Electronic Supplementary Material (ESI) for ChemComm.

Prato and Bingel-Hirsch cycloaddition to heptagon-containing $LaSc_2N@C_s$(hept)-C_{80}: importance of pentalene units

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Electronic Supporting Information

Table S1. Relative energies (ΔE, kJ/mol) and HOMO-LUMO gaps (gap_{H-L}, eV) of $LaSc_2N@C_{80}(CH_2)_2NH$ adducts.[a]

Addition site	ΔE(PBE)	gap_{H-L}	Δ*E*(PBE-D3)
2-10	0.0	1.21	0.0
15-31	29.9	1.11	31.7
11-12	29.1	1.19	32.4
20-21	35.4	1.06	35.3
9-10	34.0	1.15	36.0
17-30	35.4	0.73	37.0
13-13'	32.9	1.32	38.5
3-8	45.8	1.15	
37-38	48.2	0.96	
16-17	48.4	1.08	
33-35	50.1	0.83	
39-40	50.7	0.94	
25-43	51.1	1.04	
27-28	51.2	0.88	
19-28	52.2	0.93	
11-16	53.4	1.09	
42-43	57.1	0.97	
41-42	57.6	1.09	
40-41	58.1	0.95	
4-5	59.7	0.94	
24-24'	60.7	1.15	
9-18	61.5	1.14	
15-16	61.6	0.56	
14-34	63.1	1.12	
6-7	63.5	1.10	
23-23'	64.6	0.86	
10-11	64.6	0.57	
18-19	66.8	1.00	
24-5	66.9	0.69	
7-20	67.7	0.93	
19-20	68.4	0.61	
37-41	68.7	0.77	

Addition site	ΔE(PBE)	gap_{H-L}
1-12	69.4	0.82
1-2	69.8	0.85
22-23	69.8	1.04
29-30	70.1	1.17
33-34	70.2	0.69
26-27	70.6	0.97
8-9	71.5	0.79
35-36	71.7	0.89
6-23	72.0	0.68
30-31	72.5	0.58
2-3	72.5	0.76
14-15	74.6	0.98
38-39	75.3	0.80
32-33	76.7	1.08
34-34'	76.8	0.80
21-27	78.4	0.62
25-26	78.6	1.17
17-18	82.7	0.87
1-1	84.5	0.86
21-22	85.5	0.91
36-37	85.5	0.91
5-6	88.1	0.81
26-40	89.0	0.86
28-29	93.8	0.76
29-39	95.2	0.98
13-14	96.7	0.72
3-4	100.7	0.80
32-38	101.0	0.90
31-32	105.1	0.80
12-13	111.8	0.62
22-24	116.2	0.80
7-8	125.1	0.87

[a] PBE/TZ2P values. Table 1 in the main paper lists PBE-D3//PBE values, which are slightly different

Table S2. POAV pyramidalization angles in DFT-optimized $LaSc_2N@C_s$(hept)-C_{80}

atom	θ_p	atom	θ_p
1	7.328	**23**	10.548
2	13.498	**24**	9.297
3	7.03	**25**	10.855
4	7.103	**26**	8.864
5	9.464	**27**	10.114
6	10.129	**28**	10.366
7	8.593	**29**	8.887
8	8.34	**30**	10.355
9	13.059	**31**	9.967
10	15.961	**32**	8.693
11	14.267	**33**	10.326
12	9.735	**34**	9.942
13	7.523	**35**	10.934
14	8.249	**36**	8.952
15	10.09	**37**	10.126
16	10.573	**38**	10.332
17	11.207	**39**	10.109
18	9.345	**40**	10.306
19	9.539	**41**	9.993
20	11.367	**42**	11.619
21	10.606	**43**	12.762
22	8.911		

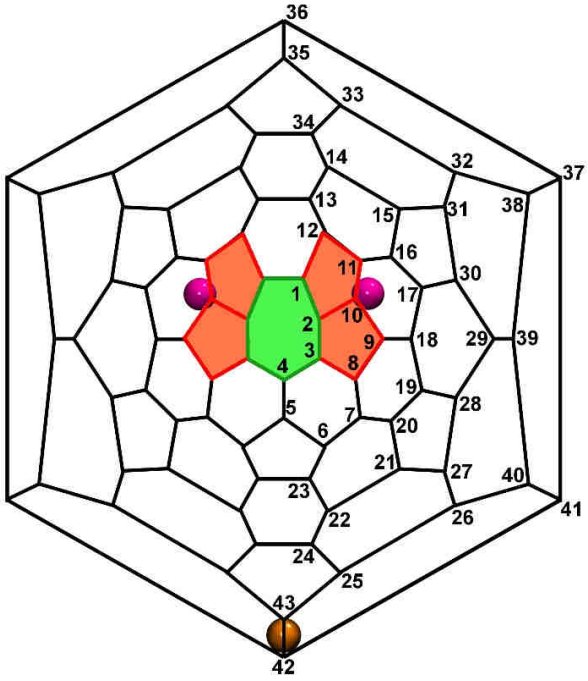

Table S3. CC bond lengths (*d*(CC), in Å) in DFT-optimized $LaSc_2N@C_s$(hept)-C_{80}

bond	*d*(CC)	bond	*d*(CC)	bond	*d*(CC)	bond	*d*(CC)
1-1'	1.403	**10-11**	1.466	**20-21**	1.436	**30-31**	1.442
1-2	1.455	**11-12**	1.465	**21-22**	1.424	**31-32**	1.427
1-12	1.453	**11-16**	1.421	**21-27**	1.445	**32-33**	1.417
2-3	1.465	**12-13**	1.465	**22-23**	1.425	**33-34**	1.449
2-10	1.445	**13-13'**	1.442	**22-24**	1.444	**33-34**	1.449
3-4	1.461	**13-14**	1.467	**23-23'**	1.434	**33-35**	1.436
3-8	1.452	**14-15**	1.440	**24-24'**	1.431	**34-34'**	1.430
4-5	1.427	**14-34**	1.418	**24-25**	1.450	**35-36**	1.434
5-6	1.446	**15-16**	1.447	**25-26**	1.445	**36-37**	1.430
6-7	1.411	**15-31**	1.436	**25-43**	1.468	**37-38**	1.435
6-23	1.442	**16-17**	1.455	**26-27**	1.435	**37-41**	1.460
7-8	1.441	**17-18**	1.449	**26-40**	1.434	**38-39**	1.436
7-20	1.428	**17-30**	1.445	**27-28**	1.440	**39-40**	1.442
8-9	1.460	**18-19**	1.432	**28-29**	1.429	**40-41**	1.457
9-10	1.450	**19-20**	1.444	**29-30**	1.428	**41-42**	1.449
9-18	1.450	**19-28**	1.440	**29-39**	1.433	**42-43**	1.469

Regiochemistry of $Sc_3N@C_{68}$

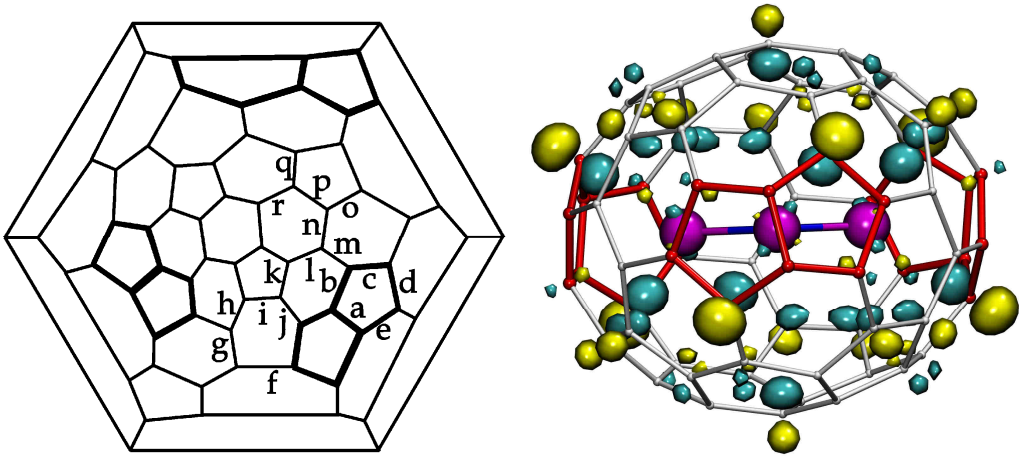

Figure S1. Schlegel diagram of $Sc_3N@C_{68}$ (left) and its LUMO isosurface (at ±0.045 a.u.). According to experimental and computational studies,[1] Bingel-Hirsch addition to $Sc_3N@C_{68}$ proceeds across the bond **m**. In the corresponding intermediate, the malonate group is added to the pentalene carbon atom with the largest LUMO contribution

