Electronic Supplementary Material (ESI) for Chemical Science
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Electronic Supplementary Information

$Sc_2S@C_2(7892)$-C_{70}: Metallic Sulfide Cluster in a Non-IPR C_{70} Cage

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Experimental Details:

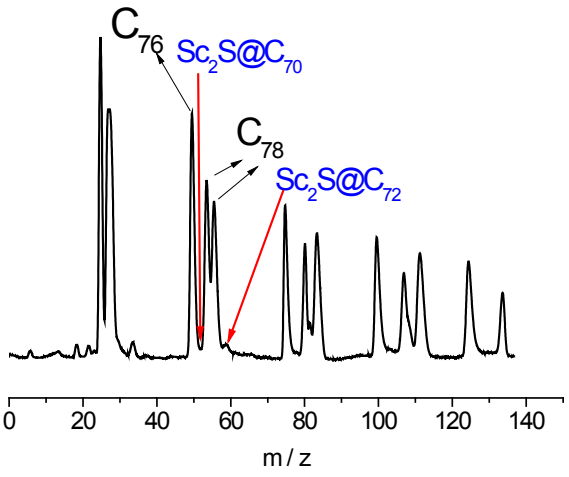

Figure S1. HPLC Chromatogram of the second-step separation of $Sc_2S@C_{70}$ obtained on a 10mm×250mm Buckyprep column using λ = 320 nm, a flow rate of 4 mL/min, and toluene as the eluent at 25℃.

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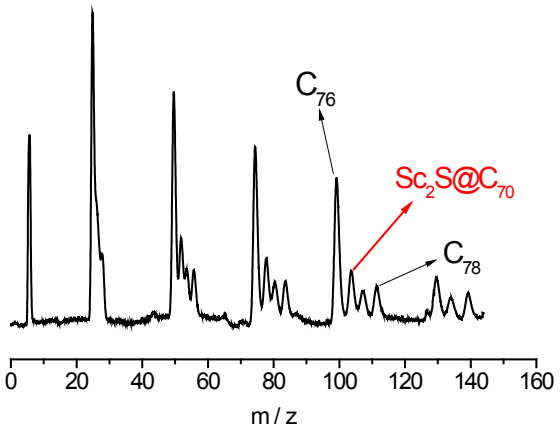

Figure S2. HPLC Chromatogram of the third-step separation of $Sc_2S@C_{70}$ obtained on a 10mm×250mm Buckyprep column using λ = 320 nm, a flow rate of 4 mL/min, and toluene as the eluent at 25℃.

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Table S1. Relative energies, in kcal mol^{-1}, for the lowest-energy isomers of C_{70}^{4-} and $Sc_2S@C_{70}$, along with their number of adjacent pentagon pairs (APP), number of pyracylenes and the IPSI values, in Å, for the tetraanionic cages.

Isomer	APP	C_{70}^{4-}	$Sc_2S@C_{70}$	Pyra.	IPSI
8149	0	0.0	20.6	20	13.4820
7892	2	3.9	0.0	11	13.7102
7957	2	4.7	19.1	10	13.7031
7851	3	6.2	20.3	6	13.8262
7852	3	6.3	23.5	5	13.8250
7887	3	7.0	21.6	6	13.8217
7854	3	8.5	26.3	4	13.8173
7893	3	9.4	19.7	7	13.8265
7886	3	10.8	21.5	6	13.8209
7924	2	11.6	18.6	12	13.7088
7846	3	13.2	29.3	7	13.8318
7960	2	14.1	21.9	11	13.7054
7922	3	14.2	27.7	7	13.8146
7921	3	14.7	29.1	8	13.8260
7850	3	14.7	33.2	6	13.8285
7847	3	15.6	28.8	8	13.8277
8008	2	16.0		13	13.7150
7853	3	16.4		6	13.8357
8094	1	16.7	26.5	17	13.6052
8064	2	17.4		14	13.7153
8005	2	17.7		13	13.7140
7849	3	18.2		6	13.8259
7848	3	18.3		7	13.8315
7889	3	18.4		8	13.8251
7888	3	18.7		9	13.8275
7925	2	18.9		13	13.7150
7911	3	19.2		8	13.8236
8111	2	19.9		14	13.7106
7904	3	20.1		9	13.8299
8044	3	20.1		9	13.8375
7950	3	20.4		8	13.8261
8090	2	20.4		14	13.7175
7890	3	20.6		9	13.8290
8148	3	22.5		9	13.8238
8147	3	22.9		9	13.8354
7787	3	23.0		10	13.8309
7891	3	23.9		9	13.8342
7983	3	24.7		10	13.8344
7883	3	24.8		9	13.8266
7927	3	26.1		10	13.8376
7982	3	26.5		9	13.8316
8142	2	26.5		15	13.7255
8043	3	26.8		9	13.8381
7858	3	27.2		10	13.8322
7903	3	27.3		9	13.8324
8104	3	27.5		10	13.8381
7915	3	28.0		9	13.8322

