

NC Unit Trapped by Fullerenes: A Density Functional Theory Study on $\text{Sc}_3\text{NC}@C_{2n}$ ($2n = 68, 78$ and 80)

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Ref.41. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 03, Gaussian, Inc., Wallingford CT, 2004.

Optimized Cartesian Coordinates and Relative Energies

Sc₃NC@C₆₈ (C₂) 0.0 kcal/mol

C	0.00000000	0.00000000	-0.09070000
Sc	-1.94110000	-0.00150000	0.96230000
Sc	1.94110000	0.00150000	0.96230000
Sc	0.00000000	0.00000000	-2.13690000
C	0.00060000	3.42840000	-0.00590000
C	-0.00060000	-3.42840000	-0.00590000
C	-1.00570000	3.22140000	-1.00320000
C	1.00570000	-3.22140000	-1.00320000
C	-0.64850000	2.75100000	-2.31450000
C	0.64850000	-2.75100000	-2.31450000
C	0.72440000	2.45990000	-2.66940000
C	-0.72440000	-2.45990000	-2.66940000
C	1.72480000	2.69720000	-1.67030000
C	-1.72480000	-2.69720000	-1.67030000
C	1.36840000	3.21680000	-0.37670000
C	-1.36840000	-3.21680000	-0.37670000
C	2.33210000	2.74870000	0.58440000
C	-2.33210000	-2.74870000	0.58440000
C	1.94610000	2.46080000	1.94750000
C	-1.94610000	-2.46080000	1.94750000
C	0.57700000	2.69520000	2.31360000

C	-0.57700000	-2.69520000	2.31360000
C	-0.36590000	3.21800000	1.35660000
C	0.36590000	-3.21800000	1.35660000
C	-1.68720000	2.75180000	1.70250000
C	1.68720000	-2.75180000	1.70250000
C	-2.68720000	2.46090000	0.69360000
C	2.68720000	-2.46090000	0.69360000
C	-2.31010000	2.70460000	-0.67220000
C	2.31010000	-2.70460000	-0.67220000
C	-2.74190000	1.83810000	-1.74730000
C	2.74190000	-1.83810000	-1.74730000
C	-1.74810000	1.93490000	-2.79160000
C	1.74810000	-1.93490000	-2.79160000
C	2.87430000	1.82920000	-1.50830000
C	-2.87430000	-1.82920000	-1.50830000
C	3.30220000	1.93220000	-0.12970000
C	-3.30220000	-1.93220000	-0.12970000
C	-0.14220000	1.83280000	3.23210000
C	0.14220000	-1.83280000	3.23210000
C	-1.54500000	1.94050000	2.89320000
C	1.54500000	-1.94050000	2.89320000
C	-2.45030000	0.86710000	3.10090000
C	2.45030000	-0.86710000	3.10090000
C	-3.61800000	0.71060000	2.22840000
C	3.61800000	-0.71060000	2.22840000
C	-3.68570000	1.43080000	0.95080000
C	3.68570000	-1.43080000	0.95080000
C	-3.97290000	0.43890000	-0.11930000
C	3.97290000	-0.43890000	-0.11930000
C	-3.41400000	0.59340000	-1.47050000
C	3.41400000	-0.59340000	-1.47050000
C	-2.96920000	-0.58980000	-2.22170000
C	2.96920000	0.58980000	-2.22170000
C	-2.02940000	-0.43450000	-3.34110000
C	2.02940000	0.43450000	-3.34110000
C	-1.49840000	0.87130000	-3.69990000
C	1.49840000	-0.87130000	-3.69990000
C	-0.15380000	0.70970000	-4.25060000
C	0.15380000	-0.70970000	-4.25060000
C	0.98050000	1.42270000	-3.64600000
C	-0.98050000	-1.42270000	-3.64600000
C	4.00240000	0.87650000	0.52710000
C	-4.00240000	-0.87650000	0.52710000

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C	3.77680000	0.71020000	1.96800000
C	-3.77680000	-0.71020000	1.96800000
C	2.66480000	1.41230000	2.64020000
C	-2.66480000	-1.41230000	2.64020000
C	1.87180000	0.43160000	3.39260000
C	-1.87180000	-0.43160000	3.39260000
C	0.43490000	0.59250000	3.67300000
C	-0.43490000	-0.59250000	3.67300000
N	0.00000000	0.00000000	1.17020000

Sc₃NC@C₆₈ (C₂) 14.6 kcal/mol

N	0.00000000	0.00000000	-0.11180000
Sc	-1.97220000	0.02170000	0.93330000
Sc	1.97220000	-0.02170000	0.93330000
Sc	0.00000000	0.00000000	-2.12350000
C	-0.00020000	3.42940000	-0.00380000
C	0.00020000	-3.42940000	-0.00380000
C	-1.00760000	3.22510000	-1.00080000
C	1.00760000	-3.22510000	-1.00080000
C	-0.65040000	2.75620000	-2.31100000
C	0.65040000	-2.75620000	-2.31100000
C	0.72290000	2.46180000	-2.66310000
C	-0.72290000	-2.46180000	-2.66310000
C	1.72440000	2.69940000	-1.66740000
C	-1.72440000	-2.69940000	-1.66740000
C	1.36910000	3.21870000	-0.37390000
C	-1.36910000	-3.21870000	-0.37390000
C	2.33190000	2.74770000	0.58470000
C	-2.33190000	-2.74770000	0.58470000
C	1.94230000	2.45530000	1.94410000
C	-1.94230000	-2.45530000	1.94410000
C	0.57410000	2.69160000	2.31200000
C	-0.57410000	-2.69160000	2.31200000
C	-0.36870000	3.21670000	1.35620000
C	0.36870000	-3.21670000	1.35620000
C	-1.69100000	2.74790000	1.70020000
C	1.69100000	-2.74790000	1.70020000
C	-2.69640000	2.46220000	0.69520000
C	2.69640000	-2.46220000	0.69520000
C	-2.31270000	2.70630000	-0.67050000
C	2.31270000	-2.70630000	-0.67050000
C	-2.74390000	1.84120000	-1.74410000

C	2.74390000	-1.84120000	-1.74410000
C	-1.74920000	1.93700000	-2.78570000
C	1.74920000	-1.93700000	-2.78570000
C	2.87280000	1.82900000	-1.50550000
C	-2.87280000	-1.82900000	-1.50550000
C	3.30470000	1.93150000	-0.12840000
C	-3.30470000	-1.93150000	-0.12840000
C	-0.14360000	1.83160000	3.23280000
C	0.14360000	-1.83160000	3.23280000
C	-1.54620000	1.93600000	2.88970000
C	1.54620000	-1.93600000	2.88970000
C	-2.45440000	0.86680000	3.09650000
C	2.45440000	-0.86680000	3.09650000
C	-3.62590000	0.71180000	2.22580000
C	3.62590000	-0.71180000	2.22580000
C	-3.70390000	1.43630000	0.95010000
C	3.70390000	-1.43630000	0.95010000
C	-3.99690000	0.44230000	-0.12500000
C	3.99690000	-0.44230000	-0.12500000
C	-3.42080000	0.59460000	-1.46600000
C	3.42080000	-0.59460000	-1.46600000
C	-2.96880000	-0.58930000	-2.21620000
C	2.96880000	0.58930000	-2.21620000
C	-2.02650000	-0.43390000	-3.33070000
C	2.02650000	0.43390000	-3.33070000
C	-1.49650000	0.87170000	-3.69060000
C	1.49650000	-0.87170000	-3.69060000
C	-0.15390000	0.70940000	-4.23720000
C	0.15390000	-0.70940000	-4.23720000
C	0.97920000	1.42290000	-3.63620000
C	-0.97920000	-1.42290000	-3.63620000
C	4.01190000	0.87690000	0.52410000
C	-4.01190000	-0.87690000	0.52410000
C	3.77940000	0.70820000	1.96360000
C	-3.77940000	-0.70820000	1.96360000
C	2.66150000	1.40620000	2.63190000
C	-2.66150000	-1.40620000	2.63190000
C	1.87090000	0.42990000	3.38700000
C	-1.87090000	-0.42990000	3.38700000
C	0.43650000	0.59190000	3.67040000
C	-0.43650000	-0.59190000	3.67040000
C	0.00000000	0.00000000	1.15250000

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Two Low-energy $\text{Sc}_3\text{NC}@C_{68}$ isomers based on C_{2v} : 6073 cage and relative energies (compared to the lowest-energy $\text{Sc}_3\text{NC}@C_{68}$ (D_3 : 6140 cage)) **$\text{Sc}_3\text{NC}@C_{68}$ (C_{2v}) 68.9 kcal/mol**

C	4.22480000	0.72420000	-1.03380000
C	4.22480000	-0.72420000	-1.03380000
C	4.08510000	1.16430000	0.34620000
C	4.08510000	-1.16430000	0.34620000
C	4.02130000	0.00000000	1.21370000
C	3.31100000	1.18230000	-2.07650000
C	3.31100000	-1.18230000	-2.07650000
C	3.19810000	0.00000000	2.40790000
C	3.19720000	2.22730000	0.64430000
C	3.19720000	-2.22730000	0.64430000
C	2.78730000	0.00000000	-2.77610000
C	2.42890000	1.16030000	2.77790000
C	2.42890000	-1.16030000	2.77790000
C	2.44020000	2.26570000	1.87740000
C	2.44020000	-2.26570000	1.87740000
C	2.39670000	2.80140000	-0.42030000
C	2.39670000	-2.80140000	-0.42030000
C	2.39220000	2.26590000	-1.77490000
C	2.39220000	-2.26590000	-1.77490000
C	1.47490000	0.00000000	-3.43410000
C	1.25180000	0.77520000	3.56490000
C	1.25180000	-0.77520000	3.56490000
C	1.19820000	2.92470000	1.60310000
C	1.19820000	-2.92470000	1.60310000
C	1.19580000	3.29080000	0.18980000
C	1.19580000	-3.29080000	0.18980000
C	1.16500000	2.31490000	-2.51850000
C	1.16500000	-2.31490000	-2.51850000
C	0.72920000	1.23210000	-3.39430000
C	0.72920000	-1.23210000	-3.39430000
C	0.00000000	1.53740000	3.42330000
C	0.00000000	2.60590000	2.32890000
C	0.00000000	-1.53740000	3.42330000
C	0.00000000	3.37220000	-0.56380000
C	0.00000000	-2.60590000	2.32890000
C	0.00000000	2.92220000	-1.93790000
C	0.00000000	-3.37220000	-0.56380000
C	0.00000000	-2.92220000	-1.93790000
C	-0.72920000	1.23210000	-3.39430000

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C	-0.72920000	-1.23210000	-3.39430000
C	-1.16500000	2.31490000	-2.51850000
C	-1.16500000	-2.31490000	-2.51850000
C	-1.19580000	3.29080000	0.18980000
C	-1.19580000	-3.29080000	0.18980000
C	-1.19820000	2.92470000	1.60310000
C	-1.19820000	-2.92470000	1.60310000
C	-1.25180000	0.77520000	3.56490000
C	-1.25180000	-0.77520000	3.56490000
C	-1.47490000	0.00000000	-3.43410000
C	-2.39220000	2.26590000	-1.77490000
C	-2.39220000	-2.26590000	-1.77490000
C	-2.39670000	2.80140000	-0.42030000
C	-2.39670000	-2.80140000	-0.42030000
C	-2.44020000	2.26570000	1.87740000
C	-2.44020000	-2.26570000	1.87740000
C	-2.42890000	1.16030000	2.77790000
C	-2.42890000	-1.16030000	2.77790000
C	-2.78730000	0.00000000	-2.77610000
C	-3.19720000	2.22730000	0.64430000
C	-3.19720000	-2.22730000	0.64430000
C	-3.19810000	0.00000000	2.40790000
C	-3.31100000	1.18230000	-2.07650000
C	-3.31100000	-1.18230000	-2.07650000
C	-4.02130000	0.00000000	1.21370000
C	-4.08510000	1.16430000	0.34620000
C	-4.08510000	-1.16430000	0.34620000
C	-4.22480000	0.72420000	-1.03380000
C	-4.22480000	-0.72420000	-1.03380000
Sc	-2.12330000	0.00000000	-0.50950000
Sc	2.12330000	0.00000000	-0.50950000
Sc	0.00000000	0.00000000	1.87360000
N	0.00000000	0.00000000	-1.27260000
C	0.00000000	0.00000000	-0.04670000