Table S4. Relative energies of $Sc_3N@C_{68}(CH_2)_2NH$ adducts (kJ/mol)

CC bond	ΔE(PBE)	gap_{H-L}	Δ*E*(PBE-D3)
a	0.0	1.29	0.0
b	20.3	1.11	19.7
g	33.2	1.35	40.9
i	39.1	0.88	43.4
e	40.1	0.82	
h	40.5	1.12	
d	41.4	1.35	
q	46.5	1.02	
o	46.7	1.12	
k	49.6	1.01	
c	49.7	1.02	
p	51.2	1.02	
j	62.0	1.18	
m	70.5	1.04	
l	71.6	1.05	
n	77.9	0.94	
r	88.5	1.09	
f	95.6	0.55	

References

1. T. Cai, L. Xu, C. Shu, J. E. Reid, H. W. Gibson and H. C. Dorn, *J. Phys. Chem. C*, 2008, **112**, 19203; N. Alegret, A. Rodríguez-Fortea and J. M. Poblet, *Chem.-Eur. J.*, 2013, **19**, 5061.

Table S5. Prato bis-adducts of $LaSc_2N@C_s$(hept)-C_{80}

Addition sites	ΔE(PBE)	gap_{H-L}	Addition sites	ΔE(PBE)	gap_{H-L}	Addition sites	ΔE(PBE)	gap_{H-L}
2'-10',2-10	0.0	1.43	**7'-20',2-10**	50.5	1.05	**4-5,2-10**	66.6	1.12
11'-12',2-10	14.0	1.24	**33-34,2-10**	50.5	0.85	**36-37,2-10**	67.0	1.05
15-31,2-10	15.2	1.24	**19-20,2-10**	50.8	0.65	**21'-22',2-10**	67.4	1.03
17-30,2-10	16.1	0.81	**10'-11',2-10**	50.9	0.64	**2'-3',2-10**	67.4	0.90
9'-10',2-10	17.5	1.19	**14-34,2-10**	51.7	1.20	**21-22,2-10**	68.0	1.01
20-21,2-10	19.6	1.16	**14'-34',2-10**	51.9	1.21	**5-6,2-10**	68.3	0.85
17'-30',2-10	20.7	0.82	**24-5,2-10**	52.4	0.79	**4'-5',2-10**	68.6	1.13
15'-31',2-10	22.4	1.15	**37-41,2-10**	53.0	0.91	**28'-29',2-10**	69.8	1.00
20'-21',2-10	24.6	1.15	**26-27,2-10**	53.0	1.15	**17'-18',2-10**	69.9	0.80
39'-40',2-10	32.3	1.11	**35'-36',2-10**	54.3	1.05	**26-40,2-10**	71.4	0.99
19-28,2-10	32.4	1.11	**30-31,2-10**	54.4	0.66	**26'-40',2-10**	72.6	0.95
37-38,2-10	34.4	1.01	**35-36,2-10**	54.6	1.05	**15-16,2-10**	75.2	0.58
25-43,2-10	34.8	1.20	**33'-34',2-10**	54.9	0.79	**11-12,2-10**	76.5	1.03
37'-38',2-10	35.4	1.14	**8'-9',2-10**	54.9	0.91	**36'-37',2-10**	77.0	0.93
39-40,2-10	36.1	1.07	**30'-31',2-10**	55.0	0.72	**32-38,2-10**	78.5	1.05
27'-28',2-10	37.1	1.04	**22'-23',2-10**	55.8	1.07	**13'-14',2-10**	80.0	0.79
33'-35',2-10	37.4	0.93	**9'-18',2-10**	56.2	1.09	**18-19,2-10**	80.5	0.83
13-13',2-10	37.5	1.30	**21-27,2-10**	56.4	0.73	**29'-39',2-10**	83.9	0.96
16'-17',2-10	37.7	1.16	**26'-27',2-10**	56.9	1.09	**8-9,2-10**	85.8	0.95
25'-43',2-10	38.5	1.06	**6'-7',2-10**	57.1	1.08	**31'-32',2-10**	85.8	0.92
16-17,2-10	39.0	1.11	**22-23,2-10**	57.1	1.06	**32'-38',2-10**	85.8	1.04
42'-43',2-10	40.2	1.11	**19'-20',2-10**	57.9	0.67	**28-29,2-10**	87.3	0.68
42-43,2-10	40.2	1.11	**29'-30',2-10**	58.3	1.21	**17-18,2-10**	87.7	1.06
27-28,2-10	40.5	0.91	**14'-15',2-10**	58.5	1.00	**12'-13',2-10**	90.0	0.68
33-35,2-10	41.9	0.87	**7-20,2-10**	60.0	0.96	**31-32,2-10**	91.6	0.84
3'-8',2-10	42.5	1.10	**11-16,2-10**	60.2	1.08	**1'-2',2-10**	92.5	0.78
41'-42',2-10	42.6	1.23	**6-7,2-10**	61.2	1.15	**1-1',2-10**	94.2	0.95
41-42,2-10	42.8	1.21	**6-23,2-10**	61.2	0.86	**3-8,2-10**	95.1	0.99
15'-16',2-10	43.9	0.59	**34-34',2-10**	61.2	0.93	**13-14,2-10**	97.3	0.70
19'-28',2-10	45.1	0.87	**38'-39',2-10**	61.6	0.93	**22-24,2-10**	97.9	1.00
18'-19',2-10	45.2	1.11	**25'-26',2-10**	61.6	1.20	**1'-12',2-10**	98.2	0.66
40'-41',2-10	45.3	0.99	**14-15,2-10**	61.6	0.96	**22'-24',2-10**	101.4	0.88
23-23',2-10	46.5	0.92	**6'-23',2-10**	61.9	0.80	**7'-8',2-10**	105.6	0.93
40-41,2-10	46.5	1.12	**21'-27,2-10**	63.6	0.76	**3'-4',2-10**	109.3	0.95
29-30,2-10	46.8	1.26	**32'-33',2-10**	64.3	1.18	**3-4,2-10**	115.6	0.68
24'-5',2-10	46.8	0.96	**32-33,2-10**	64.4	1.11	**12-13,2-10**	124.5	0.67
11'-16',2-10	47.1	1.13	**38-39,2-10**	64.5	0.90	**1-12,2-10**	135.7	0.66
9-18,2-10	47.8	1.17	**25-26,2-10**	64.8	1.16	**7-8,2-10**	138.9	0.76
37'-41',2-10	48.7	0.99	**29-39,2-10**	65.8	1.00			
24-24',2-10	49.2	1.23	**5'-6',2-10**	66.1	0.93			

