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

Electronic Supporting Information

La–La bonded dimetallofullerenes $[La_2@C_{2n}]^-$: species for stabilizing C_{2n} (2n = 92–96) besides $La_2C_2@C_{2n}$

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Note S1. Computational details for statistical thermodynamic analysis

Relative concentrations or mole fractions X_i of m isomers can be expressed through the partition functions q_i and the ground-state energies $\Delta H_{0,i}^{o}$ by the following compact formula reported by Slanina Zdeněk and co-workers[S1-2]:

$$Xi = \frac{q_i \exp[-\Delta H_{0,i}^{o}/(RT)]}{\sum_{j=1}^{m} q_j \exp[-\Delta H_{0,j}^{o}/(RT)]}$$

This equation is an exact formula that can be directly resulted from the standard Gibbs energies of the isomers and strongly temperature-dependent, simulating the conditions of the inter-isomeric thermodynamic equilibrium. In this equation, R and T represent the gas constant and the absolute temperature, respectively. $\Delta H_{0,i}^{o}$ represents the enthalpies at the absolute zero temperature or ground-state energies, i.e., the relative potential energy corrected by the vibrational zero-point energy. The rotational–vibrational partition functions can result from the calculated structural and vibrational data using the rigid rotator and harmonic oscillator approximation with no frequency scaling. The chirality contributions are considered as its partition functions q_i is doubled for an enantiomeric pair.

The encapsulate motions can be described via a modified and simplified treatment, the so called free, fluctuating, or floating encapsulate model (FEM) proposed by Slanina Zdeněk et al, which is on the basis of the findings from observation and calculations that the encapsulated atoms can exercise large amplitude motions, especially at high temperatures (unless the motions are restricted by cage derivatizations). According to this model, the encapsulate is assumed to be relatively free, then, at sufficiently high temperatures, its behavior in different fullerene cages would lead to the same contribution to the partition functions which can be cancelled out in above equation. When performing this FEM approach, two steps should be considered: firstly, the three lowest vibrational frequencies belonging to the metal motions in the cage should be removed; in addition, the symmetries of the isomers should be treated as the topologically highest possible.

REFERENCES:

[S1] Slanina, Z. *Int. Rev. Phys. Chem.* **1987**, *6*, 251-267.

[S2] Slanina, Z.; Lee, S. L.; Uhlík, F.; Adamowicz, L.; Nagase, S. *Theor. Chem. Acc.* **2007**, *117*, 315-322.

Table S1. Relative potential energies (E_{Rel}, kcal mol^{-1}) and HOMO–LUMO gaps (eV) of anionic C_{94}^{6-} model at different theory levels.

C_{94}^{6-} spiral ID	IPR ID	sym.[a]	PA[b]	AM1	M06-2X/6-31G(d)		C_{94}^{6-} spiral ID	IPR ID	sym.	PA	AM1	M06-2X/6-31G(d)	
					E_{Rel}	gap						E_{Rel}	gap
153480	**121**	C_2	0	0.0	0.0	3.35	153451	92	C_1	0	22.5	24.6	2.95
153476	**117**	C_2	0	6.8	5.9	2.64	153433	74	C_1	0	24.8	25.1	2.45
152345		C_s	1	11.1	10.3	2.68	131505		C_1	1	29.5	25.5	2.91
153485	126	C_2	0	10.1	11.2	2.97	153450	91	C_1	0	23.2	25.6	2.80
153489	130	C_2	0	10.8	11.6	2.96	153481	122	C_1	0	23.1	25.7	2.19
151381		C_2	1	16.0	12.3	3.02	152750		C_1	1	25.3	25.7	2.75
153289		C_1	1	17.9	12.4	3.28	153469	110	C_3	0	25.7	25.8	1.90
141346		C_1	1	15.5	12.4	3.17	153148		C_1	1	28.2	26.5	2.55
153488	129	C_1	0	13.3	13.5	2.87	148551		C_1	2	29.9	26.5	3.07
153491	132	C_1	0	11.7	13.5	2.46	150836		C_1	1	26.5	26.6	2.88
153413	54	C_1	0	14.4	13.9	2.28	120213		C_1	1	29.2	26.7	2.56
153474	115	C_1	0	13.7	14.0	2.51	153490	131	C_1	0	27.5	27.3	2.34
153484	125	C_1	0	14.1	14.6	2.56	152752		C_2	2	32.7	27.6	3.28
153307		C_s	1	15.7	14.9	2.65	153415	56	C_1	0	27.4	28.3	2.33
150347		C_1	1	20.7	15.5	2.99	153305		C_1	1	28.7	28.5	2.49
152749		C_1	1	18.7	15.6	2.98	153487	128	C_1	0	25.7	29.0	2.05
153477	118	C_1	0	15.6	16.4	2.22	118496		C_1	1	29.2	29.2	3.01
153478	119	C_1	0	15.0	16.7	2.71	151710		C_1	1	29.2	29.2	2.54
153479	**120**	C_s	0	21.1	16.8	2.00	153379	20	C_2	0	24.2	30.2	2.47
153471	112	C_1	0	16.0	16.8	2.71	153460	101	C_1	0	29.6	30.3	2.27
149086		C_1	1	19.6	16.8	2.85	152730		C_1	1	30.0	30.8	2.86
152655		C_1	1	20.3	17.1	2.76	149085		C_2	2	35.8	30.9	2.76
153418	59	C_1	0	15.0	18.1	2.53	153232		C_1	1	30.0	31.3	2.82
153416	57	C_1	0	18.2	18.6	2.73	153395	36	C_1	0	26.9	31.6	2.41
141360		C_1	1	20.9	18.8	2.99	153453	94	C_2	0	27.3	32.2	2.49
143831		C_1	1	19.1	18.8	2.90	153393	34	C_1	0	27.5	33.0	2.53
136631		C_1	1	23.1	19.0	2.92	153317		C_2	2	39.8	34.2	2.73
153285		C_1	1	22.4	19.3	3.01	153493	134	C_{3v}	0	32.7	35.4	2.03
153461	102	C_1	0	20.8	19.5	2.48	123227		C_2	2	41.3	35.7	3.41
153392	33	C_2	0	18.0	19.6	2.67	153402	43	C_2	0	29.6	37.1	2.63
123185		C_1	1	21.5	19.6	3.00	151095		C_2	2	46.4	37.3	3.89
153492	133	C_2	0	18.2	19.8	2.94	120155		C_2	2	44.6	37.4	3.17
153410	51	C_2	0	15.8	19.8	2.64	151090		C_2	2	42.8	37.8	2.82
153483	124	C_2	0	19.4	19.9	2.38	153377	18	C_s	0	32.6	38.8	2.04
139389		C_1	1	22.9	20.0	3.16	117086		C_2	2	44.3	39.3	3.04

153458	99	C_1	0	20.4	20.1	2.78	149087		C_s	2	46.6	39.3	2.80
123142		C_1	1	24.1	20.4	3.06	151614		C_2	2	47.2	39.9	3.37
153454	95	C_1	0	19.1	20.8	2.53	150352		C_2	2	47.1	39.9	3.08
153229		C_1	1	22.7	21.1	2.99	153326		C_2	2	45.5	40.0	2.84
149092		C_1	2	25.7	21.4	3.15	150782		C_s	2	44.6	40.9	3.29
153431	72	C_1	0	20.7	21.4	2.67	152778		C_2	2	43.9	41.3	2.82
153146		C_1	1	25.4	21.9	2.50	153328		C_2	2	49.7	41.6	3.41
152479		C_1	1	26.6	22.0	3.03	153398	39	C_s	0	39.8	42.4	2.57
117861		C_1	1	24.4	22.1	3.39	153330		C_s	2	49.6	42.4	2.84
153449	90	C_1	0	23.1	22.8	2.85	153327		C_2	2	49.2	42.9	2.73
149084		C_1	1	26.3	22.9	2.51	153390	31	C_s	0	38.8	43.1	2.18
153475	116	C_1	0	24.0	23.0	2.66	153404	45	C_s	0	36.6	43.1	2.33
122503		C_1	1	24.3	23.5	2.93	152955		C_s	1	44.3	46.7	2.39
152527		C_1	1	27.2	23.6	2.38	153312		C_2	2	48.8	47.5	2.65
153306		C_s	1	23.8	24.0	2.74	153238		C_2	2	48.1	47.8	3.20
151612		C_1	1	27.9	24.1	3.02	153411	52	C_{2v}	0	49.3	48.0	2.50
151601		C_1	1	26.9	24.2	2.98	153401	42	C_s	0	39.2	48.4	2.45
149095		C_1	1	26.8	24.3	2.81	152572		C_2	2	49.8	49.1	2.75
143646		C_1	1	26.6	24.5	2.56	153403	44	C_s	0	47.9	56.3	2.08

[a]sym.: symmetry of the original empty cage.

[b]PA: the number of pentagon adjacency.

Note S2. Computational details for anionic C_{94}^{6-} and C_{92}^{4-} models

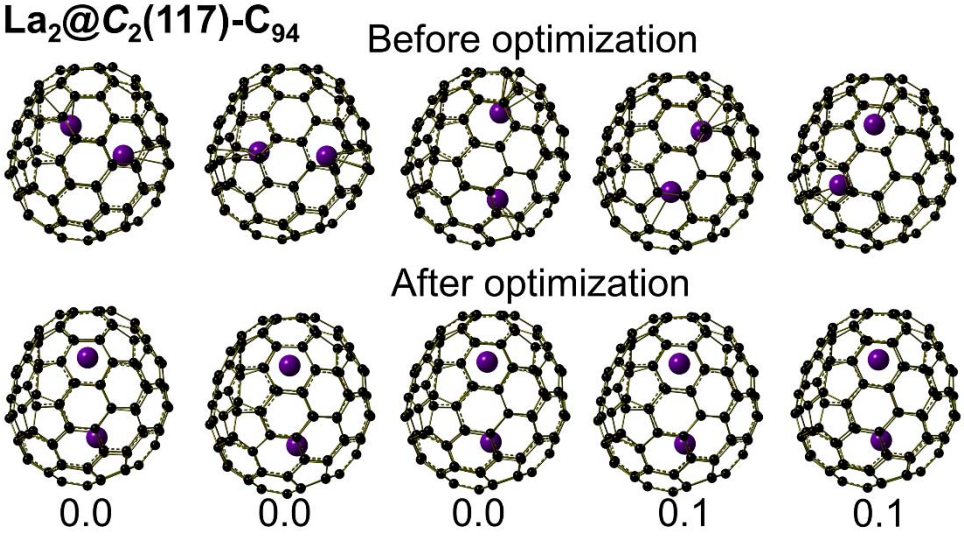
The initial screenings of anionic C_{94}^{6-} (134, 1285, and 7567 isomers for PA = 0, 1, and 2, respectively) and C_{92}^{4-} (86, 840, and 5401 isomers for PA = 0, 1, and 2, respectively) cages were performed with the semi-empirical AM1 method. Subsequent structural optimizations of selected isomers with relative potential energies less than 30.0 kcal mol^{-1} (several high-symmetry isomers with relative energies less than 50.0 kcal mol^{-1} were also considered) were carried out through the dispersion-corrected density functional theory method M06-2X with the basis set of 6-31G(d) for C. The results at the M06-2X/6-31G(d) level are basically consistent with those reported previously[S3] at the B3LYP/6-31G(d) level.

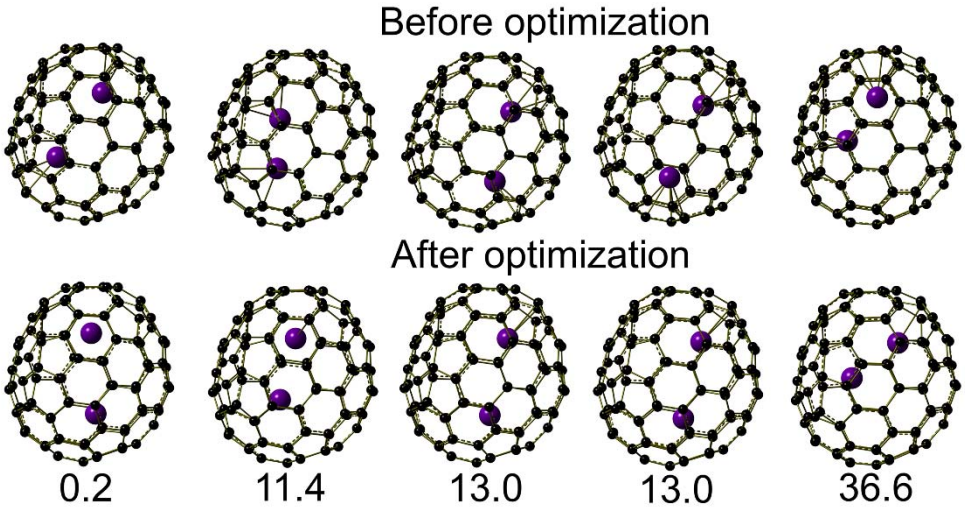
REFERENCE: [S3] Guo, Y. J.; Yang, T.; Nagase, S.; Zhao, X. *Inorg. Chem.* **2014**, *53*, 2012-2021.

Table S2. Relative potential energies (E_{Rel}, kcal mol^{-1}) and HOMO–LUMO gaps (eV) of anionic C_{92}^{4-} model at different theory levels.

