Supplementary Information

Theoretical Studies on Characterization of Classical and Non-classical C_{68} Isomers and Their Newly Synthesized Derivatives by Spectroscopy

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1. The calculated energies and relative energies of $Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ via or without the pseudopotential basis set:

Table S1. The energies (kcal/mol) of isomer $Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ at the TPSSh-D3BJ/6-311+G(3df, 3pd) or TPSSh-D3BJ/6-311+G(3df, 3pd) ~ Lanl2DZ level.

Molecule	Pseudopotential basis set	energy(au)	Relative energy(au)
$Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$	None	-4190.09	0
	Lanl2DZ	-2761.54	1428.55

2. The relative energies of singlet and triplet states of C_{68} systems：

Table S2. The relative energies (kcal/mol) of singlet and triplet states of two C_{68} isomers. The three external derivatives at the B3LYP-D3BJ/6-311+G(3df, 3pd) level, while the embedded derivative $Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ at the TPSSh-D3BJ/6-311+G(3df, 3pd) level.

Molecule	Relative energies
$C_{2v}\text{-}^{\#6073}C_{68}$ (singlet)	0.00
$C_{2v}\text{-}^{\#6073}C_{68}$ (triplet)	3.15
$C_1\text{-}C_{68}(NC3)$ (singlet)	0.00
$C_1\text{-}C_{68}(NC3)$ (triplet)	0.72
$C_1\text{-}C_{68}Cl_{28}$ (singlet)	0.00
$C_1\text{-}C_{68}Cl_{28}$ (triplet)	54.18
$C_1\text{-}C_{68}Cl_{26}(OH)_2$ (singlet)	0.00
$C_1\text{-}C_{68}Cl_{26}(OH)_2$ (triplet)	49.66
$C_1\text{-}C_{68}Cl_{25}(OH)_3$ (singlet)	0.00
$C_1\text{-}C_{68}Cl_{25}(OH)_3$ (triplet)	49.61
$Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ (singlet)	0.00
$Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ (triplet)	13.39

3. The bond lengths of C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, C_1-$C_{68}Cl_{25}(OH)_3$ and $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ are compared with previous work:

The partial bond length information of chlorinated derivative C_1-$C_{68}Cl_{28}$ with its partially hydrolyzed derivatives C_1-$C_{68}Cl_{26}(OH)_2$ and C_1-$C_{68}Cl_{25}(OH)_3$ can be seen in Table S3. The table makes it apparent that our computed bond length data are almost consistent with previous findings even if they exist a little bit high. This is mainly because different computation techniques were used. The predecessors used GAMESS (US) software to optimize derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, and C_1-$C_{68}Cl_{25}(OH)_3$ at mPW3PBE/Def2-TZVP functional level,[1] while we optimized the three derivatives at the B3LYP/6-31G(d) level and taking into account dispersion interactions (D3BJ) using the Gaussian 16 quantum chemical package. For instance, our computed findings for the R_{C-Cl} and average R_{C-Cl} in the table are only 0.02-0.03 Å longer than the prior. Similarly, for the bond lengths of O-H.... Cl as well as O-H ....Cl, our results are merely 0.06 Å and 0.08 Å longer than the earlier findings. As a consequence, our computation technique is trustworthy and logical, and it is meaningful to calculate and evaluate the geometric structures of non-classical fullerenes and their derivatives at the same theoretical level. The partial bond length statistics of $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ are presented in Figure S1 (b), and the conclusions are nearly entirely in line with prior investigations. In order to acquire the bond length data for $Sc_2C_2@C_2$-$^{\#6073}C_{68}$, predecessors employed Material Studio software to do geometric optimization at the GGA-PBE/DNP level,[2] and we optimized the derivative $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ at the TPSSh-D3BJ/6-31G(d) level using the Gaussian 16 quantum chemical package. The bond length data agreed well despite the different calculation techniques we utilized. This also demonstrates why it is reasonable to compute metallic carbide clusterfullerene $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ using the TPSSh functional.

Table S3. Statistics of Bond Lengths (Å) that compared to earlier research of the derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, and C_1-$C_{68}Cl_{25}(OH)_3$.

	[a]Average R_{C-Cl}	[b]R_{C-Cl}	[c]$R_{O-H\ldots Cl}$	[c]$R_{O-H\ldots O}$
Theory[1]	1.77	1.80–1.82	3.19-3.24	2.94
This Study	1.79	1.83-1.85	3.26-3.32	3.00

[a]the average bond length over the sites of pentagon–pentagon fusion in C_1-$C_{68}Cl_{28}$. [b] the four C–Cl bonds indicated in Figure S1.(a). [c] C_1-$C_{68}Cl_{26}(OH)_2$ and C_1-$C_{68}Cl_{25}(OH)_3$ weak intramolecular hydrogen bonds
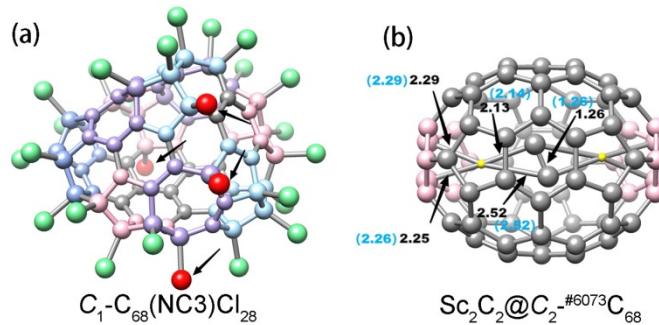
Figure S1. (a) The four chlorine atoms that C-Cl bond lengths longer than 1.8 Å in derivative C_1-$C_{68}Cl_{28}$ are indicated in red. (b) Partial bond lengths of embedded derivative $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ and the length data from earlier investigation[2] are displayed in blue.