Table S6. Relative energies of intermediates $[LaSc_2N@C_{80}CH_2Br]^-$

C-C	ΔE(PBE)	ΔE(PBE-D3)	C-C	ΔE(PBE)	C-C	ΔE(PBE)	C-C	ΔE(PBE)
1-12	0.0	0.0	**33-35**	40.9	**23-22**	60.1	**5-4**	82.4
1-2	1.8	1.6	**7-20**	42.2	**23-6**	60.3	**39-38**	83.0
1-1'	5.1	5.2	**7-6**	42.3	**25-43**	60.5	**39-40**	83.9
11-16	5.5	7.7	**12-13**	42.7	**43-25**	60.5	**5-6'**	85.2
11-12	6.8	9.3	**12-1**	43.5	**43-25'**	60.5	**5-6**	85.3
11-10	9.4	11.9	**29-28**	43.6	**43-42**	60.9	**39-29**	85.7
3-8	11.0	12.2	**29-30**	44.0	**23-23'**	61.8	**27-26**	90.1
16-17	13.3	13.4	**29-39**	44.9	**22-23**	62.2	**27-28**	90.1
16-15	15.6	15.4	**19-28**	45.9	**4-5**	62.3	**27-21**	90.7
3-4	14.6	16.2	**36-35**	46.4	**8-7**	62.8	**34-14**	92.7
16-11	17.9	17.7	**12-11**	47.0	**22-21**	63.7	**34-33**	93.9
9-18	15.7	18.1	**36-37**	47.0	**8-9**	64.5	**34-34'**	95.1
9-8	17.1	19.6	**36-37'**	47.1	**41-40**	65.4	**35-33**	98.6
3-2	17.7	19.1	**7-8**	47.6	**22-24**	65.5	**35-33'**	98.7
18-17	19.1	21.9	**19-20**	48.5	**41-37**	65.9	**35-36**	98.9
18-19	19.7	22.1	**30-29**	50.8	**24-24'**	66.2		
42-41	20.4	29.3	**19-18**	51.4	**41-42**	66.5		
42-43	20.9	29.9	**17-18**	53.2	**24-22**	67.1		
18-9	21.8	24.4	**30-31**	53.8	**37-38**	67.2		
9-10	22.2	24.4	**17-30**	54.1	**37-36**	68.3		
15-14	25.9		**17-16**	55.8	**24-25**	68.4		
15-31	26.2		**20-7**	55.9	**4-3**	69.1		
13-13'	28.8		**28-27**	56.1	**4-3'**	69.1		
13-14	28.8		**28-19**	56.2	**38-32**	69.3		
10-2	32.1		**20-21**	56.4	**38-39**	69.4		
10-9	32.1		**8-3**	56.7	**37-41**	70.3		
2-3	33.0		**30-17**	56.8	**38-37**	71.2		
13-12	34.5		**32-33**	57.1	**31-15**	72.2		
10-11	35.3		**28-29**	57.4	**31-32**	73.4		
26-27	35.4		**40-39**	58.0	**31-30**	74.6		
26-40	35.5		**20-19**	58.3	**21-30**	76.4		
14-34	35.8		**32-38**	58.6	**6-7**	76.6		
15-16	35.9		**32-31**	59.0	**21-20**	76.8		
14-15	36.4		**25-26**	59.1	**6-5**	77.4		
26-25	36.6		**40-26**	59.4	**21-27**	77.4		
14-13	37.5		**40-41**	59.5	**6-23**	77.7		
2-1	37.6		**25-24**	59.7				
2-10	37.9							
33-34	38.7							
33-32	39.0							

Table S7. Relative energies of $LaSc_2N@C_{80}CH_2$ cycloadducts

C-C	ΔE(PBE)	gap_{H-L}	C-C	ΔE(PBE)	gap_{H-L}
42-43	0.0	1.13	**13-13'**	59.2	1.30
2-3	13.2	1.05	**6-23**	61.8	1.14
41-42	16.9	1.13	**26-27**	62.3	1.11
10-11	17.4	1.10	**2-10**	62.4	1.14
9-18	17.6	1.15	**32-38**	62.9	1.13
17-18	18.2	1.14	**22-23**	63.0	1.14
12-13	19.1	1.15	**24-24'**	63.3	1.12
13-14	21.1	1.17	**19-28**	63.3	1.12
25-43	22.2	1.14	**21-27**	64.0	1.13
16-17	25.7	1.11	**39-40**	64.6	1.15
37-41	29.5	1.08	**19-20**	64.9	1.10
3-8	30.7	1.10	**29-30**	67.0	1.11
25-26	35.7	1.11	**28-29**	67.7	1.13
40-41	37.3	1.11	**27-28**	68.0	1.10
9-10	39.1	1.15	**4-5**	70.3	0.96
11-12	41.2	1.06	**17-30**	70.8	1.08
36-37	42.6	1.02	**5-6**	74.6	1.10
24-25	42.7	1.13	**37-38**	74.8	1.12
8-9	43.4	1.14	**38-39**	75.0	1.13
14-15	43.6	1.06	**33-35**	75.3	1.16
1-2	44.1	1.18	**29-39**	76.2	1.15
3-4	44.2	0.99	**14-34**	80.2	1.13
26-40	45.3	1.09	**32-33**	82.0	1.17
33-34	47.1	1.15	**18-19**	82.3	1.09
7-20	48.3	1.14	**21-30**	83.0	1.14
35-36	50.5	1.18	**6-7**	84.0	1.11
22-24	53.6	1.14	**15-16**	92.4	1.11
30-31	56.0	1.11	**23-23'**	94.5	0.91
1-12	56.8	1.09	**7-8**	96.8	1.19
20-21	58.1	1.15	**31-32**	99.7	1.12
15-31	58.2	1.17	**34-34'**	110.5	0.84
11-16	58.5	1.15	**1-1'**	113.0	1.00

PBE/TZ2P-optimized Cartesian coordinates

$LaSc_2N@C_s$(hept)-C_{80}

C	0.957059000	2.615045000	3.206585000
C	0.536177000	1.436866000	3.938019000
C	-0.888402000	1.197943000	4.064623000
C	1.406109000	0.300262000	3.880755000
C	2.158000000	2.593213000	2.402521000
C	3.746322000	1.200146000	1.150538000
C	3.012947000	1.450760000	2.355855000
C	2.642171000	0.316809000	3.142513000
C	0.896007000	-1.050806000	3.854566000
C	-0.507596000	-1.285948000	3.732639000
C	-1.385629000	-0.143824000	3.773270000
C	-0.941576000	-2.404758000	2.991073000
C	1.834909000	-1.864797000	3.133883000
C	2.156555000	-3.258630000	1.142941000
C	1.398103000	-2.959712000	2.334676000
C	0.006091000	-3.263733000	2.324715000
C	4.067113000	-0.136953000	0.715474000
C	3.619627000	-1.275414000	1.464496000
C	2.922318000	-1.022198000	2.692781000
C	3.294780000	-2.468197000	0.715606000
C	-2.156273000	-2.363371000	2.208494000
C	-2.966174000	-1.192581000	2.108459000
C	-2.580676000	-0.065045000	2.953130000
C	-3.722125000	-1.032735000	0.868933000
C	-1.974097000	-3.280111000	1.105749000
C	-1.942299000	-3.457078000	-1.328012000
C	-2.623302000	-3.079610000	-0.130502000
C	-3.566424000	-1.992656000	-0.208696000
C	1.519991000	-3.798271000	-0.019380000
C	0.100126000	-4.060100000	-0.035358000
C	-0.631680000	-3.804417000	1.160177000
C	-0.581009000	-3.912974000	-1.277446000
C	-4.242575000	0.183621000	0.240502000
C	-3.124367000	2.071311000	1.543334000
C	-2.849064000	1.364974000	2.784860000
C	-3.748619000	1.542136000	0.403566000
C	-4.402079000	-0.042483000	-1.177853000
C	-3.030882000	0.890673000	-3.001215000
C	-3.888257000	1.129501000	-1.893948000
C	-3.443155000	2.095587000	-0.904249000
C	-2.106395000	-2.677566000	-2.532880000
C	-3.054808000	-1.607498000	-2.618862000
C	-3.926848000	-1.377992000	-1.483338000
C	-2.667219000	-0.457575000	-3.411100000