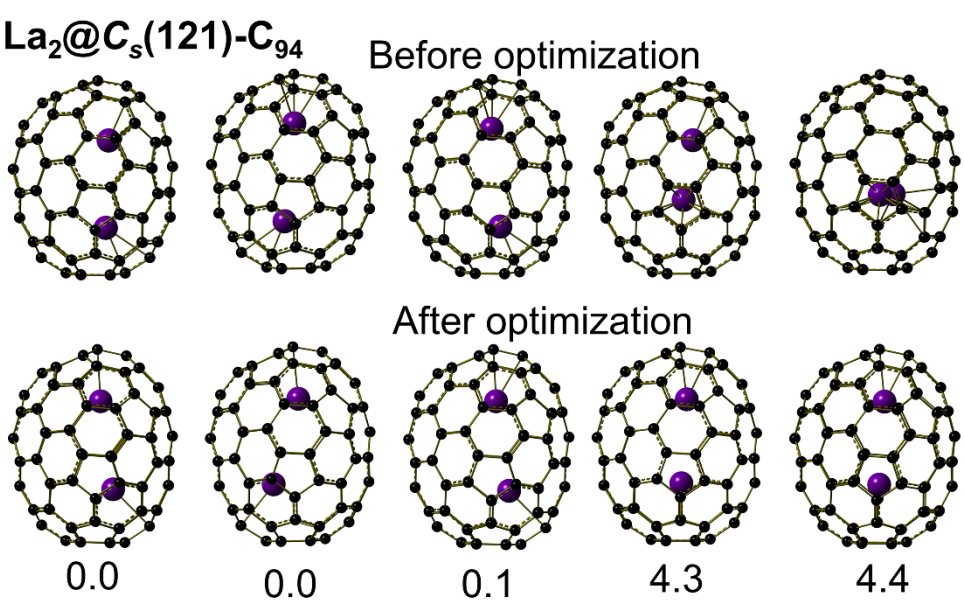
C_{92}^{4-}	IPR	sym.	PA	AM1	M06-2X/6-31G(d)		C_{92}^{4-}	IPR	sym.	PA	AM1	M06-2X/6-31G(d)	
spiral ID	ID				E_{Rel}	gap	spiral ID	ID				E_{Rel}	gap
126408	**85**	D_3	0	0.0	0.0	3.03	126395	72	C_1	0	28.2	26.1	2.64
126387	**64**	C_2	0	8.0	7.5	2.64	126404	81	D_2	0	28.9	26.3	2.90
126390	67	C_1	0	8.3	7.9	2.85	126407	84	D_2	0	22.9	26.7	1.84
126339	**16**	C_s	0	8.9	10.7	2.71	126402	79	C_2	0	29.9	26.9	2.75
126389	66	C_1	0	11.9	12.2	2.42	126332	9	C_2	0	29.0	27.6	2.39
126382	59	C_1	0	10.7	13.5	2.39	126409	86	T	0	29.6	27.9	2.31
126359	36	C_2	0	13.0	14.2	2.46	126334	11	C_1	0	28.6	28.0	2.49
126397	74	C_2	0	14.8	17.0	2.51	126394	71	D_3	0	29.8	28.5	2.58
126392	69	C_2	0	15.1	17.0	2.22	126405	82	D_2	0	24.4	28.6	1.94
126391	68	C_1	0	16.8	17.0	2.44	126406	83	D_3	0	25.9	28.9	1.92
126355	32	C_1	0	14.8	17.2	2.46	126401	78	D_3	0	29.5	29.1	2.50
126367	44	C_1	0	17.0	17.2	2.32	126337	14	C_s	0	26.0	29.4	2.15
126383	60	C_1	0	17.9	18.5	2.13	126358	35	C_{2v}	0	30.9	30.6	1.92
126400	77	C_2	0	14.2	18.5	2.15	126351	28	D_3	0	29.1	31.4	2.52
126338	**15**	C_s	0	15.2	18.5	2.20	126271		C_1	1	26.5	31.7	1.79
126393	70	C_1	0	18.0	19.6	2.19	125827		C_s	1	24.8	32.5	2.26
126399	76	C_1	0	17.6	19.9	2.30	126278		C_1	1	31.6	33.3	1.89
126388	65	C_2	0	18.0	19.9	1.94	126289		C_1	1	28.8	34.3	2.02
126385	62	C_1	0	19.1	20.2	2.25	124328		C_1	1	29.9	34.5	1.53
126333	10	C_1	0	18.0	20.7	2.27	120663		C_1	1	32.0	34.7	1.96
126354	31	C_2	0	18.7	21.1	2.46	126321		C_1	1	33.3	34.8	1.57
126398	75	C_2	0	25.6	21.7	2.55	121023		C_1	1	41.1	37.1	2.87
126384	61	C_2	0	20.0	22.1	2.32	104189		C_1	1	33.2	37.4	1.55
126396	73	C_1	0	22.6	23.2	1.95	124721		C_1	1	45.1	41.7	2.67
126386	63	C_1	0	21.2	23.3	2.17	121020		C_1	1	48.4	44.4	2.50
126347	24	C_s	0	25.6	23.5	2.40	124498		C_s	1	44.7	45.6	2.31
126365	42	C_1	0	22.9	24.6	2.01	126323		C_{2v}	1	48.3	46.2	2.93
126403	80	C_2	0	22.2	24.8	2.09	126200		C_2	2	47.1	46.8	2.01
126357	34	C_2	0	21.0	25.1	1.96	126217		C_2	2	50.6	51.7	2.26
126366	43	C_1	0	24.0	25.8	2.12	98832		C_2	2	45.4	56.2	2.01

$La_2@C_2(117)$-C_{94}





$La_2@C_s(121)$-C_{94}



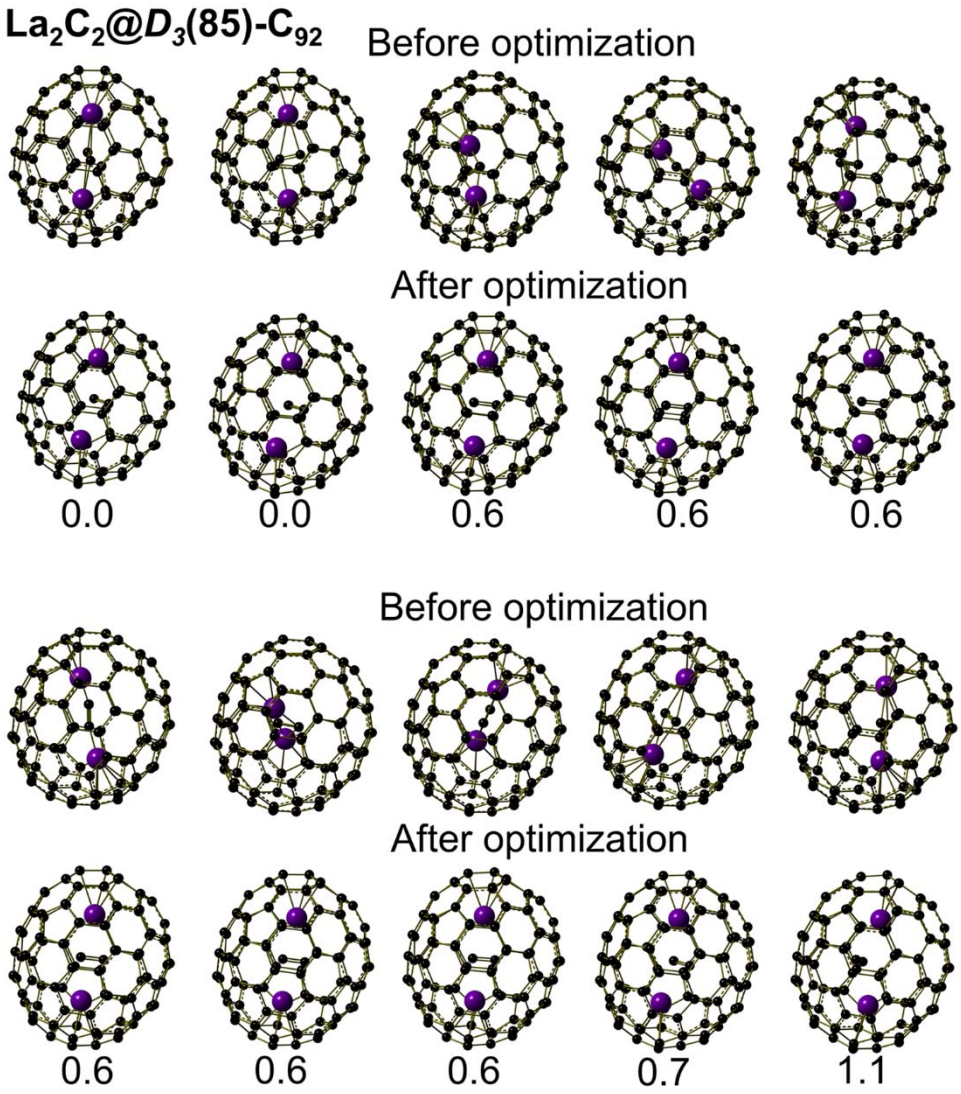


Figure S1. Geometry structures of $La_2@C_{94}$ and $La_2C_2@C_{92}$ with singlet state considering different encapsulation positions of La_2 and La_2C_2 at M06-2X/STO-3G~Lanl2dz level.

Note S3. Computational details for $La_2@C_{94}$ and $La_2C_2@C_{92}$ isomers

In this work, different positions of encaged La_2 in each C_{94} cage and La_2C_2 in each C_{92} cage were considered to explore their real energy minimum points. Herein, we just present the results of several key structures (Figure S1), though all relevant $La_2@C_{94}$ and $La_2C_2@C_{92}$ isomers considering different encapsulation positions were performed. Subsequently, several higher computational methods (see below) were adopted to further explore the lowest-energy geometry of each isomer and the relative stability of $La_2@C_{94}$, $La_2C_2@C_{92}$, and La_2C_{94} isomers, respectively.

Table S3. Relative potential energies (kcal mol^{-1}) of $La_2@C_{94}$ with respect to the lowest-energy triplet isomer $La_2@C_2(117)$-C_{94} at different theory levels.[a]

$La_2@C_{94}$	IPR	Sym.	PA	(U)M06-2X/*x*~CEP-4G				(U)B3LYP/*x*~CEP-4G			
	ID			*x* = 3-21G		*x* = 6-31G(d)		*x* = 3-21G		*x* = 6-31G(d)	
spiral ID				singlet	triplet	singlet	triplet	singlet	triplet	singlet	triplet
153476	**117**	C_2	0	15.9	0.0	16.2	0.0	8.7	0.0	8.5	0.0
153479	**120**	C_s	0	17.2	4.5	17.5	4.6	11.1	6.0	10.3	5.6
153480	**121**	C_2	0	20.3	6.4	20.4	5.5	6.2	5.6	7.3	5.0
152345		C_s	1	23.8	5.7	25.7	7.1	13.3	6.1	16.2	7.8
153413	54	C_1	0	20.9	8.6	22.1	9.0	12.6	8.2	12.8	8.4
153491	132	C_1	0	23.3	10.6	22.5	9.2	15.6	8.3	13.8	6.9
153474	115	C_1	0	26.3	10.3	25.9	9.6	16.7	9.6	15.4	9.0
153485	126	C_2	0	26.9	11.2	27.1	10.3	15.3	8.4	14.5	7.4
153307		C_s	1	28.0	9.9	30.8	11.4	17.8	10.6	20.4	12.4
153489	130	C_2	0	28.8	13.8	27.6	12.3	16.1	12.4	15.6	11.2
153484	125	C_1	0	33.2	16.0	31.4	13.4	20.2	12.7	18.1	10.5
153488	129	C_1	0	28.2	14.9	28.3	13.9	15.8	12.4	15.0	11.2
141346		C_1	1	20.2	10.6	24.7	14.5	7.9	14.6	13.7	18.8
151381		C_2	1	29.6	15.7	31.6	16.9	15.6	13.4	18.9	15.3
153289		C_1	1	21.3	13.0	26.1	17.4	10.1	17.5	16.1	21.4
153306		C_s	1	39.9	24.4	41.0	25.0	27.4	21.4	28.6	22.5
149092		C_1	2	37.6	25.0	41.4	27.9	24.7	25.5	30.0	29.1
148551		C_1	2	42.8	27.7	46.8	30.7	28.9	28.1	34.4	31.6
153493	134	C_{3v}	0	42.6	32.9	42.1	32.8	31.7	27.8	29.8	25.8
153317		C_2	2	53.5	37.5	54.4	37.5	42.0	33.8	42.9	34.4
149085		C_2	2	65.6	51.4	67.3	53.1	51.0	43.0	52.7	44.5
152752		C_2	2	79.9	65.4	79.0	64.5	61.8	54.5	60.8	53.4

[a]The influence of functionals (M06-2X and B3LYP) and basis sets (3-21G and 6-31G(d)) on the stability of $La_2@C_{94}$ isomers can be ignored.

