

Electronic supplementary information

**Scandium Carbides/Cyanides in Boron Cage: Computational
Prediction of X@B₈₀ (X = Sc₂C₂, Sc₃C₂, Sc₃CN and Sc₃C₂CN)**

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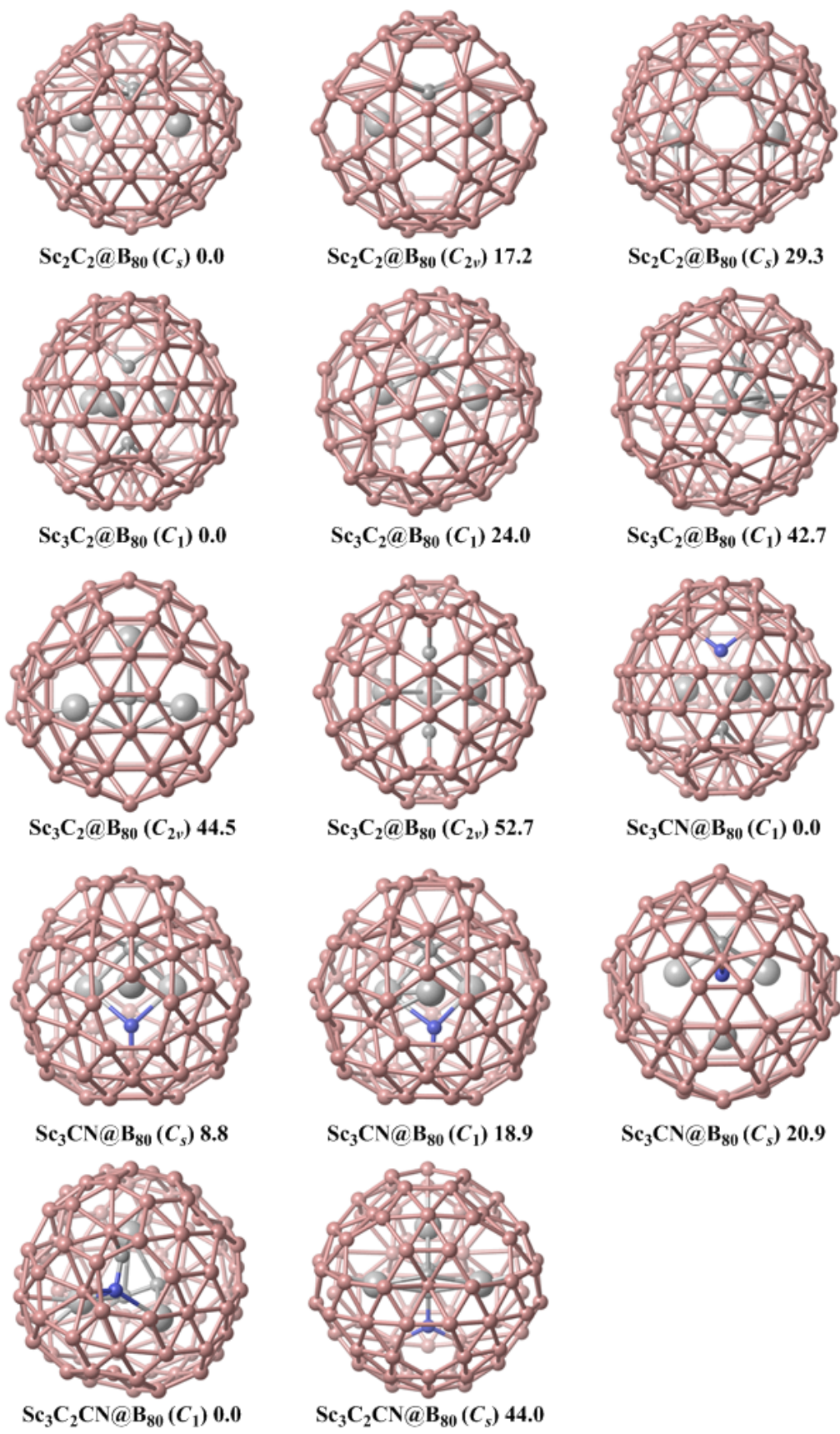


Fig. S1 Some low-energy isomers (with relative energies in kcal/mol, PBE/6-31G*~LanL2DZ level) of X@B₈₀.