4. Kohn–Sham orbitals of two C_{68} isomers and their derivatives:

Figure S2 presents the localized HOMO and LUMO of the six molecules analyzed in paper. This can be observed that the orbitals have a significant difference between the pure cages and their derivatives. This suggests that either by inserting the metal carbide or by chlorinating the pure cage, the truth is feasible to effectively modify the geometry and electrical structure of the fullerene C_{68}. It originates from electrons moving between the embedded metal carbide or chlorine atoms with the pure cage. The positive and negative aspects of the orbitals are represented in the illustration by the colors red and blue, respectively. Figure S2 shows that the hydroxyl groups or the chlorine atoms have important interactions with the pure cage in the derivatives of C_1-C_{68}(NC3). The embedded derivative $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ shows a strong interaction between the metal Sc and the carbon cage and exhibits blue electron clouds dominating the carbon cage skeleton and red electron clouds centered mostly on the embedded metal carbide Sc_2C_2 cluster. In other words, the metal carbide Sc_2C_2 contains the majority of the positive charges. This agrees with the calculation result of the NBO.
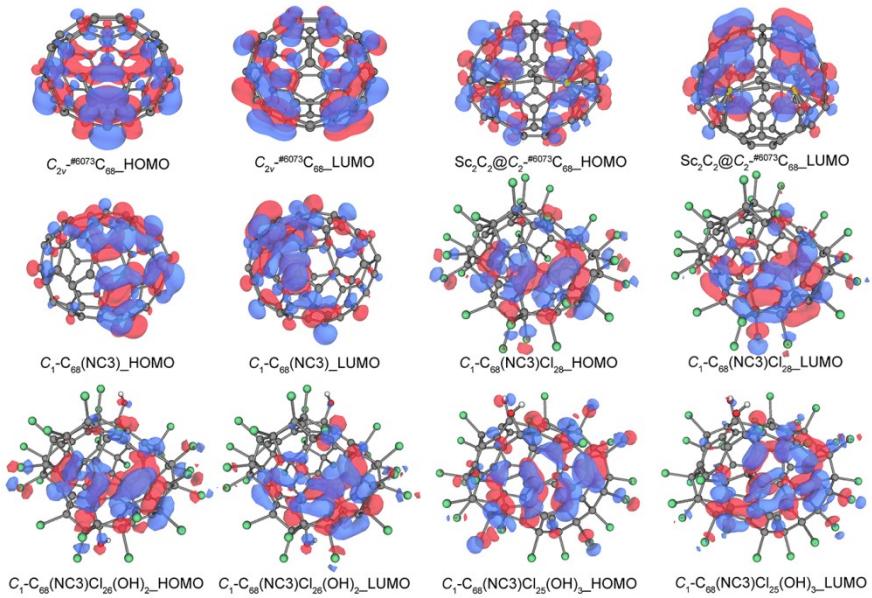
Figure S2. Isosurfaces of the HOMO and LUMO for the C_1-C_{68}(NC3) and the corresponding three derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, and C_1-$C_{68}Cl_{25}(OH)_3$, along with C_{2v}-$^{\#6073}C_{68}$ and its derivative $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ by using Multiwfn software[3].

5. UV-vis absorption spectra of $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ simulated by using functionals

with different HF%
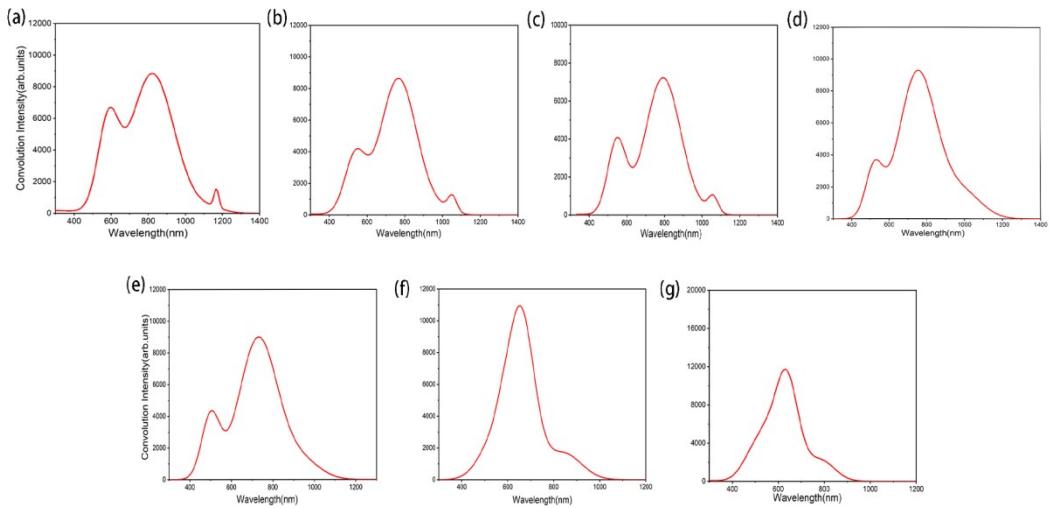
Figure S3. The calculated UV-vis absorption spectra of $Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ with (a) TPSS(0% HF), (b) TPSSh (10% HF), (c) O3LYP (11.61% HF), (d) B3LYP (20% HF), (e) PBE0 (25% HF), (f) PBE38 (37.5%HF) and (g) M06-2X (54%HF) functionals.

6. The natural charges of the derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, C_1-$C_{68}Cl_{25}(OH)_3$ as well as $Sc_2C_2@C_2$-$^{#6073}C_{68}$.

Table S4. The natural charges of carbon atoms, hydroxyl groups, and the chlorine atoms of the derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, C_1-$C_{68}Cl_{25}(OH)_3$ at the B3LYP-D3BJ/6-31G level, along with $Sc_2C_2@C_2$-$^{#6073}C_{68}$ at the TPSSh-D3BJ/6-31G level. (The carbon atoms attached to the chlorine atom are shown in blue)

$Sc_2C_2@C_2$-$^{#6073}C_{68}$		C_1-$C_{68}Cl_{28}$		C_1-$C_{68}Cl_{26}(OH)_2$		C_1-$C_{68}Cl_{25}(OH)_3$	
Atom	Natural Charge	Atom	Natural Charge	Atom	Natural Charge	Atom	Natural Charge
C(1)	-0.02431	C(1)	0.01004	Cl(1)	0.05864	Cl(1)	0.05696
C(2)	-0.02509	C(2)	-0.0484	Cl(2)	0.05305	Cl(2)	0.05254
C(3)	-0.02086	C(3)	-0.00266	Cl(3)	0.04308	Cl(3)	0.04276
C(4)	-0.03307	C(4)	0.01581	Cl(4)	0.04413	Cl(4)	0.04028
C(5)	-0.04609	C(5)	0.01767	Cl(5)	0.05544	Cl(5)	0.05428
C(6)	-0.03097	C(6)	0.01195	Cl(6)	0.05931	Cl(6)	0.05798
C(7)	-0.03776	C(7)	0.01928	Cl(7)	0.06001	Cl(7)	0.05899
C(8)	-0.04846	C(8)	-0.07076	Cl(8)	0.08589	Cl(8)	0.08559
C(9)	-0.04056	C(9)	-0.05724	Cl(9)	0.0361	Cl(9)	0.0357
C(10)	-0.02472	C(10)	-0.06373	Cl(10)	0.02903	Cl(10)	0.02161
C(11)	-0.05768	C(11)	-0.06371	Cl(11)	0.08305	Cl(11)	0.05516
C(12)	0.0094	C(12)	0.00956	Cl(12)	-0.00847	Cl(12)	0.0427
C(13)	0.00885	C(13)	0.02983	Cl(13)	0.04371	Cl(13)	0.03704
C(14)	-0.00856	C(14)	0.02504	Cl(14)	0.03763	Cl(14)	0.04585
C(15)	0.00884	C(15)	-0.00939	Cl(15)	0.04629	Cl(15)	0.05679
C(16)	-0.05267	C(16)	0.01766	Cl(16)	0.05803	Cl(16)	0.03266
C(17)	-0.02805	C(17)	0.02445	Cl(17)	0.03348	Cl(17)	0.08023
C(18)	-0.02926	C(18)	-0.00315	Cl(18)	0.08106	Cl(18)	0.03261