Sc₃NC@C₆₈ (C_{2v}) 76.5 kcal/mol

C	4.21830000	0.72290000	-1.03080000
C	4.21830000	-0.72290000	-1.03080000
C	4.08970000	1.16550000	0.34870000
C	4.08970000	-1.16550000	0.34870000
C	4.03070000	0.00000000	1.21690000
C	3.30200000	1.17870000	-2.07180000

C	3.30200000	-1.17870000	-2.07180000
C	3.19880000	0.00000000	2.40500000
C	3.19800000	2.22650000	0.64340000
C	3.19800000	-2.22650000	0.64340000
C	2.77840000	0.00000000	-2.77230000
C	2.42810000	1.16030000	2.77390000
C	2.42810000	-1.16030000	2.77390000
C	2.44090000	2.26740000	1.87670000
C	2.44090000	-2.26740000	1.87670000
C	2.39590000	2.79910000	-0.42150000
C	2.39590000	-2.79910000	-0.42150000
C	2.38810000	2.26420000	-1.77600000
C	2.38810000	-2.26420000	-1.77600000
C	1.47190000	0.00000000	-3.44200000
C	1.24970000	0.77520000	3.55990000
C	1.24970000	-0.77520000	3.55990000
C	1.19800000	2.92540000	1.60220000
C	1.19800000	-2.92540000	1.60220000
C	1.19480000	3.28710000	0.18810000
C	1.19480000	-3.28710000	0.18810000
C	1.16410000	2.31450000	-2.52500000
C	1.16410000	-2.31450000	-2.52500000
C	0.72880000	1.23460000	-3.40750000
C	0.72880000	-1.23460000	-3.40750000
C	0.00000000	1.53930000	3.42190000
C	0.00000000	2.60810000	2.32850000
C	0.00000000	-1.53930000	3.42190000
C	0.00000000	3.36820000	-0.56700000
C	0.00000000	-2.60810000	2.32850000
C	0.00000000	2.92190000	-1.94330000
C	0.00000000	-3.36820000	-0.56700000
C	0.00000000	-2.92190000	-1.94330000
C	-0.72880000	1.23460000	-3.40750000
C	-0.72880000	-1.23460000	-3.40750000
C	-1.16410000	2.31450000	-2.52500000
C	-1.16410000	-2.31450000	-2.52500000
C	-1.19480000	3.28710000	0.18810000
C	-1.19480000	-3.28710000	0.18810000
C	-1.19800000	2.92540000	1.60220000
C	-1.19800000	-2.92540000	1.60220000
C	-1.24970000	0.77520000	3.55990000
C	-1.24970000	-0.77520000	3.55990000
C	-1.47190000	0.00000000	-3.44200000

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C	-2.38810000	2.26420000	-1.77600000
C	-2.38810000	-2.26420000	-1.77600000
C	-2.39590000	2.79910000	-0.42150000
C	-2.39590000	-2.79910000	-0.42150000
C	-2.44090000	2.26740000	1.87670000
C	-2.44090000	-2.26740000	1.87670000
C	-2.42810000	1.16030000	2.77390000
C	-2.42810000	-1.16030000	2.77390000
C	-2.77840000	0.00000000	-2.77230000
C	-3.19800000	2.22650000	0.64340000
C	-3.19800000	-2.22650000	0.64340000
C	-3.19880000	0.00000000	2.40500000
C	-3.30200000	1.17870000	-2.07180000
C	-3.30200000	-1.17870000	-2.07180000
C	-4.03070000	0.00000000	1.21690000
C	-4.08970000	1.16550000	0.34870000
C	-4.08970000	-1.16550000	0.34870000
C	-4.21830000	0.72290000	-1.03080000
C	-4.21830000	-0.72290000	-1.03080000
Sc	-2.11490000	0.00000000	-0.48190000
Sc	2.11490000	0.00000000	-0.48190000
Sc	0.00000000	0.00000000	1.87470000
C	0.00000000	0.00000000	-1.24470000
N	0.00000000	0.00000000	-0.00280000

Sc₃NC@C₇₈ (C₂) 0.0 kcal/mol

C	-4.33360000	-0.15870000	0.01000000
C	-4.28990000	0.55840000	-1.25120000
C	-3.99170000	-1.56150000	-0.02780000
C	-4.01230000	0.55860000	1.21830000
C	-3.92950000	-0.13450000	-2.48860000
C	-3.60260000	1.84320000	-1.27580000
C	-3.46990000	-2.18250000	-1.24810000
C	-3.39410000	-1.48340000	-2.48660000
C	-3.51250000	1.91310000	1.17940000
C	-3.33000000	-2.19490000	1.09080000
C	-3.40930000	-0.09760000	2.34950000
C	-3.22290000	2.53850000	-0.07740000
C	-2.98090000	0.69000000	-3.18900000
C	-3.03260000	-1.46780000	2.28830000

C	-2.76040000	1.89470000	-2.46130000
C	-2.41720000	-3.08330000	-0.87500000
C	-2.63190000	2.09730000	2.29560000
C	-2.56300000	0.85540000	3.04440000
C	-2.39640000	-3.15720000	0.56560000
C	-2.09840000	-1.45910000	-3.18000000
C	-1.85600000	-0.08820000	-3.62690000
C	-2.09260000	3.38490000	-0.17960000
C	-1.86130000	-1.84520000	3.04010000
C	-1.47210000	2.51960000	-2.46950000
C	-1.49220000	2.94400000	2.19870000
C	-1.20260000	-3.19410000	-1.64840000
C	-1.43100000	0.48030000	3.85770000
C	-1.20750000	-3.49030000	1.26370000
C	-1.24090000	3.38140000	-1.36120000
C	-0.98420000	-2.30120000	-2.79470000
C	-1.25600000	3.63190000	0.96590000
C	-1.10160000	-0.94080000	3.88850000
C	-0.97260000	-2.84600000	2.52370000
C	-0.54700000	0.48140000	-3.68940000
C	-0.34790000	1.86820000	-3.16640000
C	-0.35020000	2.57300000	2.99820000
C	-0.30530000	1.40940000	3.87360000
C	-0.08120000	-3.69400000	-0.94190000
C	-0.07840000	-3.86040000	0.49390000
C	0.07840000	3.86040000	0.49390000
C	0.08120000	3.69400000	-0.94190000
C	0.30530000	-1.40940000	3.87360000
C	0.35020000	-2.57300000	2.99820000
C	0.34790000	-1.86820000	-3.16640000
C	0.54700000	-0.48140000	-3.68940000
C	0.97260000	2.84600000	2.52370000
C	1.10160000	0.94080000	3.88850000
C	1.25600000	-3.63190000	0.96590000
C	0.98420000	2.30120000	-2.79470000
C	1.24090000	-3.38140000	-1.36120000
C	1.20750000	3.49030000	1.26370000
C	1.43100000	-0.48030000	3.85770000
C	1.20260000	3.19410000	-1.64840000
C	1.49220000	-2.94400000	2.19870000
C	1.47210000	-2.51960000	-2.46950000
C	1.86130000	1.84520000	3.04010000
C	2.09260000	-3.38490000	-0.17960000

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C	1.85600000	0.08820000	-3.62690000
C	2.09840000	1.45910000	-3.18000000
C	2.39640000	3.15720000	0.56560000
C	2.56300000	-0.85540000	3.04440000
C	2.63190000	-2.09730000	2.29560000
C	2.41720000	3.08330000	-0.87500000
C	2.76040000	-1.89470000	-2.46130000
C	3.03260000	1.46780000	2.28830000
C	2.98090000	-0.69000000	-3.18900000
C	3.22290000	-2.53850000	-0.07740000
C	3.40930000	0.09760000	2.34950000
C	3.33000000	2.19490000	1.09080000
C	3.51250000	-1.91310000	1.17940000
C	3.39410000	1.48340000	-2.48660000
C	3.46990000	2.18250000	-1.24810000
C	3.60260000	-1.84320000	-1.27580000
C	3.92950000	0.13450000	-2.48860000
C	4.01230000	-0.55860000	1.21830000
C	3.99170000	1.56150000	-0.02780000
C	4.28990000	-0.55840000	-1.25120000
C	4.33360000	0.15870000	0.01000000
C	0.00000000	0.00000000	0.03960000
Sc	0.00000000	0.00000000	2.10370000
Sc	-2.07500000	-0.20150000	-1.17680000
Sc	2.07500000	0.20150000	-1.17680000
N	0.00000000	0.00000000	-1.20390000

Sc₃NC@C₇₈ (C₂) 13.4 kcal/mol

C	-4.35000000	-0.16000000	0.00890000
C	-4.30120000	0.55810000	-1.25270000
C	-4.00790000	-1.56570000	-0.03130000
C	-4.01500000	0.55810000	1.21530000
C	-3.93850000	-0.13750000	-2.49200000
C	-3.60670000	1.84070000	-1.27610000
C	-3.48840000	-2.19150000	-1.25450000
C	-3.40870000	-1.49060000	-2.49530000
C	-3.51150000	1.91190000	1.17570000
C	-3.33420000	-2.19240000	1.08670000
C	-3.41140000	-0.09670000	2.34690000
C	-3.22330000	2.53770000	-0.08030000
C	-2.98200000	0.68520000	-3.18340000
C	-3.03360000	-1.46610000	2.28420000

C	-2.76020000	1.88940000	-2.45720000
C	-2.42340000	-3.08070000	-0.87840000
C	-2.62910000	2.09640000	2.29100000
C	-2.56180000	0.85600000	3.04000000
C	-2.39850000	-3.15240000	0.56250000
C	-2.10600000	-1.46110000	-3.18000000
C	-1.85770000	-0.09070000	-3.62090000
C	-2.09120000	3.38330000	-0.18240000
C	-1.86170000	-1.84460000	3.03490000
C	-1.47170000	2.51380000	-2.46590000
C	-1.49050000	2.94560000	2.19620000
C	-1.20570000	-3.19220000	-1.64820000
C	-1.42870000	0.48090000	3.85180000
C	-1.21050000	-3.48980000	1.26080000
C	-1.23950000	3.38040000	-1.36210000
C	-0.98560000	-2.29500000	-2.79070000
C	-1.25390000	3.63160000	0.96330000
C	-1.10030000	-0.93990000	3.88250000
C	-0.97500000	-2.84800000	2.52160000
C	-0.54890000	0.47860000	-3.68240000
C	-0.34750000	1.86320000	-3.16180000
C	-0.34810000	2.57450000	2.99460000
C	-0.30400000	1.40950000	3.86890000
C	-0.08410000	-3.69400000	-0.94390000
C	-0.08090000	-3.85970000	0.49160000
C	0.08090000	3.85970000	0.49160000
C	0.08410000	3.69400000	-0.94390000
C	0.30400000	-1.40950000	3.86890000
C	0.34810000	-2.57450000	2.99460000
C	0.34750000	-1.86320000	-3.16180000
C	0.54890000	-0.47860000	-3.68240000
C	0.97500000	2.84800000	2.52160000
C	1.10030000	0.93990000	3.88250000
C	1.25390000	-3.63160000	0.96330000
C	0.98560000	2.29500000	-2.79070000
C	1.23950000	-3.38040000	-1.36210000
C	1.21050000	3.48980000	1.26080000
C	1.42870000	-0.48090000	3.85180000
C	1.20570000	3.19220000	-1.64820000
C	1.49050000	-2.94560000	2.19620000
C	1.47170000	-2.51380000	-2.46590000
C	1.86170000	1.84460000	3.03490000
C	2.09120000	-3.38330000	-0.18240000

