	C_1	7.49	3.09
230933	175	C_1	7.67	3.72
231010	252	C_2	8.17	0.00
230932	174	C_1	8.87	5.57
231004	246	C_2	11.01	8.67
230919	161	C_1	12.01	17.68
230947	189	C_2	12.48	----
230941	183	C_2	12.73	----
230839	81	C_2	14.13	8.72
230982	224	C_2	14.43	----
230942	184	C_2	14.56	----

a. Empty carbon cages C_{98}^{7-} were optimized with the method of B3LYP/6-31g(d). The top ten fullerenes were selected for the next-step optimization. Due to the complexity of computation, the calculation for some less important EMFs with higher-energy empty cages was not performed here.

b. Optimized with the method of 6-31g(d)/SDD.

Table. S4 Relative energies of the top 15 isomers of C_{98}^{8-} before and after encapsulating La_3Pt clusters.

Spiral ID	IPR code	Symmetry	Empty cage [a]	EMF [b]
230924	166	C_2	0.00	7.36
230925	167	C_{2v}	1.89	12.61
230932	174	C_2	6.42	5.57
230926	168	C_1	6.89	3.09
230933	175	C_1	8.29	3.72
230922	164	C_1	9.57	12.64
231005	247	C_1	9.72	1.21
230839	81	C_2	11.03	8.72
230947	189	C_2	11.18	----
230927	169	C_1	12.22	----
230938	180	C_1	12.36	----
231010	252	C_2	12.83	0.00
231004	246	C_2	12.87	8.67
230969	211	C_2	14.12	----
230941	183	C_2	14.33	----

a. Empty carbon cages C_{98}^{8-} were optimized with the method of B3LYP/6-31g(d). The top eight fullerenes were selected for the next-step optimization. Due to the complexity of computation, the calculation for some less important EMFs with higher-energy empty cages was not performed here.

b. Optimized with the method of 6-31g(d)/SDD.

Table. S5 Relative energies and corresponding ranks of $La_3Pt@C_{98}$ isomers based on three different methods.

Spiral ID	Method-A [a]		Method-B [b]		Method-C [c]	
	Rank [d]	ΔE (in kcal/mol)	Rank [d]	ΔE (in kcal/mol)	Rank [d]	ΔE (in kcal/mol)
231010	1	0.00	1	0.00	1	0.00
231005	2	1.21	2	1.59	2	0.25
230926	3	3.09	3	5.01	3	1.59
230933	4	3.72	4	4.38	4	3.28
230932	5	5.57	7	6.88	5	5.41
230979	6	5.58	6	6.84	6	5.43
230924	7	7.36	5	6.43	7	7.25
231004	8	8.67	8	9.06	8	9.49
230839	9	8.72	9	9.90	9	9.55
168785	10	12.59	10	11.23	10	9.76

a. Method-A: B3LYP/6-31g(d)/SDD;

b. Method-B: wB97X-D/6-31g(d)/SDD;

c. Method-C: TPSSH/6-31g(d)/SDD.

d. The relative energy order of the top 10 $La_3Pt@C_{98}$ isomers with three different methods.

Table. S6 Relative energies and corresponding ranks, together with HOMO-LUMO gaps of $La_3Pt@C_{98}$ and $La_3Pt@C_{98}^+$ isomers at the B3LYP/6-31g(d)/SDD level.

Spiral ID	$La_3Pt@C_{98}$ [a]			$La_3Pt@C_{98}^+$ [b]		
	Rank [c]	ΔE (in kcal/mol)	Gap (in eV)	Rank [c]	ΔE (in kcal/mol)	Gap (in eV)
231010	1	0.00	0.78/1.67	2	2.00	1.50
231005	2	1.21	0.92/1.73	1	0	1.57
230926	3	3.09	1.11/1.28	3	6.61	1.20
230933	4	3.72	1.10/1.30	6	8.17	1.20
230932	5	5.57	0.76/1.27	4	7.50	1.25
230979	6	5.58	1.19/1.24	5	7.51	1.24
230924	7	7.36	0.87/1.72	7	10.68	1.49
231004	8	8.67	1.02/1.68	8	10.79	1.37
230839	9	8.72	1.07/1.85	9	12.85	1.49
168785	10	12.59	1.12/2.09	10	16.28	1.58

a. Relative energies and corresponding ranks, together with HOMO-LUMO gaps of $La_3Pt@C_{98}$, which were calculated at the level of UB3LYP/6-31g(d)/SDD;

b. Relative energies and corresponding ranks, together with HOMO-LUMO gaps of $La_3Pt@C_{98}^+$, which were calculated at the level of B3LYP/6-31g(d)/SDD.

c. The relative energy order of the top 10 $La_3Pt@C_{98}$ and $La_3Pt@C_{98}^+$ isomers at the B3LYP/6-31g(d)/SDD level.

Table. S7 Comparison of La-C and Pt-C bond lengths (in Å) in $La_3Pt@C_{98}$ isomers.

Spiral ID	La-C (Carbon Cage) (in Å) [a]				Pt-C (in Å)	Coordinated Environment [b]		
	La-C	La_1-C	La_2-C	La_3-C		La_1	La_2	La_3
231010	2.52	2.52	2.53	2.51	3.10	acenaphthylene	penalene	acenaphthylene
231005	2.52	2.51	2.54	2.52	3.01	acenaphthylene	hexagon	acenaphthylene
230926	2.53	2.53	2.56	2.52	2.93	acenaphthylene	hexagon	acenaphthylene
230933	2.53	2.52	2.54	2.52	3.04	acenaphthylene	pentagon	acenaphthylene
230932	2.52	2.50	2.51	2.54	3.03	acenaphthylene	naphthalene	pentagon
230979	2.54	2.52	2.51	2.58	3.24	hexagon	hexagon	hexagon
230924	2.57	2.56	2.56	2.60	3.00	hexagon	naphthalene	pentagon
231010	2.54	2.53	2.54	2.54	3.14	acenaphthylene	pentagon	naphthalene
230839	2.51	2.51	2.50	2.51	3.37	acenaphthylene	acenaphthylene	acenaphthylene
168785	2.57	2.54	2.55	2.63	3.16	naphthalene	acenaphthylene	pentagon

a. The La_1-C, La_2-C, La_3-C bond lengths are the distances between the three La atoms and their nearest C atoms in the cages of $La_3Pt@C_{98}$ isomers, and the La-C bond lengths are the average distances of the three values.

b. The coordinated environment of La atoms has a series of types: pentagon (La atom coordinates with a pentagonal carbon ring of the cage); hexagon (La atom coordinates with a hexagonal carbon ring of the cage); naphthalene (La atom is located near the junctions of two hexagons); acenaphthylene (La atom is situated at the junctions of one pentagon and two hexagons); penalene (La atom is located near the junctions of three hexagons).