C	-2.180345000	3.166174000	1.401548000
C	-1.409803000	3.230754000	2.631605000
C	-1.844473000	2.125794000	3.492107000
C	-0.011362000	3.450608000	2.512281000
C	-1.644883000	3.519600000	0.084833000
C	0.475429000	3.731683000	-1.182643000
C	-0.229540000	3.900780000	0.035541000
C	0.559174000	3.836446000	1.239177000
C	-1.895511000	1.755335000	-3.243014000
C	-1.523737000	2.803540000	-2.327612000
C	-2.286577000	2.975551000	-1.086878000
C	-0.160587000	3.192372000	-2.343999000
C	1.867334000	3.328797000	-1.211622000
C	2.579435000	3.070512000	-0.013957000
C	1.918042000	3.373855000	1.213575000
C	3.543318000	2.009281000	-0.017870000
C	2.084630000	2.533302000	-2.387585000
C	2.666477000	0.271974000	-3.153381000
C	2.991235000	1.421856000	-2.368062000
C	3.748458000	1.189258000	-1.177716000
C	-0.900801000	0.984057000	-3.933533000
C	1.429099000	0.216866000	-3.878372000
C	0.487785000	1.297224000	-3.833225000
C	0.836486000	2.454817000	-3.093900000
C	-0.831589000	-2.628195000	-3.200390000
C	0.978788000	-1.146106000	-3.902819000
C	-0.419535000	-1.459231000	-3.911658000
C	-1.353224000	-0.383570000	-4.008714000
C	2.251278000	-3.352782000	-1.189720000
C	1.935725000	-1.943895000	-3.176312000
C	1.506036000	-3.067255000	-2.394777000
C	0.112037000	-3.404733000	-2.438650000
C	4.104533000	-0.157164000	-0.741258000
C	3.017955000	-1.078329000	-2.725252000
C	3.764627000	-1.337358000	-1.510528000
C	3.387322000	-2.534806000	-0.747916000
N	-0.501468000	0.155396000	0.132839000
La	1.443620000	-0.857550000	-0.462061000
Sc	-0.729006000	1.255702000	1.751779000
Sc	-2.178420000	0.026932000	-0.894339000

(2-10) $LaSc_2N@C_{80}(CH_2)_2NH$

C	-3.419302620	1.812038320	2.419793730
C	-3.404404630	1.158165480	3.800642860
C	-2.847316310	-0.284281700	3.749946000
C	-3.191628710	-1.405197090	2.890109350
C	-2.372145120	-2.577900580	2.986334640
C	-1.170907960	-2.600380440	3.777633780
C	-0.770551520	-1.477300720	4.527363520
C	-1.670425920	-0.346364900	4.574095460
C	-1.199032020	0.970065020	4.944155340
C	-2.279082780	2.001331640	4.587987860
C	-1.735157570	2.986665160	3.539853350
C	-2.469090910	2.882746790	2.306718840
C	-1.918389180	3.268501280	1.004154420
C	-0.521992210	3.698024730	0.973195160
C	0.245100460	3.639406890	2.181155170
C	-0.344140220	3.228337310	3.441981480
C	0.643331980	2.433778560	4.150012920
C	0.211302830	1.234065810	4.836834250
C	1.112508220	0.117247960	4.754198570
C	0.624848140	-1.234827500	4.689821380
C	1.596699980	-2.032598640	3.993390130
C	1.188325960	-3.118064130	3.168929810
C	-0.197763850	-3.447347450	3.131108150
C	1.970243080	-3.387811020	1.988051860
C	3.096299730	-2.566844780	1.592065650
C	3.392434160	-1.383289010	2.369044980
C	2.677783850	-1.165884140	3.591814030
C	2.365829720	0.164109330	4.055510160
C	2.740957670	1.320412280	3.301601810
C	1.858764340	2.440857680	3.358006980
C	1.616408210	3.225160950	2.171376000
C	2.304690610	2.958233020	0.947031460
C	1.602338950	3.219602240	-0.256866700
C	0.203467290	3.586208260	-0.240014630
C	1.851782160	2.447992520	-1.444224110
C	2.779503020	1.355413530	-1.427350460
C	3.522442490	1.120567840	-0.230092000
C	3.292353360	1.922008470	0.939979990
C	3.491699900	1.099160560	2.100681990
C	3.832672110	-0.226601360	1.648218190
C	3.887552350	-0.227390510	0.191302240
C	3.593839910	-1.402594690	-0.604298830
C	3.223418020	-2.617980080	0.132956570
C	-3.957866100	-1.277358540	1.658524130
C	-2.158214660	-3.482143080	1.882780680
C	-2.084614160	-3.632578300	-0.550317170

C	-2.795433360	-3.286819800	0.638686420
C	-3.760013350	-2.219478410	0.566115940
C	1.365858590	-3.928116020	0.808032840
C	-0.049870800	-4.215291610	0.766628560
C	-0.806483890	-3.986163650	1.953439500
C	-0.713233740	-4.062336130	-0.483044420
C	-4.487336510	-0.064938770	1.048449040
C	-4.007021590	1.290599510	1.262691120
C	-4.613854320	-0.267579500	-0.381323990
C	-3.222461760	0.717513740	-2.160037540
C	-4.102779550	0.922392470	-1.061102440
C	-3.688720880	1.869584190	-0.044584170
C	-2.243837410	-2.839273390	-1.745605540
C	-3.205813800	-1.784466170	-1.825180960
C	-4.103890730	-1.585937150	-0.699478860
C	-2.825752760	-0.614373020	-2.587205870
C	-2.102236530	1.604969720	-2.372394750
C	-1.761637810	2.636614780	-1.428839080
C	-2.536872360	2.748178440	-0.190029630
C	-0.405705130	3.053547240	-1.417832610
C	2.488099120	0.208157600	-2.235219840
C	-1.081714570	0.866482330	-3.064640070
C	1.260033260	0.141582080	-2.976605970
C	0.297848880	1.203484950	-2.931829870
C	0.615706080	2.356660510	-2.170565670
C	-0.956387710	-2.755099080	-2.391922250
C	0.838116970	-1.228965280	-3.033262020
C	-0.555359590	-1.568615970	-3.073932610
C	-1.506740970	-0.506538870	-3.168393640
C	2.113262990	-3.459818860	-0.343451320
C	1.804796280	-2.023303820	-2.314238810
C	1.382307470	-3.168632540	-1.557535720
C	-0.009511940	-3.522708830	-1.624281560
C	2.867629450	-1.141785910	-1.834426050
N	-0.700879630	0.022566970	0.993547310
La	1.219500220	-1.004266890	0.329828070
Sc	-0.925818510	1.032263500	2.641420370
Sc	-2.398692610	-0.149261310	-0.027484870
C	-4.691126650	1.394669590	4.668415840
C	-3.077740260	2.637589770	5.783818680
H	-4.774462060	0.566874950	5.389608070
H	-5.606224740	1.424761400	4.064062120
H	-2.947653530	1.989727200	6.664030490
H	-2.721633660	3.644657480	6.030987430
N	-4.484728020	2.646585250	5.391339340
H	-4.666081950	3.439218920	4.770381340

a-$Sc_3N@C_{68}(CH_2)_2NH$

C	-0.000815000	-0.028542000	3.475116000
C	-0.986543000	0.994305000	3.285218000
C	-2.308898000	0.668926000	2.822741000
C	-2.672401000	-0.689763000	2.496746000
C	-1.687734000	-1.702808000	2.716692000
C	-0.387689000	-1.388419000	3.245439000
C	0.554302000	-2.364322000	2.751846000
C	1.888766000	-1.977680000	2.374134000
C	2.279159000	-0.628823000	2.656102000
C	1.368555000	0.317933000	3.240446000
C	1.727488000	1.634605000	2.775575000
C	0.728165000	2.636238000	2.499119000
C	-0.633348000	2.289629000	2.760896000
C	-1.705713000	2.741073000	1.895844000
C	-2.763983000	1.776725000	2.003898000
C	-1.530784000	-2.814450000	1.796844000
C	-0.164664000	-3.252292000	1.871040000
C	3.156558000	0.080552000	1.762598000
C	2.875789000	1.484547000	1.906528000
C	3.104427000	2.390460000	0.842229000
C	2.243644000	3.545893000	0.712934000
C	0.984607000	3.595610000	1.447355000
C	-0.076247000	3.885275000	0.481187000
C	-1.439529000	3.411323000	0.652647000
C	-2.198101000	3.018439000	-0.532989000
C	-3.313518000	2.100892000	-0.370717000
C	-3.662933000	1.557584000	0.931902000
C	-4.225824000	0.236936000	0.754289000
C	-3.640554000	-0.907363000	1.443860000
C	-3.356979000	-1.928903000	0.432265000
C	-2.240158000	-2.856102000	0.558753000
C	-1.514982000	-3.259532000	-0.641718000
C	-0.163466000	-3.786078000	-0.514698000
C	0.467519000	-3.867141000	0.765816000
C	1.981174000	-3.925690000	0.655711000
C	2.545140000	-2.654734000	1.295529000
C	3.280410000	-1.891620000	0.308515000
C	3.542340000	-0.471207000	0.493505000
C	3.553005000	0.412437000	-0.669488000
C	3.356298000	1.841702000	-0.479908000
C	2.605745000	2.652814000	-1.441411000
C	1.959758000	3.723051000	-0.694927000
C	0.538170000	3.941761000	-0.833766000
C	-0.145499000	3.342895000	-1.919612000
C	-1.518058000	2.944359000	-1.797825000
C	-1.717904000	1.830827000	-2.704806000