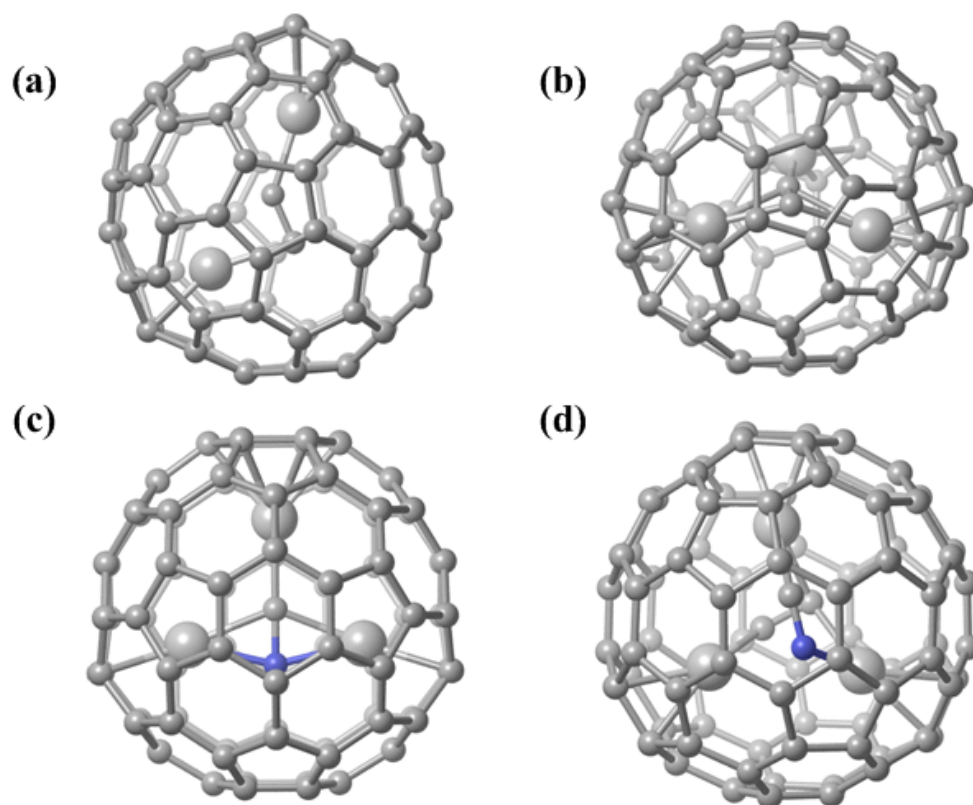


Fig. S2 Optimized structures of (a) $\text{Sc}_2\text{C}_2@C_{2v}(5)\text{-C}_{80}$, (b) $\text{Sc}_3\text{C}_2@I_h(7)\text{-C}_{80}$, (c) $\text{Sc}_3\text{CN}@I_h(7)\text{-C}_{80}$ and (d) $\text{Sc}_3\text{C}_2\text{CN}@I_h(7)\text{-C}_{80}$.

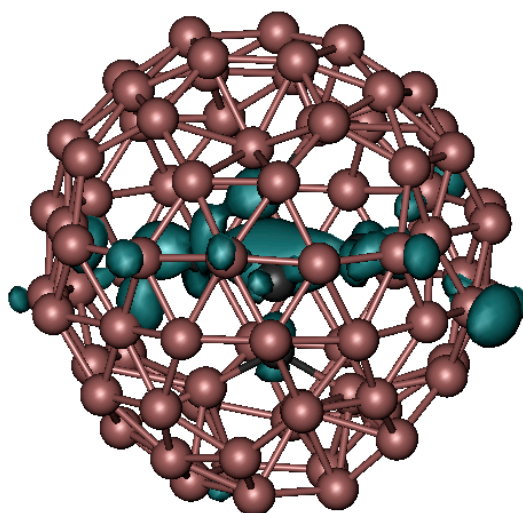


Fig. S3 Spin density distribution of $\text{Sc}_3\text{C}_2@B_{80}$ (isovalue: 0.002 a.u.).