Table. S8 Comparison of La-La distances, La-Pt and La-C bond lengths (in Å) in the cages of $La_3N@C_{88,92,96}$ and $La_3Pt@C_{98}$. *

EMFs		La-La distances (in Å) [a]				La-Pt bond lengths (in Å) [b]				La-C bond lengths (in Å) [c]			
Types [d]	IPR-code	La-La	La_1-La_2	La_2-La_3	La_3-La_1	La-Pt	La_1-Pt	La_2-Pt	La_3-Pt	La-C	La_1-C	La_2-C	La_3-C
$La_3N@C_{88}$	31	3.83	3.67	3.91	3.90	2.21	2.19	2.23	2.22	2.62	2.64	2.60	2.62
$La_3N@C_{92}$	86	3.78	3.78	3.78	3.78	2.19	2.19	2.19	2.19	2.55	2.55	2.55	2.55
$La_3N@C_{96}$	186	3.95	4.07	3.89	3.89	2.28	2.29	2.28	2.28	2.64	2.63	2.65	2.65
$La_3Pt@C_{98}$	252	4.30	4.53	4.32	4.06	2.81	2.81	2.80	2.83	2.52	2.52	2.53	2.51
	247	4.29	4.45	4.45	3.96	2.80	2.81	2.81	2.78	2.52	2.51	2.54	2.52
	168	4.36	4.33	4.39	4.35	2.79	2.80	2.75	2.81	2.53	2.53	2.56	2.52
	175	4.30	4.36	4.40	4.14	2.80	2.79	2.79	2.82	2.53	2.52	2.54	2.52

a. The distances are La-La distances between La_1 (La_2, La_3) and La_2 (La_3, La_1) atoms, together with their average values;

b. The distances are La-Pt bond lengths between La_1 (La_2, La_3) and Pt atoms, together with their average values;

c. The La_1-C, La_2-C, La_3-C bond lengths are the distances between the three La atoms and their corresponding nearest C atoms in the cages. The La-C bond lengths are the average distances between the three La atoms and their nearest C atoms in the cages;

d. These $La_3N@C_{2n}$ (2n=88, 92, 96) isomers were taken from the reference 33, 65, 66, in turn, and reoptimized at the level of B3LYP/6-31G(d).

*. A rough comparison shows that the distance between La-N is significantly shorter than the distance between La-Pt, while the distance between La-C ($La_3N@C_{2n}$) is slightly farer than the distance between La-C ($La_3Pt@C_{2n}$).

Table. S9 Relative energies and HOMO−LUMO gaps of different conformational isomers of $La_3Pt@C_{98}$ at the B3LYP/6-31g(d)/SDD level.

Rank	Isomeric spiral ID [a]	Caged IPR-code [b]	ΔE (in kcal/mol) [c]	Gap (in eV) [d]
1	231010-1	252	0.00	0.95/1.50
2	231005-1	247	1.21	0.92/1.73
3	230926-1	168	3.09	1.11/1.28
4	230933-1	175	3.72	1.10/1.30
5	231005-2	247	4.96	0.89/1.81
6	230932-1	174	5.57	1.09/1.31
7	230979-1	221	5.58	1.19/1.24
8	230932-2	174	6.32	1.22/1.25
9	230933-2	175	6.68	1.11/1.33
10	230924-1	166	7.36	0.87/1.72
11	230924-2	166	8.49	0.40/1.58
12	231004-1	246	8.67	1.02/1.68
13	230979-2	221	8.70	1.25/1.33
14	230932-3	174	8.70	0.85/1.30
15	230839-1	81	8.72	1.07/1.85
16	230933-3	175	9.20	0.83/1.68
17	231005-3	247	9.65	0.83/1.68
18	231010-2	252	9.80	0.95/1.50
19	230924-3	166	10.37	1.07/1.65

20	230926-2	168	11.23	1.01/1.42
21	168785-1	----	12.59	1.12/2.09
22	230925-1	167	12.61	1.17/1.23
23	230922-1	164	12.64	1.10/1.23
24	230919-1	161	17.68	0.97/1.56

a. Isomeric spiral ID is specific to each conformational isomer.

b. Caged IPR-code is the IPR number specific to the cage of these $La_3Pt@C_{98}$ isomers. Different conformational isomers can share a common cage;

c. The relative energy of each isomer with respect to that of the isomer 231010-1. Calculations were performed at the UB3LYP/6-31g(d)/SDD level. The order of energy ranking is shown in the first column, where the non-dominant conformational isomers are marked in red;

d. HOMO-LUMO gap for α and β spin orbitals of $La_3Pt@C_{98}$ isomers at the UB3LYP/6-31g(d)/SDD level.

Table. S10 La-La distances (in Å) and La-Pt bond lengths (in Å), La-Pt-La bond angles (in degree) of the metal cluster La_3Pt in these conformational isomers of $La_3Pt@C_{98}$ at the B3LYP/6-31g(d)/SDD level.

Isomeric spiral ID	La-La distances (in Å) [a]				La-Pt bond lengths (in Å) [b]				La-Pt-La bond angles (in degree) [c]			
	La-La	La_1-La_2	La_2-La_3	La_3-La_1	La-Pt	La_1-Pt	La_2-Pt	La_3-Pt	La-Pt-La	La_1-Pt-La_2	La_2-Pt-La_3	La_3-Pt-La_1
231005-2	4.23	4.44	4.12	4.13	2.80	2.79	2.85	2.77	98.1	104.0	94.3	96.0
230932-2	4.21	4.19	4.29	4.15	2.82	2.82	2.83	2.80	96.7	95.9	99.3	95.2
230933-2	4.25	4.29	4.43	4.03	2.81	2.81	2.82	2.81	98.4	99.4	104.0	91.7
230924-2	4.17	3.61	4.78	4.12	2.79	2.83	2.82	2.72	98.2	79.4	119.2	96.1
230979-2	4.16	3.92	4.27	4.30	2.80	2.79	2.83	2.79	96.1	88.4	98.9	101.1
230932-3	4.17	4.27	4.31	3.92	2.80	2.83	2.79	2.79	95.8	98.8	100.2	88.5
230933-3	4.24	4.53	4.01	4.17	2.81	2.80	2.77	2.86	98.4	109.0	91.0	95.1
231005-3	4.26	4.59	4.27	3.92	2.81	2.78	2.85	2.79	99.0	109.2	98.4	89.4
231010-2	4.23	4.20	4.11	4.37	2.81	2.82	2.84	2.76	97.8	95.9	94.4	103.2
230924-3	4.19	4.19	3.89	4.49	2.80	2.81	2.84	2.74	97.6	96.0	88.6	108.1
230926-2	4.26	4.13	4.40	4.24	2.80	2.82	2.78	2.79	99.4	95.4	104.6	98.2

a. The distances are La-La distances between La_1 (La_2, La_3) and La_2 (La_3, La_1) atoms, together with their average values;

b. The distances are La-Pt bond lengths between La_1 (La_2, La_3) and Pt atoms, together with their average values;

c. The angles are La-Pt-La bond angles among La_1 (La_2, La_3), Pt and La_2 (La_3, La_1) atoms, together with their average values.