C(19)	-0.01157	C(19)	0.01377	Cl(19)	0.03393	Cl(19)	0.01895
C(20)	-0.00728	C(20)	-0.00099	Cl(20)	0.01996	Cl(20)	0.06435
C(21)	-0.00119	C(21)	-0.00175	Cl(21)	0.06497	Cl(21)	0.05623
C(22)	0.00453	C(22)	0.01715	Cl(22)	0.05762	Cl(22)	0.04245
C(23)	-0.0315	C(23)	0.00247	Cl(23)	0.0432	Cl(23)	0.03918
C(24)	-0.02012	C(24)	-0.06218	Cl(24)	0.04211	Cl(24)	0.05751
C(25)	0.00385	C(25)	-0.05057	Cl(25)	0.05995	Cl(25)	0.05998
C(26)	0.01951	C(26)	-0.00447	Cl(26)	0.06078	O(26)	-0.70166
C(27)	-0.03766	C(27)	0.01809	O(27)	-0.70153	H(27)	0.48752
C(28)	-0.02324	C(28)	0.00423	H(28)	0.48757	O(28)	-0.71332
C(29)	-0.01721	C(29)	-0.0059	O(29)	-0.70892	H(29)	0.50221
C(30)	-0.01837	C(30)	0.01017	H(30)	0.48844	O(30)	-0.74097
C(31)	0.01237	C(31)	-0.06511	C(31)	-0.0498	H(31)	0.50221
C(32)	0.03011	C(32)	-0.08236	C(32)	-0.06202	C(32)	-0.04945
C(33)	0.01237	C(33)	-0.06435	C(33)	0.00441	C(33)	-0.06144
C(34)	0.01767	C(34)	-0.06761	C(34)	0.01764	C(34)	0.00393
C(35)	0.03011	C(35)	-0.06775	C(35)	-0.07158	C(35)	0.01731
C(36)	0.00503	C(36)	-0.07294	C(36)	0.01935	C(36)	-0.0715
C(37)	0.01767	C(37)	-0.05914	C(37)	-0.0042	C(37)	0.01908
C(38)	0.00503	C(38)	-0.06625	C(38)	-0.00977	C(38)	-0.00356
C(39)	-0.01837	C(39)	0.01922	C(39)	-0.05922	C(39)	-0.00855
C(40)	-0.01721	C(40)	-0.07011	C(40)	-0.05647	C(40)	-0.05947
C(41)	-0.02324	C(41)	-0.06149	C(41)	-0.02091	C(41)	-0.05499
C(42)	-0.03766	C(42)	-0.05346	C(42)	0.01114	C(42)	-0.02467
C(43)	0.01951	C(43)	-0.06213	C(43)	-0.07085	C(43)	0.00941

C(44)	0.00385	C(44)	-0.06374	C(44)	-0.06302	C(44)	-0.07059
C(45)	-0.02012	C(45)	-0.07131	C(45)	0.01382	C(45)	-0.06252
C(46)	-0.0315	C(46)	0.01489	C(46)	-0.00137	C(46)	0.01437
C(47)	0.00453	C(47)	-0.02328	C(47)	-0.00689	C(47)	-0.00123
C(48)	-0.00119	C(48)	-0.0564	C(48)	0.00262	C(48)	-0.00705
C(49)	-0.00728	C(49)	-0.05978	C(49)	0.25279	C(49)	0.0023
C(50)	-0.01157	C(50)	-0.00778	C(50)	-0.05557	C(50)	0.25274
C(51)	-0.02926	C(51)	0.01793	C(51)	-0.06471	C(51)	-0.0555
C(52)	-0.02805	C(52)	-0.06082	C(52)	0.00706	C(52)	-0.06457
C(53)	-0.05267	C(53)	0.01651	C(53)	-0.00624	C(53)	0.00755
C(54)	0.00884	C(54)	-0.00356	C(54)	0.0167	C(54)	-0.00619
C(55)	-0.00856	C(55)	0.01842	C(55)	-0.06005	C(55)	0.01746
C(56)	0.00885	C(56)	0.01511	C(56)	-0.05675	C(56)	-0.06163
C(57)	0.0094	C(57)	-0.00338	C(57)	-0.04061	C(57)	-0.05534
C(58)	-0.05768	C(58)	0.01756	C(58)	-0.0054	C(58)	0.25237
C(59)	-0.02472	C(59)	-0.07621	C(59)	0.02479	C(59)	0.0061
C(60)	-0.04056	C(60)	0.04628	C(60)	0.00655	C(60)	0.02831
C(61)	-0.04846	C(61)	-0.06813	C(61)	0.00058	C(61)	0.00441
C(62)	-0.03776	C(62)	0.01059	C(62)	-0.06198	C(62)	0.00025
C(63)	-0.03097	C(63)	-0.00229	C(63)	-0.05253	C(63)	-0.06183
C(64)	-0.04609	C(64)	0.04182	C(64)	-0.00188	C(64)	-0.05182
C(65)	-0.03307	C(65)	0.00932	C(65)	0.01372	C(65)	-0.0017
C(66)	-0.02086	C(66)	-0.06512	C(66)	-0.00491	C(66)	0.01321
C(67)	-0.02509	C(67)	-0.05586	C(67)	0.00438	C(67)	-0.00487
C(68)	-0.02431	C(68)	0.01532	C(68)	-0.00427	C(68)	0.00435