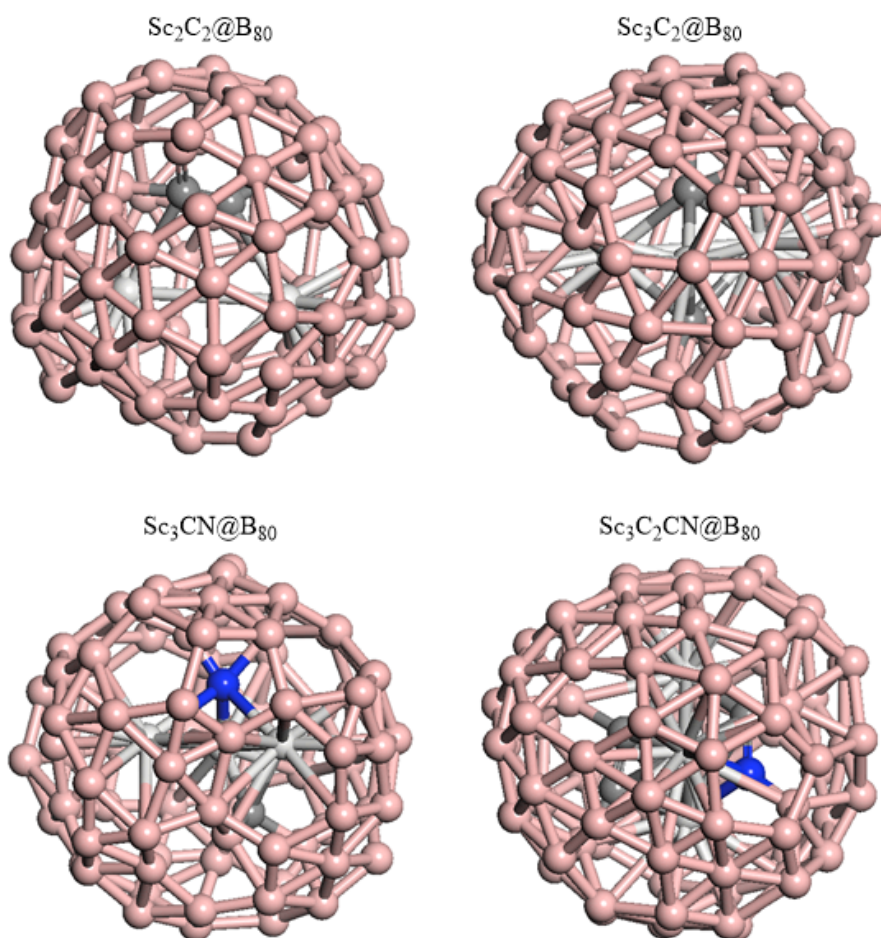


Fig. S4 The structures of $X@B_{80}$ after 3 ps BO-MD simulations at 800 K.

Table S1 Calculated ^{11}B NMR Chemical Shifts (δ : chemical shifts in ppm; M: intensity)

B_{80}		$\text{Sc}_2\text{C}_2@B_{80}$		$[\text{Sc}_3\text{C}_2@B_{80}]^-$		$\text{Sc}_3\text{CN}@B_{80}$		$\text{Sc}_3\text{C}_2\text{CN}@B_{80}$	
δ	M	δ	M	δ	M	δ	M	δ	M
15.0	12	43.3	2	72.4	1	74.0	1	80.7	1
13.9	24	40.3	2	71.3	1	58.6	1	56.1	1
13.4	24	31.9	2	43.9	1	50.8	1	52.4	1
11.9	8	31.5	2	42.0	1	48.6	1	48.7	1
-0.7	12	29.2	2	34.9	1	39.4	1	39.6	1
		28.0	2	33.3	1	38.4	1	36.1	1
		27.1	1	31.7	1	38.0	1	35.5	1
		27.0	2	31.3	1	32.1	2	33.9	1