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C	1.85770000	0.09070000	-3.62090000
C	2.10600000	1.46110000	-3.18000000
C	2.39850000	3.15240000	0.56250000
C	2.56180000	-0.85600000	3.04000000
C	2.62910000	-2.09640000	2.29100000
C	2.42340000	3.08070000	-0.87840000
C	2.76020000	-1.88940000	-2.45720000
C	3.03360000	1.46610000	2.28420000
C	2.98200000	-0.68520000	-3.18340000
C	3.22330000	-2.53770000	-0.08030000
C	3.41140000	0.09670000	2.34690000
C	3.33420000	2.19240000	1.08670000
C	3.51150000	-1.91190000	1.17570000
C	3.40870000	1.49060000	-2.49530000
C	3.48840000	2.19150000	-1.25450000
C	3.60670000	-1.84070000	-1.27610000
C	3.93850000	0.13750000	-2.49200000
C	4.01500000	-0.55810000	1.21530000
C	4.00790000	1.56570000	-0.03130000
C	4.30120000	-0.55810000	-1.25270000
C	4.35000000	0.16000000	0.00890000
N	0.00000000	0.00000000	0.09240000
Sc	0.00000000	0.00000000	2.09850000
Sc	-2.11740000	-0.24690000	-1.15620000
Sc	2.11740000	0.24690000	-1.15620000
C	0.00000000	0.00000000	-1.15420000

Three Low-energy Sc₃NC@C₇₈ isomers based on *D*_{3h} : 24109 cage and relative energies (compared to the lowest-energy Sc₃NC@C₇₈(C₂: 22010 cage))

Sc₃NC@C₇₈ (C₁) 6.0 kcal/mol

C	0.06380000	0.19600000	-0.00240000
Sc	-0.72270000	-0.13840000	-1.99400000
Sc	2.11960000	0.35250000	0.20730000
Sc	-0.74220000	-0.14120000	1.98680000
C	-2.80390000	-1.62570000	-2.41650000
C	-1.80410000	-2.66550000	-2.35740000
C	-1.79250000	-3.47410000	-1.17460000
C	-0.58580000	-4.10350000	-0.72170000
C	0.61500000	-3.91130000	-1.42870000

C	-2.62690000	-0.42140000	-3.21100000
C	-1.44130000	-0.23340000	-4.03590000
C	-0.39420000	-1.26760000	-3.93550000
C	-0.55340000	-2.47450000	-3.11600000
C	0.63820000	-3.08940000	-2.60570000
C	-2.77720000	2.73610000	-1.17350000
C	-2.53940000	1.96720000	-2.35630000
C	-3.16540000	0.66660000	-2.41300000
C	0.61470000	-3.90990000	1.42480000
C	1.84790000	-3.71070000	0.69970000
C	-0.58480000	-4.10220000	0.71810000
C	1.84510000	-3.71250000	-0.70550000
C	2.65430000	-2.76890000	-1.42520000
C	3.48160000	-1.82940000	-0.73690000
C	3.76210000	-0.57870000	-1.41320000
C	0.89790000	-0.58490000	-3.86880000
C	2.06020000	-1.14420000	-3.20600000
C	1.93020000	-2.41860000	-2.63540000
C	3.01020000	-0.24050000	-2.61360000
C	-0.39850000	-1.26840000	3.92850000
C	-0.55570000	-2.47780000	3.11410000
C	0.63650000	-3.09590000	2.60550000
C	1.92840000	-2.42410000	2.63150000
C	3.00530000	-0.24280000	2.58290000
C	2.05130000	-1.14840000	3.18970000
C	0.89240000	-0.58490000	3.85080000
C	3.50100000	-1.83400000	0.73500000
C	2.65840000	-2.76860000	1.41760000
C	3.82320000	-0.58490000	1.42330000
C	-1.80680000	-2.66660000	2.35470000
C	-1.79420000	-3.47310000	1.17250000
C	-1.44520000	-0.23390000	4.03270000
C	-2.63580000	-0.42310000	3.21210000
C	-2.80770000	-1.62640000	2.41490000
C	-0.76990000	1.07230000	3.91680000
C	-1.29450000	2.17660000	3.11110000
C	-0.35240000	3.13740000	2.60740000
C	2.78280000	1.16570000	2.58410000
C	1.59560000	1.72870000	3.19190000
C	0.66840000	0.82910000	3.84830000
C	1.08370000	2.90540000	2.63660000
C	-3.60310000	-1.29780000	1.23750000
C	-3.44110000	-2.01270000	-0.00200000

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C	-2.57330000	-3.12550000	-0.00120000
C	-3.60340000	-1.29760000	-1.24220000
C	-3.82710000	0.10860000	1.23850000
C	-3.40970000	2.16330000	-0.00080000
C	-3.89200000	0.83580000	-0.00180000
C	-3.82800000	0.10870000	-1.24370000
C	-2.54160000	1.96730000	2.35380000
C	-3.16760000	0.66590000	2.41110000
C	-2.77890000	2.73470000	1.17180000
C	0.60580000	4.09820000	0.69920000
C	-0.62740000	3.90050000	1.42450000
C	-1.82570000	3.70890000	0.71820000
C	0.60290000	4.09970000	-0.70530000
C	3.45700000	1.74360000	1.42640000
C	2.76020000	2.82970000	0.73590000
C	1.66870000	3.45500000	1.41810000
C	3.40210000	1.72090000	-1.41660000
C	4.11830000	0.65370000	-0.72210000
C	4.18840000	0.66420000	0.73820000
C	1.66510000	3.45460000	-1.42550000
C	2.74330000	2.81910000	-0.73820000
C	0.67340000	0.83010000	-3.86590000
C	1.08680000	2.89820000	-2.63770000
C	1.60630000	1.72670000	-3.20870000
C	2.79060000	1.16560000	-2.61630000
C	-1.82710000	3.71020000	-0.72190000
C	-0.62780000	3.90240000	-1.42880000
C	-0.34950000	3.13130000	-2.60670000
C	-1.29150000	2.17380000	-3.11210000
C	-0.76530000	1.07250000	-3.92300000
N	-1.16250000	-0.14400000	-0.00430000

Sc₃NC@C₇₈ (C_s) 6.7 kcal/mol

N	0.63910000	-0.30980000	0.00000000
Sc	-0.02920000	-0.91850000	-1.86640000
Sc	-0.09850000	2.07970000	0.00000000
Sc	-0.02920000	-0.91850000	1.86640000
C	1.21250000	-3.01350000	-2.42840000
C	2.40310000	-2.18320000	-2.36260000
C	3.20260000	-2.28970000	-1.18020000
C	3.99500000	-1.18510000	-0.72110000
C	3.97630000	0.02920000	-1.42470000
C	0.03690000	-2.69120000	-3.23780000

C	0.01930000	-1.45960000	-4.00370000
C	1.18410000	-0.58230000	-3.87110000
C	2.38550000	-0.91480000	-3.10440000
C	3.17370000	0.17240000	-2.60850000
C	-3.13100000	-2.34340000	-1.17950000
C	-2.33850000	-2.22610000	-2.36690000
C	-1.12980000	-3.03330000	-2.43040000
C	3.97630000	0.02920000	1.42470000
C	3.96190000	1.27690000	0.70290000
C	3.99500000	-1.18510000	0.72110000
C	3.96190000	1.27690000	-0.70290000
C	3.14450000	2.21130000	-1.42410000
C	2.32690000	3.15770000	-0.73560000
C	1.12710000	3.62360000	-1.40850000
C	0.70420000	0.78620000	-3.81710000
C	1.44290000	1.84720000	-3.18480000
C	2.69750000	1.54590000	-2.63790000
C	0.67660000	2.90600000	-2.58380000
C	1.18410000	-0.58230000	3.87110000
C	2.38550000	-0.91480000	3.10440000
C	3.17370000	0.17240000	2.60850000
C	2.69750000	1.54590000	2.63790000
C	0.67660000	2.90600000	2.58380000
C	1.44290000	1.84720000	3.18480000
C	0.70420000	0.78620000	3.81710000
C	2.32690000	3.15770000	0.73560000
C	3.14450000	2.21130000	1.42410000
C	1.12710000	3.62360000	1.40850000
C	2.40310000	-2.18320000	2.36260000
C	3.20260000	-2.28970000	1.18020000
C	0.01930000	-1.45960000	4.00370000
C	0.03690000	-2.69120000	3.23780000
C	1.21250000	-3.01350000	2.42840000
C	-1.17500000	-0.60560000	3.89190000
C	-2.35820000	-0.96090000	3.11370000
C	-3.16860000	0.11220000	2.60720000
C	-0.74940000	2.89800000	2.59050000
C	-1.48820000	1.82390000	3.19170000
C	-0.72580000	0.77340000	3.82310000
C	-2.73530000	1.49610000	2.64160000
C	0.76410000	-3.68740000	1.23120000
C	1.50360000	-3.65720000	0.00000000
C	2.74680000	-3.00430000	0.00000000

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C	0.76410000	-3.68740000	-1.23120000
C	-0.66430000	-3.70030000	1.23110000
C	-2.65250000	-3.03750000	0.00000000
C	-1.39730000	-3.67250000	0.00000000
C	-0.66430000	-3.70030000	-1.23110000
C	-2.33850000	-2.22610000	2.36690000
C	-1.12980000	-3.03330000	2.43040000
C	-3.13100000	-2.34340000	1.17950000
C	-3.98610000	1.19720000	0.70210000
C	-3.96870000	-0.05180000	1.42430000
C	-3.96020000	-1.26440000	0.72180000
C	-3.98610000	1.19720000	-0.70210000
C	-1.21580000	3.61330000	1.41190000
C	-2.40920000	3.12460000	0.73560000
C	-3.19610000	2.15250000	1.42560000
C	-1.21580000	3.61330000	-1.41190000
C	-0.04920000	4.15780000	-0.72620000
C	-0.04920000	4.15780000	0.72620000
C	-3.19610000	2.15250000	-1.42560000
C	-2.40920000	3.12460000	-0.73560000
C	-0.72580000	0.77340000	-3.82310000
C	-2.73530000	1.49610000	-2.64160000
C	-1.48820000	1.82390000	-3.19170000
C	-0.74940000	2.89800000	-2.59050000
C	-3.96020000	-1.26440000	-0.72180000
C	-3.96870000	-0.05180000	-1.42430000
C	-3.16860000	0.11220000	-2.60720000
C	-2.35820000	-0.96090000	-3.11370000
C	-1.17500000	-0.60560000	-3.89190000
C	-0.65300000	0.01350000	0.00000000

Sc₃NC@C₇₈ (C_{2v}) 17.9 kcal/mol

N	0.00000000	0.00000000	-0.10970000
Sc	0.00000000	-2.00250000	0.67710000
Sc	0.00000000	0.00000000	-2.14430000
Sc	0.00000000	2.00250000	0.67710000
C	1.16000000	-2.40500000	3.02300000
C	2.34290000	-2.35170000	2.19890000
C	3.14370000	-1.17220000	2.31760000
C	3.95810000	-0.71970000	1.22590000
C	3.95460000	-1.42510000	0.01070000
C	0.00000000	-3.19330000	2.64920000