Table. S11 La-C, Pt-C bond lengths (in Å), and the coordinated environment of three La atoms in the cages of these conformational isomers of $La_3Pt@C_{98}$ at the B3LYP/6-31g(d)/SDD level.

Isomeric spiral ID	La-C (Carbon Cage) (in Å) [a]				Pt-C (in Å)	Coordinated Environment [b]		
	La-C	La_1-C	La_2-C	La_3-C		La_1	La_2	La_3
231005-2	2.53	2.57	2.51	2.50	3.03	hexagon	acenaphthylene	acenaphthylene
230932-2	2.53	2.51	2.55	2.54	3.27	naphthalene	hexagon	pentagon
230933-2	2.53	2.53	2.53	2.52	3.05	naphthalene	naphthalene	acenaphthylene
230924-2	2.56	2.58	2.54	2.56	3.04	pentagon	naphthalene	naphthalene
230979-2	2.52	2.52	2.50	2.55	3.02	acenaphthylene	naphthalene	hexagon
230932-3	2.52	2.51	2.54	2.52	3.03	naphthalene	naphthalene	naphthalene
230933-3	2.51	2.54	2.51	2.49	3.35	naphthalene	naphthalene	acenaphthylene
231005-3	2.52	2.52	2.53	2.52	3.06	acenaphthylene	naphthalene	pentagon
231010-2	2.53	2.52	2.55	2.51	3.04	acenaphthylene	hexagon	acenaphthylene
230924-3	2.52	2.56	2.50	2.50	2.94	hexagon	acenaphthylene	acenaphthylene
230926-2	2.52	2.52	2.52	2.51	3.11	naphthalene	acenaphthylene	naphthalene

a. The La_1-C, La_2-C, La_3-C bond lengths are the distances between the three La atoms and their nearest C atoms in the cages, and the La-C bond lengths are the average distances of three values.

b. The coordinated environment of La atoms has a series of types: pentagon; hexagon; naphthalene; acenaphthylene. (See footnote to **Table. S6** for descriptions)

Table. S12 Mulliken charge distributions of the top 10 $La_3Pt@C_{98}$ isomers

Spiral ID	Mulliken Charge Distribution				
	La_1	La_2	La_3	Pt	Carbon Cage [a]
231010	0.49	0.52	0.50	-0.24	-1.27
231005	0.53	0.51	0.51	-0.29	-1.26
230926	0.48	0.49	0.52	-0.22	-1.26
230933	0.52	0.49	0.51	-0.24	-1.28
230932	0.51	0.48	0.48	-0.18	-1.29
230979	0.48	0.48	0.51	-0.18	-1.29
230924	0.53	0.50	0.51	-0.45	-1.09
231004	0.49	0.50	0.52	-0.23	-1.28
230839	0.51	0.47	0.47	-0.19	-1.26
168785	0.44	0.41	0.34	-0.18	-1.01

a. The sum of Mulliken charges of all C atoms.

Table. S13 Hirshfeld charge distributions of the top 10 $La_3Pt@C_{98}$ isomers

Spiral ID	Hirshfeld Charge Distribution				
	La_1	La_2	La_3	Pt	Carbon Cage [a]
231010	0.45	0.48	0.47	-0.16	-1.24
231005	0.44	0.46	0.49	-0.16	-1.23
230926	0.46	0.46	0.47	-0.16	-1.23
230933	0.48	0.47	0.46	-0.16	-1.25
230932	0.47	0.47	0.47	-0.16	-1.25
230979	0.48	0.47	0.47	-0.15	-1.27
230924	0.47	0.37	0.35	-0.15	-1.04
231004	0.46	0.48	0.47	-0.16	-1.25
230839	0.46	0.48	0.48	-0.16	-1.24
168785	0.38	0.36	0.45	-0.18	-1.01

a. The sum of Hirshfeld charges of all C atoms.

Table. S14 Voronoi deformation density (VDD) charge distributions of the top 10 $La_3Pt@C_{98}$ isomers

Spiral ID	Voronoi Deformation Density (VDD) Charge Distribution				
	La_1	La_2	La_3	Pt	Carbon Cage [a]
231010	0.31	0.33	0.33	-0.35	-0.62
231005	0.31	0.31	0.34	-0.36	-0.60
230926	0.32	0.32	0.32	-0.36	-0.60
230933	0.34	0.33	0.32	-0.35	-0.64
230932	0.33	0.37	0.31	-0.30	-0.71
230979	0.34	0.33	0.33	-0.35	-0.65
230924	0.32	0.21	0.21	-0.34	-0.40
231004	0.34	0.32	0.30	-0.34	-0.60
230839	0.31	0.34	0.32	-0.29	-0.66
168785	0.23	0.21	0.30	-0.37	-0.37

a. The sum of Voronoi deformation density (VDD) charges of all C atoms.

Table. S15 Total Mayer Bond Orders between La (Pt) and C atoms coordinated to them in $La_3Pt@C_{98}$ isomers.

Spiral ID	Mayer Bond Order			
	La_1-Cage	La_2-Cage	La_3-Cage	Pt-Cage
231010	2.68	2.52	2.75	0
231005	2.83	2.72	2.41	0
230926	2.82	2.57	2.21	0
230933	2.50	2.78	2.74	0
230932	2.97	2.53	2.48	0
230979	2.68	2.64	2.59	0
230924	2.64	2.44	2.19	0
231004	2.71	2.74	2.78	0
230839	2.68	2.56	2.51	0
168785	2.54	3.10	3.09	0