C(69)	-0.46659	Cl(69)	-0.00083	C(69)	-0.01666	C(69)	-0.00418
C(70)	-0.46659	Cl(70)	0.04611	C(70)	0.01022	C(70)	-0.01649
Sc(71)	1.02267	Cl(71)	0.08146	C(71)	-0.06231	C(71)	0.01003
Sc(72)	1.02267	Cl(72)	0.03899	C(72)	-0.06515	C(72)	-0.06238
Total	0.00000	Cl(73)	0.04618	C(73)	0.01083	C(73)	-0.06496
		Cl(74)	0.05291	C(74)	0.01703	C(74)	0.00964
		Cl(75)	0.05939	C(75)	-0.00526	C(75)	0.01736
		Cl(76)	0.05918	C(76)	0.01776	C(76)	-0.00705
		Cl(77)	0.06592	C(77)	-0.00345	C(77)	0.00872
		Cl(78)	0.05904	C(78)	0.01051	C(78)	-0.01799
		Cl(79)	0.04472	C(79)	0.24215	C(79)	0.01505
		Cl(80)	0.0433	C(80)	0.06308	C(80)	0.24364
		Cl(81)	0.06231	C(81)	-0.06949	C(81)	0.06342
		Cl(82)	0.05939	C(82)	-0.06103	C(82)	-0.06976
		Cl(83)	0.02287	C(83)	-0.0693	C(83)	-0.0609
		Cl(84)	0.03799	C(84)	0.00894	C(84)	-0.06983
		Cl(85)	0.08282	C(85)	-0.06402	C(85)	0.00912
		Cl(86)	0.04028	C(86)	0.02547	C(86)	-0.06414
		Cl(87)	0.04441	C(87)	0.01626	C(87)	0.02587
		Cl(88)	0.06214	C(88)	-0.00927	C(88)	0.01638
		Cl(89)	0.0613	C(89)	0.02249	C(89)	-0.00913
		Cl(90)	0.0572	C(90)	0.02968	C(90)	0.02241
		Cl(91)	0.04423	C(91)	-0.08214	C(91)	0.02933
		Cl(92)	0.02905	C(92)	-0.06405	C(92)	-0.08207
		Cl(93)	0.02016	C(93)	-0.06703	C(93)	-0.06363

Cl(94)	0.03175	C(94)	-0.06735	C(94)	-0.06657
Cl(95)	0.02895	C(95)	0.01614	C(95)	-0.06663
Cl(96)	0.08393	C(96)	-0.00584	C(96)	0.01364
Total	0.00000	C(97)	-0.05748	C(97)	-0.00898
		C(98)	-0.07281	C(98)	-0.0566
		Total	0.00000	C(99)	-0.07237
				Total	0.00000

7. Binding Energies:

Table S5. The bond C-Cl or C-OH energies of three derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, and C_1-$C_{68}Cl_{25}(OH)_3$ at different stages in the chlorination process.

C_1-$C_{68}Cl_{28}$	B3LYP-D3BJ/6-311G*	C_1-$C_{68}Cl_{26}(OH)_2$	B3LYP-D3BJ/6-311G*	C_1-$C_{68}Cl_{25}(OH)_3$	B3LYP-D3BJ/6-311G*
C_{68}	-	C_{68}	-	C_{68}	-
$C_{68}Cl_1$	-60.2462	$C_{68}Cl_1$	-60.2462	$C_{68}Cl_1$	-60.2462
$C_{68}Cl_2$	-58.4299	$C_{68}Cl_2$	-58.4299	$C_{68}Cl_2$	-58.4299
$C_{68}Cl_3$	-33.2734	$C_{68}Cl_3$	-33.2734	$C_{68}Cl_3$	-33.2734
$C_{68}Cl_4$	-46.9754	$C_{68}Cl_4$	-46.9754	$C_{68}Cl_4$	-46.9754
$C_{68}Cl_5$	-31.446	$C_{68}Cl_5$	-31.446	$C_{68}Cl_5$	-31.446
$C_{68}Cl_6$	-40.6254	$C_{68}Cl_6$	-40.6254	$C_{68}Cl_6$	-40.6254
$C_{68}Cl_7$	-58.0864	$C_{68}Cl_7$	-58.0864	$C_{68}Cl_7$	-58.0864
$C_{68}Cl_8$	-65.2498	$C_{68}Cl_8$	-65.2498	$C_{68}Cl_8$	-65.2498
$C_{68}Cl_9$	-64.9965	$C_{68}Cl_9$	-64.9965	$C_{68}Cl_9$	-64.9965
$C_{68}Cl_{10}$	-40.0167	$C_{68}Cl_{10}$	-40.0167	$C_{68}Cl_{10}$	-40.0167
$C_{68}Cl_{11}$	-49.2163	$C_{68}Cl_{11}$	-49.2163	$C_{68}Cl_{11}$	-49.2163
$C_{68}Cl_{12}$	-46.1849	$C_{68}Cl_{12}$	-46.1849	$C_{68}Cl_{12}$	-46.1849
$C_{68}Cl_{13}$	-69.5757	$C_{68}Cl_{13}$	-69.5757	$C_{68}Cl_{13}$	-69.5757
$C_{68}Cl_{14}$	-40.8461	$C_{68}Cl_{14}$	-40.8461	$C_{68}Cl_{14}$	-40.8461
$C_{68}Cl_{15}$	-64.9033	$C_{68}Cl_{15}$	-64.9033	$C_{68}Cl_{15}$	-64.9033
$C_{68}Cl_{16}$	-39.216	$C_{68}Cl_{16}$	-39.216	$C_{68}Cl_{16}$	-39.216
$C_{68}Cl_{17}$	-47.4303	$C_{68}Cl_{17}$	-47.4303	$C_{68}Cl_{17}$	-47.4303
$C_{68}Cl_{18}$	-33.8997	$C_{68}Cl_{18}$	-33.8997	$C_{68}Cl_{18}$	-33.8997
$C_{68}Cl_{19}$	-63.3696	$C_{68}Cl_{19}$	-63.3696	$C_{68}Cl_{19}$	-63.3696
$C_{68}Cl_{20}$	-64.1627	$C_{68}Cl_{20}$	-64.1627	$C_{68}Cl_{20}$	-64.1627
$C_{68}Cl_{21}$	-22.7062	$C_{68}Cl_{21}$	-22.7062	$C_{68}Cl_{21}$	-22.7062
$C_{68}Cl_{22}$	-57.4764	$C_{68}Cl_{22}$	-57.4764	$C_{68}Cl_{22}$	-57.4764
$C_{68}Cl_{23}$	-64.3502	$C_{68}Cl_{23}$	-64.3502	$C_{68}Cl_{23}$	-64.3502
$C_{68}Cl_{24}$	-46.2432	$C_{68}Cl_{24}$	-46.2432	$C_{68}Cl_{24}$	-46.2432
$C_{68}Cl_{25}$	-69.7772	$C_{68}Cl_{25}$	-69.7772	$C_{68}Cl_{25}$	-69.7772
$C_{68}Cl_{26}$	-41.4487	$C_{68}Cl_{26}$	-20.2058	$C_{68}Cl_{25}(OH)_1$	-63.0314
$C_{68}Cl_{27}$	-31.2763	$C_{68}Cl_{26}(OH)_1$	-67.5141	$C_{68}Cl_{25}(OH)_2$	-49.6422
$C_{68}Cl_{28}$	-44.7067	$C_{68}Cl_{26}(OH)_2$	-72.1625	$C_{68}Cl_{25}(OH)_3$	-72.9658
Total BE	-1396.14	Total BE	-1439.59	Total BE	-1464.34

8. Optimized coordinates of C_{2v}-[#6073] C_{68} in gas phase:

Table S6. Coordinates of optimized structure of C_{2v}-[#6073]C_{68} in gas phase at the B3LYP-D3BJ/6-31G* level.