Isomer	APP	C_{70}^{4-}	$Sc_2S@C_{70}$	Pyra.	IPSI
7915	3	28.0		9	13.8322
7956	3	29.0		9	13.8272
7780	3	29.1		9	13.8287
8042	2	29.2		14	13.7251
7926	3	29.5		10	13.8280
8041	3	29.6		11	13.8400
8055	3	29.6		11	13.8299
8116	3	29.7		11	13.8362
8103	3	29.9		11	13.8328
8009	2	30.2		15	13.7248
7790	2	31.4		15	13.7229
7782	3	31.9		9	13.8349
7966	3	31.9		10	13.8302
8006	3	32.1		11	13.8338
7975	3	32.3		10	13.8312
7841	3	32.6		9	13.8293
7759	3	32.8		11	13.8351
7929	3	32.8		11	13.8269
8144	2	33.6		15	13.7239
7860	3	33.6		10	13.8231
7961	3	33.6		10	13.8310
7963	3	34.3		11	13.8456
7793	3	35.1		10	13.8360
8007	3	35.1		11	13.8331
8010	3	35.2		11	13.8328
8065	3	35.3		12	13.8350
8002	3	35.5		11	13.8360
8125	3	36.4		12	13.8379
7974	3	36.5		12	13.8343
7777	3	36.6		11	13.8361
8061	3	37.0		12	13.8381
7761	3	37.2		11	13.8349
7837	3	37.7		10	13.8395
7958	3	38.0		10	13.8306
8095	3	38.2		10	13.8309
7913	2	38.3		15	13.7244
8089	3	38.8		11	13.8265
7698	3	38.8		13	13.8569
7930	3	39.0		11	13.8320
7711	3	39.2		12	13.8539
7912	3	39.5		11	13.8328
8093	3	39.5		11	13.8325
7901	3	39.6		11	13.8414
8003	3	40.4		12	13.8401
8067	3	40.8		13	13.8371
7969	3	41.3		12	13.8430
8092	3	41.6		11	13.8249

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Isomer	APP	C_{72}^{4-}	$Sc_2S@C_{72}$	Pyra.	IPSI
8141	3	41.6		12	13.8437
8013	3	42.2		11	13.8256
8128	3	42.9		13	13.8419
8011	3	43.0		12	13.8447
8091	2	43.2		16	13.7262
7671	3	45.7		13	13.8584
7959	3	46.7		11	13.8392
7726	3	47.4		12	13.8540
8097	3	47.6		12	13.8245
7670	3	47.8		12	13.8523
7755	3	48.3		11	13.8393
8087	3	48.6		12	13.8404
7716	2	49.5		18	13.7536
7805	3	51.7		12	13.8357
7724	3	55.1		14	13.8625
7766	3	55.2		13	13.8501
7661	3	55.6		13	13.8627
7906	3	58.2		13	13.8365

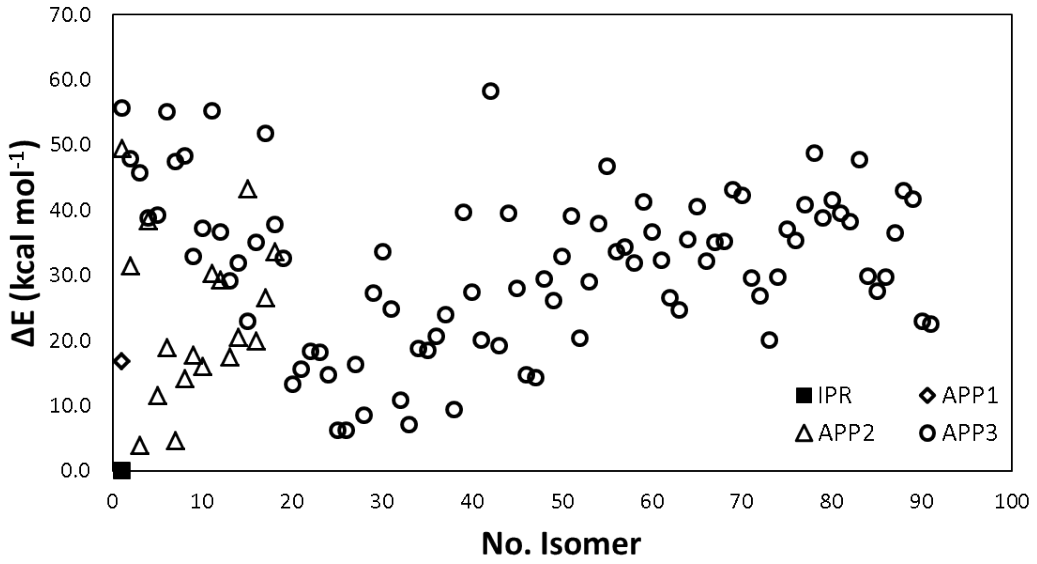

Figure S3. Relative energies for all computed tetraanions, 1 IPR, 1 APP1, 18 APP2 and 91 APP3.