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C	0.00000000	-4.02600000	1.45690000
C	1.18580000	-3.93270000	0.58720000
C	2.35360000	-3.11480000	0.93560000
C	3.15330000	-2.60490000	-0.14290000
C	-3.14370000	-1.17220000	2.31760000
C	-2.34290000	-2.35170000	2.19890000
C	-1.16000000	-2.40500000	3.02300000
C	3.95460000	1.42510000	0.01070000
C	3.95570000	0.70280000	-1.23870000
C	3.95810000	0.71970000	1.22590000
C	3.95570000	-0.70280000	-1.23870000
C	3.15350000	-1.42310000	-2.18770000
C	2.36020000	-0.73610000	-3.15760000
C	1.16950000	-1.41430000	-3.64720000
C	0.71700000	-3.87690000	-0.79920000
C	1.45780000	-3.20460000	-1.85060000
C	2.69680000	-2.63590000	-1.52520000
C	0.71090000	-2.59330000	-2.92320000
C	1.18580000	3.93270000	0.58720000
C	2.35360000	3.11480000	0.93560000
C	3.15330000	2.60490000	-0.14290000
C	2.69680000	2.63590000	-1.52520000
C	0.71090000	2.59330000	-2.92320000
C	1.45780000	3.20460000	-1.85060000
C	0.71700000	3.87690000	-0.79920000
C	2.36020000	0.73610000	-3.15760000
C	3.15350000	1.42310000	-2.18770000
C	1.16950000	1.41430000	-3.64720000
C	2.34290000	2.35170000	2.19890000
C	3.14370000	1.17220000	2.31760000
C	0.00000000	4.02600000	1.45690000
C	0.00000000	3.19330000	2.64920000
C	1.16000000	2.40500000	3.02300000
C	-1.18580000	3.93270000	0.58720000
C	-2.35360000	3.11480000	0.93560000
C	-3.15330000	2.60490000	-0.14290000
C	-0.71090000	2.59330000	-2.92320000
C	-1.45780000	3.20460000	-1.85060000
C	-0.71700000	3.87690000	-0.79920000
C	-2.69680000	2.63590000	-1.52520000
C	0.71280000	1.24190000	3.77640000
C	1.43940000	0.00000000	3.72150000
C	2.67350000	0.00000000	3.02950000

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C	0.71280000	-1.24190000	3.77640000
C	-0.71280000	1.24190000	3.77640000
C	-2.67350000	0.00000000	3.02950000
C	-1.43940000	0.00000000	3.72150000
C	-0.71280000	-1.24190000	3.77640000
C	-2.34290000	2.35170000	2.19890000
C	-1.16000000	2.40500000	3.02300000
C	-3.14370000	1.17220000	2.31760000
C	-3.95570000	0.70280000	-1.23870000
C	-3.95460000	1.42510000	0.01070000
C	-3.95810000	0.71970000	1.22590000
C	-3.95570000	-0.70280000	-1.23870000
C	-1.16950000	1.41430000	-3.64720000
C	-2.36020000	0.73610000	-3.15760000
C	-3.15350000	1.42310000	-2.18770000
C	-1.16950000	-1.41430000	-3.64720000
C	0.00000000	-0.73060000	-4.20340000
C	0.00000000	0.73060000	-4.20340000
C	-3.15350000	-1.42310000	-2.18770000
C	-2.36020000	-0.73610000	-3.15760000
C	-0.71700000	-3.87690000	-0.79920000
C	-2.69680000	-2.63590000	-1.52520000
C	-1.45780000	-3.20460000	-1.85060000
C	-0.71090000	-2.59330000	-2.92320000
C	-3.95810000	-0.71970000	1.22590000
C	-3.95460000	-1.42510000	0.01070000
C	-3.15330000	-2.60490000	-0.14290000
C	-2.35360000	-3.11480000	0.93560000
C	-1.18580000	-3.93270000	0.58720000
C	0.00000000	0.00000000	1.17980000

Sc₃NC@C₈₀ (C_{2v}) 0.0 kcal/mol

C	0.00000000	2.70070000	-3.09620000
C	1.16710000	3.18800000	-2.40180000
C	0.00000000	1.45170000	-3.83610000
C	1.22170000	0.72120000	-3.89090000
C	2.38130000	1.16850000	-3.15910000
C	2.36090000	2.35990000	-2.37400000
C	-1.16710000	3.18800000	-2.40180000

C	0.73940000	4.03260000	-1.28000000
C	-1.22170000	0.72120000	-3.89090000
C	1.22170000	-0.72120000	-3.89090000
C	3.09170000	0.00000000	-2.70040000
C	-0.73940000	4.03260000	-1.28000000
C	3.13300000	2.38030000	-1.17420000
C	2.38130000	-1.16850000	-3.15910000
C	-2.36090000	2.35990000	-2.37400000
C	-2.38130000	1.16850000	-3.15910000
C	-1.22170000	-0.72120000	-3.89090000
C	1.46900000	3.88470000	-0.01580000
C	0.00000000	-1.45170000	-3.83610000
C	2.66600000	3.09990000	-0.00820000
C	3.85190000	1.22410000	-0.72460000
C	3.79800000	0.00000000	-1.46340000
C	-1.46900000	3.88470000	-0.01580000
C	-3.09170000	0.00000000	-2.70040000
C	-2.38130000	-1.16850000	-3.15910000
C	-3.13300000	2.38030000	-1.17420000
C	2.36090000	-2.35990000	-2.37400000
C	3.12150000	2.38430000	1.16480000
C	0.72170000	3.87390000	1.21910000
C	3.83780000	1.22280000	0.71390000
C	0.00000000	-2.70070000	-3.09620000
C	-2.66600000	3.09990000	-0.00820000
C	3.85190000	-1.22410000	-0.72460000
C	-0.72170000	3.87390000	1.21910000
C	1.16710000	-3.18800000	-2.40180000
C	3.13300000	-2.38030000	-1.17420000
C	-3.85190000	1.22410000	-0.72460000
C	-3.79800000	0.00000000	-1.46340000
C	-2.36090000	-2.35990000	-2.37400000
C	-1.16710000	-3.18800000	-2.40180000
C	1.16400000	3.14930000	2.38760000
C	2.34760000	2.36600000	2.35900000
C	3.78090000	0.00000000	1.44340000
C	3.83780000	-1.22280000	0.71390000
C	-3.12150000	2.38430000	1.16480000
C	-1.16400000	3.14930000	2.38760000
C	0.73940000	-4.03260000	-1.28000000
C	-3.83780000	1.22280000	0.71390000
C	2.66600000	-3.09990000	-0.00820000
C	0.00000000	2.68950000	3.11680000

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C	-3.85190000	-1.22410000	-0.72460000
C	-0.73940000	-4.03260000	-1.28000000
C	-3.13300000	-2.38030000	-1.17420000
C	-2.34760000	2.36600000	2.35900000
C	3.12150000	-2.38430000	1.16480000
C	2.34630000	1.16270000	3.15290000
C	3.03210000	0.00000000	2.66890000
C	1.46900000	-3.88470000	-0.01580000
C	-3.78090000	0.00000000	1.44340000
C	-3.83780000	-1.22280000	0.71390000
C	-2.66600000	-3.09990000	-0.00820000
C	0.00000000	1.51150000	3.96260000
C	-1.46900000	-3.88470000	-0.01580000
C	1.23970000	0.74230000	3.99980000
C	2.34630000	-1.16270000	3.15290000
C	2.34760000	-2.36600000	2.35900000
C	-2.34630000	1.16270000	3.15290000
C	-3.12150000	-2.38430000	1.16480000
C	0.72170000	-3.87390000	1.21910000
C	-3.03210000	0.00000000	2.66890000
C	-1.23970000	0.74230000	3.99980000
C	1.23970000	-0.74230000	3.99980000
C	-0.72170000	-3.87390000	1.21910000
C	1.16400000	-3.14930000	2.38760000
C	-2.34760000	-2.36600000	2.35900000
C	-2.34630000	-1.16270000	3.15290000
C	-1.23970000	-0.74230000	3.99980000
C	0.00000000	-1.51150000	3.96260000
C	-1.16400000	-3.14930000	2.38760000
C	0.00000000	-2.68950000	3.11680000
C	0.00000000	0.00000000	0.14360000
Sc	0.00000000	2.04120000	-0.65230000
Sc	0.00000000	-2.04120000	-0.65230000
Sc	0.00000000	0.00000000	2.22290000
N	0.00000000	0.00000000	-1.12750000

Sc₃NC@C₈₀ (C₁) 0.8 kcal/mol

C	0.00680000	3.24880000	2.86100000
C	1.21480000	2.50900000	3.31920000
C	-0.00910000	3.86330000	1.52470000
C	1.19570000	3.83820000	0.74070000
C	2.37400000	3.13300000	1.18260000

C	2.38850000	2.40710000	2.43270000
C	-1.15800000	2.41840000	3.19900000
C	0.74030000	1.25220000	3.92670000
C	-1.20860000	3.81740000	0.74180000
C	1.19150000	3.82930000	-0.71100000
C	3.08160000	2.68380000	0.00600000
C	-0.70320000	1.22610000	3.87900000
C	3.12040000	1.17480000	2.39430000
C	2.36840000	3.13560000	-1.16790000
C	-2.35880000	2.34420000	2.38240000
C	-2.38810000	3.11220000	1.17630000
C	-1.21580000	3.82340000	-0.71220000
C	1.45920000	-0.00660000	3.83310000
C	-0.01420000	3.83780000	-1.48450000
C	2.68830000	-0.00910000	3.11190000
C	3.84500000	0.72680000	1.22600000
C	3.80530000	1.45580000	0.00120000
C	-1.45020000	-0.01600000	3.82590000
C	-3.11340000	2.68370000	0.01340000
C	-2.39540000	3.12560000	-1.14950000
C	-3.13220000	1.14610000	2.40600000
C	2.39050000	2.42240000	-2.43090000
C	3.14780000	-1.16430000	2.39690000
C	0.71980000	-1.23340000	3.87110000
C	3.84710000	-0.70690000	1.22410000
C	0.00390000	3.20850000	-2.80400000
C	-2.68580000	-0.02060000	3.12230000
C	3.83720000	0.72880000	-1.22370000
C	-0.71420000	-1.23510000	3.87090000
C	1.20970000	2.50810000	-3.30610000
C	3.10840000	1.18060000	-2.39300000
C	-3.85550000	0.70240000	1.23720000
C	-3.81120000	1.43230000	0.01020000
C	-2.36480000	2.34690000	-2.34860000
C	-1.15560000	2.39360000	-3.14850000
C	1.16610000	-2.39060000	3.13740000
C	2.35830000	-2.35690000	2.35660000
C	3.79550000	-1.44000000	-0.00290000
C	3.83630000	-0.70340000	-1.22840000
C	-3.13190000	-1.18930000	2.39630000
C	-1.16520000	-2.40550000	3.14670000
C	0.73520000	1.25980000	-3.93820000
C	-3.84940000	-0.73050000	1.23070000

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C	2.67650000	-0.00090000	-3.11700000
C	0.00320000	-3.13260000	2.69470000
C	-3.85140000	0.70040000	-1.21060000
C	-0.70640000	1.21930000	-3.85870000
C	-3.13190000	1.15000000	-2.37930000
C	-2.37690000	-2.40610000	2.38370000
C	3.12980000	-1.15660000	-2.40000000
C	2.37520000	-3.13030000	1.15850000
C	3.08610000	-2.68170000	-0.00590000
C	1.45100000	-0.00450000	-3.85340000
C	-3.80220000	-1.46370000	0.00840000
C	-3.84360000	-0.73720000	-1.21430000
C	-2.68830000	-0.01420000	-3.10560000
C	-0.00590000	-3.93490000	1.48810000
C	-1.45590000	-0.02070000	-3.82190000
C	1.20420000	-3.85650000	0.71500000
C	2.38040000	-3.13580000	-1.17520000
C	2.34440000	-2.35180000	-2.37340000
C	-2.43690000	-3.26720000	1.20140000
C	-3.13030000	-1.18210000	-2.38710000
C	0.71330000	-1.22990000	-3.89760000
C	-3.07550000	-2.71420000	0.01840000
C	-1.27320000	-4.06320000	0.75370000
C	1.21890000	-3.85210000	-0.73720000
C	-0.72690000	-1.24140000	-3.90030000
C	1.15920000	-2.39060000	-3.16280000
C	-2.34430000	-2.36830000	-2.37360000
C	-2.34990000	-3.14260000	-1.14880000
C	-1.22700000	-3.93420000	-0.71510000
C	0.00430000	-3.83750000	-1.48370000
C	-1.17100000	-2.41200000	-3.17780000
C	-0.00400000	-3.12670000	-2.72490000
C	0.14750000	0.03680000	0.11870000
Sc	-0.72540000	-1.95790000	0.50370000
Sc	0.33770000	1.48120000	1.60750000
Sc	0.46820000	1.35930000	-1.60290000
N	-0.12800000	-0.56740000	-0.95960000