Table S4. Relative potential energies (kcal mol^{-1}) of $La_2C_2@C_{92}$ with respect to the lowest-energy singlet isomer $La_2C_2@D_3(85)$-C_{92} at different theory levels.[a]

$La_2C_2@C_{92}$ spiral ID	IPR ID	sym.	PA	(U)M06-2X/*x*~CEP-4G			(U)B3LYP/*x*~CEP-4G		
				x = 3-21G		*x* = 6-31G(d)	*x* = 3-21G		*x* = 6-31G(d)
				singlet	triplet	singlet	singlet	triplet	singlet
126408	**85**	D_3	0	0.0	27.6	0.0	0.0	22.1	0.0
126387	**64**	C_2	0	7.7	27.7	7.5	6.6	23.3	6.4
126390	67	C_1	0	14.6	31.1	13.2	12.1	35.6	11.0
126359	36	C_2	0	8.7	19.3	13.3	10.1	28.9	13.7
126338	**15**	C_s	0	11.1	15.8	13.7	10.0	13.9	13.2
126339	**16**	C_s	0	12.2	24.5	13.8	9.8	20.0	13.0
126389	66	C_1	0	18.0	35.6	17.0	15.0	28.0	14.2
126382	59	C_1	0	17.9	26.5	18.3	16.6	28.8	16.4
126347	24	C_s	0	16.1	19.6	19.4	15.1	18.0	19.1
126271		C_1	1	20.5	37.6	20.3	18.0	31.8	18.4
125827		C_s	1	20.9	35.3	21.1	18.8	30.0	20.1
126407	84	D_2	0	30.9	42.2	29.3	25.5	32.9	24.3
98832		C_2	2	25.2	46.4	37.2	27.1	44.7	39.3
126394	71	D_3	0	40.7	44.9	39.0	35.2	38.7	33.0
126406	83	D_3	0	46.1	49.5	42.4	39.0	46.0	35.4
126404	81	D_2	0	47.0	49.8	43.9	38.9	43.8	36.5
126409	86	T	0	49.7	56.8	46.5	43.9	47.6	40.5
126405	82	D_2	0	54.3	53.5	51.5	44.6	44.9	42.3
126200		C_2	2	57.8	78.0	56.8	51.3	67.5	51.7
126217		C_2	2	75.0	89.2	73.3	66.9	78.9	66.6

[a]The influence of functionals (M06-2X and B3LYP) and basis sets (3-21G and 6-31G(d)) on the stability of $La_2C_2@C_{92}$ isomers can be ignored.

Table S5. Relative potential energies (E_{Rel}, kcal mol^{-1}) and HOMO/SOMO–LUMO gaps (eV) of La_2C_{94} at different theory levels.

La_2C_{94} (spiral ID)	IPR ID	PA	(U)M06-2X/*x*~CEP-4G					(U)B3LYP/*x*~CEP-4G				
			spin[a]	*x* = 3-21G		*x* = 6-31G(d)		spin	*x* = 3-21G		*x* = 6-31G(d)	
				E_{Rel}	gap	E_{Rel}	gap		E_{Rel}	gap	E_{Rel}	gap
$La_2@C_2$(153476)-C_{94}	**117**	0	3et	0.0	1.34	0.0	1.46	3et	0.0	0.74	0.0	0.75
$La_2@C_s$(153479)-C_{94}	**120**	0	3et	4.5	1.06	4.6	1.17	3et	6.0	0.71	5.6	0.72
$La_2@C_2$(153480)-C_{94}	**121**	0	3et	6.4	1.92	5.5	1.93	3et	5.6	0.80	5.0	0.83
$La_2@C_s$(152345)-C_{94}		1	3et	5.7	1.46	7.1	1.55	3et	6.1	0.78	7.8	0.79
$La_2@C_1$(153413)-C_{94}	54	0	3et	8.6	1.39	9.0	1.50	3et	8.2	0.75	8.4	0.76
$La_2@C_1$(153491)-C_{94}	132	0	3et	10.6	1.69	9.2	1.80	3et	8.3	0.73	6.9	0.74
$La_2@C_1$(153474)-C_{94}	115	0	3et	10.3	1.58	9.6	1.69	3et	9.6	0.71	9.0	0.72
$La_2@C_2$(153485)-C_{94}	126	0	3et	11.2	1.63	10.3	1.68	3et	8.4	0.76	7.4	0.77
$La_2@C_s$(153307)-C_{94}		1	3et	9.9	1.07	11.4	1.13	3et	10.6	0.78	12.4	0.79
$La_2@C_2$(153489)-C_{94}	130	0	3et	13.8	1.92	12.3	1.94	3et	12.4	0.82	11.2	0.83
$La_2@C_1$(153484)-C_{94}	125	0	3et	16.0	1.60	13.4	1.66	3et	12.7	0.77	10.5	0.78
$La_2@C_1$(153488)-C_{94}	129	0	3et	14.9	1.51	13.9	1.57	3et	12.4	0.71	11.2	0.72
$La_2@C_1$(141346)-C_{94}		1	3et	10.6	1.75	14.5	1.77	1et	7.9	1.36	13.7	1.29
$La_2@C_2$(151381)-C_{94}		1	3et	15.7	1.63	16.9	1.69	3et	13.4	0.74	15.3	0.74
$La_2@C_1$(153289)-C_{94}		1	3et	13.0	1.71	17.4	1.72	1et	10.1	1.34	16.1	1.27
$La_2C_2@D_3$(126408)-C_{92}	**85**	0	1et	4.9	3.04	20.1	2.97	1et	10.9	1.71	23.1	1.65
$La_2@C_s$(153306)-C_{94}		1	3et	24.4	1.77	25.0	1.78	3et	21.4	0.77	22.5	0.78
$La_2C_2@C_2$(126387)-C_{92}	64	0	1et	12.6	2.91	27.5	2.86	1et	17.5	1.60	29.6	1.57
$La_2@C_1$(149092)-C_{94}		2	3et	25.0	1.76	27.9	1.82	3et	25.5	0.75	29.1	0.76
$La_2@C_1$(148551)-C_{94}		2	3et	27.7	1.87	30.7	1.88	3et	28.1	0.77	31.6	0.78
$La_2@C_{3v}$(153493)-C_{94}	134	0	3et	32.9	1.30	32.8	1.48	3et	27.8	0.82	25.8	0.83
$La_2C_2@C_1$(126390)-C_{92}	67	0	1et	19.5	3.13	33.2	3.11	1et	23.1	1.85	34.1	1.81
$La_2C_2@C_2$(126359)-C_{92}	36	0	1et	13.6	2.81	33.4	2.88	1et	21.0	1.63	36.9	1.60
$La_2C_2@C_s$(126338)-C_{92}	**15**	0	1et	16.1	2.31	33.8	2.34	1et	20.9	1.05	36.4	1.08
$La_2C_2@C_s$(126339)-C_{92}	**16**	0	1et	17.2	2.46	33.9	2.44	1et	20.7	1.22	36.1	1.20
$La_2C_2@C_1$(126389)-C_{92}	66	0	1et	22.9	2.62	37.0	2.56	1et	25.9	1.32	37.4	1.29
$La_2@C_2$(153317)-C_{94}		2	3et	37.5	1.39	37.5	1.44	3et	33.8	0.76	34.4	0.77
$La_2C_2@C_1$(126382)-C_{92}	59	0	1et	22.9	2.52	38.3	2.47	1et	27.5	1.28	39.5	1.24
$La_2C_2@C_s$(126347)-C_{92}	24	0	1et	21.0	2.24	39.5	2.27	1et	26.0	0.97	42.2	1.01
$La_2C_2@C_1$(126271)-C_{92}		1	1et	25.4	2.53	40.3	2.52	1et	28.9	1.31	41.5	1.29

$La_2C_2@C_s$(125827)-C_{92}		1	1et	25.8	2.51	41.1	2.51	1et	29.8	1.27	43.3	1.26
$La_2C_2@D_2$(126407)-C_{92}	84	0	1et	35.9	2.31	49.3	2.29	1et	36.4	1.05	47.5	1.03
$La_2@C_2$(149085)-C_{94}		2	3et	51.4	1.72	53.1	1.72	3et	43.0	0.70	44.5	0.71
$La_2C_2@C_2$(98832)-C_{92}		2	1et	30.1	2.72	57.3	2.68	1et	38.0	1.48	62.5	1.44
$La_2C_2@D_3$(126394)-C_{92}	71	0	1et	45.6	2.21	59.1	2.20	1et	46.1	1.01	56.1	1.06
$La_2C_2@D_3$(126406)-C_{92}	83	0	1et	51.0	2.13	62.4	2.13	1et	49.9	1.02	58.6	1.02
$La_2C_2@D_2$(126404)-C_{92}	81	0	1et	51.9	2.27	64.0	2.28	1et	49.9	1.01	59.6	1.01
$La_2@C_2$(152752)-C_{94}		2	3et	65.4	1.79	64.5	1.80	3et	54.5	0.75	53.4	0.76
$La_2C_2@T$(126409)-C_{92}	86	0	1et	54.6	2.22	66.6	2.18	1et	54.8	0.95	63.6	0.93
$La_2C_2@D_2$(126405)-C_{92}	82	0	1et	59.2	1.85	71.5	1.85	1et	55.5	0.79	65.4	0.79
$La_2C_2@C_2$(126200)-C_{92}		2	1et	62.7	2.66	76.8	2.64	1et	62.2	1.42	74.9	1.39
$La_2C_2@C_2$(126217)-C_{92}		2	1et	79.9	2.47	93.4	2.48	1et	77.8	1.26	89.8	1.27

[a]spin multiplicity: 1et = singlet; 3et = triplet.

Table S6. Relative potential energies (E_{Rel}, kcal mol^{-1}) of La_2C_{94} isomers at *x*/6-311G(d)~CEP-4G (*x* = (U)M06-2X and (U)B3LYP) levels.

La_2C_{94} (IPR ID) single-point energy calculations	PA	spin	E_{Rel} (kcal mol^{-1})	
			M06-2X	B3LYP
$La_2@C_2$(117)-C_{94}	0	3et	0.0	0.0
$La_2@C_s$(120)-C_{94}	0	3et	4.7	5.4
$La_2C_2@D_3$(85)-C_{92}	0	1et	17.0	21.1
$La_2C_2@C_s$(15)-C_{92}	0	1et	30.6	34.8
$La_2C_2@C_s$(16)-C_{92}	0	1et	31.2	34.8

Note S4. The influence of functionals and basis sets on the stability of La_2C_{94} isomers

Different from the slight effect of functionals (M06-2X and B3LYP, as shown in Table S5), there is a large influence of basis sets on the energy difference between $La_2@C_{94}$ and $La_2C_2@C_{92}$. For example, the energy difference of $La_2@C_2$(117)-C_{94} and $La_2C_2@D_3$(85)-C_{92} is 4.9~10.9 kcal mol^{-1} at the basis set of 3-21G, which increases to 20.1~23.1 kcal mol^{-1} when using the basis set of 6-31G(d). Since the results at a larger 6-311G(d) basis set show the same order in relative energy as that calculated using

the 6-31G(d) basis set. The relative stability of La_2C_{94} isomers were discussed on the basis of results calculated using the 6-31G(d) basis set in the main text considering the computational efficiency and accuracy.

Table S7. Zero-point corrected relative potential energies (z-E_{Rel}, kcal mol^{-1}) of La_2C_{94} isomers at *x*/6-31G(d)~CEP-4G (*x* = (U)M06-2X and (U)B3LYP) levels.

La_2C_{94} (spiral ID)	IPR ID	PA	M06-2X		B3LYP	
			spin	z-E_{Rel}	spin	z-E_{Rel}
$La_2@C_2$(153476)-C_{94}	117	0	3et	0.0	3et	0.0
$La_2@C_2$(153480)-C_{94}	121	0	3et	4.8	3et	4.6
$La_2@C_s$(153479)-C_{94}	120	0	3et	4.4	3et	5.3
$La_2@C_1$(153491)-C_{94}	132	0	3et	8.9	3et	6.6
$La_2@C_2$(153485)-C_{94}	126	0			3et	7.2
$La_2@C_s$(152345)-C_{94}		1	3et	6.9	3et	7.8
$La_2@C_1$(153413)-C_{94}	54	0	3et	8.9	3et	8.1
$La_2@C_1$(153474)-C_{94}	115	0	3et	9.5	3et	8.7
$La_2C_2@D_3$(126408)-C_{92}	85	0	1et	17.5	1et	20.3
$La_2C_2@C_2$(126387)-C_{92}	64	0	1et	25.1	1et	26.8
$La_2C_2@C_1$(126390)-C_{92}	67	0	1et	30.4	1et	31.0
$La_2C_2@C_s$(126339)-C_{92}	16	0	1et	30.2	1et	32.1
$La_2C_2@C_s$(126338)-C_{92}	15	0	1et	30.2	1et	32.5
$La_2C_2@C_2$(126359)-C_{92}	36	0	1et	30.9	1et	33.9
$La_2C_2@C_1$(126389)-C_{92}	66	0			1et	34.1

Note S5. The influence of zero-point correction on the stability of La_2C_{94} isomers

As shown in Table S5 and Table S7, the zero-point correction influences little on the stability order of La_2C_{94} isomers. However, relative potential energy for each isomer becomes smaller after the zero-point correction (z-E_{Rel}) than that without correction (E_{Rel}) by 0.0–3.7 kcal mol^{-1} (M06-2X) and 0.0–4.1 kcal mol^{-1} (B3LYP).