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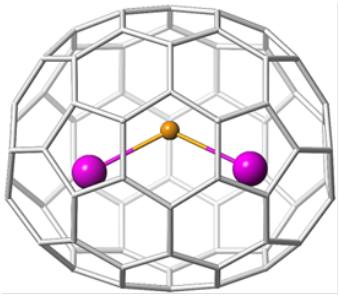

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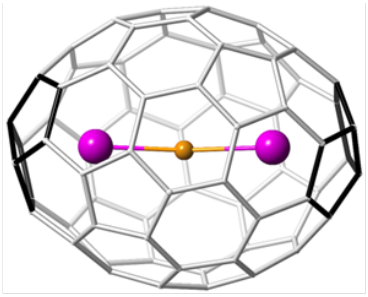

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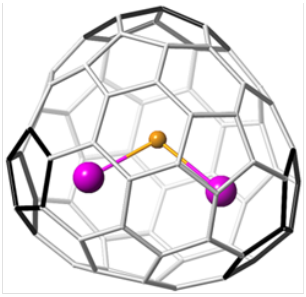

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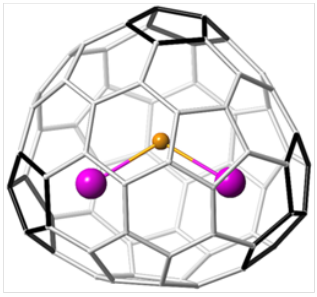

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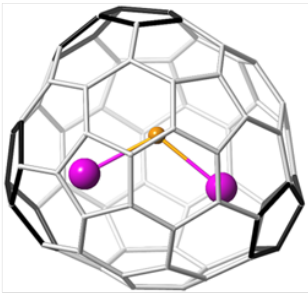

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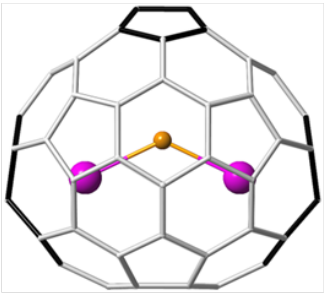

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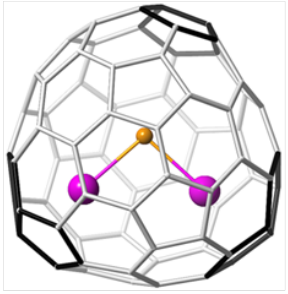

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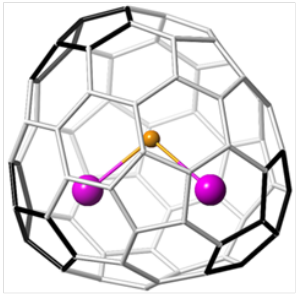

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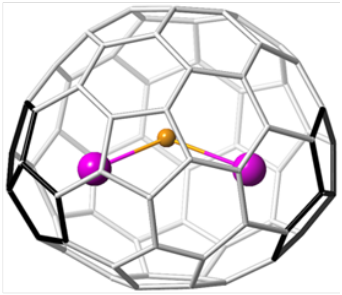

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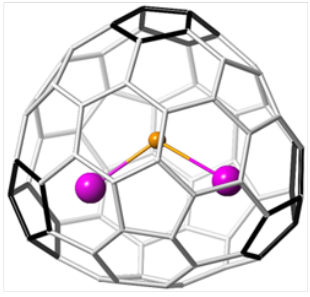

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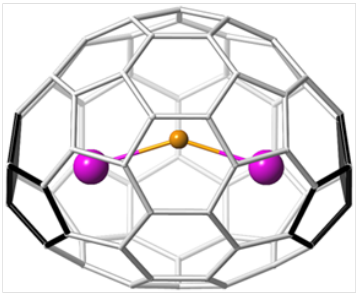

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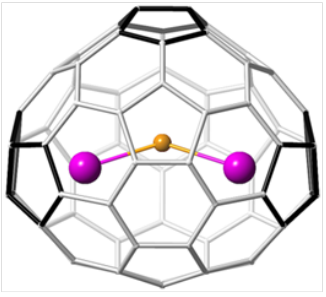