C	-2.717694000	0.841519000	-2.455388000
C	-3.639337000	1.083060000	-1.368669000
C	-4.242240000	-0.040763000	-0.664592000
C	-3.715481000	-1.371821000	-0.859313000
C	-2.858860000	-1.612968000	-1.961024000
C	-1.813491000	-2.594188000	-1.878931000
C	-0.765993000	-2.185828000	-2.779034000
C	0.592869000	-2.591898000	-2.552791000
C	0.852638000	-3.571073000	-1.536532000
C	2.254820000	-3.757507000	-0.916159000
C	3.026192000	-2.440954000	-0.998390000
C	2.768523000	-1.515472000	-2.037311000
C	3.110725000	-0.118980000	-1.918309000
C	2.232445000	0.628816000	-2.795313000
C	1.890096000	1.989612000	-2.508484000
C	0.539704000	2.406060000	-2.789783000
C	-0.442960000	1.471812000	-3.271948000
C	-2.400598000	-0.522929000	-2.796161000
C	-1.102961000	-0.889741000	-3.303518000
C	1.605625000	-1.620861000	-2.887442000
C	1.267848000	-0.287360000	-3.337305000
C	-0.095565000	0.105331000	-3.524419000
N	-0.047149000	0.040267000	-0.050751000
Sc	0.942550000	-1.638429000	-0.217545000
Sc	-2.045728000	0.053060000	0.040612000
Sc	0.999458000	1.742549000	0.005194000
C	2.664947000	-5.296005000	0.994805000
H	2.132733000	-5.842920000	1.782541000
H	3.691953000	-5.094369000	1.337034000
N	2.707835000	-6.058287000	-0.250988000
H	1.788247000	-6.469416000	-0.430229000
C	3.015124000	-5.079816000	-1.292940000
H	2.735644000	-5.450700000	-2.286175000
H	4.095515000	-4.866869000	-1.287388000

Bis (2-10, 2'-10') $LaSc_2N@C_{80}[(CH_2)_2NH]_2$

C	-3.407246740	1.766877180	2.415381130
C	-3.380671570	1.143627300	3.813158540
C	-2.812966500	-0.287512290	3.763048850
C	-3.131316080	-1.382487340	2.862528790
C	-2.306317770	-2.555505550	2.978061680
C	-1.115055520	-2.586949970	3.780124840
C	-0.721549890	-1.469650310	4.542220720
C	-1.632053740	-0.347809810	4.590031940
C	-1.164350490	0.968543310	4.951003900
C	-2.248104400	1.994188760	4.589648580
C	-1.709522000	2.961256730	3.530223740
C	-2.439253010	2.835086790	2.301305030
C	-1.875908510	3.200724040	1.006791050
C	-0.492875240	3.666749920	0.972257400
C	0.272022600	3.627440260	2.180147000
C	-0.318791170	3.213404110	3.435074180
C	0.673306680	2.431992120	4.147498320
C	0.248843040	1.236645240	4.840798110
C	1.157164950	0.128556510	4.768490930
C	0.673585270	-1.223504560	4.702806650
C	1.650824300	-2.018263560	4.006541980
C	1.250231850	-3.106402210	3.184248080
C	-0.136393820	-3.436255100	3.140350150
C	2.040318270	-3.375669420	2.006151320
C	3.171619050	-2.559409470	1.613085220
C	3.459007830	-1.370502720	2.387237650
C	2.730395960	-1.148542440	3.604293160
C	2.413824560	0.180054850	4.068803470
C	2.783125970	1.333820330	3.313563780
C	1.894242010	2.450379420	3.363130960
C	1.650202810	3.229300230	2.175420000
C	2.337922930	2.959501430	0.951952460
C	1.639258670	3.214899420	-0.256143360
C	0.236541530	3.561008840	-0.241087740
C	1.898094640	2.444060150	-1.442333790
C	2.832828660	1.358383600	-1.423573870
C	3.575557290	1.126795710	-0.221276510
C	3.330071670	1.927416210	0.948109980
C	3.534253170	1.109874760	2.110563920
C	3.896470970	-0.212614530	1.662690580
C	3.963261260	-0.213632270	0.201031450
C	3.667402890	-1.393375500	-0.593670300
C	3.295811310	-2.606478170	0.148627440
C	-3.895739340	-1.260286300	1.633171100
C	-2.082129350	-3.453662440	1.879164710
C	-1.997905180	-3.616089010	-0.545022820

C	-2.709504810	-3.251848890	0.634832680
C	-3.687280290	-2.190785150	0.552459390
C	1.437619480	-3.913247690	0.824181930
C	0.024323490	-4.203649950	0.776926420
C	-0.737034830	-3.974712460	1.960781400
C	-0.631627950	-4.062808590	-0.476605830
C	-4.748041380	-0.082811620	1.123582850
C	-3.990995730	1.237580780	1.264926280
C	-4.826064210	-0.312083830	-0.472870730
C	-3.164605670	0.666316230	-2.154626300
C	-4.047868560	0.864801720	-1.065435410
C	-3.625816250	1.766638920	-0.032025520
C	-2.159767940	-2.840065110	-1.744517820
C	-3.149122330	-1.803762560	-1.828956960
C	-4.053385350	-1.617761050	-0.719598100
C	-2.771142980	-0.650917510	-2.615813100
C	-2.041853590	1.554902920	-2.364071840
C	-1.710987790	2.576299040	-1.418920490
C	-2.481495820	2.658069470	-0.181310080
C	-0.363412560	3.023026760	-1.418532700
C	2.550866330	0.210951570	-2.231675860
C	-1.021503820	0.836249800	-3.071678870
C	1.328626060	0.135319060	-2.985676640
C	0.357680370	1.186020940	-2.938073540
C	0.663442120	2.340752000	-2.172268980
C	-0.877920340	-2.766830110	-2.394829390
C	0.911965680	-1.237884020	-3.041157650
C	-0.479482670	-1.587622090	-3.094258120
C	-1.442038880	-0.537074730	-3.188699550
C	2.181346040	-3.438970150	-0.324867460
C	1.873023810	-2.020289930	-2.304562290
C	1.453653950	-3.160619740	-1.544422410
C	0.069402240	-3.530989500	-1.620509380
C	2.929718370	-1.134276560	-1.817354600
N	-0.648394020	0.019650490	0.959797380
La	1.344728090	-0.944369280	0.409171940
Sc	-0.915097780	0.997468320	2.640433980
Sc	-2.289065800	-0.239474470	-0.085617330
C	-4.654440470	1.386187010	4.700268970
C	-3.034469970	2.643142130	5.785156950
H	-4.721565030	0.565794360	5.431787740
H	-5.582560820	1.410941010	4.116077940
H	-2.895376970	2.006569950	6.672166380
H	-2.676879010	3.653498300	6.016388030
N	-4.445935520	2.646487380	5.407832030
H	-4.631267130	3.430450770	4.776891970
C	-6.369096420	-0.382112130	-0.752088970
H	-6.610602620	-1.069476950	-1.571090880