Atoms	Coordinates		
	X	Y	Z
C	0.728067	4.15495	-1.016761
C	-0.728067	4.15495	-1.016761
C	1.181986	4.061635	0.33108
C	-1.181986	4.061635	0.33108
C	0	4.048205	1.200222
C	1.176853	3.260036	-2.006213
C	-1.176853	3.260036	-2.006213
C	0	3.251284	2.337416
C	2.280271	3.243785	0.632047
C	-2.280271	3.243785	0.632047
C	0	2.74994	-2.705435
C	1.167352	2.451714	2.674141
C	-1.167352	2.451714	2.674141
C	2.282285	2.455027	1.847223
C	-2.282285	2.455027	1.847223
C	2.867127	2.426839	-0.402658
C	-2.867127	2.426839	-0.402658
C	2.296486	2.390026	-1.726246
C	-2.296486	2.390026	-1.726246
C	0	1.460865	-3.263591
C	0.71654	1.204474	3.269035
C	-0.71654	1.204474	3.269035
C	2.975204	1.207797	1.582985
C	-2.975204	1.207797	1.582985
C	3.375944	1.215002	0.201814
C	-3.375944	1.215002	0.201814
C	2.349503	1.156371	-2.411625
C	-2.349503	1.156371	-2.411625
C	1.222603	0.701492	-3.241442
C	-1.222603	0.701492	-3.241442
C	1.456206	0	3.125201
C	2.633266	0	2.249499
C	-1.456206	0	3.125201
C	3.47236	0	-0.529429
C	-2.633266	0	2.249499
C	3.00266	0	-1.880644
C	-3.47236	0	-0.529429
C	-3.00266	0	-1.880644

C	1.222603	-0.701492	-3.241442
C	-1.222603	-0.701492	-3.241442
C	2.349503	-1.156371	-2.411625
C	-2.349503	-1.156371	-2.411625
C	3.375944	-1.215002	0.201814
C	-3.375944	-1.215002	0.201814
C	2.975204	-1.207797	1.582985
C	-2.975204	-1.207797	1.582985
C	0.71654	-1.204474	3.269035
C	-0.71654	-1.204474	3.269035
C	0	-1.460865	-3.263591
C	2.296486	-2.390026	-1.726246
C	-2.296486	-2.390026	-1.726246
C	2.867127	-2.426839	-0.402658
C	-2.867127	-2.426839	-0.402658
C	2.282285	-2.455027	1.847223
C	-2.282285	-2.455027	1.847223
C	1.167352	-2.451714	2.674141
C	-1.167352	-2.451714	2.674141
C	0	-2.74994	-2.705435
C	2.280271	-3.243785	0.632047
C	-2.280271	-3.243785	0.632047
C	0	-3.251284	2.337416
C	1.176853	-3.260036	-2.006213
C	-1.176853	-3.260036	-2.006213
C	0	-4.048205	1.200222
C	1.181986	-4.061635	0.33108
C	-1.181986	-4.061635	0.33108
C	0.728067	-4.15495	-1.016761
C	-0.728067	-4.15495	-1.016761

9. Optimized coordinates of C_1-C_{68}(NC3) in gas phase:

Table S7. Coordinates of optimized structure of C_1-C_{68}(NC3) in gas phase at the B3LYP-D3BJ/6-31G* level.

Atoms	Coordinates		
	X	Y	Z
C	-1.29548	-3.43751	-0.12187
C	-2.01272	-2.89555	-1.20775
C	-1.48221	-2.12244	-2.34769
C	-0.17103	-1.97144	-2.71858
C	0.970262	-2.71111	-2.2561
C	1.16641	-3.32612	-0.9419
C	0.170366	-3.65568	-0.02017
C	0.530104	-3.5453	1.357337
C	-0.67953	-3.24108	2.096248
C	-1.79967	-3.15635	1.220348
C	-2.80537	-2.17183	1.478232
C	-3.65684	-1.86037	0.382129
C	-3.27177	-2.29683	-0.90789
C	-3.5564	-1.2231	-1.85111
C	-2.3964	-1.00901	-2.60909
C	-1.89823	0.332748	-2.82266
C	-0.4364	0.529675	-2.97341
C	0.326713	-0.63652	-3.14892
C	1.73641	-0.6391	-2.98898
C	2.124664	-1.97342	-2.56824
C	3.072309	-2.13395	-1.52676
C	2.463073	-2.87159	-0.44774
C	2.63782	-2.3918	0.913154
C	1.592445	-2.73161	1.815517
C	1.01052	-1.88105	2.888294
C	-0.39393	-2.28051	3.03861
C	-1.22875	-1.13391	3.131389
C	-2.48058	-1.09387	2.446051
C	-2.99997	0.194912	2.208367
C	-4.0245	0.421852	1.194474
C	-4.29266	-0.5535	0.234596
C	-4.23534	-0.17333	-1.18589
C	-3.90576	1.142665	-1.55819
C	-2.70296	1.378833	-2.35277
C	-2.03329	2.573171	-1.81888
C	-0.59394	2.711627	-1.83332
C	0.242566	1.724125	-2.4982
C	1.686029	1.700978	-2.22798

C	2.453362	0.503896	-2.54734
C	3.720565	0.242022	-1.88435
C	3.952834	-1.10029	-1.27447
C	4.416935	-0.89508	0.055458
C	3.535909	-1.27749	1.137624
C	3.293244	-0.03167	1.923718
C	2.087325	0.410497	2.578901
C	1.046802	-0.49315	3.004319
C	-0.36306	-0.00381	3.169617
C	-0.78953	1.284288	2.757421
C	-2.18242	1.403002	2.347124
C	-2.76799	2.393762	1.476515
C	-3.93177	1.785493	0.798503
C	-3.91947	2.149236	-0.54481
C	-2.78764	3.048024	-0.74176
C	-2.13704	3.257189	0.535623
C	-0.77428	3.535296	0.493676
C	-0.04957	3.462871	-0.77356
C	1.350112	3.417014	-0.47091
C	2.255787	2.622976	-1.23861
C	3.481318	2.285333	-0.57119
C	4.281062	1.172649	-0.99947
C	4.807381	0.469555	0.17246
C	4.106331	0.99331	1.262703
C	3.509147	2.249071	0.888546
C	2.403274	2.674127	1.593843
C	1.67698	1.787342	2.479095
C	0.277268	2.207319	2.435173
C	0.187214	3.332959	1.524097
C	1.483938	3.521544	0.941372

10. Optimized coordinates of C_1-$C_{68}Cl_{28}$ in gas phase:

Table S8. Coordinates of optimized structure of C_1-$C_{68}Cl_{28}$ in gas phase at the B3LYP-D3BJ/6-31G* level.