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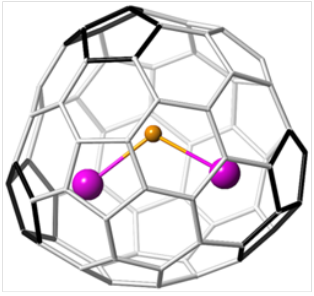

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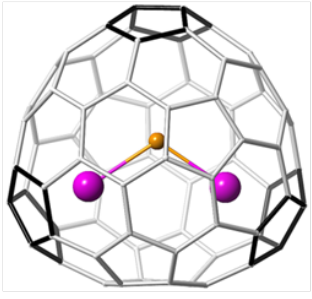

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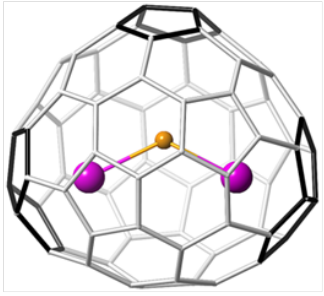

7847 (28.8)

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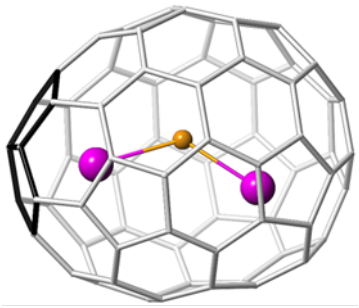

Figure S4. Optimized structures for different cages isomers of $Sc_2S@C_{70}$ with their relative energies (in parenthesis), in kcal mol^{-1}, with respect to the lowest-energy $Sc_2S@C_{70}$ isomer. The adjacent pentagon pairs are colored in black.

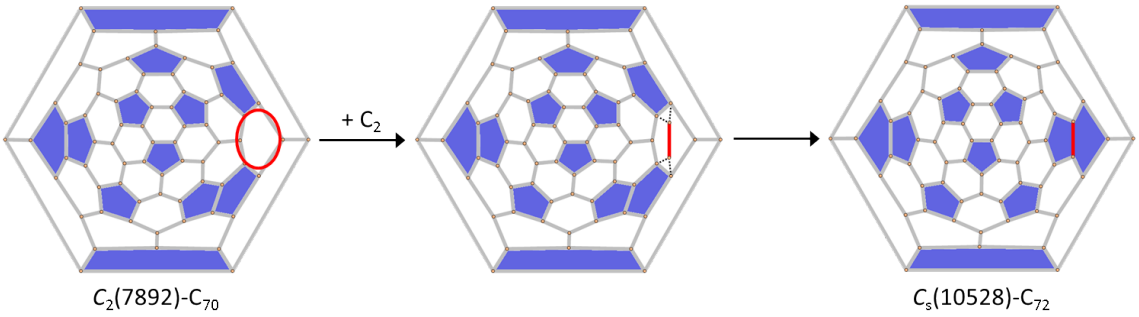

Figure S5. Schlegel diagrams showing the $C_2(7892)$-C_{70} to $C_s(10528)$-C_{72} conversion by means of single C_2 addition. The added C_2 unit which forms the new bond is highlighted in red.