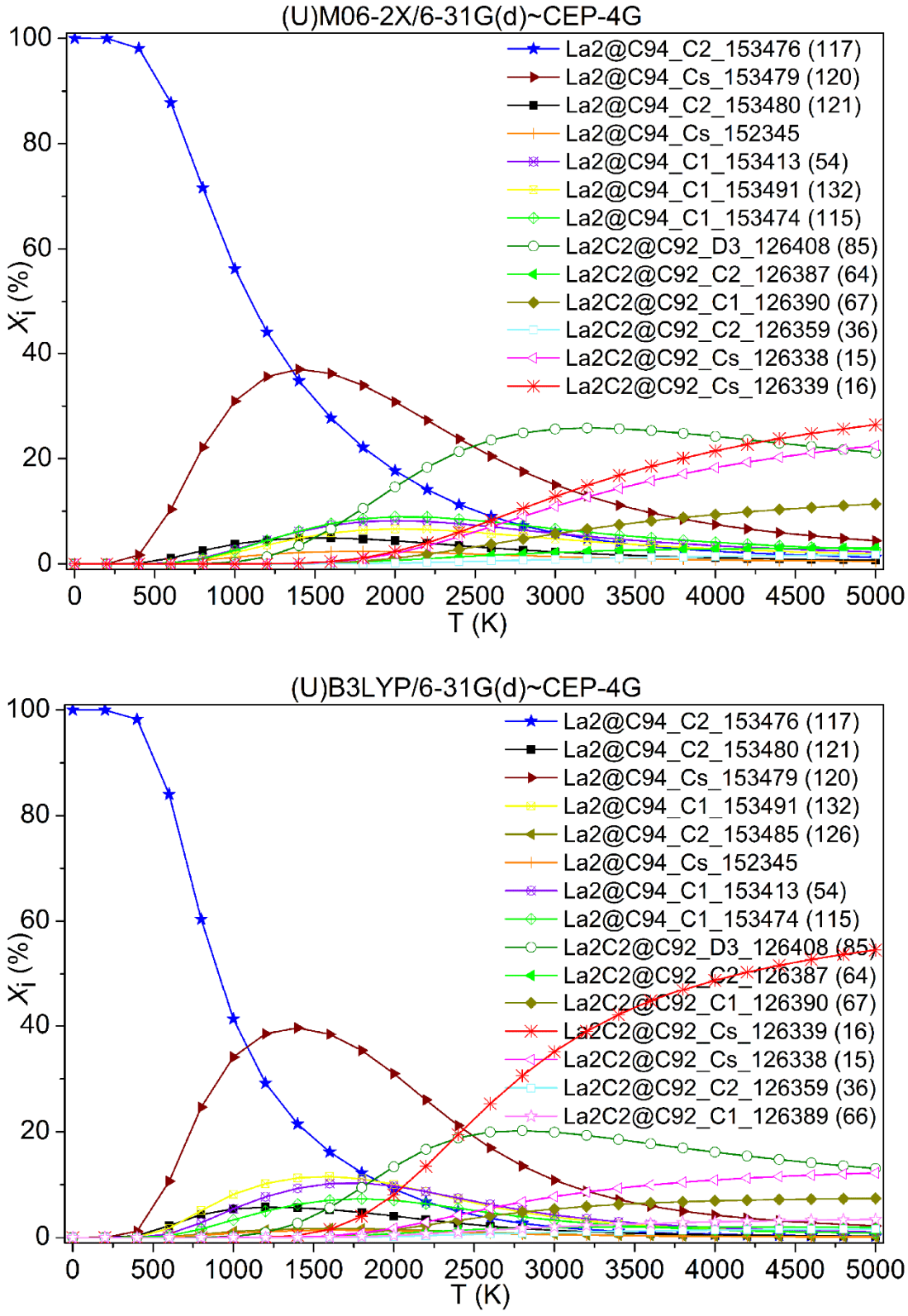


Figure S2. Relative concentrations of La_2C_{94} isomers at *x*/6-31G(d)~CEP-4G (*x* = (U)M06-2X and (U)B3LYP) levels.

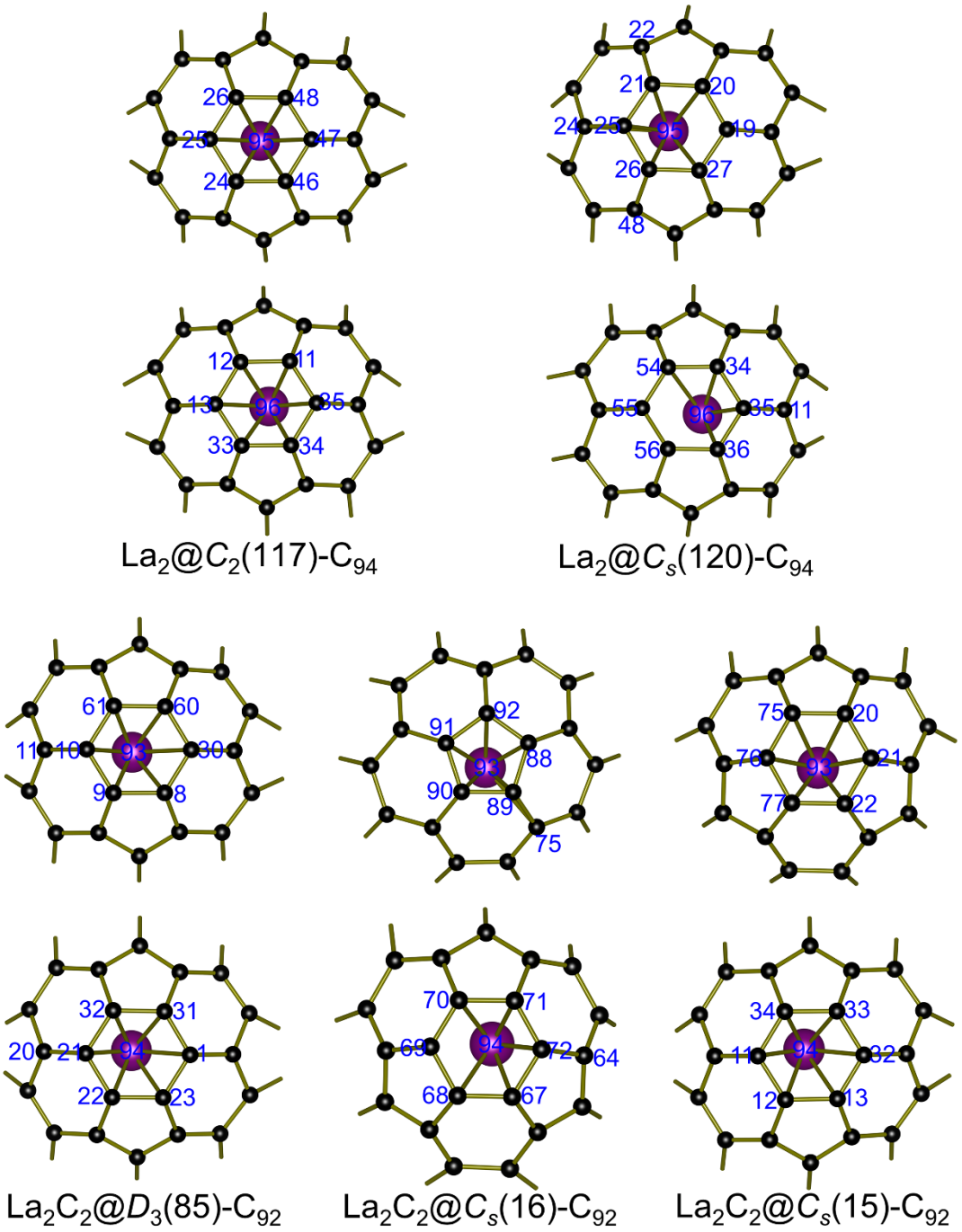


Figure S3. La–cage coordination fragments for five promising La_2C_{94} isomers at the (U)B3LYP/6-31G(d)~CEP-4G level.

Table S8. Mayer bond order, bond length (Å), and bond critical point (a.u.) parameters of La–C and La–La for five promising La_2C_{94} (IPR ID) isomers at the (U)B3LYP/6-31G(d)~CEP-4G level.

$La_2@C_2(117)$-C_{94}	Mayer bond order	Bond length (Å)	Bond critical point (BCP) parameter[a]				
			ρ_{bcp}	$\nabla^2\rho_{bcp}$	G_{bcp}/ρ_{bcp}	H_{bcp}/ρ_{bcp}	$\lvert V_{bcp}\rvert/G_{bcp}$
La95–C24	0.233	2.620	0.046	0.137	0.827	−0.090	1.109
La95–C26	0.219	2.646	0.043	0.133	0.829	−0.062	1.075
La95–C46	0.214	2.667					
La95–C48	0.212	2.687	0.041	0.130	0.824	−0.029	1.035
La95–C25	0.189	2.646	0.042	0.145	0.904	−0.035	1.039
La95–C47	0.148	2.756					
La96–C11	0.232	2.625	0.046	0.136	0.827	−0.087	1.105
La96–C12	0.217	2.658					
La96–C34	0.217	2.650	0.043	0.133	0.829	−0.060	1.073
La96–C33	0.216	2.676	0.041	0.128	0.817	−0.043	1.053
La96–C35	0.185	2.657					
La96–C13	0.153	2.738					
La95–La96	0.610	4.601	0.011	−0.005	0.052	−0.156	3.984

$La_2@C_s(120)$-C_{94}	Mayer bond order	Bond length (Å)	Bond critical point (BCP) parameter				
			ρ_{bcp}	$\nabla^2\rho_{bcp}$	G_{bcp}/ρ_{bcp}	H_{bcp}/ρ_{bcp}	$\lvert V_{bcp}\rvert/G_{bcp}$
La95–C21	0.245	2.615	0.047	0.139	0.828	−0.086	1.104
La95–C26	0.225	2.636	0.045	0.140	0.844	−0.060	1.071
La95–C25	0.222	2.578	0.048	0.156	0.906	−0.087	1.096
La95–C24	0.190	2.780					
La95–C27	0.182	2.760					
La95–C20	0.172	2.780					
La95–C22	0.145	2.858					
La95–C48	0.127	2.926					
La95–C19	0.111	2.901					
La96–C34	0.241	2.623	0.046	0.136	0.821	−0.078	1.095
La96–C36	0.231	2.642	0.045	0.134	0.819	−0.075	1.091
La96–C35	0.199	2.599	0.045	0.153	0.914	−0.067	1.073
La96–C54	0.195	2.719					
La96–C11	0.178	2.851					
La96–C56	0.163	2.803					

La96–C55	0.145	2.833					
La95–La96	0.606	4.665	0.011	−0.004	0.049	−0.152	4.098

$La_2C_2@D_3(85)$-C_{92}	Mayer bond order	Bond length (Å)	Bond critical point (BCP) parameter				
			ρ_{bcp}	$\nabla^2\rho_{bcp}$	G_{bcp}/ρ_{bcp}	H_{bcp}/ρ_{bcp}	$\lvert V_{bcp}\rvert/G_{bcp}$
L93–C9	0.204	2.654	0.043	0.138	0.866	−0.054	1.062
L93–C61	0.203	2.666	0.042	0.135	0.855	−0.045	1.053
L93–C10	0.182	2.619	0.042	0.150	0.929	−0.046	1.050
L93–C60	0.181	2.730					
L93–C8	0.169	2.731					
L93–C11	0.140	2.888					
L93–C30	0.133	2.798					
L94–C22	0.204	2.658	0.042	0.137	0.863	−0.052	1.060
L94–C32	0.203	2.662	0.042	0.136	0.856	−0.048	1.056
L94–C31	0.183	2.722					
L94–C21	0.181	2.622	0.042	0.149	0.927	−0.044	1.048
L94–C23	0.170	2.732					
L94–C20	0.138	2.895					
L94–C1	0.133	2.793					
L93–C95	0.595	2.571	0.048	0.169	0.905	−0.018	1.020
L93–C96	0.553	2.605					
L94–C95	0.556	2.597	0.047	0.170	0.907	−0.010	1.011
L94–C96	0.592	2.579					

$La_2C_2@C_s(16)$-C_{92}	Mayer bond order	Bond length (Å)	Bond critical point (BCP) parameter				
			ρ_{bcp}	$\nabla^2\rho_{bcp}$	G_{bcp}/ρ_{bcp}	H_{bcp}/ρ_{bcp}	$\lvert V_{bcp}\rvert/G_{bcp}$
La93–C89	0.211	2.608	0.046	0.152	0.903	−0.081	1.090
La93–C90	0.208	2.660	0.042	0.144	0.890	−0.042	1.048
La93–C88	0.193	2.694					
La93–C91	0.163	2.775					
La93–C75	0.161	2.706					
La93–C92	0.149	2.790					
La94–C72	0.167	2.702	0.038	0.131	0.887	−0.025	1.028
La94–C71	0.161	2.727	0.037	0.129	0.889	−0.009	1.010
La94–C67	0.151	2.745					
La94–C70	0.147	2.781					

La94–C64	0.134	2.812					
La94–C68	0.130	2.796					
La94–C69	0.126	2.824					
L93–C95	0.562	2.566	0.047	0.170	0.914	−0.013	1.014
L93–C96	0.504	2.610					
L94–C95	0.575	2.605	0.050	0.170	0.897	−0.042	1.047
L94–C96	0.650	2.536					

$La_2C_2@C_s(15)$-C_{92}	Mayer bond order	Bond length (Å)	Bond critical point (BCP) parameter				
			ρ_{bcp}	$\nabla^2\rho_{bcp}$	G_{bcp}/ρ_{bcp}	H_{bcp}/ρ_{bcp}	$\lvert V_{bcp}\rvert/G_{bcp}$
La93–C22	0.187	2.687	0.040	0.134	0.881	−0.033	1.037
La93–C21	0.173	2.689	0.038	0.132	0.881	−0.023	1.027
La93–C77	0.163	2.718	0.037	0.131	0.891	−0.015	1.016
La93–C75	0.151	2.783					
La93–C20	0.147	2.756					
La93–C76	0.146	2.744					
La94–C34	0.203	2.638	0.044	0.139	0.859	−0.068	1.079
La94–C33	0.190	2.696					
La94–C11	0.179	2.660					
La94–C12	0.166	2.739					
La94–C13	0.161	2.759	0.035	0.114	0.833	−0.005	1.006
La94–C32	0.147	2.771					
L93–C95	0.692	2.457	0.057	0.155	0.850	−0.165	1.194
L93–C96	0.354	2.951					
L94–C95	0.514	2.578	0.048	0.171	0.901	−0.019	1.021
L94–C96	0.674	2.580					

[a]Bond critical point (BCP) parameters: electronic density ρ_{bcp}; Laplacian of electron density $\nabla^2\rho_{bcp}$, kinetic energy density G_{bcp}, total energy density H_{bcp}, and potential energy density V_{bcp}.