H	-6.719432720	0.626852730	-1.020850470
N	-6.998324330	-0.798005030	0.498381720
H	-6.890339770	-1.808721450	0.616442070
C	-6.263790360	-0.101111240	1.549998170
H	-6.416261370	-0.582963890	2.523601500
H	-6.622138290	0.939408610	1.609060950

Intermediate (1–12)-[$LaSc_2N@C_{80}CH_2Br$]$^-$

C	-0.145850000	-1.673911000	3.420893000
C	-1.334267000	-0.823513000	3.570534000
C	-1.479307000	0.571550000	3.913017000
C	-0.522846000	1.774385000	4.018047000
C	0.224754000	3.025191000	-2.683144000
C	0.084063000	1.928803000	-3.597575000
C	-0.245723000	-0.981751000	-4.192044000
C	-0.302001000	-2.848730000	2.618284000
C	-0.359129000	3.860418000	-0.580998000
C	-0.381264000	-2.336219000	-3.642130000
C	-0.369583000	3.352285000	1.856128000
C	-0.880676000	3.450354000	-1.868676000
C	-1.094529000	3.681271000	0.619251000
C	-1.130040000	2.686292000	2.895302000
C	-1.171141000	-3.813991000	0.667103000
C	-1.190413000	-3.536210000	-1.768947000
C	-1.208816000	1.337096000	-3.747415000
C	-1.369519000	-0.090066000	-3.997745000
C	-1.516852000	-3.156517000	1.902578000
C	-1.578683000	-2.684922000	-2.871294000
C	-1.917848000	-3.573857000	-0.522950000
C	-2.151031000	2.831605000	-1.980604000
C	-2.316421000	1.791504000	-2.953548000
C	-2.457503000	3.250999000	0.464115000
C	-2.522120000	2.347330000	2.765100000
C	-2.574974000	-1.197872000	2.886418000
C	-2.585969000	-0.492160000	-3.303142000
C	-2.644998000	-2.309070000	1.977224000
C	-2.691744000	-1.780778000	-2.688237000
C	-2.744529000	1.049198000	3.425735000
C	-2.953298000	2.781012000	-0.801606000
C	-3.096827000	-2.778497000	-0.423040000
C	-3.163585000	2.545083000	1.511508000
C	-3.172670000	0.669376000	-2.685763000
C	-3.425251000	-0.031161000	2.739294000
C	-3.474128000	-1.883395000	-1.492730000
C	-3.478650000	-2.176411000	0.825262000
C	-3.851626000	1.681800000	-0.552494000
C	-3.912618000	0.576816000	-1.458406000
C	-3.978308000	1.513023000	0.881065000
C	-4.073378000	0.185973000	1.453178000
C	-4.090123000	-0.723360000	-0.896086000
C	-4.113383000	-0.909464000	0.534065000
C	4.121427000	0.617396000	0.700131000
C	3.949782000	-0.696977000	1.276651000
C	3.348631000	-0.783713000	2.592523000

C	3.748859000	-1.783710000	0.363492000
C	4.000444000	0.824265000	-0.722679000
C	3.021648000	-0.017399000	-2.814859000
C	3.775358000	-0.266999000	-1.622766000
C	3.691549000	-1.577972000	-1.063135000
C	2.867442000	-2.876949000	0.686147000
C	2.078675000	-2.842110000	1.881995000
C	2.293980000	-1.758544000	2.803725000
C	0.787587000	-3.414611000	1.851421000
C	2.304307000	-3.371861000	-0.542520000
C	0.232287000	-3.704813000	-1.808279000
C	0.981768000	-3.898908000	-0.588067000
C	0.253776000	-3.979954000	0.635810000
C	2.185443000	-1.025999000	-3.431498000
C	2.038370000	-2.317728000	-2.818934000
C	2.813941000	-2.570712000	-1.633211000
C	0.750895000	-2.969376000	-2.948648000
C	1.199178000	-1.155262000	3.560441000
C	0.880027000	1.447541000	3.632081000
C	1.618732000	0.221688000	3.852551000
C	1.674895000	2.342394000	2.829372000
C	2.981296000	1.721901000	2.650972000
C	2.951151000	0.422552000	3.307439000
C	3.573039000	1.796247000	1.358231000
C	1.074590000	3.240025000	1.828943000
C	1.063218000	3.711948000	-0.610418000
C	1.792145000	3.382241000	0.568186000
C	3.028783000	2.666572000	0.351567000
C	1.425909000	3.198226000	-1.911366000
C	2.529203000	2.316816000	-2.073869000
C	3.351093000	2.094581000	-0.932548000
C	2.414460000	1.265340000	-3.042249000
C	1.210572000	1.066944000	-3.801773000
C	1.061444000	-0.358298000	-4.083780000
Sc	1.579490000	0.326692000	1.551314000
Sc	-1.647748000	0.692969000	1.478306000
La	-0.014166000	-0.760883000	-1.610587000
N	-0.061279000	0.101387000	0.473053000
H	0.017881000	3.415927000	5.357147000
C	-0.632460000	2.534840000	5.356082000
Br	-0.069142000	1.459424000	6.922031000
H	-1.670002000	2.819226000	5.558388000

Intermediate (11–16)-[$LaSc_2N@C_{80}CH_2Br]^-$

C	-0.126502000	-1.738383000	3.387894000
C	-1.320205000	-0.900361000	3.556993000
C	-1.462823000	0.503722000	3.910996000
C	-0.487025000	1.565685000	3.671171000
C	0.249577000	3.061895000	-2.632203000
C	0.100411000	1.977395000	-3.558409000
C	-0.242871000	-0.927419000	-4.199453000
C	-0.284463000	-2.902162000	2.577347000
C	-0.328939000	3.878847000	-0.510464000
C	-0.383028000	-2.290501000	-3.669489000
C	-0.343796000	3.341036000	1.913725000
C	-0.851904000	3.486223000	-1.799580000
C	-1.060707000	3.708887000	0.700101000
C	-1.097854000	2.642374000	2.966005000
C	-1.162000000	-3.836769000	0.617708000
C	-1.190691000	-3.521052000	-1.815319000
C	-1.194345000	1.385439000	-3.710070000
C	-1.369176000	-0.034155000	-3.999850000
C	-1.504185000	-3.194360000	1.861968000
C	-1.584864000	-2.661215000	-2.911731000
C	-1.913044000	-3.575127000	-0.565849000
C	-2.112782000	2.851485000	-1.902143000
C	-2.288622000	1.826419000	-2.890927000
C	-2.416456000	3.227865000	0.562277000
C	-2.648381000	2.472391000	3.028951000
C	-2.555721000	-1.249966000	2.883700000
C	-2.579303000	-0.448426000	-3.297983000
C	-2.631897000	-2.346991000	1.954568000
C	-2.694758000	-1.751988000	-2.705564000
C	-2.748359000	0.990405000	3.489531000
C	-2.899995000	2.770346000	-0.716271000
C	-3.088679000	-2.778325000	-0.448497000
C	-3.131302000	2.519440000	1.587393000
C	-3.146975000	0.703093000	-2.641874000
C	-3.408420000	-0.070239000	2.772184000
C	-3.464582000	-1.865824000	-1.502978000
C	-3.472643000	-2.197041000	0.811559000
C	-3.794147000	1.672952000	-0.488181000
C	-3.879690000	0.589861000	-1.413072000
C	-3.914985000	1.488853000	0.944252000
C	-4.059264000	0.157982000	1.486643000
C	-4.081032000	-0.715508000	-0.879339000
C	-4.107083000	-0.923712000	0.547260000
C	4.151432000	0.591791000	0.702580000
C	3.980182000	-0.733612000	1.259529000
C	3.374915000	-0.835597000	2.575941000