4 Supplementary Data

Data S1 The XYZ coordinates of $La_3Pt@C2(231010)$-C_{98}-1

Element	X	Y	Z
C	-3.04222721	0.14700493	3.05921861
C	-1.87930044	0.90478389	3.48160302
C	-0.71693524	0.15577604	3.91333501
C	0.49495217	0.86384289	4.08924248
C	1.75628830	0.23245662	3.93668148
C	2.70069374	1.23077004	3.49020389
C	3.72892458	0.88318122	2.53477245
C	4.04655389	1.81572941	1.46232618
C	4.41006472	1.25785354	0.14712734
C	4.09702475	2.03379870	-1.01992830
C	3.76234429	1.41424186	-2.26541662
C	2.67843884	2.17591973	-2.85292043
C	1.62824952	1.53072624	-3.55045349
C	0.27800746	2.00643262	-3.44196554
C	-0.79342986	1.06744205	-3.75590236
C	-2.11795598	1.43613836	-3.40454018
C	-3.16029124	0.48893021	-3.19374783
C	-4.15675356	1.09322136	-2.30096963
C	-4.86707299	0.28269682	-1.32275554
C	-4.97142074	0.83604963	0.02553181
C	-4.73069502	-0.01385902	1.18762460
C	-3.99140501	0.73936263	2.16429898
C	-3.00446536	-1.26761568	3.06568881
C	-3.74209288	-2.05227285	2.09359303
C	-4.53865742	-1.43096181	1.09434561
C	-4.53594512	-1.99051930	-0.22694031
C	-4.59237470	-1.12680897	-1.39611014
C	-3.67682913	-1.71793819	-2.37389335
C	-2.85423090	-0.91376092	-3.21460014
C	-1.52488111	-1.35804240	-3.57876261
C	-0.54890859	-0.34187341	-3.96426050
C	0.80379513	-0.74774680	-4.10046313
C	1.86826353	0.17246493	-3.90898234
C	3.03400263	-0.56859188	-3.48111254
C	3.90399346	0.02009387	-2.47399615
C	4.39968341	-0.79873091	-1.39394735
C	4.58211389	-0.18201177	-0.05639145
C	4.43759901	-1.01099215	1.09372990

C	3.93920053	-0.49797394	2.32990598
C	3.04067205	-1.50407105	2.88619406
C	1.86487230	-1.14142954	3.56718189
C	0.66152567	-1.93895246	3.42712899
C	-0.61750295	-1.29516672	3.72467981
C	-1.79950666	-1.97065358	3.36316883
C	-1.77664376	-3.18356003	2.60119968
C	-2.97528023	-3.22782130	1.80556500
C	-2.93616964	-3.76083707	0.48669151
C	-3.70527937	-3.10916105	-0.52535594
C	-3.16702054	-2.93241981	-1.85151949
C	-1.88375286	-3.43581526	-2.22395718
C	-1.04285157	-2.68106313	-3.13654628
C	0.37502114	-3.03673412	-3.23162542
C	1.27963743	-2.07918968	-3.84349552
C	2.69286490	-1.97266232	-3.51642797
C	3.27173099	-2.83541557	-2.52898714
C	4.10282199	-2.23622571	-1.48983394
C	3.82008260	-2.96046997	-0.28027689
C	3.98125356	-2.37002903	0.97778768
C	3.05753207	-2.64247788	2.03324590
C	1.90205593	-3.45640398	1.83777654
C	0.69781240	-3.14534004	2.59411766
C	-0.55610395	-3.74923979	2.16525214
C	-0.60454938	-4.48972472	0.93968789
C	-1.74967678	-4.40641570	0.07479254
C	-1.26837282	-4.31208280	-1.28323997
C	0.13978597	-4.49714977	-1.26506584
C	0.97919785	-3.95888319	-2.27301463
C	2.39111852	-3.81705022	-1.90699834
C	2.75679909	-3.88650915	-0.49458797
C	1.80412078	-4.14994442	0.55666165
C	0.54783751	-4.61497020	0.12498239
C	-2.40593460	2.61912511	-2.66938571
C	-3.63937114	2.41267836	-1.95874897
C	-3.75716385	2.95878182	-0.63338138
C	-4.39271109	2.13527350	0.35344574
C	-3.79767998	2.05541687	1.66750660
C	-2.68824173	2.85118293	2.09533163
C	-1.72145738	2.30506925	3.03164992
C	-0.43029821	2.97312333	3.14303727
C	0.63815104	2.25846032	3.77061865
C	2.03565663	2.50003806	3.48329945
C	2.43042151	3.50566330	2.54282961

C	3.43876559	3.15371857	1.54379006
C	3.03035312	3.81376484	0.32447315
C	3.34276598	3.24473299	-0.92439961
C	2.39939827	3.28005087	-2.00646054
C	1.07715707	3.78532644	-1.83438094
C	0.00132020	3.19179271	-2.61463739
C	-1.35852586	3.48204855	-2.22431412
C	-1.61635194	4.19854921	-1.02234483
C	-2.74200495	3.84086267	-0.18963707
C	-2.28063820	3.86362829	1.18220073
C	-0.96230372	4.39344644	1.20521489
C	-0.03682607	4.05046284	2.21807197
C	1.37652968	4.27251463	1.90780989
C	1.77174670	4.46464475	0.50397427
C	0.79205850	4.46480904	-0.56948249
C	-0.55150570	4.60768740	-0.17903617
Pt	-0.14619197	-0.56403796	0.75185323
La	1.58970160	-1.44187920	-1.27841565
La	-2.48777731	0.35955909	-0.47339691
La	1.26429621	1.87147167	1.03721489

Data S2 The XYZ coordinates of $La_3Pt@C1(231005)$-C_{98}-1

Element	X	Y	Z
C	-2.48446500	-0.96040400	3.57570400
C	-2.04822000	0.39872700	3.71154000
C	-0.65308600	0.68504800	3.87427700
C	-0.14821400	2.01447500	3.51436300
C	1.27276800	2.22352700	3.44923900
C	1.77959100	3.29020800	2.64083200
C	3.01796700	3.11160800	1.92914600
C	2.88774100	3.77837800	0.65757400
C	3.40129200	3.11676200	-0.53794700
C	2.58047400	3.12856200	-1.74318500
C	2.56011900	1.96095200	-2.62239000
C	1.35740000	1.62521300	-3.40504200
C	1.10672600	0.25313900	-3.81217200
C	-0.26258700	-0.25949500	-3.95885200
C	-0.60710600	-1.64167900	-3.60708100
C	-1.95167300	-1.94323600	-3.09693300
C	-2.11861200	-3.08737100	-2.22269400