Atoms	Coordinates		
	X	Y	Z
C	0.015273	-1.60557	-2.72228
C	1.461573	-1.71928	-3.05811
C	2.197625	-0.49386	-2.58595
C	1.537961	0.779448	-2.55933
C	0.108129	0.856649	-2.74152
C	-0.65239	-0.3664	-2.78749
C	-0.50853	-2.68434	-2.03629
C	0.605475	-3.62854	-1.64574
C	1.931717	-3.11536	-2.42352
C	2.992695	-2.92975	-1.25468
C	4.075471	-1.84276	-1.47428
C	3.469228	-0.60257	-2.07041
C	4.131624	0.525498	-1.58046
C	3.50522	1.732466	-1.45066
C	2.213519	1.907498	-1.98119
C	1.472004	3.047045	-1.57671
C	0.127312	3.119817	-1.79033
C	-0.57935	2.049433	-2.41169
C	-1.99808	2.025606	-2.30238
C	-2.70335	0.862611	-2.30787
C	-2.03419	-0.37312	-2.471
C	-2.60242	-1.52949	-1.90212
C	-1.80563	-2.58019	-1.47019
C	-2.49142	-3.34787	-0.33893
C	-1.55337	-3.55558	0.998583
C	-0.08955	-3.16176	0.811459
C	0.856816	-3.24858	-0.21509
C	2.110191	-2.64744	-0.07155
C	2.442021	-1.80234	1.002365
C	3.525868	-0.86033	0.838801
C	4.659853	-1.20554	-0.10959
C	5.136909	0.233927	-0.51073
C	4.624458	1.252337	0.580894
C	4.06036	2.488988	-0.26652
C	2.929248	3.27329	0.454619
C	1.939076	4.009814	-0.49897
C	0.558946	4.136993	0.311544

C	-0.53292	4.096765	-0.83944
C	-1.93358	3.627521	-0.54739
C	-2.78294	3.184051	-1.7588
C	-4.11426	2.490975	-1.19584
C	-4.13138	1.014113	-1.88235
C	-4.5766	-0.18311	-0.96219
C	-4.02075	-1.60412	-1.39591
C	-3.7397	-2.41386	-0.05565
C	-3.36129	-1.2601	0.832691
C	-2.43888	-1.26872	1.882013
C	-1.92518	-2.60848	2.338079
C	-0.54759	-2.45202	3.087418
C	0.368758	-2.52048	1.942923
C	1.518987	-1.77429	2.047254
C	1.413874	-0.81783	3.191434
C	1.329364	0.551905	2.573896
C	2.313334	1.138529	1.751168
C	3.484814	0.454285	1.201447
C	1.970647	2.379758	1.196758
C	0.658267	2.888531	1.193583
C	-0.34223	2.23065	1.91494
C	-1.83049	2.538637	1.86239
C	-2.43878	3.100688	0.570585
C	-3.80619	2.463346	0.350463
C	-3.52196	1.122328	0.91368
C	-3.89506	-0.07264	0.356892
C	-2.53356	1.161959	1.881575
C	-2.02095	-0.03442	2.411013
C	-0.904	0.175534	3.399149
C	-0.06625	-1.10599	3.820792
C	0.059971	1.105226	2.673863
Cl	1.604466	-1.64605	-4.90869
Cl	0.228701	-5.36856	-1.85493
Cl	2.495665	-4.2493	-3.66126
Cl	3.779825	-4.52732	-0.851
Cl	5.406125	-2.42591	-2.54578
Cl	-3.07189	-4.9087	-1.04749
Cl	-1.58133	-5.28721	1.505437
Cl	5.872682	-2.22236	0.715545
Cl	6.841327	0.387582	-0.98184
Cl	5.813063	1.689	1.84041
Cl	5.402504	3.571671	-0.80143
Cl	3.629446	4.405371	1.689485
Cl	2.599413	5.526466	-1.17039

Cl	0.399645	5.57301	1.369258
Cl	-0.66423	5.779973	-1.56395
Cl	-3.08993	4.37511	-3.07708
Cl	-5.58789	3.399259	-1.56529
Cl	-5.10673	0.991637	-3.4145
Cl	-6.36465	-0.16414	-0.72219
Cl	-5.04395	-2.44661	-2.5957
Cl	-5.17082	-3.27344	0.588753
Cl	-3.19756	-3.31882	3.390463
Cl	-0.19719	-3.89624	4.129811
Cl	2.811475	-0.95729	4.326196
Cl	-2.24178	3.723381	3.214647
Cl	-5.09069	3.228761	1.396985
Cl	-1.66033	1.004127	4.845908
Cl	0.011537	-1.29614	5.581843

11. Optimized coordinates of C_1-$C_{68}Cl_{26}(OH)_2$ in gas phase:

Table S9. Coordinates of optimized structure of C_1-$C_{68}Cl_{26}(OH)_2$ in gas phase at the B3LYP-D3BJ/6-31G* level.

Atoms	Coordinates		
	X	Y	Z
Cl	-1.78107	-5.26212	1.260959
Cl	-3.31295	-4.69289	-1.23265
Cl	-0.0471	-5.25034	-2.13948
Cl	-0.28537	-4.05655	3.927183
Cl	-3.27434	-3.32932	3.278292
Cl	-5.30659	-3.05542	0.528238
Cl	-5.21281	-2.07084	-2.61163
Cl	2.210243	-4.10729	-3.96446
Cl	3.547014	-4.61719	-1.19153
Cl	2.844322	-1.27665	4.20184
Cl	0.043708	-1.53349	5.493416
Cl	-1.49587	0.900884	4.905918
Cl	-6.38887	0.167817	-0.59321
Cl	-5.14082	1.411849	-3.25172
Cl	5.231907	-2.50092	-2.80798
Cl	5.779533	-2.48613	0.444249
Cl	-4.89977	3.396382	1.680316
Cl	-5.47184	3.737636	-1.26589
Cl	-2.96542	4.676394	-2.79417
Cl	-0.4445	5.895909	-1.27254
Cl	6.825556	0.163078	-1.14363
Cl	5.920593	1.364128	1.763293
Cl	5.533969	3.39496	-0.76894
Cl	3.853486	4.176123	1.803211
Cl	0.658747	5.485692	1.630451
Cl	2.810473	5.486359	-0.96874
O	1.464576	-1.6181	-4.62566
H	1.189694	-0.74445	-4.95145
O	-1.98185	3.424122	3.114532
H	-1.83299	2.936494	3.943614
C	-1.69294	-3.50913	0.840212
C	-2.65184	-3.19473	-0.46285
C	-1.95822	-2.40131	-1.5714
C	-0.67975	-2.5317	-2.17164
C	0.404227	-3.5383	-1.85356
C	0.701631	-3.24284	-0.41226
C	-0.21772	-3.16695	0.639223