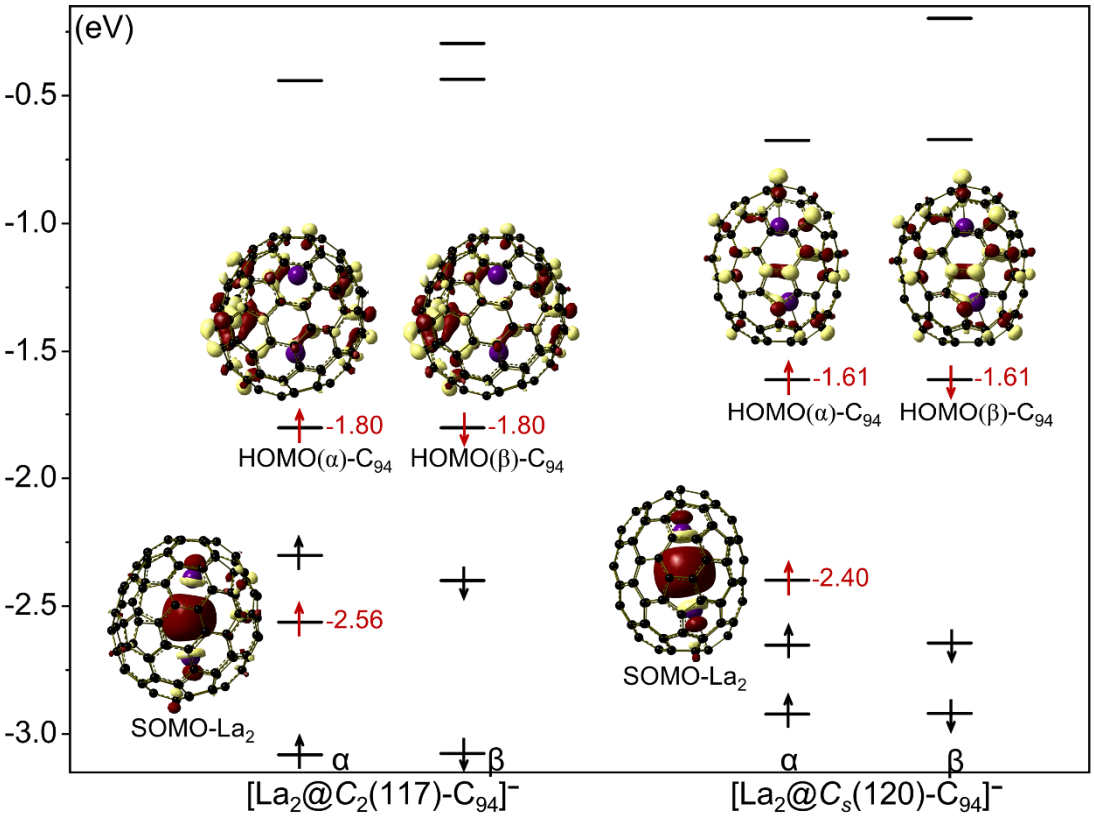


Figure S4. Diagram of the main frontier orbitals (isosurface value = 0.035) for $[La_2@C_2(117)\text{-}C_{94}]^-$ and $[La_2@C_s(120)\text{-}C_{94}]^-$ isomers at the (U)B3LYP/6-31G(d)~CEP-4G level.

Table S9. Potential energy differences between singlet and triplet La_2C_{2n} isomers (ΔE(singlet − triplet), kcal mol^{-1}) at the (U)B3LYP/3-21G~CEP-4G level.

La_2C_{2n} (spiral ID)	IPR ID	PA	ground state	ΔE(singlet − triplet)
$La_2@D_3(85)$-C_{92}	85	0	triplet	6.6
$La_2C_2@D_3(85)$-C_{92}	85	0	singlet	−22.1
$La_2@C_s(153479)$-C_{94}	120	0	triplet	5.1
$La_2C_2@C_s(153479)$-C_{94}	120	0	singlet	−21.7
$La_2@D_2(191838)$-C_{96}	186	0	triplet	4.3
$La_2C_2@D_2(191838)$-C_{96}	186	0	singlet	−5.8
$La_2@C_2(191809)$-C_{96}	157	0	triplet	7.9
$La_2C_2@C_2(191809)$-C_{96}	157	0	singlet	−21.6
$La_2@D_5(285913)$-C_{100}	450	0	singlet	−11.2
$La_2C_2@D_5(285913)$-C_{100}	450	0	singlet	−4.2

Note S6. Thermodynamic stabilities and experimental characterization of above La_2C_{2n} isomers

For dimetallofullerene (di-EMF) isomers $La_2@D_3(85)$-C_{92},[S4] $La_2@D_2(186)$-C_{96},[S5] and the experimentally characterized $La_2@D_5(450)$-C_{100},[S6-S8] they all exhibit the lowest potential energies in their La_2C_{92}, La_2C_{96}, and La_2C_{100} series, respectively, resulting in the most relative concentrations at low temperatures of the fullerene formation temperature region (500–3000 K). In addition, another two di-EMFs $La_2@C_s(120)$-C_{94} and $La_2@C_2(157)$-C_{96}[S5] are the second and third lowest-energy La_2C_{94} and La_2C_{96} isomers, possessing some relative concentrations at above temperature region, respectively. For carbide cluster metallofullerene (CCMF) isomers, except for the experimentally characterized $La_2C_2@D_3(85)$-C_{92},[S7] $La_2C_2@C_2(157)$-C_{96},[S7,S9] and $La_2C_2@D_5(450)$-C_{100},[S10] another two isomers $La_2C_2@C_s(120)$-C_{94}[S5] and $La_2C_2@D_2(186)$-C_{96}[S9] also show favorable relative concentrations in their corresponding statistical thermodynamic curves.

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2017) in advance. Herein, the relevant results (Table R[S4] and Figure R[S4]) are reproduced below for convenience with the permission of all authors (Copyright Sciencepaper Online).

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Table R[S4]. Relative potential energies (E_{Rel}, kcal mol^{-1}) of La_2C_{92} isomers at *x*/6-31G(d)~CEP-4G (*x* = (U)M06-2X and (U)B3LYP) levels.

La_2C_{92} (spiral ID)	IPR ID	PA	ground state	E_{Rel} (kcal mol^{-1})	
				M06-2X	B3LYP
$La_2@D_3$-(126408)-C_{92}	**85**	0	triplet	0.0	0.0
$La_2@C_1$-(126389)-C_{92}	66	0	triplet	8.4	10.0
$La_2@C_2$-(126387)-C_{92}	64	0	triplet	10.8	11.4
$La_2@C_2$-(126359)-C_{92}	36	0	triplet	13.5	15.7
$La_2@C_2$-(126388)-C_{92}	65	0	triplet	14.6	17.6
$La_2@C_1$-(126367)-C_{92}	44	0	triplet	14.8	17.5
$La_2@C_2$-(126400)-C_{92}	77	0	triplet	15.1	14.0
$La_2@C_1$-(126390)-C_{92}	67	0	triplet	16.0	18.5
$La_2@C_s$-(126339)-C_{92}	16	0	triplet	17.8	17.6
$La_2@C_1$-(103625)-C_{92}		1	triplet	27.1	26.9
$La_2@C_2$-(126261)-C_{92}		2	triplet	53.2	40.9
$La_2C_2@C_2$-(99915)-C_{90}	43	0	singlet	36.9	35.3
$La_2C_2@C_2$-(99913)-C_{90}	41	0	singlet	39.4	39.6
$La_2C_2@C_1$-(84069)-C_{90}		1	singlet	48.1	45.3

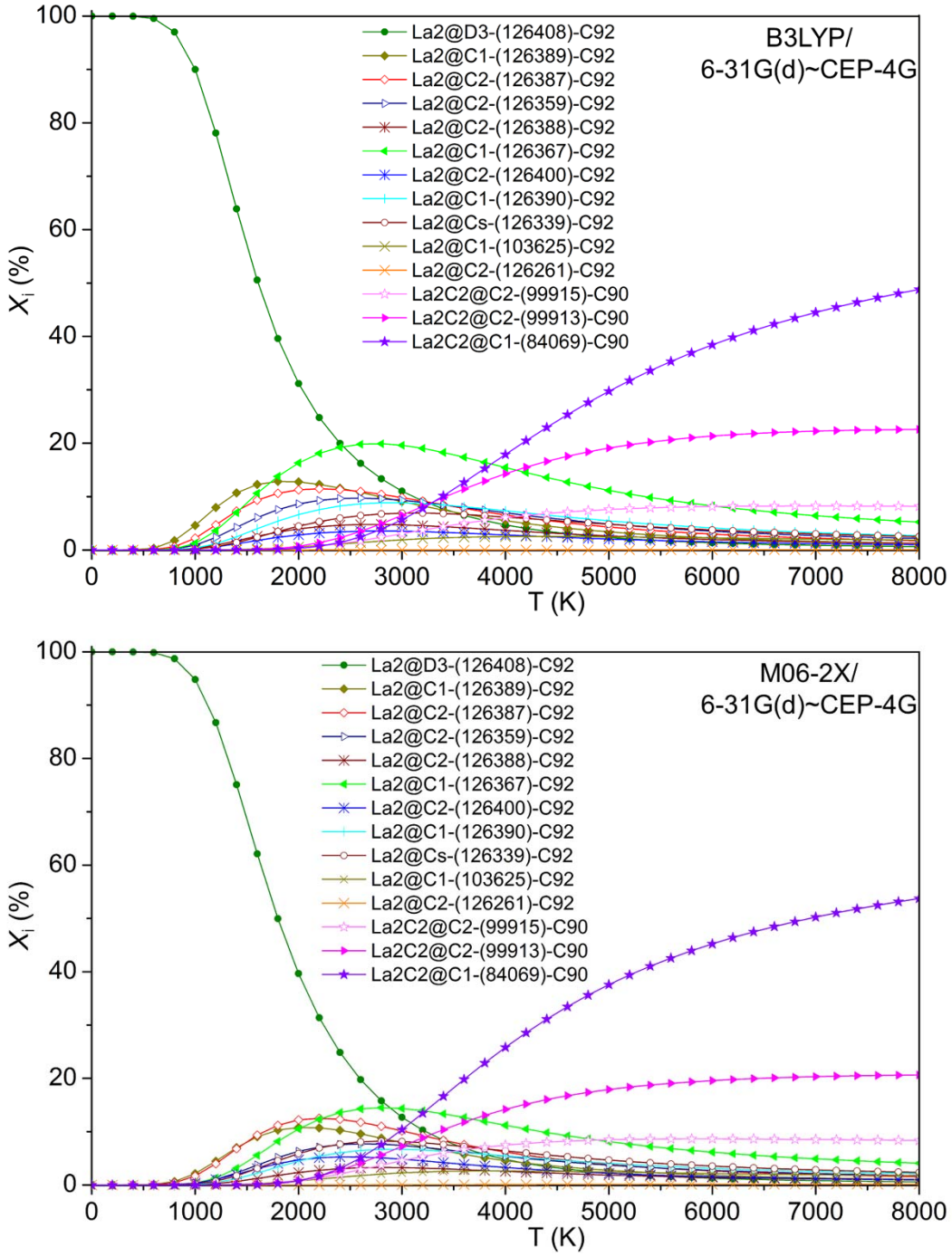

Figure R[S4]. Relative concentrations of several La_2C_{92} isomers at *x*/6-31G(d)~CEP-4G (*x* = (U)M06-2X and (U)B3LYP) levels.