Sc₃NC@C₈₀ (Cs) 1.4 kcal/mol

C	-3.65510000	1.40340000	1.21690000
C	-2.93320000	2.65960000	1.21370000
C	-3.65510000	1.40340000	-1.21690000

C	-2.93320000	2.65960000	-1.21370000
C	-2.60490000	3.39210000	0.00000000
C	-3.27830000	0.65260000	2.38070000
C	-2.07340000	2.63780000	2.39170000
C	-3.27830000	0.65260000	-2.38070000
C	-2.07340000	2.63780000	-2.39170000
C	-2.30080000	1.40980000	3.11260000
C	-1.33660000	4.14930000	0.00000000
C	-2.30080000	1.40980000	-3.11260000
C	-3.21720000	-0.77410000	2.34400000
C	-3.64750000	-1.43820000	1.16450000
C	-3.64750000	-1.43820000	-1.16450000
C	-0.79520000	3.26910000	2.37400000
C	-3.21720000	-0.77410000	-2.34400000
C	-0.44380000	4.02090000	1.17700000
C	-0.44380000	4.02090000	-1.17700000
C	-0.79520000	3.26910000	-2.37400000
C	-1.24260000	0.76290000	3.83710000
C	-3.02250000	-2.65900000	0.71970000
C	-3.02250000	-2.65900000	-0.71970000
C	-2.18000000	-1.40890000	3.12000000
C	-1.24260000	0.76290000	-3.83710000
C	0.92190000	3.90320000	0.71820000
C	0.24640000	2.65590000	3.14740000
C	0.92190000	3.90320000	-0.71820000
C	-2.18000000	-1.40890000	-3.12000000
C	-1.23630000	-0.68600000	3.93960000
C	0.24640000	2.65590000	-3.14740000
C	0.01970000	1.42000000	3.86260000
C	-1.23630000	-0.68600000	-3.93960000
C	0.01970000	1.42000000	-3.86260000
C	-1.56600000	-2.63290000	2.68830000
C	-1.95530000	-3.26040000	1.44760000
C	-1.95530000	-3.26040000	-1.44760000
C	-1.56600000	-2.63290000	-2.68830000
C	1.61480000	2.65580000	2.71230000
C	1.97250000	3.25080000	1.46440000
C	1.97250000	3.25080000	-1.46440000
C	1.61480000	2.65580000	-2.71230000
C	-0.00330000	-1.48830000	4.06930000
C	1.25970000	0.66010000	3.89710000
C	-0.00330000	-1.48830000	-4.06930000
C	-0.22640000	-2.69100000	3.22670000

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C	1.25970000	0.66010000	-3.89710000
C	2.23400000	1.43570000	3.15360000
C	-0.94880000	-3.95430000	0.72130000
C	-0.22640000	-2.69100000	-3.22670000
C	-0.94880000	-3.95430000	-0.72130000
C	1.29430000	-0.79140000	3.98560000
C	2.23400000	1.43570000	-3.15360000
C	3.03400000	2.66920000	0.72090000
C	3.03400000	2.66920000	-0.72090000
C	1.29430000	-0.79140000	-3.98560000
C	0.80170000	-3.27850000	2.38240000
C	0.41860000	-3.95270000	1.17320000
C	0.41860000	-3.95270000	-1.17320000
C	3.23440000	0.79740000	2.35530000
C	0.80170000	-3.27850000	-2.38240000
C	3.66870000	1.45420000	1.16660000
C	3.66870000	1.45420000	-1.16660000
C	3.23440000	0.79740000	-2.35530000
C	2.30350000	-1.40430000	3.14420000
C	1.26190000	-3.93530000	0.00000000
C	2.30350000	-1.40430000	-3.14420000
C	2.08240000	-2.63820000	2.39580000
C	3.27320000	-0.63170000	2.38780000
C	2.08240000	-2.63820000	-2.39580000
C	3.27320000	-0.63170000	-2.38780000
C	2.50420000	-3.23680000	0.00000000
C	2.92050000	-2.62330000	1.22690000
C	3.64680000	-1.38350000	1.22530000
C	2.92050000	-2.62330000	-1.22690000
C	3.64680000	-1.38350000	-1.22530000
C	-4.00440000	0.73490000	0.00000000
C	-4.04750000	-0.68630000	0.00000000
C	4.03720000	0.69560000	0.00000000
C	3.99600000	-0.72880000	0.00000000
C	-0.05180000	0.09880000	0.00000000
Sc	0.17670000	-0.71980000	2.03020000
Sc	0.17670000	-0.71980000	-2.03020000
Sc	-0.83210000	2.04130000	0.00000000
N	0.28180000	-1.12850000	0.00000000

Sc₃NC@C₈₀ (C₁) 3.6 kcal/mol

C	0.00460000	3.12030000	2.67700000
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C	1.17360000	2.40630000	3.13150000
C	0.00110000	3.83860000	1.44720000
C	1.23050000	3.88260000	0.71270000
C	2.40590000	3.17480000	1.16720000
C	2.39090000	2.39840000	2.37310000
C	-1.16330000	2.40440000	3.12820000
C	0.71930000	1.23950000	3.85090000
C	-1.23250000	3.89000000	0.71150000
C	1.22980000	3.86890000	-0.72260000
C	3.15180000	2.72200000	-0.00620000
C	-0.71720000	1.23890000	3.84410000
C	3.23280000	1.20590000	2.41450000
C	2.38770000	3.14350000	-1.16750000
C	-2.36160000	2.38630000	2.34590000
C	-2.39470000	3.17740000	1.16100000
C	-1.23240000	3.87490000	-0.72590000
C	1.44210000	0.01740000	3.78620000
C	-0.00030000	3.81600000	-1.45890000
C	2.67980000	0.02740000	3.05090000
C	4.04990000	0.76680000	1.26190000
C	3.97070000	1.51720000	-0.00100000
C	-1.44300000	0.01410000	3.77880000
C	-3.14000000	2.71190000	-0.00770000
C	-2.39110000	3.15550000	-1.17270000
C	-3.18390000	1.19160000	2.36670000
C	2.35190000	2.35920000	-2.36620000
C	3.10550000	-1.13630000	2.32380000
C	0.71590000	-1.21260000	3.84160000
C	3.89980000	-0.69740000	1.20690000
C	0.00080000	3.10080000	-2.69170000
C	-2.67270000	0.02220000	3.03440000
C	3.87050000	0.73070000	-1.21410000
C	-0.72190000	-1.21360000	3.83230000
C	1.16630000	2.39000000	-3.14970000
C	3.13100000	1.16050000	-2.38120000
C	-4.04460000	0.76770000	1.25340000
C	-3.99170000	1.53540000	-0.00300000
C	-2.35380000	2.36580000	-2.36380000
C	-1.16600000	2.38970000	-3.14830000
C	1.15940000	-2.37200000	3.11890000
C	2.33280000	-2.35130000	2.33060000
C	3.79290000	-1.44810000	-0.01880000
C	3.86440000	-0.72800000	-1.23610000

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C	-3.13490000	-1.14050000	2.33470000
C	-1.17070000	-2.37790000	3.11080000
C	0.71960000	1.21720000	-3.85750000
C	-3.95120000	-0.70820000	1.22330000
C	2.69180000	-0.00450000	-3.09940000
C	-0.00630000	-3.10350000	2.65930000
C	-3.91460000	0.74580000	-1.22260000
C	-0.71920000	1.21670000	-3.85300000
C	-3.14160000	1.16880000	-2.37720000
C	-2.35940000	-2.35630000	2.33280000
C	3.15010000	-1.17530000	-2.39680000
C	2.34960000	-3.17150000	1.14270000
C	3.04090000	-2.68640000	-0.01640000
C	1.45230000	-0.00240000	-3.81200000
C	-3.84490000	-1.46190000	-0.00670000
C	-3.88050000	-0.71650000	-1.22320000
C	-2.69170000	0.00220000	-3.08510000
C	-0.00090000	-3.89840000	1.46390000
C	-1.45380000	-0.00270000	-3.80300000
C	1.25540000	-4.04210000	0.72150000
C	2.36930000	-3.20070000	-1.18500000
C	2.35320000	-2.36970000	-2.37190000
C	-2.38990000	-3.15070000	1.15100000
C	-3.15150000	-1.16320000	-2.38330000
C	0.71440000	-1.23100000	-3.86380000
C	-3.10840000	-2.70270000	-0.00850000
C	-1.23000000	-3.89990000	0.71040000
C	1.27070000	-4.08720000	-0.76550000
C	-0.72120000	-1.23110000	-3.84950000
C	1.16200000	-2.38690000	-3.14480000
C	-2.37220000	-2.36430000	-2.36150000
C	-2.39390000	-3.15350000	-1.17270000
C	-1.23510000	-3.91800000	-0.74240000
C	-0.00080000	-3.95960000	-1.50710000
C	-1.17110000	-2.39040000	-3.12870000
C	-0.00660000	-3.12220000	-2.67790000
C	0.01750000	-0.11580000	-0.13180000
Sc	-2.07150000	0.45110000	0.31310000
Sc	0.44820000	-2.16120000	-0.16030000
Sc	1.95610000	0.68920000	0.55820000
N	-0.07990000	1.11220000	0.17040000

Sc₃NC@C₈₀ (C_{2v}) 10.9 kcal/mol

C	0.00000000	2.69210000	-3.08710000
C	1.16410000	3.17910000	-2.39250000
C	0.00000000	1.45020000	-3.83630000
C	1.22250000	0.72110000	-3.89420000
C	2.38120000	1.16800000	-3.16080000
C	2.35940000	2.35640000	-2.37200000
C	-1.16410000	3.17910000	-2.39250000
C	0.73970000	4.03320000	-1.27890000
C	-1.22250000	0.72110000	-3.89420000
C	1.22250000	-0.72110000	-3.89420000
C	3.09340000	0.00000000	-2.70300000
C	-0.73970000	4.03320000	-1.27890000
C	3.13410000	2.38030000	-1.17500000
C	2.38120000	-1.16800000	-3.16080000
C	-2.35940000	2.35640000	-2.37200000
C	-2.38120000	1.16800000	-3.16080000
C	-1.22250000	-0.72110000	-3.89420000
C	1.47310000	3.89380000	-0.01620000
C	0.00000000	-1.45020000	-3.83630000
C	2.66690000	3.10190000	-0.01010000
C	3.85350000	1.22430000	-0.72660000
C	3.80000000	0.00000000	-1.46630000
C	-1.47310000	3.89380000	-0.01620000
C	-3.09340000	0.00000000	-2.70300000
C	-2.38120000	-1.16800000	-3.16080000
C	-3.13410000	2.38030000	-1.17500000
C	2.35940000	-2.35640000	-2.37200000
C	3.12340000	2.38500000	1.16240000
C	0.72290000	3.88380000	1.21890000
C	3.83950000	1.22290000	0.71150000
C	0.00000000	-2.69210000	-3.08710000
C	-2.66690000	3.10190000	-0.01010000
C	3.85350000	-1.22430000	-0.72660000
C	-0.72290000	3.88380000	1.21890000
C	1.16410000	-3.17910000	-2.39250000
C	3.13410000	-2.38030000	-1.17500000
C	-3.85350000	1.22430000	-0.72660000
C	-3.80000000	0.00000000	-1.46630000
C	-2.35940000	-2.35640000	-2.37200000
C	-1.16410000	-3.17910000	-2.39250000
C	1.16420000	3.14930000	2.38240000
C	2.34910000	2.36600000	2.35500000