C	-3.17623000	-3.09217700	-1.24540400
C	-3.01254600	-3.65499300	0.07920300
C	-3.92264800	-2.97759900	0.97267900
C	-3.44128100	-2.67820800	2.30499400
C	-3.68851900	-1.35149400	2.84988400
C	-1.52652200	-2.00551200	3.44902300
C	-2.08127000	-3.04990600	2.63759700
C	-1.18341700	-3.79912600	1.77470700
C	-1.71502700	-4.16083100	0.47591600
C	-0.81590600	-4.43109600	-0.57508500
C	-1.01875600	-3.91121300	-1.91383800
C	0.25576500	-3.69228500	-2.49732700
C	0.47678800	-2.56272300	-3.33202700
C	1.82391800	-2.08724800	-3.38553500
C	2.12082400	-0.71049300	-3.60123100
C	3.32775700	-0.38836500	-2.91488400
C	3.54356500	0.91088700	-2.39022500
C	4.41271300	0.97382300	-1.26394300
C	4.28984800	2.02811300	-0.31804100
C	4.57651800	1.48960900	0.99054400
C	3.84310000	1.96239100	2.11284700
C	3.44383100	1.01635800	3.09108300
C	2.15963500	1.14505600	3.72123900
C	1.65084500	-0.16774600	3.92721800
C	0.27359200	-0.44068100	3.94926500
C	-0.13188300	-1.77860200	3.58071500
C	0.79215400	-2.70996700	2.93622400
C	0.25303200	-3.67857100	1.96775300
C	1.13954200	-4.16719900	0.91916900
C	0.58248500	-4.50679100	-0.34324900
C	1.26354900	-4.15932700	-1.57404500
C	2.57554600	-3.63656200	-1.57338800
C	2.86265700	-2.63184400	-2.54629600
C	3.82004100	-1.58890700	-2.26565400
C	4.57763400	-1.54624300	-1.04500600
C	4.84996200	-0.22696900	-0.56712300
C	4.89132400	0.09430000	0.84345400
C	4.48509900	-0.87679300	1.81456800
C	3.72951100	-0.38465500	2.92605700
C	2.60183200	-1.11872900	3.44472000
C	2.19584700	-2.37377900	2.91233500
C	3.08813500	-2.95705500	1.92720300
C	2.53947100	-3.79758500	0.91234600
C	3.29243100	-3.58763500	-0.31240300

C	4.33220600	-2.59831100	-0.04779100
C	4.21960300	-2.22888500	1.36544400
C	-4.13562700	-2.05503900	-1.16381900
C	-4.60831700	-1.95622000	0.21507100
C	-4.92016900	-0.64077400	0.76449400
C	-4.43058400	-0.32787000	2.11705500
C	-4.06292800	1.02678200	2.38995100
C	-2.91007300	1.38702300	3.18812200
C	-2.38804000	2.62464300	2.69707400
C	-1.02293300	2.96945200	2.82444500
C	-0.50567600	4.00034800	1.91622800
C	0.93310700	4.18822600	1.89546300
C	1.67581300	4.54849800	0.68707300
C	0.95556000	4.71998400	-0.53535600
C	1.42307000	4.00929300	-1.72359900
C	0.26608900	3.65731200	-2.48417800
C	0.22306900	2.52470600	-3.35802400
C	-1.05976100	2.06801800	-3.71364600
C	-1.29948100	0.68639500	-3.98864300
C	-2.64398100	0.36249300	-3.58458200
C	-2.97206100	-0.90320600	-3.05204900
C	-4.06201400	-0.94262400	-2.06218200
C	-4.65484500	0.25841100	-1.59969400
C	-5.02331300	0.42109700	-0.18647000
C	-4.71550300	1.77425800	0.15367000
C	-4.22326100	2.07596300	1.42112800
C	-3.18900000	3.05385300	1.58689100
C	-2.58440300	3.73345400	0.48231500
C	-1.27637900	4.31826900	0.68871900
C	-0.49021400	4.65208400	-0.51162000
C	-0.90288900	4.09264300	-1.76930600
C	-2.17782100	3.49837000	-1.99183200
C	-2.25865600	2.59667000	-3.08126300
C	-3.24025100	1.56575300	-3.08752200
C	-4.20302100	1.52262200	-2.07948400
C	-4.15783200	2.45973600	-0.98852400
C	-3.09054300	3.38914800	-0.86438600
Pt	-0.14249300	-0.18444800	-0.95200700
La	0.53725300	2.32921900	0.10640800
La	-2.18588400	-1.13286300	0.73413900
La	2.20846300	-1.25538600	0.07045200

Data S3 The XYZ coordinates of $La_3Pt@C1(230926)$-C_{98}-1

Element	X	Y	Z
C	-2.84089800	-0.08766800	3.27279200
C	-1.68035400	0.72521200	3.57578500
C	-0.44278000	0.04123800	3.93610500
C	0.71692400	0.81812200	4.03461500
C	2.01497100	0.25147400	3.88960100
C	2.89247400	1.28925500	3.41137700
C	3.95357100	0.97440900	2.52866600
C	4.27131100	1.90248500	1.51035900
C	4.62760900	1.41343900	0.18321200
C	4.04774800	2.31544500	-0.76949900
C	3.46082900	1.84810300	-1.98530600
C	2.28858900	2.56004900	-2.50612500
C	1.30813500	1.88273200	-3.32846000
C	-0.11112700	2.26488800	-3.30044800
C	-1.11201900	1.23826200	-3.60464900
C	-2.45277000	1.47697200	-3.23619300
C	-3.35289100	0.40566200	-2.93017000
C	-4.27781400	0.87955500	-1.92360000
C	-4.79200300	0.00717000	-0.91595700
C	-4.91954300	0.50342600	0.41671600
C	-4.63382100	-0.36479800	1.54321900
C	-3.89575400	0.45048800	2.50013300
C	-2.72450800	-1.52254000	3.24142800
C	-3.53295700	-2.38495500	2.37684800
C	-4.45979900	-1.78089300	1.42911000
C	-4.45471200	-2.31183000	0.06999900
C	-4.51521300	-1.38852400	-1.05169600
C	-3.61735500	-1.84337300	-2.07678400
C	-2.93039700	-0.94708800	-2.96481300
C	-1.59772600	-1.27478400	-3.41620000
C	-0.72743800	-0.16149100	-3.81814800
C	0.63810100	-0.42247900	-4.00224600
C	1.64415000	0.58539200	-3.76536800
C	2.83964900	-0.08727100	-3.33763800
C	3.70705600	0.46569300	-2.34617200
C	4.44739300	-0.43784500	-1.43352500
C	4.83768100	0.04173500	-0.11255900
C	4.79061500	-0.88750600	1.03040900
C	4.21632200	-0.41066700	2.27021200
C	3.37257900	-1.44027800	2.80126300
C	2.17747700	-1.11198200	3.52768600