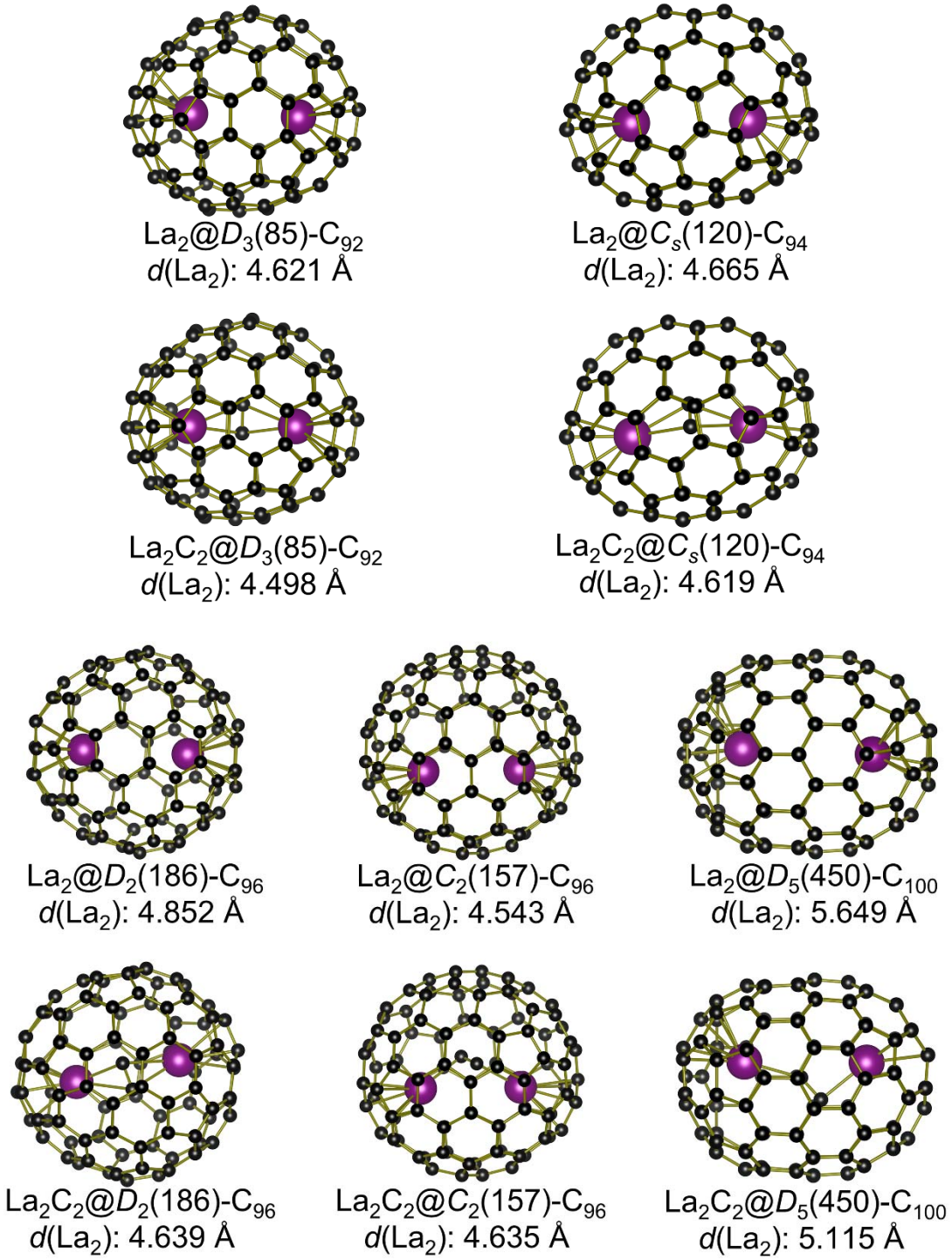

Figure S5. Optimized ground state structures and the distances of two La atoms ($d(La_2)$, Å) for $La_2@C_{2n}$ and $La_2C_2@C_{2n}$ isomers at the (U)B3LYP/6-31G(d)~CEP-4G level.

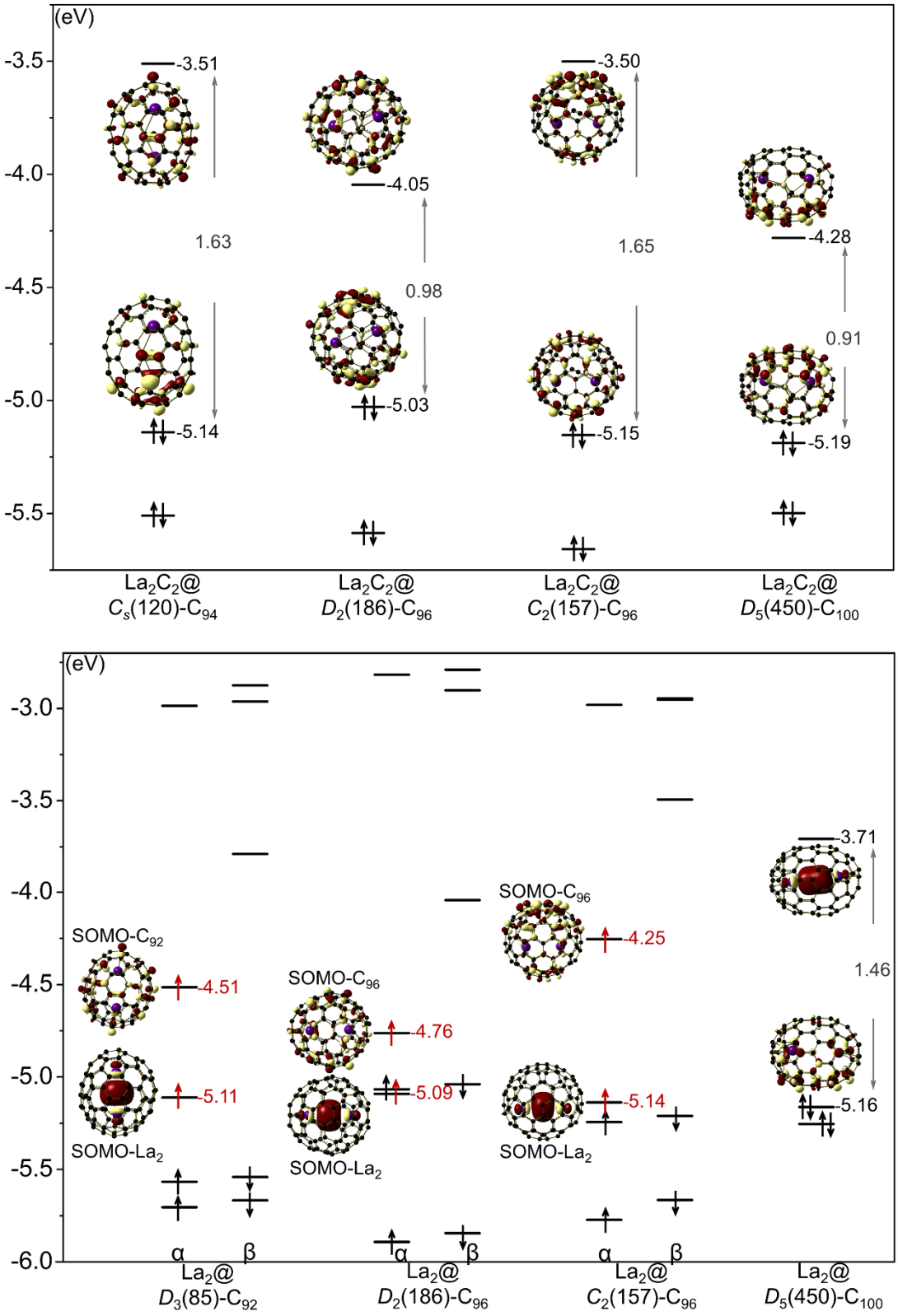

Figure S6. Diagram of the main frontier orbitals (isosurface value = 0.035) for $La_2@C_{2n}$ and $La_2C_2@C_{2n}$ isomers at the (U)B3LYP/6-31G(d)~CEP-4G level.

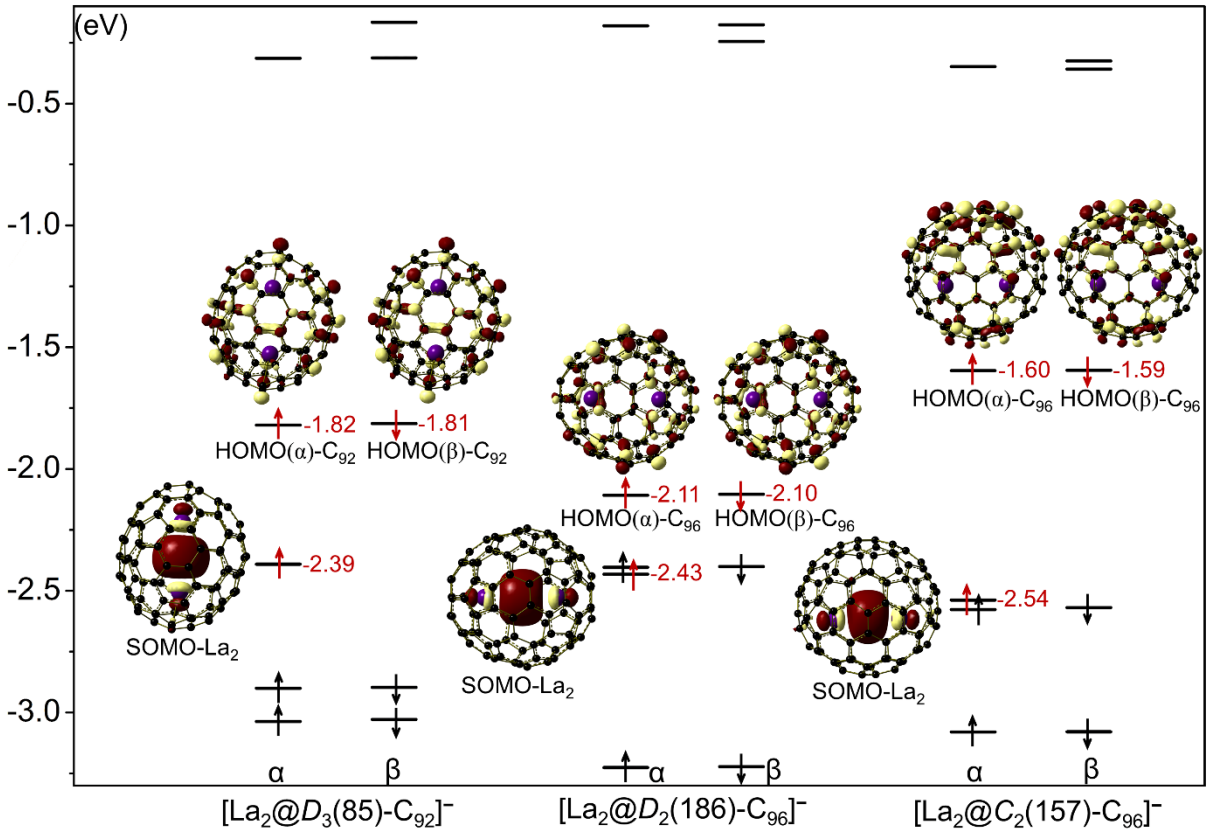

Figure S7. Diagram of the main frontier orbitals (isosurface value = 0.035) for anionic $[La_2@C_{2n}]^-$ isomers at the UB3LYP/6-31G(d)~CEP-4G level.

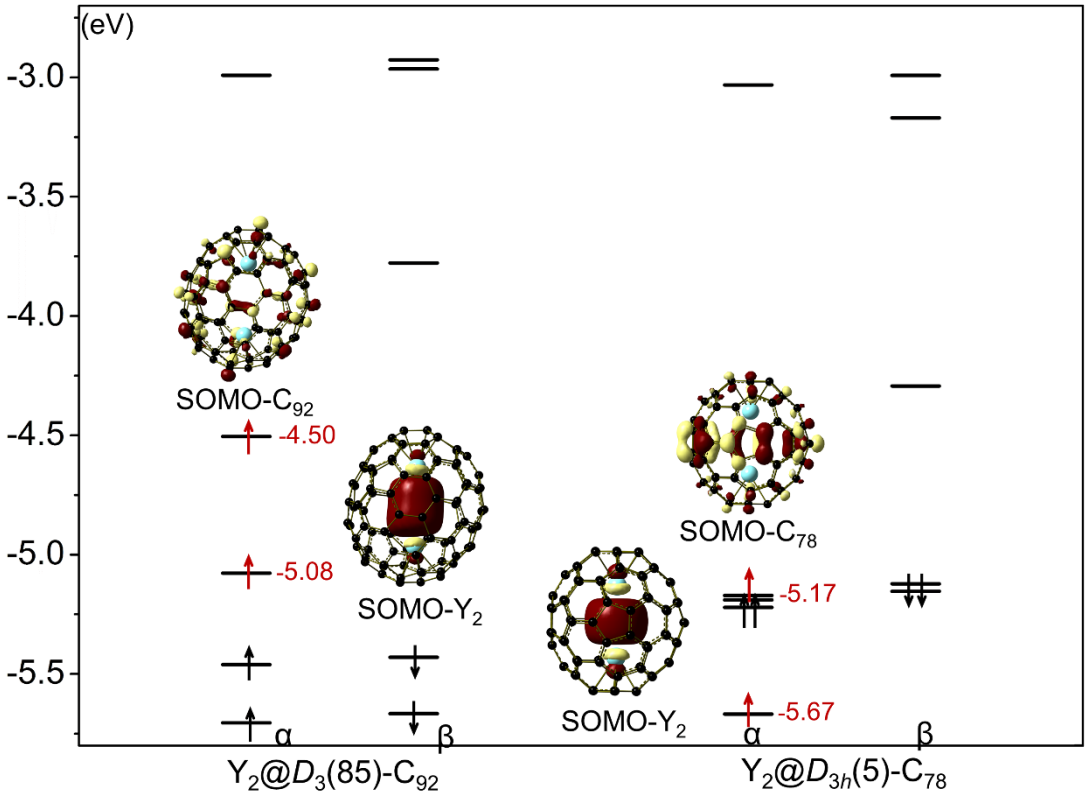

Figure S8. Diagram of the main frontier orbitals (isosurface value = 0.035) for $Y_2@D_3(85)$-C_{92} and $Y_2@D_{3h}(5)$-C_{78} at the UB3LYP/6-31G(d)~CEP-4G level.