C	3.78410000	0.00000000	1.44150000
C	3.83950000	-1.22290000	0.71150000
C	-3.12340000	2.38500000	1.16240000
C	-1.16420000	3.14930000	2.38240000
C	0.73970000	-4.03320000	-1.27890000
C	-3.83950000	1.22290000	0.71150000
C	2.66690000	-3.10190000	-0.01010000
C	0.00000000	2.68580000	3.10710000
C	-3.85350000	-1.22430000	-0.72660000
C	-0.73970000	-4.03320000	-1.27890000
C	-3.13410000	-2.38030000	-1.17500000
C	-2.34910000	2.36600000	2.35500000
C	3.12340000	-2.38500000	1.16240000
C	2.34850000	1.16240000	3.14780000
C	3.03630000	0.00000000	2.66630000
C	1.47310000	-3.89380000	-0.01620000
C	-3.78410000	0.00000000	1.44150000
C	-3.83950000	-1.22290000	0.71150000
C	-2.66690000	-3.10190000	-0.01010000
C	0.00000000	1.50640000	3.95070000
C	-1.47310000	-3.89380000	-0.01620000
C	1.23900000	0.74050000	3.98970000
C	2.34850000	-1.16240000	3.14780000
C	2.34910000	-2.36600000	2.35500000
C	-2.34850000	1.16240000	3.14780000
C	-3.12340000	-2.38500000	1.16240000
C	0.72290000	-3.88380000	1.21890000
C	-3.03630000	0.00000000	2.66630000
C	-1.23900000	0.74050000	3.98970000
C	1.23900000	-0.74050000	3.98970000
C	-0.72290000	-3.88380000	1.21890000
C	1.16420000	-3.14930000	2.38240000
C	-2.34910000	-2.36600000	2.35500000
C	-2.34850000	-1.16240000	3.14780000
C	-1.23900000	-0.74050000	3.98970000
C	0.00000000	-1.50640000	3.95070000
C	-1.16420000	-3.14930000	2.38240000
C	0.00000000	-2.68580000	3.10710000
C	0.00000000	0.00000000	-1.11540000
Sc	0.00000000	2.06400000	-0.58640000
Sc	0.00000000	-2.06400000	-0.58640000
Sc	0.00000000	0.00000000	2.20830000
N	0.00000000	0.00000000	0.16810000

Sc₃NC@C₈₀ (C₁) 12.1 kcal/mol

C	0.01020000	3.12080000	2.69360000
C	1.17950000	2.40820000	3.14810000
C	0.00300000	3.83800000	1.46080000
C	1.23180000	3.89020000	0.72310000
C	2.39410000	3.17020000	1.17030000
C	2.37830000	2.38940000	2.36770000
C	-1.15530000	2.40460000	3.14980000
C	0.72870000	1.23790000	3.86090000
C	-1.22920000	3.88700000	0.72550000
C	1.23000000	3.87630000	-0.71410000
C	3.13100000	2.70490000	0.00060000
C	-0.70820000	1.23660000	3.86260000
C	3.21720000	1.20070000	2.39770000
C	2.38080000	3.14380000	-1.16320000
C	-2.34810000	2.37320000	2.36920000
C	-2.38360000	3.15770000	1.17280000
C	-1.22570000	3.87650000	-0.71160000
C	1.45650000	0.01700000	3.79370000
C	-0.00140000	3.82640000	-1.44800000
C	2.68950000	0.02490000	3.05250000
C	4.05550000	0.76730000	1.26420000
C	3.95990000	1.51680000	0.00360000
C	-1.43890000	0.01070000	3.81180000
C	-3.12150000	2.70960000	0.00930000
C	-2.39960000	3.16230000	-1.16700000
C	-3.12490000	1.17280000	2.38680000
C	2.34480000	2.36230000	-2.35800000
C	3.14460000	-1.13890000	2.34320000
C	0.73500000	-1.21500000	3.84460000
C	3.95090000	-0.70600000	1.22780000
C	-0.01170000	3.10210000	-2.67650000
C	-2.67760000	0.00690000	3.10240000
C	3.87340000	0.73480000	-1.21390000
C	-0.70100000	-1.21800000	3.86020000
C	1.15020000	2.39150000	-3.14090000
C	3.13000000	1.16730000	-2.37990000
C	-3.84860000	0.73000000	1.22020000
C	-3.90230000	1.49480000	-0.00100000
C	-2.41780000	2.40130000	-2.39120000
C	-1.18240000	2.38450000	-3.12230000

C	1.18120000	-2.37480000	3.11730000
C	2.36830000	-2.35860000	2.34030000
C	3.83290000	-1.45840000	-0.00460000
C	3.85930000	-0.71980000	-1.22150000
C	-3.12840000	-1.16600000	2.39690000
C	-1.14840000	-2.37870000	3.14640000
C	0.70800000	1.22290000	-3.85270000
C	-3.84100000	-0.72010000	1.23330000
C	2.68590000	0.00120000	-3.09290000
C	0.01350000	-3.10700000	2.67450000
C	-4.03540000	0.76630000	-1.26740000
C	-0.72700000	1.21990000	-3.85280000
C	-3.28160000	1.21900000	-2.46160000
C	-2.33680000	-2.35560000	2.36980000
C	3.14240000	-1.16530000	-2.38770000
C	2.39700000	-3.15620000	1.16080000
C	3.10640000	-2.70190000	-0.00100000
C	1.44350000	-0.00240000	-3.80060000
C	-3.78490000	-1.44040000	0.01610000
C	-3.88700000	-0.69140000	-1.21240000
C	-2.71800000	0.02700000	-3.09450000
C	0.00590000	-3.91610000	1.48800000
C	-1.46210000	0.00500000	-3.80550000
C	1.23380000	-3.91140000	0.72590000
C	2.37940000	-3.14210000	-1.16220000
C	2.35720000	-2.35810000	-2.35610000
C	-2.34170000	-3.16110000	1.16810000
C	-3.11730000	-1.13690000	-2.34350000
C	0.70860000	-1.22700000	-3.84780000
C	-3.03090000	-2.67170000	0.00490000
C	-1.25570000	-4.04440000	0.74590000
C	1.22840000	-3.91250000	-0.72850000
C	-0.73000000	-1.22680000	-3.85850000
C	1.15570000	-2.38670000	-3.12400000
C	-2.34150000	-2.35490000	-2.34540000
C	-2.35600000	-3.17990000	-1.15800000
C	-1.26690000	-4.07150000	-0.74290000
C	-0.00710000	-3.94940000	-1.49310000
C	-1.17250000	-2.38610000	-3.14000000
C	-0.00470000	-3.12100000	-2.67370000
C	-0.06750000	1.07200000	0.29570000
Sc	-1.86420000	0.65580000	-0.82750000
Sc	-0.39280000	-2.18020000	-0.06680000

Sc	2.00510000	0.49210000	0.52440000
N	-0.00990000	-0.16850000	-0.02060000

Five Low-energy $\text{Sc}_3\text{C}_2@\text{C}_{79}\text{N}$ isomers and relative energies (compared to the lowest-energy $\text{Sc}_3\text{NC}@\text{C}_{80}(\text{C}_{2v})$)

$\text{Sc}_3\text{C}_2@\text{C}_{79}\text{N}$ (C_1) 51.2kcal/mol

C	-3.67000000	1.39200000	1.19300000
C	-2.92510000	2.62270000	1.18380000
C	-3.67580000	1.38020000	-1.25450000
C	-2.93380000	2.60390000	-1.25920000
C	-2.51770000	3.21710000	-0.05040000
C	-3.29310000	0.64090000	2.36420000
C	-2.08160000	2.64610000	2.35290000
C	-3.28840000	0.62570000	-2.41660000
C	-2.07720000	2.61200000	-2.41570000
C	-2.31810000	1.41220000	3.07980000
C	-1.24760000	3.86590000	-0.04030000
C	-2.30650000	1.38760000	-3.14770000
C	-3.23990000	-0.78850000	2.33780000
C	-3.66540000	-1.44470000	1.15330000
C	-3.64430000	-1.45620000	-1.16870000
C	-0.82060000	3.33250000	2.38550000
C	-3.21750000	-0.79670000	-2.36240000
C	-0.43030000	3.94190000	1.12590000
C	-0.78800000	3.18580000	-2.36200000
C	-1.25110000	0.78180000	3.76730000
C	-3.02450000	-2.67240000	0.73230000
C	-3.01430000	-2.66930000	-0.71310000
C	-2.22750000	-1.45610000	3.12690000
C	-1.24880000	0.74190000	-3.86650000
C	0.94130000	3.95000000	0.68040000
C	0.23790000	2.80540000	3.25040000
C	0.92890000	3.88890000	-0.74500000
C	-2.18570000	-1.43590000	-3.13540000
C	-1.23260000	-0.66250000	3.79630000
C	0.24330000	2.63870000	-3.17290000
C	0.00290000	1.49070000	3.85880000
C	-1.24040000	-0.70960000	-3.95560000
C	0.01440000	1.41010000	-3.89590000

C	-1.67190000	-2.77220000	2.82630000
C	-2.01460000	-3.33200000	1.51230000
C	-1.95340000	-3.27360000	-1.43960000
C	-1.56500000	-2.65220000	-2.68430000
C	1.64620000	2.80460000	2.78390000
C	1.99570000	3.34230000	1.46870000
C	1.95990000	3.25210000	-1.49260000
C	1.60740000	2.64020000	-2.73150000
C	-0.02490000	-1.44010000	3.87990000
C	1.21690000	0.71780000	3.81480000
C	-0.00040000	-1.50400000	-4.04310000
C	-0.26330000	-2.77980000	3.31760000
C	1.25220000	0.64460000	-3.89340000
C	2.21500000	1.50350000	3.13410000
C	-0.96300000	-3.97160000	0.75550000
C	-0.22030000	-2.69630000	-3.20350000
C	-0.94890000	-3.95580000	-0.69610000
C	1.23190000	-0.72680000	3.79770000
C	2.22910000	1.42270000	-3.15470000
C	3.01880000	2.68990000	0.71130000
C	3.02050000	2.67730000	-0.73190000
C	1.28460000	-0.80160000	-3.94520000
C	0.80500000	-3.33340000	2.46860000
C	0.41720000	-3.95730000	1.21310000
C	0.41650000	-3.93830000	-1.13900000
C	3.22250000	0.82740000	2.35230000
C	0.80500000	-3.26740000	-2.35290000
C	3.65750000	1.47000000	1.15990000
C	3.65890000	1.46180000	-1.16530000
C	3.23500000	0.79420000	-2.35520000
C	2.29790000	-1.36750000	3.12240000
C	1.25810000	-3.91150000	0.03070000
C	2.30060000	-1.40550000	-3.11310000
C	2.05720000	-2.61560000	2.41280000
C	3.27660000	-0.60400000	2.40110000
C	2.08140000	-2.63190000	-2.36580000
C	3.27950000	-0.63170000	-2.37570000
C	2.50920000	-3.22080000	0.02220000
C	2.90750000	-2.59760000	1.24320000
C	3.64680000	-1.36510000	1.23770000
C	2.92900000	-2.61730000	-1.20290000
C	3.65740000	-1.37940000	-1.20870000
C	-4.01120000	0.72990000	-0.02440000

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C	-4.04640000	-0.69990000	-0.01430000
C	4.03660000	0.71120000	0.00200000
C	3.99670000	-0.71810000	0.01200000
C	-0.10080000	0.96470000	-0.57920000
C	0.15810000	-0.15440000	0.09850000
Sc	-0.32700000	-1.60730000	1.46720000
Sc	0.05930000	-0.61810000	-1.99450000
Sc	0.37660000	1.53060000	1.41810000
N	-0.41580000	3.88160000	-1.18360000