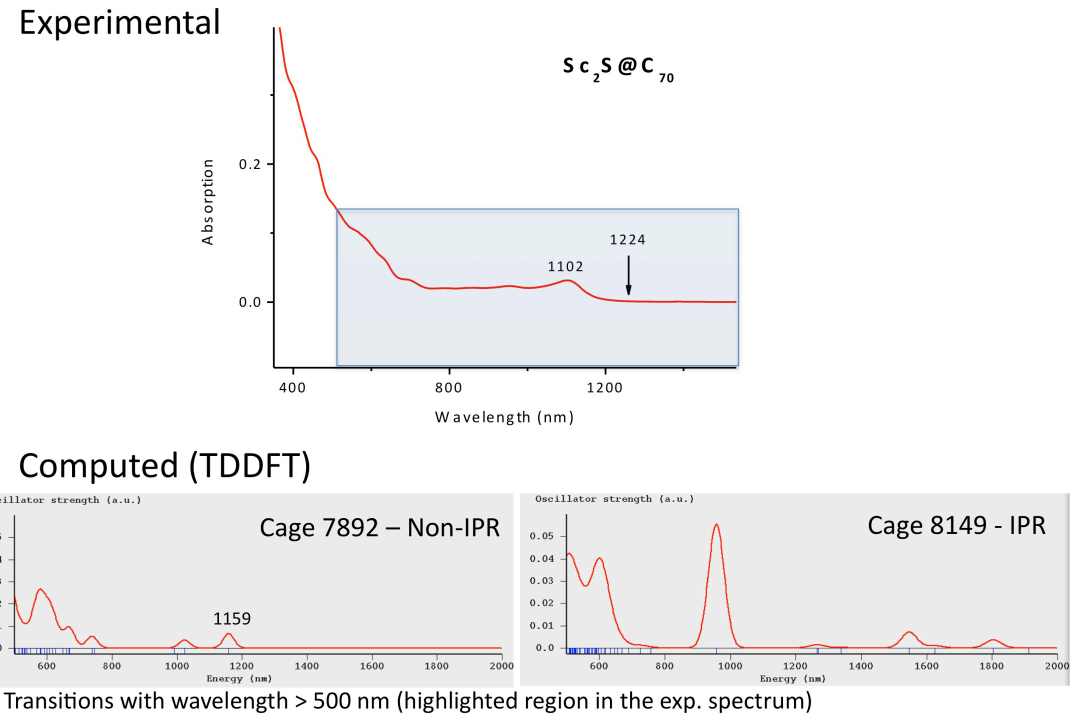

Figure S6. Experimental (top) and predicted UV-Vis-NIR spectra (bottom) for $Sc_2S@C_2(7892)$-C_{70} and $Sc_2S@D_{5h}(8149)$-C_{70} (using TDDFT methodology, at BP86/TZP level).

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Optimized cartesian coordinates of $Sc_2S@C_2(7892)$-C_{70}:

C	3.886362415	1.070823260	1.051745723
C	3.517697912	0.521061213	2.339359635
C	2.444339650	1.345539389	2.884129228
C	2.216663364	2.436807652	1.937364125
C	3.082641570	2.237373096	0.787824787
C	3.940011025	0.013782534	0.078311337
C	3.607048495	-1.234264785	0.768397693
C	3.339431867	-0.905898419	2.164143942
C	2.196719206	-1.512974050	2.766462477
C	1.224848768	-0.720535454	3.502012968
C	1.284940246	0.721925906	3.491787001
C	0.034702850	1.426405213	3.452918460
C	-0.143836875	2.583702947	2.609488649
C	0.922478755	3.053012017	1.780921929
C	0.598816506	3.581907189	0.508732082
C	1.463224097	3.362569150	-0.635278198
C	2.622885711	2.535599623	-0.546837173
C	2.919490421	1.571892690	-1.630399922
C	3.508609864	0.255101538	-1.280140407
C	3.132390534	-0.901032244	-2.009759551
C	2.820779305	-2.166847258	-1.332605197
C	2.895019088	-2.293672643	0.078978162
C	1.831880649	-3.025470003	0.797116340
C	1.505801126	-2.602996610	2.137907080
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C	-0.034702850	-1.426405213	3.452918460
C	-1.284940246	-0.721925906	3.491787001
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C	2.106432511	1.630603115	-2.794319257
C	1.782027144	0.443118710	-3.550654749
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C	-3.339431867	0.905898419	2.164143942
C	-3.607048495	1.234264785	0.768397693
C	-2.895019088	2.293672643	0.078978162
C	-2.820779305	2.166847258	-1.332605197
C	-1.762638375	2.799837800	-2.072305142
C	-1.419105731	1.970499373	-3.200400426
C	-0.087093483	1.847229170	-3.619636132
C	0.419056774	0.560695237	-4.040598001
C	-0.419056774	-0.560695237	-4.040598001
C	0.087093483	-1.847229170	-3.619636132
C	-0.959076127	-2.512085278	-2.876474855
C	-0.628293247	-3.335534695	-1.801811001

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C	-1.463224097	-3.362569150	-0.635278198
C	-2.622885711	-2.535599623	-0.546837173
C	-3.082641570	-2.237373096	0.787824787
C	-3.886362415	-1.070823260	1.051745723
C	-3.940011025	-0.013782534	0.078311337
C	-3.508609864	-0.255101538	-1.280140407
C	-3.132390534	0.901032244	-2.009759551
C	-2.271543704	0.801010588	-3.153014383
C	-1.782027144	-0.443118710	-3.550654749
C	-2.106432511	-1.630603115	-2.794319257
C	-2.919490421	-1.571892690	-1.630399922
S	0.000000000	0.000000000	-0.598201283
Sc	1.755620853	0.239092623	0.948150841
Sc	-1.755620853	-0.239092623	0.948150841

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Optimized cartesian coordinates of $Sc_2S@C_{2v}(7854)$-C_{70}:

C	4.184736000	-1.152410000	0.724194000
C	4.186405000	-1.154997000	-0.712857000
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C	2.764651000	-2.876173000	0.007695000
C	3.283793000	-2.187144000	1.186310000
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C	3.871346000	1.100277000	0.001925000
C	3.999782000	0.228932000	-1.161151000
C	3.150863000	0.453205000	-2.253427000
C	2.413926000	-0.623018000	-2.882115000
C	2.393809000	-1.941792000	-2.293039000
C	1.166102000	-2.660064000	-2.331166000
C	0.720028000	-3.479975000	-1.216844000
C	1.455404000	-3.495307000	0.008270000
C	0.718265000	-3.475903000	1.232504000
C	1.162488000	-2.652084000	2.344493000
C	2.389891000	-1.933673000	2.304898000
C	2.409427000	-0.613349000	2.890338000
C	3.146914000	0.460513000	2.258488000
C	2.371327000	1.681775000	2.349705000
C	2.335631000	2.618930000	1.260373000
C	2.999519000	2.271526000	-0.000123000
C	2.337481000	2.614891000	-1.262503000
C	2.375002000	1.674117000	-2.348718000
C	1.230876000	1.390041000	-3.161493000
C	1.225998000	-0.032789000	-3.431511000
C	0.004822000	-0.774304000	-3.493355000
C	0.004275000	-2.110000000	-2.973680000
C	-1.158526000	-2.659598000	-2.332301000
C	-0.714371000	-3.479750000	-1.217570000
C	-1.451548000	-3.495152000	0.006721000
C	-0.716145000	-3.475919000	1.231816000
C	-1.162019000	-2.652220000	2.343448000
C	-0.000119000	-2.100268000	2.984167000
C	-0.000406000	-0.762907000	3.499678000
C	1.220867000	-0.021517000	3.436745000
C	1.226129000	1.400436000	3.162278000
C	0.000243000	2.105083000	2.964098000
C	0.001093000	3.173546000	2.037389000
C	1.169912000	3.453779000	1.221870000
C	0.717158000	4.008336000	-0.004187000
C	1.171718000	3.449771000	-1.227903000
C	0.004086000	3.166815000	-2.043849000
C	0.004725000	2.095290000	-2.966975000
C	-1.221296000	1.390291000	-3.162938000
C	-1.216286000	-0.032493000	-3.432834000
C	-2.405014000	-0.622395000	-2.884611000
C	-2.385933000	-1.940939000	-2.295068000
C	-3.280101000	-2.190770000	-1.175771000
C	-2.760908000	-2.875995000	0.005179000
C	-3.282156000	-2.187351000	1.183375000
C	-2.389583000	-1.933851000	2.302991000
C	-2.409544000	-0.613143000	2.888046000
C	-1.221470000	-0.021349000	3.435513000
C	-1.226122000	1.400701000	3.160895000
C	-2.370163000	1.682311000	2.347040000
C	-2.332533000	2.619622000	1.257713000
C	-1.166489000	3.454083000	1.220448000
C	-0.711751000	4.008508000	-0.005089000
C	-1.164636000	3.450022000	-1.229349000

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C	-2.330638000	2.615417000	-1.265292000
C	-2.366460000	1.674564000	-2.351473000
C	-3.142450000	0.453775000	-2.256542000
C	-3.992683000	0.229661000	-1.165119000
C	-4.180571000	-1.154011000	-0.717015000
C	-4.181796000	-1.151798000	0.720004000
C	-3.994694000	0.233429000	1.163699000
C	-3.146071000	0.461124000	2.255493000
C	-3.866467000	1.101054000	-0.002110000
C	-2.994642000	2.272253000	-0.003666000
S	0.002207000	0.452685000	0.000966000
Sc	-2.082346000	-0.551359000	0.002448000
Sc	2.086896000	-0.551082000	0.001915000

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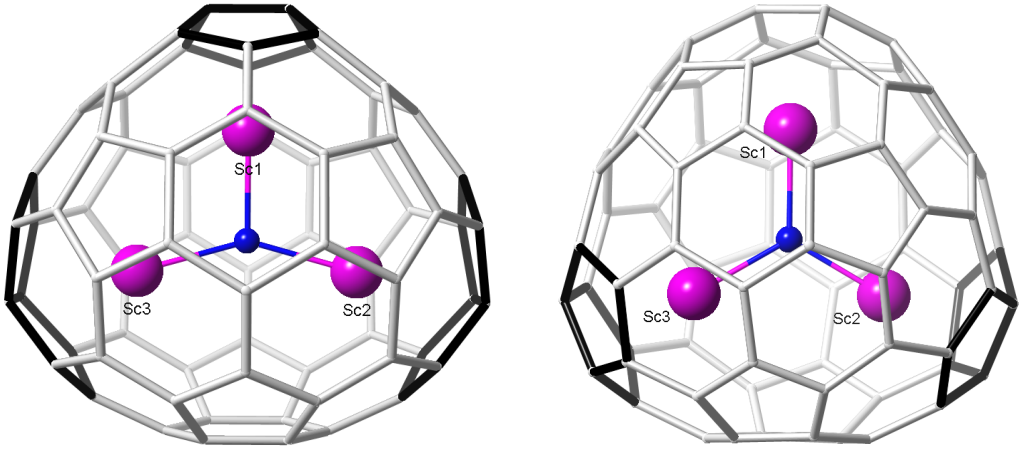

Figure S7. Optimized structures for $Sc_3N@C_{2v}(7854)$-C_{70} (left) and $Sc_3N@C_2(7892)$-C_{70} (right). The adjacent pentagon pairs are highlighted in black.