C	0.292569	-2.60523	1.790549
C	-0.59715	-2.55437	2.957033
C	-1.99585	-2.61878	2.232165
C	-2.46154	-1.23888	1.855162
C	-3.40498	-1.13544	0.830459
C	-3.85288	-2.22454	-0.10467
C	-4.12657	-1.3355	-1.396
C	-2.71788	-1.29621	-1.93145
C	-2.1125	-0.1379	-2.45435
C	-0.73764	-0.17695	-2.80404
C	-0.1231	-1.44414	-2.81555
C	1.31482	-1.60594	-3.20852
C	1.730154	-3.03847	-2.63403
C	2.824838	-2.96626	-1.48825
C	1.98492	-2.70769	-0.26799
C	2.377855	-1.93367	0.839146
C	1.478849	-1.91908	1.906225
C	1.440054	-1.01658	3.097952
C	-0.04395	-1.26534	3.742258
C	-0.82257	0.065849	3.384875
C	-1.97737	-0.05017	2.430019
C	-2.44199	1.190699	1.971657
C	-3.45264	1.245836	1.031546
C	-3.89364	0.098026	0.426756
C	-4.60915	0.084433	-0.87835
C	-4.1313	1.309424	-1.74433
C	-2.72133	1.116712	-2.21264
C	-1.96399	2.245325	-2.16348
C	-0.54736	2.212576	-2.30414
C	0.078863	1.009808	-2.708
C	1.510407	0.862876	-2.56767
C	2.109673	-0.4356	-2.66755
C	3.38864	-0.62197	-2.19657
C	3.951013	-1.91728	-1.67777
C	4.594232	-1.37684	-0.29872
C	3.499422	-1.03218	0.694955
C	3.52671	0.263258	1.122671
C	2.39993	0.968664	1.733366
C	1.408389	0.382966	2.546708
C	0.165832	0.984571	2.691401
C	-0.20641	2.161791	2.003192
C	-1.68929	2.558035	2.041308
C	-2.29329	3.199065	0.773662
C	-3.68872	2.62886	0.551923

C	-4.03199	2.747544	-0.98241
C	-2.68302	3.407315	-1.54308
C	-1.78957	3.751466	-0.33149
C	-0.37589	4.173849	-0.63416
C	0.220101	3.219238	-1.64812
C	1.565495	3.080363	-1.47309
C	2.24835	1.93288	-1.95234
C	3.542303	1.674848	-1.46342
C	4.111898	0.449521	-1.6683
C	5.126517	0.05989	-0.63922
C	4.685046	1.042669	0.513633
C	4.156934	2.34489	-0.25677
C	3.077778	3.139319	0.529906
C	2.098696	2.249738	1.249048
C	0.809275	2.811955	1.300677
C	0.742478	4.108028	0.489201
C	2.098324	3.966413	-0.35981

12. Optimized coordinates of C_1-$C_{68}Cl_{25}(OH)_3$ in gas phase:

Table S10. Coordinates of optimized structure of C_1-$C_{68}Cl_{25}(OH)_3$ in gas phase at the B3LYP-D3BJ/6-31G* level.

Atoms	Coordinates		
	X	Y	Z
Cl	-1.83648	-5.2455	1.281709
Cl	-3.39168	-4.63903	-1.19453
Cl	-0.14566	-5.21815	-2.13685
Cl	-0.31246	-4.04961	3.980658
Cl	-3.30059	-3.31697	3.318234
Cl	-5.36207	-2.99591	0.586436
Cl	-5.27636	-1.97352	-2.54385
Cl	2.101912	-4.08314	-3.97711
Cl	3.462703	-4.63854	-1.22445
Cl	2.831983	-1.34485	4.236509
Cl	-0.00482	-1.47703	5.529728
Cl	-6.41673	0.255679	-0.49326
Cl	-5.16621	1.529199	-3.13651
Cl	5.153776	-2.52849	-2.84311
Cl	5.744632	-2.55334	0.400126
Cl	-4.86552	3.43055	1.824811
Cl	-5.44984	3.833845	-1.11564
Cl	-2.94294	4.748994	-2.65582
Cl	-0.39999	5.923706	-1.14912
Cl	6.802815	0.096779	-1.17652
Cl	5.953388	1.282916	1.75339
Cl	5.559764	3.34246	-0.75496
Cl	3.923983	4.12452	1.845504
Cl	0.740233	5.470769	1.733057
Cl	2.858427	5.47319	-0.90069
O	1.379035	-1.57889	-4.6048
H	1.107488	-0.69985	-4.91868
O	-1.91949	3.282289	3.305705
H	-1.85624	2.6431	4.042351
O	-1.37174	0.742684	4.557647
H	-0.70536	0.746586	5.267981
C	-1.74013	-3.48941	0.872802
C	-2.7119	-3.1523	-0.42026
C	-2.02022	-2.35375	-1.5263
C	-0.7483	-2.49182	-2.13773
C	0.327376	-3.51366	-1.84013
C	0.644708	-3.23642	-0.3992

C	-0.26236	-3.16255	0.66301
C	0.266951	-2.62257	1.816735
C	-0.61629	-2.55876	2.990081
C	-2.02189	-2.61085	2.269574
C	-2.47441	-1.22608	1.899762
C	-3.43495	-1.09982	0.894805
C	-3.90343	-2.17322	-0.04568
C	-4.17556	-1.26501	-1.32521
C	-2.76982	-1.23541	-1.8681
C	-2.15485	-0.07725	-2.38027
C	-0.78382	-0.12929	-2.74297
C	-0.1852	-1.40375	-2.7751
C	1.245791	-1.57906	-3.18577
C	1.650002	-3.02226	-2.63034
C	2.758298	-2.97551	-1.49665
C	1.936357	-2.71909	-0.26325
C	2.352476	-1.96293	0.848453
C	1.464387	-1.95282	1.926409
C	1.439575	-1.0547	3.121607
C	-0.05117	-1.27237	3.756466
C	-0.81133	0.073931	3.425203
C	-1.95788	-0.05118	2.463399
C	-2.41052	1.193682	2.024963
C	-3.44314	1.281421	1.115094
C	-3.91313	0.145317	0.510508
C	-4.63973	0.155823	-0.78735
C	-4.14951	1.389142	-1.63718
C	-2.74527	1.182349	-2.1164
C	-1.97172	2.299421	-2.05682
C	-0.55793	2.250896	-2.21536
C	0.048453	1.045956	-2.64208
C	1.479579	0.880463	-2.52225
C	2.061139	-0.42439	-2.64289
C	3.342997	-0.6321	-2.18962
C	3.89516	-1.93951	-1.69047
C	4.562557	-1.42181	-0.31486
C	3.485411	-1.07379	0.69768
C	3.537725	0.218279	1.134593
C	2.428694	0.932494	1.762385
C	1.433402	0.34729	2.570985
C	0.200392	0.958274	2.716041
C	-0.16503	2.149163	2.056821
C	-1.64821	2.538902	2.136531
C	-2.26533	3.23754	0.901568