Sc₃C₂@C₇₉N (C₁) 52.5kcal/mol

C	0.00300000	2.84060000	-3.21280000
C	1.16170000	3.18040000	-2.38670000
C	0.01920000	1.51530000	-3.83730000
C	1.22420000	0.74120000	-3.81080000
C	2.39670000	1.17720000	-3.09330000
C	2.36510000	2.37390000	-2.32050000
C	-1.20980000	3.32970000	-2.50810000
C	0.70580000	3.87420000	-1.20750000
C	-1.19090000	0.74150000	-3.83390000
C	1.22720000	-0.70680000	-3.81620000
C	3.11800000	0.01230000	-2.65810000
C	-0.73840000	3.94020000	-1.25200000
C	3.13850000	2.40200000	-1.11750000
C	2.39540000	-1.14950000	-3.10220000
C	-2.39040000	2.44840000	-2.42030000
C	-2.37240000	1.18980000	-3.13700000
C	-1.19380000	-0.70580000	-3.83300000
C	1.45110000	3.83120000	0.03500000
C	0.01660000	-1.46290000	-3.80900000
C	2.69140000	3.12460000	0.04110000
C	3.84530000	1.22910000	-0.66510000
C	3.80520000	0.00760000	-1.40560000
C	-1.46020000	3.84390000	0.00610000
C	-3.08230000	0.01110000	-2.68980000
C	-2.37840000	-1.16860000	-3.14860000
C	-3.12200000	2.40210000	-1.18290000
C	2.35420000	-2.33590000	-2.31440000
C	3.14100000	2.41100000	1.21790000
C	0.71580000	3.88780000	1.25030000
C	3.86600000	1.22910000	0.77790000
C	-0.01140000	-2.75650000	-3.14780000

C	-2.68970000	3.11570000	0.00100000
C	3.84010000	-1.21060000	-0.66600000
C	-0.72300000	3.88290000	1.23060000
C	1.14010000	-3.11590000	-2.34800000
C	3.12530000	-2.37520000	-1.11680000
C	-3.85430000	1.23010000	-0.73900000
C	-3.82380000	0.00720000	-1.46890000
C	-2.42140000	-2.44490000	-2.45280000
C	-1.21970000	-3.29380000	-2.49980000
C	1.15690000	3.15940000	2.42000000
C	2.37450000	2.40290000	2.42910000
C	3.89580000	0.00270000	1.54960000
C	3.84220000	-1.21180000	0.77720000
C	-3.14880000	2.39590000	1.15540000
C	-1.17990000	3.15680000	2.39000000
C	0.69080000	-3.84440000	-1.19170000
C	-3.85710000	1.22680000	0.69470000
C	2.67790000	-3.10620000	0.04130000
C	-0.02780000	2.70790000	3.11760000
C	-3.85920000	-1.22380000	-0.74760000
C	-0.75070000	-3.94060000	-1.25250000
C	-3.13940000	-2.40120000	-1.20230000
C	-2.36370000	2.36740000	2.34640000
C	3.12530000	-2.40070000	1.20880000
C	2.44960000	1.19780000	3.25920000
C	3.21790000	0.00380000	2.84590000
C	1.43790000	-3.81680000	0.04390000
C	-3.81520000	-0.00340000	1.41830000
C	-3.85480000	-1.22730000	0.68620000
C	-2.69050000	-3.11370000	-0.01160000
C	-0.01920000	1.45470000	3.79630000
C	-1.46860000	-3.85480000	0.00360000
C	1.21630000	0.72820000	3.85140000
C	2.39910000	-1.16850000	3.18640000
C	2.34780000	-2.38840000	2.40260000
C	-2.37800000	1.15100000	3.10270000
C	-3.14970000	-2.39300000	1.14540000
C	0.71070000	-3.90330000	1.26580000
C	-3.08480000	-0.00680000	2.64750000
C	-1.22290000	0.70270000	3.78960000
C	1.19140000	-0.70830000	3.82300000
C	-0.73040000	-3.91200000	1.24260000
C	1.15650000	-3.17870000	2.43540000

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C	-2.34950000	-2.36950000	2.33130000
C	-2.35900000	-1.14940000	3.06680000
C	-0.02920000	-1.45580000	3.75240000
C	-1.18300000	-3.17510000	2.38440000
C	-0.02700000	-2.71670000	3.12270000
C	-0.27040000	0.17030000	0.07850000
C	0.03410000	-0.97240000	0.67570000
Sc	1.54700000	0.25520000	1.37600000
Sc	-0.45430000	1.60260000	-1.39610000
Sc	-0.70060000	-1.58070000	-1.20310000
N	-1.22280000	-0.71640000	3.78330000

Sc₃C₂@C₇₉N (C₁) 53.1kcal/mol

C	4.08290000	0.80160000	-0.02780000
C	3.85780000	1.49370000	-1.30620000
C	3.45340000	0.70270000	-2.50140000
C	3.30600000	-0.75750000	-2.39660000
C	3.66640000	-1.40170000	-1.15520000
C	4.04000000	-0.63610000	0.00990000
C	2.97580000	2.66810000	-1.26130000
C	2.48920000	3.25510000	-0.01680000
C	2.89050000	2.64170000	1.21060000
C	3.62920000	1.40700000	1.19380000
C	3.66220000	-1.40120000	1.19060000
C	3.28180000	-0.78990000	2.43830000
C	3.24090000	0.64310000	2.37250000
C	3.04470000	-2.62160000	-0.69600000
C	3.04580000	-2.62350000	0.74360000
C	2.35280000	1.42840000	-3.15870000
C	2.08310000	2.63190000	-2.40370000
C	2.04880000	2.64950000	2.37540000
C	2.26160000	1.42490000	3.09080000
C	2.24750000	-1.40040000	-3.12380000
C	1.25190000	-0.65770000	-3.86620000
C	1.24880000	0.76740000	-3.83490000
C	-0.02610000	1.42440000	-3.88480000
C	-0.26580000	2.64420000	-3.16360000
C	0.76790000	3.23600000	-2.37110000
C	0.38180000	3.92130000	-1.18390000
C	1.23050000	3.92210000	-0.01920000
C	0.37580000	3.92490000	1.14850000
C	0.75700000	3.25040000	2.33860000

C	-0.27950000	2.62430000	3.10610000
C	-0.05640000	1.40390000	3.79560000
C	1.21400000	0.76240000	3.80590000
C	1.27220000	-0.67500000	3.92770000
C	2.33210000	-1.48560000	3.32320000
C	1.67520000	-2.72200000	2.83760000
C	2.00660000	-3.26450000	1.51950000
C	1.62890000	-2.62620000	-2.67370000
C	1.98890000	-3.23390000	-1.43350000
C	0.97560000	-3.90150000	-0.68610000
C	0.97210000	-3.89580000	0.75830000
C	-4.07550000	-0.75810000	0.00360000
C	-3.71080000	-1.40740000	1.23660000
C	-3.32830000	-0.64270000	2.38990000
C	-3.27440000	0.77260000	2.34980000
C	-3.70650000	1.43670000	1.15550000
C	-4.09760000	0.67400000	-0.00800000
C	-2.93910000	-2.62780000	1.25350000
C	-2.49380000	-3.21010000	0.03620000
C	-2.90440000	-2.58090000	-1.19660000
C	-3.75300000	-1.41010000	-1.25220000
C	-3.72970000	1.43340000	-1.20440000
C	-3.37980000	0.80000000	-2.46300000
C	-3.43640000	-0.66530000	-2.48890000
C	-3.07540000	2.64180000	0.69440000
C	-3.07140000	2.63930000	-0.74080000
C	-2.32960000	-1.38680000	3.12320000
C	-2.09300000	-2.62560000	2.42140000
C	-2.04950000	-2.57830000	-2.34670000
C	-2.33280000	-1.39740000	-3.12310000
C	-2.23010000	1.40930000	3.08250000
C	-1.25770000	-0.73360000	3.76820000
C	0.01560000	-1.39070000	3.86730000
C	0.25570000	-2.64310000	3.18820000
C	-0.79810000	-3.22810000	2.38790000
C	-0.40630000	-3.90450000	1.19580000
C	-1.24280000	-3.89500000	0.02950000
C	-0.38850000	-3.89110000	-1.13160000
C	-0.75980000	-3.21320000	-2.32890000
C	0.26770000	-2.62900000	-3.12540000
C	0.03100000	-1.41550000	-3.86440000
C	-1.24030000	-0.75880000	-3.82470000
C	-1.24910000	0.66400000	-3.87110000

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C	-2.26630000	1.41810000	-3.15590000
C	-1.63090000	2.64240000	-2.71040000
C	-2.00050000	3.24930000	-1.47350000
C	-1.63530000	2.62620000	2.66070000
C	-2.01450000	3.25260000	1.42930000
C	-0.99290000	3.92630000	0.69950000
C	-0.98810000	3.93410000	-0.73840000
C	-0.78190000	-0.20750000	0.81150000
C	0.12720000	-0.09200000	-0.14930000
Sc	1.06020000	-0.94490000	1.60120000
Sc	1.88730000	0.59070000	-0.97200000
Sc	-1.82110000	-0.08120000	-1.05320000
N	-1.27110000	0.67350000	3.81520000

Sc₃C₂@C₇₉N (C₁) 54.0kcal/mol

C	4.04680000	-0.11600000	0.03550000
C	3.34690000	-0.07010000	-2.32860000
C	3.05240000	-1.46320000	-2.31560000
C	3.32300000	-2.18700000	-1.11980000
C	3.84390000	-1.51530000	0.03910000
C	3.36640000	1.90980000	-1.18180000
C	3.10940000	2.61530000	0.02700000
C	3.39060000	1.95010000	1.25330000
C	3.87730000	0.60010000	1.24710000
C	3.31100000	-2.17510000	1.21490000
C	3.04670000	-1.47230000	2.43780000
C	3.34630000	-0.06760000	2.41720000
C	2.46240000	-3.24710000	-0.68300000
C	2.45270000	-3.24410000	0.75220000
C	2.59320000	0.87130000	-3.09490000
C	2.60360000	2.11430000	-2.36720000
C	2.55180000	2.13400000	2.39680000
C	2.51410000	0.88520000	3.12140000
C	1.93870000	-1.87070000	-3.11260000
C	1.13660000	-0.91730000	-3.84340000
C	1.44710000	0.47910000	-3.89910000
C	0.34150000	1.43540000	-4.04080000
C	0.36590000	2.70890000	-3.28260000
C	1.48390000	3.03120000	-2.40200000
C	1.21990000	3.72980000	-1.17870000
C	2.03290000	3.55210000	-0.00280000
C	1.19760000	3.74690000	1.15440000
C	1.41780000	3.00470000	2.35240000