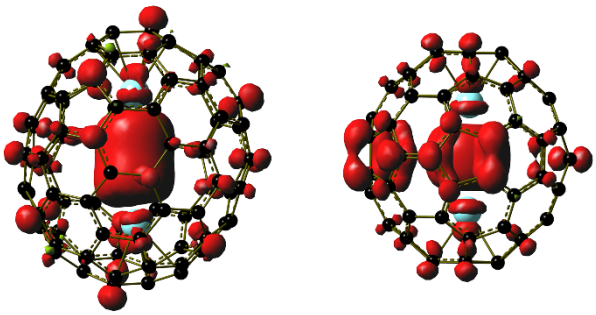

Figure S9. Spin density plots (isosurface value = 0.002) for $Y_2@D_3(85)$-C_{92} and $Y_2@D_{3h}(5)$-C_{78} at the UB3LYP/6-31G(d)~CEP-4G level.

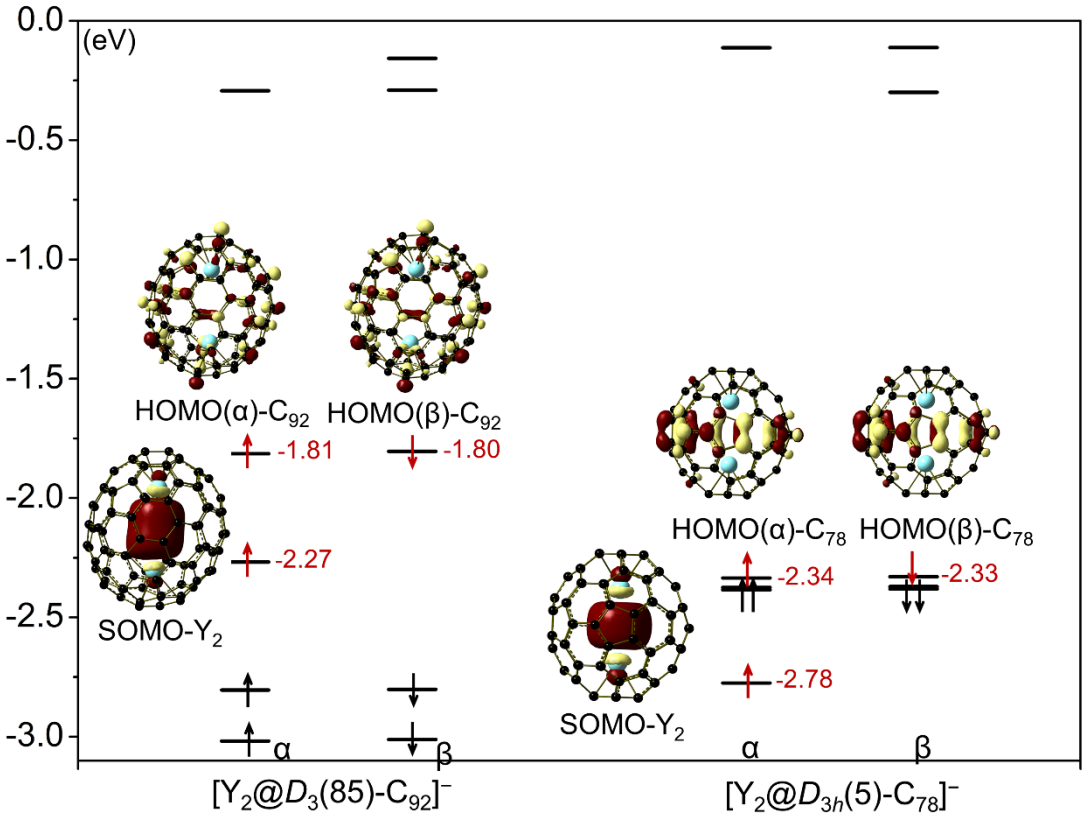

Figure S10. Diagram of the main frontier orbitals (isosurface value = 0.035) for $[Y_2@D_3(85)\text{-}C_{92}]^-$ and $[Y_2@D_{3h}(5)\text{-}C_{78}]^-$ at the UB3LYP/6-31G(d)~CEP-4G level.

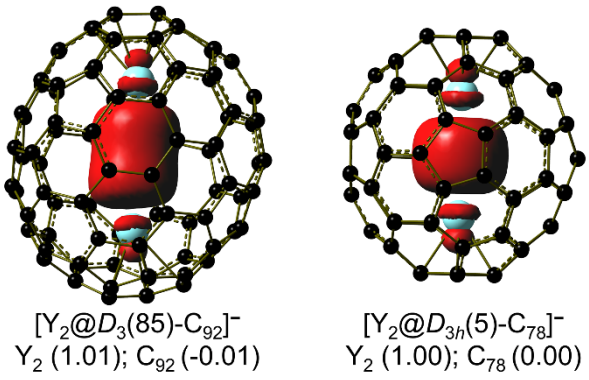

Figure S11. Spin density plots (isosurface value = 0.002) for $[Y_2@D_3(85)\text{-}C_{92}]^-$ and $[Y_2@D_{3h}(5)\text{-}C_{78}]^-$ at the UB3LYP/6-31G(d)~CEP-4G level.

Cartesian coordinates and absolute energies at the (U)B3LYP/6-31G(d)~CEP-4G level

$La_2@C_2(117)$-C_{94}: −3645.05362879 a.u.

C	3.457796	-1.746689	-2.628427	C	2.642191	3.347276	0.104416
C	2.404281	-2.680828	-2.750075	C	1.312640	3.871041	0.037724
C	1.181269	-2.356394	-3.447754	C	0.413271	3.644144	1.149624
C	0.125511	-3.097219	-2.849467	C	-1.012007	3.723042	0.876576
C	-1.206307	-2.629152	-2.879543	C	-1.903835	3.218215	1.868292
C	-2.052161	-3.194187	-1.892380	C	-3.202580	2.702065	1.568023
C	-3.264551	-2.565216	-1.495719	C	-3.657753	2.622973	0.215831
C	-3.503613	-2.883254	-0.111119	C	-4.510697	1.523550	-0.085020
C	-4.190479	-1.978267	0.729269	C	-4.461984	0.919314	-1.377603
C	-3.767624	-1.910531	2.101075	C	-3.709305	1.504304	-2.385338
C	-3.885191	-0.699237	2.896344	C	-2.917768	0.684576	-3.272637
C	-2.783894	-0.718533	3.851080	C	-1.826474	1.485892	-3.747125
C	-2.064320	0.485159	4.217538	C	-0.571161	0.928690	-4.080411
C	-0.695707	0.349178	4.530921	C	0.590707	1.820746	-3.982316
C	0.302370	1.353760	4.166621	C	0.462180	3.086602	-3.343974
C	1.570137	0.714329	4.068328	C	1.486201	3.563813	-2.433639
C	2.547762	1.144324	3.132898	C	0.795894	4.100321	-1.261480
C	3.516883	0.149633	2.640578	C	-0.605296	4.072653	-1.512111
C	4.272739	0.408814	1.423095	C	-1.542083	3.848740	-0.469119
C	4.692434	-0.664419	0.586955	C	-2.833669	3.230582	-0.820028
C	4.726786	-0.517232	-0.865554	C	-3.000251	2.725434	-2.145325
C	4.222328	-1.762489	-1.429648	C	-1.927337	2.765929	-3.096259
C	3.301200	-0.489400	-3.307517	C	-0.794626	3.506625	-2.823187
C	3.905162	0.741921	-2.822916	C	4.257566	-1.995366	0.865895
C	4.580028	0.738921	-1.521776	C	3.882780	-2.648493	-0.351122
C	4.298749	1.874483	-0.652742	C	2.709846	-3.473928	-0.400540
C	4.084937	1.666266	0.770757	C	2.056418	-3.546737	-1.651697
C	3.068766	2.569082	1.212855	C	0.663049	-3.821606	-1.728195
C	2.225740	2.311404	2.333451	C	-0.117277	-4.059557	-0.568587
C	0.905018	2.918024	2.334706	C	-1.506028	-3.874176	-0.747051
C	-0.046900	2.425813	3.308327	C	-2.367891	-3.642693	0.359577
C	-1.444249	2.612304	3.067288	C	-1.826226	-3.472977	1.655148
C	-2.468207	1.705096	3.547929	C	-2.612230	-2.647740	2.539625
C	-3.566964	1.742276	2.597351	C	-2.022470	-1.935344	3.621400

C	-4.312112	0.541126	2.241922	C	-0.629729	-2.067434	3.905130
C	-4.729999	0.453213	0.883326	C	-0.022785	-0.936642	4.520809
C	-4.723576	-0.799559	0.139733	C	1.367768	-0.683604	4.352525
C	-4.501995	-0.505503	-1.248619	C	2.162257	-1.632123	3.739777
C	-3.658866	-1.331946	-2.063649	C	3.309576	-1.221137	2.983891
C	-2.779986	-0.707373	-3.068618	C	3.567332	-2.265316	2.038522
C	-1.518278	-1.330147	-3.455364	C	2.434624	-3.161711	2.028411
C	-0.419292	-0.519930	-3.983359	C	1.914662	-3.684257	0.822292
C	0.930558	-1.069816	-3.979806	C	0.479062	-3.940280	0.753006
C	2.060466	-0.173496	-3.964704	C	-0.392029	-3.602695	1.881627
C	1.893280	1.239397	-3.931301	C	0.174372	-2.965608	3.066942
C	3.014184	1.826198	-3.217830	C	1.575049	-2.785437	3.112978
C	2.760905	2.964468	-2.357796	La	1.977629	0.668084	-1.050235
C	3.404143	2.944626	-1.060464	La	-1.794583	0.092814	1.520961

$La_2@C_s(120)$-C_{94}: −3645.04467413 a.u.

C	2.347729	2.602550	-2.981483	C	-2.213456	-0.942239	-3.672747
C	3.089728	2.646182	-1.784405	C	-2.139581	-2.118366	-2.857102
C	3.801251	1.485723	-1.309175	C	-2.801925	-2.130967	-1.562704
C	3.870835	1.564899	0.109614	C	-2.330665	-3.100303	-0.587979
C	3.955627	0.404959	0.904134	C	-2.740552	-2.912806	0.761188
C	3.566919	0.591630	2.259992	C	-2.040083	-3.450745	1.895886
C	3.184623	-0.507510	3.084380	C	-0.768972	-4.091092	1.704701
C	2.225991	-0.031102	4.057125	C	0.192779	-3.885529	2.761648
C	1.188682	-0.869193	4.537448	C	1.578447	-3.758837	2.414653
C	-0.071044	-0.261631	4.814405	C	2.034198	-4.051777	1.134299
C	-1.316454	-0.974396	4.557737	C	3.033991	-3.208668	0.517342
C	-2.305645	0.029829	4.175035	C	2.845273	-3.279347	-0.903055
C	-3.220138	-0.214196	3.105615	C	3.150870	-2.195389	-1.759415
C	-3.649528	0.871820	2.238510	C	2.423235	-2.134919	-3.036428
C	-4.036832	0.593674	0.846634	C	1.299387	-2.985361	-3.246993
C	-4.081754	1.682571	-0.061117	C	0.103194	-2.497894	-3.886931
C	-3.888384	1.494668	-1.459636	C	-1.028252	-2.958164	-3.090641
C	-3.214894	2.676983	-1.996550	C	-0.538019	-3.836736	-2.078906
C	-2.395027	2.609903	-3.140757	C	-1.153331	-3.922537	-0.805346
C	-1.188441	3.395491	-3.150451	C	-0.315491	-4.334657	0.339440

C	0.006612	2.975096	-3.874707	C	1.100173	-4.450678	0.128608
C	1.138300	3.371653	-3.042368	C	1.694533	-4.109756	-1.131537
C	2.403485	1.401338	-3.748795	C	0.888603	-3.897180	-2.229146
C	1.269771	0.967285	-4.554248	C	-3.517345	2.960514	0.278434
C	0.043585	1.733282	-4.643164	C	-2.871162	3.512611	-0.869784
C	-1.187210	0.941541	-4.625062	C	-1.578209	4.091250	-0.752705
C	-2.350844	1.364960	-3.857792	C	-0.777034	4.048823	-1.931333
C	-2.950794	0.194510	-3.262672	C	0.642312	4.014074	-1.853377
C	-3.639845	0.214317	-2.006642	C	1.324040	3.953608	-0.586316
C	-3.558459	-0.944588	-1.129813	C	2.603026	3.357509	-0.622006
C	-3.834846	-0.725721	0.278286	C	3.129671	2.723786	0.534932
C	-3.461787	-1.759858	1.179125	C	2.442338	2.761612	1.767270
C	-3.214070	-1.543528	2.571300	C	2.821452	1.742538	2.681314
C	-2.337611	-2.600365	3.049034	C	1.978658	1.357969	3.768703
C	-1.336854	-2.321897	4.068937	C	0.706689	1.947881	3.932134
C	-0.056980	-2.974137	3.887079	C	-0.286552	1.138112	4.588042
C	1.182611	-2.237657	4.105755	C	-1.675102	1.305975	4.287625
C	2.166978	-2.696312	3.161908	C	-2.086970	2.359818	3.482837
C	3.119260	-1.805892	2.544982	C	-3.156052	2.177004	2.553819
C	3.504086	-2.028817	1.137797	C	-2.979616	3.168768	1.528845
C	3.877908	-0.907909	0.285055	C	-1.683077	3.773030	1.676763
C	3.730144	-0.997946	-1.169261	C	-0.899965	4.114522	0.549675
C	3.720603	0.230607	-1.958632	C	0.544249	3.958818	0.649054
C	3.086356	0.241515	-3.247236	C	1.126470	3.373544	1.855112
C	2.424165	-0.911999	-3.759468	C	0.278888	2.989969	2.980967
C	1.298429	-0.483774	-4.545149	C	-1.107115	3.235123	2.875065
C	0.091193	-1.245597	-4.529346	La	-0.187128	0.988053	-2.186514
C	-1.136394	-0.504021	-4.517160	La	-0.389922	-1.289196	1.879466

La_2C_2@D_3(85)-C_{92}: −3645.01674793 a.u.