C	1.01884800	-1.96090800	3.40539400
C	-0.27363200	-1.38541500	3.73018500
C	-1.44458300	-2.12429000	3.40586200
C	-1.39704500	-3.32964900	2.65366000
C	-2.67163800	-3.50129100	1.98859300
C	-2.66504300	-4.01757100	0.63144300
C	-3.54199400	-3.38207500	-0.32031300
C	-3.02127500	-3.05476400	-1.64120400
C	-1.72719800	-3.43615900	-2.11203100
C	-1.00030400	-2.56235100	-3.02822200
C	0.43151400	-2.75822600	-3.15829000
C	1.20691000	-1.71091900	-3.74084300
C	2.57586300	-1.49355800	-3.39489700
C	3.22798200	-2.35150700	-2.49977800
C	4.21332800	-1.87182900	-1.56570300
C	4.16536700	-2.77781600	-0.42247500
C	4.41654900	-2.27655800	0.89339000
C	3.47122600	-2.59986000	1.96166400
C	2.29612300	-3.43587300	1.76696300
C	1.09373700	-3.16643800	2.55051600
C	-0.14422400	-3.81955400	2.15860800
C	-0.21540200	-4.52449500	0.92856800
C	-1.42691600	-4.49255100	0.13237000
C	-1.01054400	-4.31440900	-1.24945900
C	0.39999800	-4.40511400	-1.30540900
C	1.13241300	-3.67902300	-2.26832100
C	2.50864600	-3.44212900	-1.93821600
C	3.05711800	-3.68096100	-0.61437000
C	2.16488800	-4.07625700	0.45838100
C	0.90000800	-4.55619500	0.05179200
C	-2.83296300	2.62279200	-2.46193300
C	-3.94524400	2.23544900	-1.62021600
C	-4.00874900	2.70281800	-0.27976700
C	-4.48859000	1.82725100	0.73308500
C	-3.82709300	1.78447500	2.01642900
C	-2.72583900	2.62331700	2.33319800
C	-1.63298300	2.11962700	3.12749400
C	-0.35657200	2.85649400	3.09208800
C	0.76621100	2.19323600	3.63102300
C	2.10552500	2.48177400	3.22628200
C	2.36915300	3.41406200	2.18507900
C	3.52256200	3.11527100	1.36497100
C	3.47409400	3.39454200	-0.03302800
C	2.40066100	4.10796900	-0.55508300

C	1.84724500	3.73680000	-1.82164900
C	0.49627700	4.22432300	-1.87282800
C	-0.52233600	3.47325500	-2.58579900
C	-1.88899400	3.60379700	-2.09459400
C	-2.11776700	4.26854200	-0.80823800
C	-3.06090400	3.68938200	0.11156400
C	-2.46678300	3.70683300	1.42273500
C	-1.22519700	4.42039300	1.36039400
C	-0.10451500	3.98791300	2.18903000
C	1.25355100	4.19945600	1.66254300
C	1.37731500	4.68048800	0.27543600
C	0.24105600	4.90036600	-0.59421100
C	-1.06052300	4.84775900	-0.03134400
Pt	-0.09678700	-0.16341500	-0.95944000
La	-0.15662600	2.46753300	-0.01274000
La	-2.06353100	-1.38392500	0.52979200
La	2.29885300	-1.12376300	0.14802400

Data S4 The XYZ coordinates of $La_3Pt@C1(230933)\text{-}C_{98}$ (-1)

Element	X	Y	Z
C	4.83091000	0.36971300	0.71472200
C	4.44617300	-0.41671700	1.82885100
C	3.60451900	0.12527200	2.88711100
C	2.83618400	-0.94560200	3.42527600
C	1.48884300	-0.75059600	3.84127100
C	0.54366400	-1.86211100	3.70568000
C	-0.87588100	-1.62209700	3.64865900
C	-1.77532900	-2.46934100	2.85783100
C	-3.03294400	-1.87788400	2.38008800
C	-3.65071800	-2.47420100	1.25639800
C	-4.43082700	-1.70793900	0.33273300
C	-4.19739400	-2.25568700	-0.98924000
C	-4.07916200	-1.38694900	-2.11987800
C	-3.10081800	-1.68791800	-3.10624300
C	-2.32657800	-0.63667000	-3.72443800
C	-1.01463000	-1.15013800	-3.96125500
C	0.12434000	-0.32485800	-3.94954400
C	1.40754600	-0.92427400	-3.58230200
C	2.52241400	-0.02941400	-3.34603700

C	3.61480700	-0.46253700	-2.55499600
C	4.40864400	0.45390200	-1.74853800
C	4.79748200	-0.27758800	-0.56246100
C	4.56723600	1.79579700	0.75812300
C	4.30917100	2.57215000	-0.45475100
C	4.17782700	1.87658800	-1.74808600
C	3.11542000	2.30506300	-2.61799100
C	2.33780000	1.37760000	-3.42731900
C	1.03445900	1.92895900	-3.61120900
C	-0.10726300	1.11798500	-3.81172300
C	-1.40613800	1.64696700	-3.41519100
C	-2.53294500	0.72983000	-3.39970100
C	-3.66415300	1.02098500	-2.58861600
C	-4.39952400	-0.01866800	-1.92153200
C	-4.81444200	0.48482500	-0.63942200
C	-4.69891600	-0.33210700	0.54451000
C	-4.30279400	0.27979700	1.81059900
C	-3.42284800	-0.49583500	2.68997300
C	-2.56897100	0.21813700	3.58563500
C	-1.30257400	-0.31849300	3.98280000
C	-0.37574200	0.77018400	4.09052900
C	1.00535500	0.60740300	3.87771800
C	1.75963700	1.72090300	3.30068000
C	3.09457200	1.44800100	2.80981400
C	3.68879100	2.29796300	1.80483400
C	2.94791700	3.39741300	1.28638800
C	3.32145700	3.58334400	-0.10039200
C	2.30860700	4.04451100	-1.02339700
C	2.23987300	3.41025100	-2.29866100
C	0.96379100	3.17507800	-2.92470900
C	-0.26306600	3.63718900	-2.37614800
C	-1.47565200	2.88824900	-2.62444800
C	-2.61196100	3.11538800	-1.72872400
C	-3.69409700	2.18549400	-1.76274300
C	-4.47903600	1.87566200	-0.59788200
C	-4.27145500	2.54237500	0.63367800
C	-4.23885300	1.76368300	1.86637200
C	-3.26501700	2.43235900	2.70861500
C	-2.43803900	1.65022900	3.54584200
C	-1.05881000	1.97747300	3.75582400
C	-0.40113300	3.02711100	3.04228100
C	1.04010800	2.91036600	2.82655800
C	1.64675700	3.73592000	1.80318900
C	0.80282300	4.47606300	0.92500800