C	3.760262000	-1.801193000	0.331754000
C	4.019612000	0.817105000	-0.719707000
C	3.035612000	0.011803000	-2.820763000
C	3.791098000	-0.261241000	-1.635371000
C	3.705036000	-1.578751000	-1.093981000
C	2.879227000	-2.903193000	0.639672000
C	2.095000000	-2.889157000	1.835918000
C	2.310468000	-1.812443000	2.766747000
C	0.803263000	-3.459712000	1.801526000
C	2.314451000	-3.379441000	-0.593556000
C	0.233373000	-3.683291000	-1.854167000
C	0.988929000	-3.901616000	-0.643723000
C	0.263565000	-4.003820000	0.580000000
C	2.184998000	-0.982112000	-3.430374000
C	2.036021000	-2.278639000	-2.836523000
C	2.825021000	-2.563146000	-1.672006000
C	0.746913000	-2.920614000	-2.973956000
C	1.217934000	-1.220528000	3.522201000
C	0.907801000	1.380096000	3.633594000
C	1.646451000	0.147132000	3.832498000
C	1.723982000	2.297644000	2.851120000
C	3.025354000	1.680223000	2.675991000
C	2.977445000	0.358949000	3.301553000
C	3.618864000	1.765860000	1.380252000
C	1.092209000	3.168703000	1.863281000
C	1.093524000	3.723165000	-0.554485000
C	1.823102000	3.361602000	0.602151000
C	3.053392000	2.637786000	0.382449000
C	1.454399000	3.222999000	-1.874949000
C	2.547136000	2.338017000	-2.047694000
C	3.373865000	2.088964000	-0.910807000
C	2.432231000	1.300084000	-3.033355000
C	1.222938000	1.115913000	-3.780411000
C	1.058920000	-0.307830000	-4.065921000
Sc	1.659485000	0.317836000	1.492300000
Sc	-1.590126000	0.691344000	1.552807000
La	-0.160911000	-0.732398000	-1.613559000
N	-0.034361000	0.074972000	0.502223000
H	-3.241438000	4.520084000	3.463550000
C	-3.414189000	3.513414000	3.857625000
Br	-2.872429000	3.595161000	5.768657000
H	-4.483967000	3.279492000	3.863493000

Intermediate (3–8)-[$LaSc_2N@C_{80}CH_2Br$]$^-$

C	-0.152520000	-1.639283000	3.457630000
C	-1.453489000	-0.933034000	3.960691000
C	-1.471303000	0.614675000	3.906706000
C	-0.487758000	1.605419000	3.616875000
C	0.252209000	3.034316000	-2.707975000
C	0.101713000	1.932736000	-3.613915000
C	-0.250806000	-0.980925000	-4.183816000
C	-0.317399000	-2.792754000	2.641303000
C	-0.323666000	3.892679000	-0.611300000
C	-0.395899000	-2.332077000	-3.627310000
C	-0.335818000	3.396688000	1.816099000
C	-0.849856000	3.474901000	-1.894189000
C	-1.059652000	3.735084000	0.593176000
C	-1.098192000	2.688743000	2.849256000
C	-1.195519000	-3.766490000	0.701960000
C	-1.211145000	-3.514035000	-1.742286000
C	-1.195219000	1.349367000	-3.757135000
C	-1.367279000	-0.078983000	-3.997701000
C	-1.543074000	-3.127089000	1.943287000
C	-1.594359000	-2.666869000	-2.853168000
C	-1.936520000	-3.535466000	-0.497884000
C	-2.125175000	2.863180000	-1.999834000
C	-2.298439000	1.818227000	-2.966684000
C	-2.429888000	3.301266000	0.442605000
C	-2.512628000	2.390330000	2.752672000
C	-2.631424000	-1.175409000	2.938533000
C	-2.584687000	-0.467092000	-3.300289000
C	-2.661107000	-2.251293000	2.010690000
C	-2.699492000	-1.752857000	-2.677461000
C	-2.736806000	1.113102000	3.416748000
C	-2.930849000	2.827211000	-0.822288000
C	-3.106092000	-2.727078000	-0.403289000
C	-3.141870000	2.607542000	1.486851000
C	-3.162876000	0.703148000	-2.691283000
C	-3.415344000	0.016810000	2.736681000
C	-3.479085000	-1.838873000	-1.479739000
C	-3.477098000	-2.111981000	0.838720000
C	-3.838579000	1.738297000	-0.567517000
C	-3.898214000	0.624295000	-1.461852000
C	-3.956512000	1.575735000	0.868251000
C	-4.055396000	0.249917000	1.455705000
C	-4.085882000	-0.671027000	-0.892084000
C	-4.103508000	-0.849502000	0.538725000
C	4.136518000	0.622471000	0.686022000
C	3.955633000	-0.687462000	1.271856000
C	3.352953000	-0.759036000	2.589857000

C	3.740912000	-1.777439000	0.367033000
C	4.018095000	0.819998000	-0.741017000
C	3.025084000	-0.029640000	-2.823011000
C	3.778600000	-0.276234000	-1.629339000
C	3.685804000	-1.582617000	-1.061790000
C	2.856112000	-2.864516000	0.698194000
C	2.062694000	-2.803984000	1.891400000
C	2.281699000	-1.717884000	2.799862000
C	0.766458000	-3.356451000	1.862327000
C	2.287086000	-3.363137000	-0.523862000
C	0.211757000	-3.695658000	-1.786635000
C	0.958630000	-3.877309000	-0.565052000
C	0.229978000	-3.934370000	0.660089000
C	2.179129000	-1.035379000	-3.426775000
C	2.023187000	-2.323392000	-2.805539000
C	2.800825000	-2.573344000	-1.621999000
C	0.732850000	-2.968433000	-2.930298000
C	1.180413000	-1.102554000	3.551899000
C	0.924484000	1.485621000	3.624617000
C	1.651603000	0.262375000	3.852928000
C	1.724202000	2.384106000	2.809644000
C	3.025305000	1.753682000	2.638364000
C	2.983148000	0.451911000	3.301843000
C	3.608763000	1.811024000	1.337351000
C	1.102571000	3.239610000	1.789953000
C	1.097699000	3.728205000	-0.641613000
C	1.829574000	3.398435000	0.530481000
C	3.060987000	2.672229000	0.322705000
C	1.456708000	3.205391000	-1.944493000
C	2.550591000	2.313603000	-2.098403000
C	3.377759000	2.092037000	-0.958900000
C	2.428608000	1.256239000	-3.060748000
C	1.221212000	1.060926000	-3.812900000
C	1.059942000	-0.365808000	-4.081516000
Sc	1.601191000	0.372960000	1.543594000
Sc	-1.614053000	0.760945000	1.494554000
La	-0.029547000	-0.751181000	-1.599390000
N	-0.037754000	0.165810000	0.459484000
H	-2.868098000	-1.053173000	5.620202000
C	-1.920139000	-1.506257000	5.313548000
Br	-0.667788000	-1.137314000	6.810299000
H	-2.007971000	-2.596423000	5.270521000

Transition state (11–16)-[$LaSc_2N@C_{80}CH_2Br]^-$

C	-0.151922000	-1.703442000	3.382790000
C	-1.342346000	-0.863401000	3.531372000
C	-1.478596000	0.543416000	3.875038000
C	-0.498672000	1.600945000	3.644819000
C	0.273034000	3.039555000	-2.679924000
C	0.129575000	1.947000000	-3.597585000
C	-0.212084000	-0.962520000	-4.210267000
C	-0.306055000	-2.872946000	2.581313000
C	-0.322676000	3.868456000	-0.568173000
C	-0.359022000	-2.319534000	-3.669281000
C	-0.353775000	3.362540000	1.869626000
C	-0.834109000	3.466788000	-1.858161000
C	-1.069933000	3.707783000	0.637792000
C	-1.100269000	2.679006000	2.930874000
C	-1.172511000	-3.824053000	0.624696000
C	-1.183640000	-3.532275000	-1.811104000
C	-1.164887000	1.355193000	-3.756559000
C	-1.339128000	-0.066446000	-4.032636000
C	-1.521944000	-3.167466000	1.859644000
C	-1.568642000	-2.683846000	-2.920661000
C	-1.914773000	-3.572720000	-0.566151000
C	-2.096534000	2.838941000	-1.973306000
C	-2.266100000	1.805440000	-2.953176000
C	-2.425735000	3.254257000	0.472333000
C	-2.608745000	2.458704000	2.957811000
C	-2.572755000	-1.209197000	2.850022000
C	-2.555447000	-0.472657000	-3.337428000
C	-2.647606000	-2.317439000	1.935529000
C	-2.676637000	-1.769877000	-2.731569000
C	-2.758885000	1.028904000	3.447082000
C	-2.893534000	2.774633000	-0.794573000
C	-3.088454000	-2.770937000	-0.465135000
C	-3.220978000	2.608078000	1.503049000
C	-3.127693000	0.686299000	-2.699278000
C	-3.421290000	-0.028197000	2.725129000
C	-3.454728000	-1.870084000	-1.532300000
C	-3.479152000	-2.174859000	0.785316000
C	-3.798382000	1.677945000	-0.561306000
C	-3.870681000	0.586198000	-1.475957000
C	-3.949439000	1.510842000	0.862460000
C	-4.066301000	0.192992000	1.430487000
C	-4.068728000	-0.711132000	-0.924155000
C	-4.106562000	-0.903371000	0.503888000
C	4.145740000	0.595829000	0.706614000
C	3.969487000	-0.724558000	1.274435000
C	3.355799000	-0.813704000	2.586089000