C	0.27840000	2.63390000	3.13070000
C	0.24240000	1.38370000	3.84690000
C	1.36280000	0.48030000	3.88420000
C	1.10420000	-0.94720000	4.02370000
C	1.94480000	-1.92240000	3.29240000
C	1.04120000	-2.92980000	2.74360000
C	1.27570000	-3.59630000	1.47910000
C	1.07250000	-2.93520000	-2.67540000
C	1.29230000	-3.60020000	-1.42970000
C	0.14970000	-4.04470000	-0.70090000
C	0.13920000	-4.04030000	0.73790000
C	-4.25590000	0.11490000	-0.03470000
C	-3.94810000	-0.60670000	1.19620000
C	-3.39310000	0.06100000	2.36700000
C	-3.08530000	1.46250000	2.35420000
C	-3.43870000	2.22530000	1.15670000
C	-4.04600000	1.57650000	-0.03570000
C	-3.41740000	-1.95490000	1.20050000
C	-3.10320000	-2.64620000	-0.01410000
C	-3.38020000	-1.95900000	-1.23640000
C	-3.88520000	-0.60240000	-1.23860000
C	-3.33990000	2.15150000	-1.19540000
C	-2.97870000	1.40900000	-2.38240000
C	-3.33510000	0.03820000	-2.42840000
C	-2.45050000	3.18630000	0.69110000
C	-2.41240000	3.15780000	-0.74320000
C	-2.57310000	-0.89450000	3.09040000
C	-2.60510000	-2.13700000	2.37550000
C	-2.54550000	-2.14200000	-2.38970000
C	-2.51650000	-0.90870000	-3.12880000
C	-1.93160000	1.86610000	3.11180000
C	-1.12180000	0.91150000	3.83060000
C	-1.40940000	-0.48110000	3.81300000
C	-0.28440000	-1.39370000	3.90990000
C	-0.31210000	-2.60940000	3.14120000
C	-1.45770000	-2.99210000	2.34810000
C	-1.20610000	-3.74400000	1.16940000
C	-2.02680000	-3.57810000	-0.00200000
C	-1.18460000	-3.75220000	-1.15530000
C	-1.40800000	-3.01120000	-2.34990000
C	-0.26210000	-2.64960000	-3.13040000
C	-0.23010000	-1.41090000	-3.84770000
C	-1.32690000	-0.50520000	-3.82560000

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C	-1.02200000	0.90430000	-3.91760000
C	-1.82400000	1.82810000	-3.14890000
C	-0.97430000	2.91490000	-2.74100000
C	-1.23540000	3.55720000	-1.47780000
C	-1.05400000	2.92710000	2.67940000
C	-1.27570000	3.57910000	1.43470000
C	-0.13870000	4.03740000	0.70270000
C	-0.12580000	4.03060000	-0.73460000
C	1.11880000	-0.15050000	-0.24270000
C	-0.19910000	-0.16490000	-0.05810000
Sc	0.80140000	-0.70330000	1.78280000
Sc	0.30280000	0.93160000	-1.86780000
Sc	-2.08160000	0.63870000	0.22560000
N	3.85540000	0.58400000	-1.18280000

Sc₃C₂@C₇₉N (C₁) 54.2kcal/mol

C	0.03660000	2.67870000	-3.13370000
C	1.20870000	3.12670000	-2.42710000
C	0.02670000	1.43840000	-3.85020000
C	1.24820000	0.70000000	-3.90310000
C	2.42180000	1.14410000	-3.19350000
C	2.41230000	2.35000000	-2.41800000
C	-1.11750000	3.13110000	-2.40350000
C	0.77830000	3.86370000	-1.24220000
C	-1.20510000	0.70290000	-3.89050000
C	1.22660000	-0.74330000	-3.89980000
C	3.11010000	-0.04170000	-2.72560000
C	-0.66990000	3.84260000	-1.23900000
C	3.22150000	2.41870000	-1.21240000
C	2.37000000	-1.19260000	-3.16730000
C	-2.31720000	2.35220000	-2.37010000
C	-2.35310000	1.15800000	-3.15530000
C	-1.22180000	-0.73600000	-3.89660000
C	1.55410000	3.91670000	-0.02460000
C	-0.00270000	-1.47890000	-3.85470000
C	2.84110000	3.21950000	-0.03040000
C	3.82410000	1.18780000	-0.73540000
C	3.74150000	-0.03710000	-1.46620000
C	-1.41310000	3.81010000	-0.01790000
C	-3.09340000	-0.00060000	-2.71110000
C	-2.40130000	-1.18510000	-3.18070000
C	-3.09510000	2.38380000	-1.17410000

C	2.32650000	-2.36320000	-2.36230000
C	3.19380000	2.41120000	1.14520000
C	0.77300000	3.86040000	1.19750000
C	3.81790000	1.20040000	0.69900000
C	-0.01690000	-2.70160000	-3.11400000
C	-2.65380000	3.11010000	-0.01160000
C	-0.66990000	3.86170000	1.20450000
C	1.14020000	-3.15940000	-2.38890000
C	3.06540000	-2.37080000	-1.14670000
C	-3.82570000	1.22600000	-0.72660000
C	-3.83290000	0.00270000	-1.47910000
C	-2.43960000	-2.41930000	-2.42500000
C	-1.19240000	-3.13760000	-2.39190000
C	1.19910000	3.11540000	2.36750000
C	2.39650000	2.35130000	2.35650000
C	3.78580000	-0.01930000	1.44600000
C	3.78090000	-1.22370000	0.70250000
C	-3.10340000	2.40290000	1.16210000
C	-1.12400000	3.15620000	2.37300000
C	0.69590000	-3.86750000	-1.22000000
C	-3.82690000	1.24120000	0.71730000
C	2.65530000	-3.09580000	0.00090000
C	0.02850000	2.68390000	3.09810000
C	-3.96360000	-1.25250000	-0.75570000
C	-0.73780000	-3.85600000	-1.21320000
C	-3.28340000	-2.47640000	-1.22160000
C	-2.31580000	2.37570000	2.34930000
C	3.11020000	-2.38610000	1.15670000
C	2.41230000	1.15650000	3.14350000
C	3.11320000	-0.01930000	2.70600000
C	1.42420000	-3.82070000	0.00500000
C	-3.76750000	0.02630000	1.44280000
C	-3.84100000	-1.19800000	0.69190000
C	-2.73390000	-3.11670000	-0.02040000
C	0.01650000	1.48180000	3.89270000
C	-1.46960000	-3.81430000	0.00580000
C	1.23870000	0.72450000	3.88550000
C	2.38390000	-1.17370000	3.15670000
C	2.34980000	-2.36350000	2.37060000
C	-2.33200000	1.17450000	3.16230000
C	-3.10730000	-2.34530000	1.14300000
C	0.69930000	-3.85420000	1.23550000
C	-3.03100000	0.01150000	2.68240000

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C	-1.24430000	0.74840000	4.03360000
C	1.22780000	-0.72920000	3.91050000
C	-0.73790000	-3.86710000	1.24260000
C	1.15290000	-3.13300000	2.39650000
C	-2.33890000	-2.34060000	2.36570000
C	-2.36810000	-1.15840000	3.20030000
C	-1.26810000	-0.74100000	4.08580000
C	-0.00670000	-1.49410000	3.96630000
C	-1.17570000	-3.15220000	2.40820000
C	-0.00820000	-2.68150000	3.13660000
C	0.17570000	-0.23910000	0.17280000
C	0.15990000	0.04360000	-1.12510000
Sc	-1.66500000	-1.02830000	-0.71410000
Sc	-0.42870000	-0.16140000	2.14140000
Sc	1.27770000	1.61470000	-0.20380000
N	3.77730000	-1.22990000	-0.71690000

Table S1 Computed IR-Active Vibrational Wavenumbers (ν , cm⁻¹, Unscaled) and the Relative Intensities (I) for the C₂ Sc₃NC@C₆₈ Isomer at the PBE/DNP Level of Theory.^a

ν	I	ν	I
503	0.13	1322	0.14
524	0.13	1332	0.12
592	0.11	1335	0.20
627	0.14	1360	0.35
699	0.12	1374	0.63
1018	0.11	1375	0.15
1156	0.11	1384	0.12
1180	0.15	1428	0.27
1214	0.10	1434	0.12
1262	1.00	1476	0.18
1269	0.10		

^a Only those with relative intensities larger than 0.1 are presented.

Table S2 Computed ^{13}C NMR Chemical Shifts (δ , ppm) and Relative Intensities of the $\text{C}_2\text{Sc}_3\text{NC@C}_{68}$ Isomer at the B3LYP/6-31G* Level of Theory.

No.	δ	intensity	No.	δ	intensity
1	132.4	2	19	145.9	2
2	136.7	2	20	146.1	2
3	137.6	2	21	146.3	2
4	137.7	2	22	146.9	2
5	137.9	2	23	147.1	2
6	139.0	2	24	149.5	2
7	139.2	2	25	150.7	2
8	140.7	2	26	151.0	2
9	140.7	2	27	151.82	2
10	140.9	2	28	152.0	2
11	141.3	2	29	152.2	2
12	144.0	2	30	152.2	2
13	144.3	2	31	153.1	2
14	144.5	2	32	155.8	2
15	145.2	2	33	158.3	2
16	145.3	2	34	159.8	2
17	145.4	2	35	326.8	1
18	145.8	2			

Table S3 Computed IR-Active Vibrational Wavenumbers (ν , cm⁻¹, Unscaled) and the Relative Intensities (I) for the C₂ Sc₃NC@C₇₈ Isomer at the PBE/DNP Level of Theory.^a

ν	I	ν	I
285	0.24	1339	1.00
397	0.35	1340	0.78
524	0.26	1350	0.23
527	0.28	1356	0.26
544	0.40	1360	0.50
549	0.30	1378	0.98
637	0.28	1392	0.98
648	0.28	1393	0.40
779	0.38	1398	0.72
794	0.25	1423	0.39
874	0.27	1445	0.23
1046	0.37	1448	0.21
1183	0.24	1485	0.25
1241	0.34	1491	0.36
1277	0.34	1524	0.20
1319	0.47		

^a Only those with relative intensities larger than 0.2 are presented.

Table S4 Computed ^{13}C NMR Chemical Shifts (δ , ppm) and Relative Intensities of the $\text{C}_2\text{Sc}_3\text{NC@C}_{78}$ Isomer at the B3LYP/6-31G* Level of Theory.

No.	δ	intensity	No.	δ	intensity
1	132.7	2	21	142.1	2
2	133.4	2	22	143.1	2
3	134.8	2	23	143.2	2
4	135.0	2	24	145.2	2
5	135.3	2	25	145.4	2
6	135.5	2	26	145.5	2
7	137.4	2	27	145.5	2
8	137.5	2	28	145.9	2
9	138.1	2	29	147.0	2
10	138.5	2	30	147.4	2
11	138.5	2	31	147.4	2
12	138.6	2	32	147.9	2
13	138.7	2	33	148.7	2
14	140.0	2	34	148.7	2
15	140.3	2	35	151.2	2
16	140.3	2	36	154.0	2
17	140.8	2	37	154.2	2
18	140.9	2	38	155.9	2
19	141.1	2	39	157.4	2
20	141.8	2	40	282.4	1

Supplementary Material for PCCP

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Table S5 Computed IR-Active Vibrational Wavenumbers (ν , cm⁻¹, Unscaled) and the Relative Intensities (I) for the C_{2v} Sc₃NC@C₈₀ Isomer at the PBE/DNP Level of Theory.^a

ν	I	ν	I
364	0.10	1377	0.15
501	0.17	1381	0.75
651	0.25	1381	0.19
702	0.13	1395	0.11
754	0.12	1423	0.72
1252	0.15	1426	0.12
1272	0.20	1429	0.29
1307	0.45	1445	0.24
1309	0.34	1456	0.13
1342	1.00	1492	0.14
1357	0.17	1522	0.34
1366	0.35		

^a Only those with relative intensities larger than 0.1 are presented.

Table S6 Computed ^{13}C NMR Chemical Shifts (δ , ppm) and Relative Intensities of the C_{2v} $\text{Sc}_3\text{NC}@C_{80}$ Isomer at the B3LYP/6-31G* Level of Theory.

No.	δ	intensity	No.	δ	intensity
1	132.6	2	14	141.6	2
2	134.4	2	15	142.2	4
3	135.8	4	16	142.8	4
4	136.3	4	17	143.3	4
5	136.9	4	18	143.4	4
6	137.8	4	19	146.5	2
7	138.0	4	20	148.1	2
8	138.2	4	21	148.4	4
9	139.3	2	22	151.3	4
10	139.4	4	23	153.4	4
11	140.7	4	24	157.9	4
12	140.8	2	25	306.6	1
13	141.1	2			