26.9	2	30.5	1	31.7	1	33.3	1
26.2	2	29.9	1	28.7	1	30.0	2
22.5	2	27.9	1	28.6	1	28.9	1
20.9	2	27.3	1	26.9	1	25.2	1
20.8	2	24.9	1	26.4	1	24.3	1
19.9	2	24.2	1	25.9	1	23.2	1
19.8	2	23.5	1	24.5	1	22.8	1
17.7	2	23.5	1	24.2	1	22.0	1
17.2	3	23.3	2	23.0	1	21.9	1
16.9	2	22.3	1	22.4	1	21.8	1
16.7	2	21.6	1	22.0	1	21.6	1
15.4	2	20.9	1	21.3	1	21.4	2
14.9	2	19.3	1	20.5	1	21.2	1
14.0	2	18.3	1	20.3	1	20.1	1
12.0	2	17.5	1	18.8	1	19.9	1
11.6	2	16.5	1	18.6	1	19.3	1
9.8	2	16.4	1	18.0	1	19.1	2
8.8	2	15.9	1	17.9	1	17.5	1
8.2	2	15.5	1	16.8	1	17.1	1
8.0	2	14.1	1	16.1	1	16.8	1
7.0	2	13.9	3	15.2	1	16.2	1
4.1	2	13.7	1	14.9	2	16.1	2
3.6	4	13.4	1	14.3	1	15.5	1
1.4	2	13.0	1	14.2	1	15.4	1
1.3	2	12.6	1	13.5	1	14.9	1
0.8	1	12.4	1	13.4	1	14.7	1
0.0	2	11.3	3	12.4	1	14.2	1

-1.6	2	11.0	1	12.0	1	12.7	1
-4.0	2	10.9	2	11.1	1	12.6	1
-10.7	1	10.1	1	10.9	2	12.0	1
-12.4	1	10.0	1	10.4	1	11.4	1
-13.9	1	9.3	1	9.9	1	11.1	1
-14.2	1	9.1	1	9.3	1	10.7	1
-14.4	1	8.7	1	9.1	3	10.4	1
		8.6	1	9.0	1	10.1	1
		8.2	1	8.2	1	9.8	1
		7.1	1	7.1	1	9.7	1
		6.4	2	6.7	1	8.7	1
		6.3	1	6.3	1	7.8	1
		5.9	1	6.1	1	7.6	1
		5.5	1	5.6	1	7.0	1
		5.4	1	5.5	3	6.5	1
		5.2	1	5.4	1	6.4	1
		5.0	2	4.9	1	6.3	1
		4.5	1	4.8	1	6.0	1
		4.1	1	4.7	1	5.4	1
		3.8	1	4.1	1	5.3	1
		3.8	1	3.9	2	5.0	1
		3.6	1	3.8	1	4.7	1
		3.2	1	3.6	1	4.1	1
		3.1	1	3.5	1	3.1	1
		2.3	1	3.2	1	1.6	1
		1.5	1	2.6	1	0.8	1
		0.7	1	1.9	1	0.7	1

0.6	1	1.5	1	0.3	1
-0.1	1	1.2	1	-0.3	1
-3.2	1	-1.0	1	-1.2	1
-4.7	1	-1.4	1	-1.5	2
-7.2	1	-2.9	1	-1.6	1
-9.8	1	-4.2	1	-2.3	1
-12.0	1	-4.6	1	-3.5	1
-12.6	1	-8.2	1	-5.4	1
-18.1	1	-9.3	1	-6.0	1
-18.9	1	-33.7	1	-6.6	1
				-9.7	1
				-10.4	1
				-16.8	1

Optimized Cartesian coordinates (PBE/6-31G*~LanL2DZ level)

Sc₂C₂@B₈₀(C_s)