C	3.754539000	-1.800038000	0.355597000
C	4.025064000	0.809153000	-0.718048000
C	3.056575000	-0.013638000	-2.818400000
C	3.801292000	-0.276821000	-1.624350000
C	3.709169000	-1.589767000	-1.071628000
C	2.870079000	-2.898023000	0.667497000
C	2.077543000	-2.872001000	1.857664000
C	2.288456000	-1.786819000	2.779573000
C	0.785298000	-3.440634000	1.819710000
C	2.313266000	-3.384495000	-0.564947000
C	0.240029000	-3.694614000	-1.836310000
C	0.987191000	-3.904406000	-0.619450000
C	0.252654000	-3.994080000	0.599176000
C	2.208062000	-1.011771000	-3.422281000
C	2.051631000	-2.301434000	-2.817469000
C	2.832494000	-2.577996000	-1.646376000
C	0.763179000	-2.942371000	-2.958347000
C	1.193319000	-1.185208000	3.522350000
C	0.894494000	1.416781000	3.616065000
C	1.626366000	0.182703000	3.827209000
C	1.710490000	2.325131000	2.825618000
C	3.010366000	1.701908000	2.660551000
C	2.958300000	0.387039000	3.298673000
C	3.609363000	1.774898000	1.368942000
C	1.084232000	3.187624000	1.825551000
C	1.098044000	3.712806000	-0.598772000
C	1.821255000	3.364850000	0.567025000
C	3.052911000	2.640957000	0.360314000
C	1.469620000	3.203757000	-1.911554000
C	2.564824000	2.318434000	-2.069863000
C	3.382920000	2.080393000	-0.925150000
C	2.456599000	1.273186000	-3.046971000
C	1.251872000	1.083232000	-3.801097000
C	1.087760000	-0.342837000	-4.070796000
Sc	1.640563000	0.329007000	1.487359000
Sc	-1.603801000	0.772874000	1.515972000
La	-0.175864000	-0.742822000	-1.622531000
N	-0.056694000	0.108362000	0.486859000
H	-3.373587000	4.524860000	2.842190000
C	-3.625181000	3.495426000	3.058070000
Br	-3.607638000	4.363811000	5.552634000
H	-4.643973000	3.209788000	3.284038000

Cycloadduct (11–16)-$LaSc_2N@C_{80}CH_2$

C	-0.106468310	-1.756740480	3.391212820
C	-1.292051920	-0.929388290	3.559942270
C	-1.397648800	0.472746620	3.916432300
C	-0.428171300	1.523338490	3.693831730
C	0.253744630	3.046948730	-2.629222730
C	0.108319980	1.964487550	-3.562061760
C	-0.230419230	-0.939505320	-4.189972920
C	-0.264250990	-2.916294210	2.580983300
C	-0.332649980	3.843571560	-0.498489110
C	-0.372143510	-2.299326860	-3.660338700
C	-0.340943350	3.344280250	1.947818590
C	-0.845257860	3.452714870	-1.796170850
C	-1.080908410	3.680339590	0.709558520
C	-1.061347050	2.642296120	3.029608430
C	-1.149523270	-3.843355780	0.623907160
C	-1.182213260	-3.531156690	-1.807999460
C	-1.183849800	1.371234130	-3.724545260
C	-1.356873420	-0.049370870	-4.005459470
C	-1.487603710	-3.197127340	1.867491710
C	-1.576923480	-2.673755040	-2.908936840
C	-1.901595980	-3.580578560	-0.556845790
C	-2.104280230	2.827749940	-1.923018290
C	-2.280821420	1.810526700	-2.913777730
C	-2.452523280	3.268986770	0.515891850
C	-2.506840170	2.400291660	3.152575880
C	-2.527493120	-1.246021640	2.884153810
C	-2.567513990	-0.463916830	-3.307118230
C	-2.610184020	-2.345382000	1.962619350
C	-2.680676190	-1.763228440	-2.704984260
C	-2.685984010	0.984330950	3.534221530
C	-2.896523330	2.760118430	-0.747156130
C	-3.070465650	-2.775068670	-0.437163170
C	-3.354689970	2.694546650	1.517757420
C	-3.137320120	0.688979580	-2.659730020
C	-3.372009180	-0.050775160	2.775581010
C	-3.446534460	-1.869516460	-1.494794530
C	-3.444746470	-2.183188490	0.819298580
C	-3.800996810	1.665726540	-0.514511630
C	-3.860492750	0.579987930	-1.428523980
C	-3.989780160	1.515208640	0.909243270
C	-4.032040790	0.189076690	1.491817920
C	-4.047846410	-0.716107800	-0.873410270
C	-4.068092530	-0.908790830	0.554970160
C	4.164034820	0.582139640	0.701475420
C	3.994954180	-0.744969710	1.256542280
C	3.394801560	-0.848029750	2.569181290

C	3.768798100	-1.810912240	0.330309320
C	4.025730980	0.809525070	-0.717144530
C	3.042520980	0.007431760	-2.816213170
C	3.795482890	-0.265552090	-1.630263140
C	3.710688170	-1.586411300	-1.091078360
C	2.891796450	-2.916221510	0.639701760
C	2.110108440	-2.903342240	1.835239830
C	2.328729880	-1.824254650	2.763727550
C	0.819633300	-3.474385170	1.804753780
C	2.325057110	-3.390309320	-0.591770350
C	0.240261440	-3.688683600	-1.845683650
C	0.999406060	-3.911040850	-0.639327630
C	0.274986980	-4.012346880	0.583525750
C	2.191682450	-0.986953880	-3.420272810
C	2.041169020	-2.282409440	-2.826875550
C	2.833147730	-2.571120760	-1.668123980
C	0.753972440	-2.923798250	-2.963395370
C	1.242783240	-1.228475520	3.518616910
C	0.958202790	1.367591680	3.654712440
C	1.688613000	0.129756830	3.842950370
C	1.750522850	2.289605460	2.863574490
C	3.047185840	1.665010390	2.671320820
C	3.008441880	0.341648090	3.297547500
C	3.628797470	1.750555060	1.379559980
C	1.100229280	3.161526580	1.879900070
C	1.085864950	3.691210480	-0.541336530
C	1.823145570	3.341959410	0.615182270
C	3.055332480	2.627612390	0.385688860
C	1.451105120	3.202544200	-1.860604830
C	2.550781330	2.327484730	-2.041029500
C	3.376580330	2.082681000	-0.905035190
C	2.439362860	1.294157370	-3.028581370
C	1.230169050	1.107513290	-3.776819340
C	1.067133940	-0.316317540	-4.053366880
Sc	1.655737530	0.302769750	1.498184920
Sc	-1.596556450	0.852352480	1.555091140
La	-0.198088830	-0.743327350	-1.592704510
N	-0.063218590	0.141005100	0.517009690
H	-4.568056550	3.065930150	3.305680310
C	-3.617252120	3.327576820	2.839439020
H	-3.384960120	4.392487090	2.891258730