C	-3.66861	2.677487	0.672596
C	-4.0225	2.819394	-0.8561
C	-2.66834	3.464533	-1.41734
C	-1.76013	3.785642	-0.208
C	-0.34309	4.194239	-0.52856
C	0.228972	3.242575	-1.56054
C	1.57575	3.087229	-1.40799
C	2.23839	1.935621	-1.9068
C	3.535485	1.655858	-1.43753
C	4.086316	0.424928	-1.66084
C	5.109367	0.011641	-0.64951
C	4.697062	0.988887	0.517285
C	4.175357	2.306393	-0.23354
C	3.117122	3.108133	0.574259
C	2.136295	2.22261	1.295138
C	0.853742	2.800866	1.363973
C	0.793469	4.10622	0.573337
C	2.135796	3.95685	-0.29509

13. Optimized coordinates of $Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ in gas phase:

Table S11. Coordinates of optimized structure of $Sc_2C_2@C_2\text{-}^{\#6073}C_{68}$ in gas phase at the B3LYP-D3BJ/6-31G* level.

Atoms	Coordinates		
	X	Y	Z
C	-0.67934	4.253771	-1.00528
C	0.761111	4.197599	-0.9917
C	-1.13398	4.151142	0.381072
C	1.21846	4.077089	0.379556
C	0.044556	4.071137	1.238752
C	-1.14716	3.314948	-2.00878
C	1.208662	3.247924	-1.97483
C	0.041119	3.251313	2.414368
C	-2.19906	3.250905	0.650514
C	2.286178	3.188441	0.651135
C	0.02773	2.744109	-2.65352
C	-1.12398	2.465636	2.731122
C	1.190652	2.442368	2.729703
C	-2.23543	2.459747	1.876503
C	2.306054	2.410091	1.880162
C	-2.81432	2.456021	-0.39144
C	2.912322	2.401553	-0.39027
C	-2.26228	2.426467	-1.72802
C	2.331056	2.366007	-1.71142
C	0.016193	1.440753	-3.27597
C	-0.7006	1.207518	3.328891
C	0.732387	1.193895	3.327011
C	-2.96631	1.246298	1.618087
C	3.010764	1.181637	1.623762
C	-3.32824	1.249677	0.222854
C	3.387099	1.184587	0.225028
C	-2.31725	1.189014	-2.43052
C	2.352841	1.137054	-2.42897
C	-1.21846	0.727512	-3.25842
C	1.237526	0.706078	-3.25522
C	-1.45849	0.015508	3.164355
C	-2.63894	0.026501	2.277104
C	1.458493	-0.01551	3.164355
C	-3.43659	0.034525	-0.51386
C	2.638935	-0.0265	2.277104
C	-2.96029	0.032713	-1.86932
C	3.436586	-0.03453	-0.51386

C	2.960294	-0.03271	-1.86932
C	-1.23753	-0.70608	-3.25522
C	1.21846	-0.72751	-3.25842
C	-2.35284	-1.13705	-2.42897
C	2.317254	-1.18901	-2.43052
C	-3.3871	-1.18459	0.225028
C	3.328244	-1.24968	0.222854
C	-3.01076	-1.18164	1.623762
C	2.966306	-1.2463	1.618087
C	-0.73239	-1.1939	3.327011
C	0.700604	-1.20752	3.328891
C	-0.01619	-1.44075	-3.27597
C	-2.33106	-2.36601	-1.71142
C	2.262277	-2.42647	-1.72802
C	-2.91232	-2.40155	-0.39027
C	2.814319	-2.45602	-0.39144
C	-2.30605	-2.41009	1.880162
C	2.235433	-2.45975	1.876503
C	-1.19065	-2.44237	2.729703
C	1.123983	-2.46564	2.731122
C	-0.02773	-2.74411	-2.65352
C	-2.28618	-3.18844	0.651135
C	2.199059	-3.25091	0.650514
C	-0.04112	-3.25131	2.414368
C	-1.20866	-3.24792	-1.97483
C	1.147157	-3.31495	-2.00878
C	-0.04456	-4.07114	1.238752
C	-1.21846	-4.07709	0.379556
C	1.133984	-4.15114	0.381072
C	-0.76111	-4.1976	-0.9917
C	0.679339	-4.25377	-1.00528
C	0.586601	0.235598	0.175641
C	-0.5866	-0.2356	0.175641
Sc	0.115226	-2.19602	-0.28802
Sc	-0.11523	2.196022	-0.28802

14. The details of calculation:

The non-classical isomer C_1-C_{68}(NC3), the non-IPR isomer C_{2v}-$^{\#6073}C_{68}$, with their derivatives C_1-$C_{68}Cl_{28}$, C_1-$C_{68}Cl_{26}(OH)_2$, C_1-$C_{68}Cl_{25}(OH)_3$ and $Sc_2C_2@C_2$-$^{\#6073}C_{68}$ have been optimized by Gaussian 16 program at the B3LYP-D3BJ/6-31G* level, with eight-cores CPU (Intel Xeon X5450, 3.0GHz) and 6000MB memory. And then, the single point energies have been calculated by using the 6-311+G (3df, 3pd) basis set. The total CPU times are listed in Table S12.

Table S12. The total CPU times (hour) for the optimization and single point calculations of the non-classical isomer C_1-C_{68}(NC3), the non-IPR isomers C_{2v}-$^{\#6073}C_{68}$, with their derivatives.

Molecule	CPU time (h)
C_{2v}-$^{\#6073}C_{68}$	71.6
$Sc_2C_2@C_2$-$^{\#6073}C_{68}$	240.6
C_1-C_{68}(NC3)	260.0
C_1-$C_{68}Cl_{28}$	569.5
C_1-$C_{68}Cl_{26}(OH)_2$	583.2
C_1-$C_{68}Cl_{25}(OH)_3$	583.8

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