C	1.09950100	4.54487100	-0.48890500
C	-0.15451100	4.43925700	-1.19760000
C	-1.20564500	4.48616100	-0.24670900
C	-2.46573400	3.89690500	-0.49986100
C	-3.27979200	3.58800200	0.67672800
C	-2.65415600	3.53217400	2.00329500
C	-1.23684700	3.83914400	2.16951100
C	-0.60628500	4.48454000	1.08040600
C	-3.03469400	-3.55907500	0.54080200
C	-3.36346900	-3.39666000	-0.86239100
C	-2.38356000	-3.69634000	-1.85626500
C	-2.26817000	-2.84386100	-2.98436500
C	-0.96669100	-2.50833000	-3.51293000
C	0.22656800	-3.05683900	-2.99975900
C	1.44496800	-2.27658900	-3.02104200
C	2.51587300	-2.65945100	-2.09584500
C	3.57768600	-1.73331600	-1.90908100
C	4.30848800	-1.63405300	-0.68728800
C	3.97206100	-2.44473000	0.42989400
C	4.14374400	-1.82407700	1.71261200
C	3.23942200	-2.14310600	2.76188000
C	2.33004000	-3.19001900	2.61008200
C	1.01244500	-3.09901200	3.15727700
C	0.15786000	-4.01303800	2.44403400
C	-1.24833700	-3.68673000	2.23353200
C	-1.85733200	-4.18595200	0.99770200
C	-0.99101000	-4.76353400	-0.04293400
C	-1.20406400	-4.35962600	-1.41718500
C	0.07585500	-4.09875200	-2.01532300
C	1.09777500	-4.44216700	-1.07140000
C	2.32884800	-3.66929200	-1.05070200
C	2.99895600	-3.51407300	0.23805300
C	2.29199400	-3.99753300	1.42690000
C	0.99403100	-4.63174100	1.40327000
C	0.42535400	-4.93093400	0.13347300
Pt	-0.19899500	0.02787800	-0.94883900
La	2.24763100	1.15234000	-0.20574800
La	-2.00601000	1.33998300	0.72883900
La	0.23799400	-2.42529100	0.36796500

Data S5 The XYZ coordinates of $La_3Pt@C2(231010)$-C_{98}-2

Element	X	Y	Z
C	-3.26838200	-0.93081300	-2.62242400
C	-2.09735000	-1.67340400	-3.02962400
C	-1.03593900	-0.95265400	-3.73191800
C	0.18574000	-1.61213100	-3.92081800
C	1.41469000	-0.89479600	-4.01944300
C	2.46396400	-1.73388800	-3.48383900
C	3.52174700	-1.17708400	-2.70510000
C	3.99331400	-1.86373800	-1.50799000
C	4.48443300	-1.07695100	-0.37008800
C	4.35730400	-1.65181600	0.93173800
C	4.10363400	-0.83536200	2.08042900
C	3.13215500	-1.54396800	2.90115200
C	2.11532300	-0.84358900	3.57990700
C	0.79959500	-1.40863100	3.70187700
C	-0.30543200	-0.48728600	3.95395900
C	-1.61647200	-0.98429600	3.84165200
C	-2.71927900	-0.13616400	3.53329400
C	-3.70086200	-0.92636200	2.83461900
C	-4.49279000	-0.35556300	1.79633300
C	-4.74528900	-1.13882000	0.63675900
C	-4.76137600	-0.49969600	-0.66040000
C	-4.08710700	-1.40806900	-1.57242900
C	-3.33674400	0.48457700	-2.85546300
C	-4.09626600	1.40702100	-2.02180700
C	-4.77505800	0.91884000	-0.84128300
C	-4.68637500	1.74498600	0.36264800
C	-4.42788000	1.07171900	1.62034800
C	-3.47568400	1.84836100	2.36478100
C	-2.52363100	1.24536500	3.25795100
C	-1.21585100	1.82171500	3.40708600
C	-0.14014000	0.95020000	3.86647800
C	1.18431400	1.44260200	3.78232400
C	2.29725200	0.57173700	3.66839900
C	3.37232700	1.29247800	3.01219100
C	4.19501400	0.57745000	2.03748300
C	4.52875200	1.21962000	0.77330800
C	4.58550600	0.38112500	-0.44506100
C	4.26587900	0.97503300	-1.71042800
C	3.67125700	0.22597100	-2.76923700
C	2.66620600	1.06091300	-3.39622800
C	1.45933100	0.51794300	-3.89592400

C	0.21796700	1.26823000	-3.76349300
C	-1.02028200	0.51380000	-3.78765200
C	-2.20795100	1.17615100	-3.37641400
C	-2.21410300	2.50795300	-2.87537600
C	-3.38601300	2.67810700	-2.02715700
C	-3.28020100	3.49422400	-0.83007000
C	-3.92627800	2.99576800	0.37352400
C	-3.16372100	3.01995100	1.62533300
C	-1.86546300	3.62410400	1.76923700
C	-0.88270600	3.06475500	2.68944800
C	0.50612700	3.49288200	2.56103500
C	1.53265900	2.72329400	3.23907500
C	2.91954200	2.65323500	2.81919500
C	3.33424000	3.35353700	1.63568000
C	4.13421100	2.64048000	0.63981000
C	3.65933800	3.10572700	-0.64372800
C	3.72201500	2.30165400	-1.78506300
C	2.68937200	2.33998100	-2.77417900
C	1.50183300	3.11387800	-2.60151100
C	0.25170300	2.61475000	-3.16691600
C	-0.98541500	3.21309100	-2.70665300
C	-0.97604900	4.16472600	-1.64274100
C	-2.04658800	4.17548700	-0.65869100
C	-1.40700700	4.35621700	0.63990800
C	-0.02688600	4.60389400	0.43327200
C	0.94246500	4.26156500	1.41375300
C	2.31573600	4.12450600	0.94006700
C	2.54395700	3.98009000	-0.48583900
C	1.47897400	4.01589900	-1.46353000
C	0.23506000	4.48981200	-0.98812900
C	-1.88991500	-2.30424100	3.36499100
C	-3.17653900	-2.25903300	2.71527000
C	-3.39342800	-3.02197100	1.54011300
C	-4.17332700	-2.44963500	0.49856700
C	-3.75255200	-2.60294100	-0.87256000
C	-2.62979100	-3.38520200	-1.25059600
C	-1.79130300	-2.94612000	-2.35041400
C	-0.46367000	-3.54607500	-2.47947000
C	0.45961100	-2.90721200	-3.34141600
C	1.87103200	-2.98073000	-3.13084600
C	2.38840700	-3.70887000	-2.05506200
C	3.46473200	-3.17346800	-1.26992200
C	3.27070500	-3.66879700	0.06249600
C	3.69029100	-2.90201500	1.13965500