Table S2. Structural parameters of the Sc_3N unit encapsulated in $C_{2v}(7854)$-C_{70} and $C_{2v}(7854)$-C_{70}.

		$C_{2v}(7854)$-C_{70}	$C_2(7892)$-C_{70}
Bond Angle	Sc1-Sc2	105.6	119.8
	Sc2-Sc3	149.0	120.4
	Sc3-Sc1	105.4	119.8
[a] Bond Length	Sc1-N	1.977	1.979
	Sc2-N	2.038	1.991
	Sc3-N	2.037	1.989

a) Bond lengths in angstroms (Å).

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Optimized cartesian coordinates of $Sc_3N@C_{2v}(7854)$-C_{70}:

C	1.161700000	4.156550000	-0.720470000
C	1.161700000	4.156550000	0.720470000
C	-0.197459000	3.962725000	-1.162016000
C	-0.197459000	3.962725000	1.162016000
C	-1.057812000	3.827675000	0.000000000
C	2.211935000	3.273722000	-1.184031000
C	2.211935000	3.273722000	1.184031000
C	-0.440560000	3.135376000	-2.273559000
C	-0.440560000	3.135376000	2.273559000
C	-2.226430000	2.967509000	0.000000000
C	2.903190000	2.762515000	0.000000000
C	1.956408000	2.387692000	-2.299559000
C	1.956408000	2.387692000	2.299559000
C	0.636957000	2.400704000	-2.895606000
C	0.636957000	2.400704000	2.895606000
C	-1.656012000	2.383299000	-2.375307000
C	-1.656012000	2.383299000	2.375307000
C	-2.586818000	2.324223000	-1.276606000
C	-2.586818000	2.324223000	1.276606000
C	3.514317000	1.450049000	0.000000000
C	0.056419000	1.219677000	-3.470333000
C	0.056419000	1.219677000	3.470333000
C	-1.360863000	1.221495000	-3.186663000
C	-1.360863000	1.221495000	3.186663000
C	2.679833000	1.159223000	-2.342482000
C	2.679833000	1.159223000	2.342482000
C	-3.476244000	1.182402000	-1.251016000
C	-3.476244000	1.182402000	1.251016000
C	3.495147000	0.718162000	-1.228350000
C	3.495147000	0.718162000	1.228350000
C	-4.035832000	0.725848000	0.000000000
C	-3.161147000	0.000438000	-2.050473000
C	-2.062068000	-0.000179000	-2.985895000
C	0.796442000	-0.000318000	-3.522129000
C	-3.161147000	0.000438000	2.050473000
C	-2.062068000	-0.000179000	2.985895000
C	2.132055000	-0.000281000	-2.988949000
C	0.796442000	-0.000318000	3.522129000
C	2.132055000	-0.000281000	2.988949000
C	-4.034051000	-0.724425000	0.000000000
C	3.495175000	-0.718497000	-1.228346000
C	3.495175000	-0.718497000	1.228346000
C	-3.473630000	-1.180823000	-1.249900000
C	-3.473630000	-1.180823000	1.249900000
C	2.679832000	-1.159697000	-2.342421000
C	2.679832000	-1.159697000	2.342421000
C	-1.360655000	-1.222073000	-3.186092000
C	-1.360655000	-1.222073000	3.186092000
C	0.056591000	-1.220319000	-3.470179000
C	0.056591000	-1.220319000	3.470179000
C	3.514296000	-1.450459000	0.000000000
C	-2.585443000	-2.323857000	-1.275987000
C	-2.585443000	-2.323857000	1.275987000
C	-1.655534000	-2.383808000	-2.374945000
C	-1.655534000	-2.383808000	2.374945000
C	0.637221000	-2.401520000	-2.895658000
C	0.637221000	-2.401520000	2.895658000
C	1.956703000	-2.388418000	-2.299540000
C	1.956703000	-2.388418000	2.299540000
C	2.903526000	-2.763220000	0.000000000