C	3.184824	-1.515716	-3.081860	C	4.026609	0.439310	-1.779269
C	2.395611	-0.590153	-3.808222	C	4.368185	0.603658	-0.406960
C	2.415236	0.839043	-3.527783	C	3.909997	1.725193	0.345650
C	1.161761	1.396928	-3.922390	C	3.794427	1.519229	1.747969
C	0.569704	2.479299	-3.231994	C	2.853241	2.264806	2.513978
C	-0.894351	2.589632	-3.314828	C	2.190343	3.320877	1.935189

C	-1.580534	3.400115	-2.359363	C	0.868900	3.641989	2.362776
C	-2.927183	3.137371	-1.890097	C	0.212005	4.281904	1.251668
C	-3.034371	3.658584	-0.529443	C	1.086676	4.166551	0.096007
C	-3.778021	2.933784	0.506152	C	2.310493	3.568569	0.516722
C	-3.185203	2.910570	1.821219	C	3.060626	2.716850	-0.321148
C	-3.249558	1.745288	2.694746	C	-4.319990	1.193509	-1.281002
C	-2.053999	1.684744	3.478355	C	-4.453961	1.707913	0.083855
C	-1.454108	0.434852	3.856356	C	-4.474155	0.544860	0.955919
C	-0.002173	0.310355	3.938846	C	-3.906010	0.552765	2.276978
C	0.612353	-1.000068	3.785471	C	-3.426125	-0.666098	2.792394
C	2.034182	-1.091960	3.467887	C	-2.231468	-0.716449	3.613942
C	2.554762	-2.256626	2.806467	C	-1.618941	-1.993191	3.435368
C	3.617942	-2.174100	1.852579	C	-0.224109	-2.171792	3.482441
C	3.408723	-3.182341	0.821107	C	0.316840	-3.315126	2.728759
C	3.797471	-2.984865	-0.553911	C	1.701912	-3.334506	2.416699
C	2.897306	-3.539150	-1.569356	C	2.209515	-3.904947	1.203200
C	2.595533	-2.807215	-2.796964	C	1.314068	-4.412611	0.216450
C	1.190662	-3.007268	-3.095321	C	1.654248	-4.179697	-1.159699
C	0.379331	-2.061843	-3.793399	C	0.619512	-3.842300	-2.094516
C	-1.053870	-1.983750	-3.473687	C	-0.769102	-3.742394	-1.719265
C	-1.729527	-0.811894	-3.884167	C	-1.626201	-2.762099	-2.369379
C	-2.902246	-0.340634	-3.220275	C	-2.810373	-2.274191	-1.669390
C	-2.907217	1.114728	-3.265211	C	-3.446166	-1.041927	-2.124747
C	-3.565966	1.900137	-2.287747	C	-4.228958	-0.250441	-1.209282
C	4.090844	-0.972707	-2.097998	C	-4.364012	-0.639349	0.153780
C	4.420500	-1.699673	-0.869651	C	-3.812506	-1.862383	0.637246
C	4.583016	-0.693575	0.167020	C	-3.485055	-1.884671	2.020950
C	4.218339	-0.921903	1.539353	C	-2.448473	-2.732954	2.505975
C	3.837286	0.191141	2.311927	C	-1.893295	-3.673294	1.671310
C	2.780748	0.093149	3.301214	C	-0.526507	-4.042607	1.838031
C	2.163887	1.374334	3.425411	C	-0.051380	-4.484055	0.552101
C	0.793995	1.525901	3.708754	C	-1.087939	-4.194521	-0.425299
C	0.159859	2.768996	3.239268	C	-2.227778	-3.689011	0.265307
C	-1.255919	2.821555	3.145289	C	-3.084702	-2.722304	-0.301413
C	-1.932978	3.575873	2.130838	C	1.062707	-0.911271	-4.280385
C	-1.189323	4.248962	1.117122	C	0.367215	0.318746	-4.458532

C	-1.735530	4.239006	-0.212077	C	-1.010785	0.348640	-4.351314
C	-0.856038	4.069375	-1.333389	C	-1.656598	1.524709	-3.873678
C	0.572007	3.926676	-1.191933	La	-1.828945	1.321098	-0.172125
C	1.309908	3.074717	-2.113631	La	1.797391	-1.293119	-0.667654
C	2.578832	2.493431	-1.686909	C	0.412009	0.418760	0.708172
C	3.124959	1.359504	-2.426298	C	-0.306291	-0.619817	0.663252

$La_2C_2@C_s(16)$-C_{92}: −3644.99606379 a.u.

C	0.919061	3.980995	-2.017240	C	-2.319431	-3.658168	0.414271
C	2.159250	3.841812	-1.329439	C	-1.564603	-3.735340	1.596031
C	3.018357	2.715362	-1.619664	C	-0.149251	-4.076516	1.560882
C	3.636723	2.313053	-0.407436	C	0.504725	-4.340598	0.348762
C	3.915310	0.940513	-0.156964	C	1.807351	-3.712085	0.129776
C	3.947507	0.560516	1.213505	C	2.209148	-3.546013	-1.235439
C	3.613801	-0.767216	1.629973	C	2.926467	-2.363601	-1.635944
C	3.026906	-0.695184	2.936354	C	2.527106	-1.989685	-2.964404
C	2.054179	-1.637189	3.344522	C	2.456948	-0.613719	-3.324206
C	1.063912	-1.147984	4.253852	C	1.358371	-0.231826	-4.221897
C	-0.263447	-1.674966	4.203359	C	0.370677	-1.200053	-4.589263
C	-1.212162	-0.608361	4.309186	C	-1.034247	-0.861626	-4.549476
C	-2.361675	-0.590913	3.450369	C	-1.757800	-2.062481	-4.180020
C	-2.831851	0.686812	3.079628	C	-2.850364	-1.911648	-3.302134
C	-3.458941	0.901238	1.805493	C	-3.054097	-2.874594	-2.224406
C	-3.174434	2.245205	1.386950	C	-2.155196	-3.964801	-2.085699
C	-3.035880	2.592289	0.016203	C	-1.744534	-4.296869	-0.737366
C	-2.184909	3.696701	-0.265324	C	-0.345364	-4.641897	-0.774670
C	-1.504898	3.789085	-1.512855	C	0.105633	-4.526334	-2.149354
C	-0.215451	4.397518	-1.271665	C	1.391998	-3.953770	-2.356606
C	0.688404	3.128536	-3.121388	C	1.592778	-2.988399	-3.434922
C	-0.628206	2.652627	-3.445779	C	0.497533	-2.609533	-4.256565
C	-1.713343	2.832711	-2.531367	C	-0.823365	-3.174939	-4.048727
C	-2.651281	1.731071	-2.311050	C	-1.024948	-4.134655	-2.986581
C	-3.261472	1.579081	-0.991884	C	2.265893	4.141381	0.063274
C	-3.684547	0.257938	-0.535190	C	3.227953	3.219616	0.646952
C	-3.644872	-0.129304	0.879041	C	3.191807	2.830626	2.020205
C	-3.313143	-1.502313	1.281601	C	3.591922	1.473710	2.279561

C	-2.631242	-1.711608	2.554499	C	2.994301	0.684303	3.341350
C	-1.786013	-2.853220	2.683831	C	1.920922	1.202024	4.140700
C	-0.543183	-2.764090	3.405281	C	0.951074	0.255161	4.569064
C	0.493548	-3.391719	2.626989	C	-0.470811	0.584114	4.602388
C	1.750249	-2.750954	2.449336	C	-0.922617	1.857399	4.170674
C	2.387805	-2.850773	1.136564	C	-2.153133	1.895037	3.452510
C	3.274073	-1.768583	0.703602	C	-2.383189	2.867895	2.410012
C	3.412629	-1.427669	-0.709007	C	-1.406108	3.851525	2.088544
C	3.609059	-0.055228	-1.159617	C	-1.360367	4.297988	0.747533
C	3.065318	0.367798	-2.449263	C	-0.111521	4.693814	0.125912
C	2.719378	1.774803	-2.639257	C	1.130276	4.571123	0.823749
C	1.637571	2.113070	-3.504382	C	1.095437	4.208329	2.236559
C	0.930428	1.109732	-4.208902	C	2.144812	3.410489	2.871964
C	-0.480474	1.445535	-4.169358	C	1.499115	2.580203	3.887733
C	-1.466195	0.440491	-4.145356	C	0.078132	2.870085	3.865912
C	-2.582075	0.588971	-3.197744	C	-0.167072	3.861944	2.851757
C	-3.237300	-0.610222	-2.813408	La	0.822802	1.632723	1.496189
C	-3.709827	-0.782458	-1.469063	La	-0.336485	-1.852634	-1.713976
C	-3.569794	-2.169893	-1.085916	C	-0.203437	0.474411	-0.550624
C	-3.222277	-2.515787	0.255856	C	-0.371279	-0.388288	0.356087

La_2C_2@C_s(15)-C_{92}: −3644.99569778 a.u.

C	2.457507	0.526776	4.216473	C	1.422372	2.557332	-3.391124
C	1.819771	-0.738769	4.327167	C	0.685191	1.623555	-4.186169
C	2.091680	-1.781571	3.411142	C	1.142035	0.285693	-4.341007
C	0.845302	-2.506733	3.187677	C	0.107184	-0.700011	-4.530321
C	0.586301	-3.231707	2.017296	C	0.277225	-2.038230	-4.063862
C	-0.797724	-3.379383	1.580178	C	1.485376	-2.464445	-3.404556
C	-1.027589	-3.892734	0.238075	C	1.335677	-3.512676	-2.461109
C	-2.256723	-3.608411	-0.431322	C	2.203263	-3.599409	-1.326560
C	-2.321382	-3.396396	-1.847242	C	3.279848	-2.747432	-1.218294
C	-3.342757	-2.395081	-2.121037	C	3.655192	-2.242987	0.075685
C	-3.219623	-1.448715	-3.204071	C	4.258682	-0.952168	-0.122306
C	-3.675817	-0.096408	-2.916794	C	4.189121	-0.669776	-1.536785
C	-2.919981	1.072392	-3.374077	C	4.027475	0.622727	-1.974726
C	-2.963511	2.061245	-2.322020	C	3.185244	0.891972	-3.105153

C	-1.884070	2.961764	-2.040687	C	2.409045	-0.125143	-3.736812
C	-1.641147	3.398727	-0.677004	C	2.582889	-1.506083	-3.268627
C	-0.303690	3.854320	-0.347398	C	3.514415	-1.740810	-2.217297
C	0.026913	4.041216	1.013408	C	-3.253122	-2.802401	0.188431
C	1.365674	3.913385	1.517510	C	-3.925758	-2.051855	-0.843790
C	1.274914	3.617907	2.918183	C	-4.385153	-0.734005	-0.579225
C	2.207289	2.723159	3.514084	C	-4.206160	0.238518	-1.615200
C	1.772102	1.761344	4.524459	C	-3.775695	1.567853	-1.265254
C	3.327841	0.728530	3.064636	C	-3.594087	1.996406	0.082523
C	3.177359	2.084541	2.630603	C	-2.542013	2.962381	0.398967
C	3.322110	2.426804	1.232005	C	-2.135649	3.101123	1.778160
C	2.402485	3.387961	0.663530	C	-0.904314	3.765694	2.076720
C	2.157636	3.420684	-0.756649	C	-0.147620	3.551456	3.283333
C	0.812673	3.711049	-1.273178	C	-0.580117	2.588092	4.246886
C	0.507682	3.333992	-2.594978	C	0.349405	1.704318	4.889297
C	-0.815869	2.948518	-2.970231	C	-0.303150	0.396146	4.926902
C	-0.721115	1.923263	-3.999362	C	0.395170	-0.790441	4.672624
C	-1.736909	0.947429	-4.186918	C	-0.201130	-1.873562	3.927245
C	-1.310346	-0.393369	-4.536458	C	-1.525799	-1.819222	3.408500
C	-2.035512	-1.574250	-4.056577	C	-1.851906	-2.623852	2.250531
C	-1.019114	-2.572032	-3.747497	C	-3.074256	-2.299621	1.503680
C	-1.152951	-3.496755	-2.649248	C	-3.778081	-1.100180	1.805342
C	0.029105	-3.958140	-2.023325	C	-4.332501	-0.282418	0.756705
C	0.080808	-4.171750	-0.597273	C	-4.050171	1.096526	1.081232
C	1.431758	-3.942084	-0.162951	C	-3.494238	1.128544	2.387681
C	1.710706	-3.395019	1.094826	C	-2.616634	2.154978	2.795686
C	2.904943	-2.546201	1.233632	C	-1.812750	1.859707	3.940968
C	3.023961	-1.627111	2.338216	C	-1.645274	0.498720	4.383560
C	3.649020	-0.328077	2.149631	C	-2.274130	-0.591972	3.700880
C	4.135193	0.066032	0.840513	C	-3.325822	-0.232266	2.836582
C	3.966368	1.454634	0.378506	La	0.518502	1.051937	2.255890
C	3.925021	1.698693	-1.013346	La	-1.177503	-0.422012	-1.843574
C	3.045943	2.677157	-1.573435	C	0.144481	-0.477118	0.369098
C	2.652454	2.206814	-2.879926	C	0.962094	0.001517	-0.465838