C	2.86094300	-2.80791900	2.30911300
C	1.58095500	-3.44245100	2.39142700
C	0.53171400	-2.75889100	3.15349600
C	-0.84582000	-3.19885000	2.99541500
C	-1.17334800	-4.17123100	1.96258300
C	-2.36956600	-3.95612400	1.17427400
C	-2.05439100	-4.22334200	-0.20853900
C	-0.72555700	-4.74629400	-0.27313800
C	0.08776700	-4.42647200	-1.42615500
C	1.49306900	-4.43396200	-1.21245300
C	2.06441400	-4.42935200	0.14896300
C	1.22573500	-4.39167300	1.30902300
C	-0.16293000	-4.73536100	1.09920200
Pt	0.25457900	0.03444200	-0.98117400
La	1.83158600	1.50492700	0.82859300
La	-2.22037200	1.19204700	-0.22083800
La	-0.19891100	-2.33485200	0.35791300

Data S6 The XYZ coordinates of $La_3Pt@C1(231005)$-C_{98}-2

Element	X	Y	Z
C	-2.38683500	1.52316900	-3.33272700
C	-2.07485300	0.15522200	-3.63846100
C	-0.70120600	-0.22347900	-3.87572300
C	-0.30285600	-1.61344600	-3.66052100
C	1.10897400	-1.95177200	-3.63968800
C	1.53507300	-3.12441400	-2.95335300
C	2.79229500	-3.14065500	-2.24379500
C	2.60028700	-3.87765000	-1.02077200
C	3.14805900	-3.41195400	0.22170500
C	2.33771000	-3.48323300	1.43494100
C	2.44383500	-2.43546000	2.43303000
C	1.24974400	-2.11561000	3.25227300
C	1.10617300	-0.74351900	3.74924300
C	-0.18669100	-0.13878500	3.97461000
C	-0.41828300	1.29372400	3.78512600
C	-1.73461300	1.75738100	3.33678700
C	-1.82255900	3.01314600	2.61687000
C	-2.89825200	3.22960600	1.68765600
C	-2.70331500	3.92729400	0.41959700
C	-3.66523900	3.40171500	-0.52133000

C	-3.19351200	3.16898400	-1.87306000
C	-3.52684600	1.92026400	-2.52562400
C	-1.35380600	2.47709200	-3.13898700
C	-1.80934000	3.46671000	-2.20114600
C	-0.85697700	4.05338300	-1.29117200
C	-1.35623000	4.33974200	0.05021400
C	-0.42097500	4.41429700	1.10414900
C	-0.65568400	3.77673300	2.38809900
C	0.59482800	3.38741100	2.91806300
C	0.72714400	2.14774800	3.59934400
C	2.03452100	1.56395400	3.57078700
C	2.20197900	0.15212600	3.61189700
C	3.41673500	-0.18694800	2.95696600
C	3.51321000	-1.45833600	2.30197000
C	4.36263500	-1.47425300	1.16434500
C	4.14599500	-2.40511900	0.11639500
C	4.45130400	-1.75035700	-1.13568100
C	3.69301100	-2.04767500	-2.31036800
C	3.36032300	-0.96900400	-3.17850500
C	2.06973800	-0.92266700	-3.81012900
C	1.66877500	0.44791500	-3.88966600
C	0.31521300	0.83392200	-3.86500700
C	0.01696200	2.16069900	-3.33562300
C	1.00715100	2.93563900	-2.61138200
C	0.56457100	3.83472000	-1.52909200
C	1.48963700	4.12821200	-0.44252900
C	0.97728900	4.38583300	0.85728800
C	1.64125500	3.85251000	2.03064300
C	2.92969100	3.26069100	1.98923700
C	3.16785800	2.13682300	2.87075900
C	4.05491600	1.04024000	2.49236100
C	4.76471900	1.04469200	1.22157200
C	4.88484800	-0.23437200	0.59105800
C	4.87787700	-0.42104200	-0.84878000
C	4.51479400	0.66484500	-1.70796600
C	3.75194700	0.37529500	-2.87053800
C	2.69306700	1.25950900	-3.31327000
C	2.37436200	2.45280200	-2.62164800
C	3.26781500	2.80977200	-1.55525700
C	2.82956200	3.61412500	-0.47061800
C	3.59740400	3.25293100	0.71096500
C	4.52323600	2.18309200	0.33481600
C	4.31499000	1.94201100	-1.08630600
C	-3.93612900	2.27615000	1.51585000

C	-4.42748000	2.36022700	0.14055900
C	-4.81468900	1.11946700	-0.53204800
C	-4.35672200	0.90127200	-1.90955600
C	-4.12851500	-0.44048600	-2.34961500
C	-3.00517600	-0.80236900	-3.19727500
C	-2.57697000	-2.12068500	-2.84788000
C	-1.24502200	-2.53557200	-3.02864000
C	-0.78492500	-3.62948900	-2.17611100
C	0.60377500	-3.92362200	-2.21972500
C	1.28792600	-4.42006700	-1.06504500
C	0.57925200	-4.67296000	0.11225400
C	1.10935800	-4.25790300	1.38163900
C	-0.00318900	-4.08508900	2.28232400
C	0.07076900	-2.96974700	3.21513300
C	-1.18175400	-2.37602100	3.54573300
C	-1.30142300	-0.99629600	3.93064700
C	-2.60772800	-0.53134700	3.61199900
C	-2.83713900	0.82062500	3.20730300
C	-3.93213000	1.06346900	2.28328900
C	-4.64028700	-0.04444000	1.71446700
C	-4.99662700	-0.02301200	0.30171100
C	-4.79337400	-1.36201800	-0.18891100
C	-4.35652600	-1.55944000	-1.49220400
C	-3.39470300	-2.59724400	-1.76666300
C	-2.85623300	-3.42620100	-0.74363000
C	-1.56620500	-4.04698300	-1.00060400
C	-0.85655800	-4.62415300	0.14049600
C	-1.24932600	-4.36709500	1.51828100
C	-2.46319200	-3.61978600	1.76134600
C	-2.43882600	-2.75456200	2.91472800
C	-3.30769700	-1.62447000	3.01561200
C	-4.28205600	-1.38529300	2.04320000
C	-4.31756800	-2.21242000	0.86713600
C	-3.32408600	-3.23306200	0.64363900
Pt	0.24891500	-0.07394600	-0.97580600
La	2.26728800	0.99406500	0.63371500
La	-2.03840000	1.49745400	-0.34868600
La	-0.43501000	-2.13302600	0.74255000

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