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C	-2.225716000	-2.967953000	0.000000000
C	-0.440156000	-3.136293000	-2.273590000
C	-0.440156000	-3.136293000	2.273590000
C	2.212341000	-3.274588000	-1.184009000
C	2.212341000	-3.274588000	1.184009000
C	-1.057375000	-3.828661000	0.000000000
C	-0.196977000	-3.963538000	-1.162015000
C	-0.196977000	-3.963538000	1.162015000
C	1.162159000	-4.157447000	-0.720442000
C	1.162159000	-4.157447000	0.720442000
Sc	-1.865921000	0.004582000	0.000000000
Sc	0.655075000	1.963478000	0.000000000
Sc	0.655488000	-1.964517000	0.000000000
N	0.111266000	-0.000063000	0.000000000

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Optimized cartesian coordinates of $Sc_3N@C_2(7892)$-C_{70}:

C	-1.152745000	3.961039000	-0.750479000
C	-2.431955000	3.537592000	-0.226549000
C	-2.978143000	2.540474000	-1.131599000
C	-2.044636000	2.409767000	-2.244407000
C	-0.896028000	3.262654000	-1.978278000
C	-0.174053000	3.935433000	0.302257000
C	-0.857257000	3.490053000	1.523225000
C	-2.247026000	3.241626000	1.175666000
C	-2.852761000	2.058090000	1.688026000
C	-3.598664000	1.159339000	0.824606000
C	-3.601504000	1.336754000	-0.609210000
C	-3.559233000	0.156375000	-1.414248000
C	-2.716776000	0.074741000	-2.590897000
C	-1.887313000	1.172617000	-2.966791000
C	-0.613648000	0.899641000	-3.529993000
C	0.525897000	1.734645000	-3.234370000
C	0.438179000	2.824943000	-2.312098000
C	1.506205000	3.036861000	-1.320110000
C	1.172959000	3.527867000	0.017700000
C	1.927552000	3.045904000	1.144578000
C	1.248974000	2.612502000	2.375223000
C	-0.164363000	2.682261000	2.510515000
C	-0.884039000	1.569422000	3.162323000
C	-2.228361000	1.280805000	2.721601000
C	-2.714681000	-0.069093000	2.604687000
C	-3.558212000	-0.150215000	1.428917000
C	-3.602195000	-1.330730000	0.623887000
C	-3.600314000	-1.153223000	-0.809901000
C	-2.855808000	-2.052145000	-1.673891000
C	-2.231786000	-1.275424000	-2.708305000
C	-0.888261000	-1.564810000	-3.150324000
C	-0.132144000	-0.470930000	-3.661212000
C	1.295428000	-0.448620000	-3.564085000
C	1.695423000	0.893914000	-3.285354000
C	2.763359000	1.156937000	-2.405420000
C	2.684505000	2.210782000	-1.445545000
C	3.507221000	1.807989000	-0.305343000
C	3.064224000	2.207767000	0.975435000
C	3.118044000	1.251433000	2.096012000
C	1.992523000	1.517278000	2.936211000
C	1.299060000	0.451496000	3.573203000
C	-0.128407000	0.474847000	3.672020000
C	-0.611400000	-0.895420000	3.541675000
C	-1.886011000	-1.167726000	2.979925000
C	-2.045593000	-2.405384000	2.258613000
C	-2.979729000	-2.535107000	1.145992000
C	-2.434381000	-3.532329000	0.240200000
C	-2.250728000	-3.235991000	-1.161990000
C	-0.861600000	-3.485486000	-1.510947000
C	-0.168982000	-2.678063000	-2.498902000
C	1.244525000	-2.609584000	-2.365572000
C	1.988471000	-1.514873000	-2.927292000
C	3.114999000	-1.249864000	-2.088398000
C	3.566374000	0.076069000	-1.836683000
C	4.109650000	0.497520000	-0.554480000
C	4.108416000	-0.496478000	0.560541000
C	3.566993000	-0.074798000	1.843251000
C	2.764338000	-1.155426000	2.413298000
C	1.697509000	-0.891370000	3.294054000
C	0.527109000	-1.731080000	3.244638000

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C	0.437421000	-2.821337000	2.322570000
C	-0.897567000	-3.259184000	1.991162000
C	-1.155568000	-3.957358000	0.763224000
C	-0.177809000	-3.931951000	-0.290681000
C	1.169765000	-3.524646000	-0.008048000
C	1.923860000	-3.043808000	-1.135874000
C	3.061126000	-2.206243000	-0.967846000
C	3.504531000	-1.806179000	0.312158000
C	2.683755000	-2.209191000	1.453755000
C	1.504653000	-3.033653000	1.329367000
Sc	1.951740000	0.004094000	0.001697000
Sc	-1.017247000	1.725516000	-0.101282000
Sc	-1.014962000	-1.721673000	0.115497000
N	-0.026802000	0.001639000	0.006937000