B	-2.84733600	0.72766600	3.13682500	B	1.12715200	-4.19776000	0.00000000
B	-2.76169200	-1.04497000	3.14844800	B	3.31998400	-2.60545700	0.86852900
B	-3.55147000	-1.59099200	1.74796500	B	1.93410900	-3.52984300	1.34845300
B	-3.66410300	1.19868100	1.73823100	B	4.22522400	0.21915000	0.85268400
B	-4.13051900	-0.20620200	0.83942800	B	3.75071300	-1.20012500	1.71238300
B	-1.47316700	1.61052200	3.44580700	B	2.85255800	-0.71117700	3.11329000
B	-0.98520800	2.98766400	2.63234700	B	3.61990700	1.58482200	1.71288000
B	0.72957200	3.10486500	2.67566300	B	2.76180500	1.01154500	3.11245200
B	-0.02617700	0.83689600	4.08076300	B	1.34566800	1.78942900	-3.60971800
B	1.34566800	1.78942900	3.60971800	B	0.72957200	3.10486500	-2.67566300
B	-1.31730900	-1.75748900	3.50213600	B	-0.98520800	2.98766400	-2.63234700
B	0.05741600	-0.82486300	4.08685300	B	-0.02617700	0.83689600	-4.08076300
B	1.51949200	-1.62869400	3.61339700	B	-1.47316700	1.61052200	-3.44580700
B	-0.67919900	-3.01163600	2.62370500	B	3.05028800	2.93165400	-0.86340600
B	1.03677800	-2.99489700	2.67841000	B	3.05028800	2.93165400	0.86340600
B	-2.84925600	-2.82067000	0.89025100	B	1.55930900	3.69856100	1.32679900
B	-1.49269600	-3.68771600	1.32546100	B	1.55930900	3.69856100	-1.32679900
B	-0.58000200	-4.33664400	0.00000000	B	0.70431000	4.31289200	0.00000000
B	-2.84925600	-2.82067000	-0.89025100	B	2.15919700	2.36067500	-2.21233400

B	-1.49269600	-3.68771600	-1.32546100	B	-0.21762600	3.94807300	-1.46620000
B	-2.94950400	2.45357300	0.88445300	B	-1.88381800	1.05215400	-1.63462300
B	-2.94950400	2.45357300	-0.88445300	B	-1.48166200	-0.06817300	-3.79819200
B	-1.85693700	3.63483200	-1.34582600	B	-1.72227700	-1.47294800	-1.66216700
B	-1.85693700	3.63483200	1.34582600	B	0.18226500	-3.91505200	-1.46678100
B	-1.02661800	4.35404800	0.00000000	B	0.18226500	-3.91505200	1.46678100
B	-4.13051900	-0.20620200	-0.83942800	B	-1.72227700	-1.47294800	1.66216700
B	-3.55147000	-1.59099200	-1.74796500	B	-1.48166200	-0.06817300	3.79819200
B	-2.76169200	-1.04497000	-3.14844800	B	1.38661500	0.08048300	3.59919300
B	-3.66410300	1.19868100	-1.73823100	B	2.34265500	-2.07386400	2.17400400
B	-2.84733600	0.72766600	-3.13682500	B	3.77731200	-1.18690200	0.00000000
B	2.85255800	-0.71117700	-3.11329000	B	3.57412200	1.54978900	0.00000000
B	3.75071300	-1.20012500	-1.71238300	B	2.15919700	2.36067500	2.21233400
B	4.22522400	0.21915000	-0.85268400	B	-0.21762600	3.94807300	1.46620000
B	2.76180500	1.01154500	-3.11245200	B	-3.89370600	1.29471400	0.00000000
B	3.61990700	1.58482200	-1.71288000	B	-3.79518700	-1.68674900	0.00000000
B	1.51949200	-1.62869400	-3.61339700	B	2.34265500	-2.07386400	-2.17400400
B	0.05741600	-0.82486300	-4.08685300	B	1.38661500	0.08048300	-3.59919300
B	-1.31730900	-1.75748900	-3.50213600	B	-1.88381800	1.05215400	1.63462300
B	1.03677800	-2.99489700	-2.67841000	Sc	0.14132300	-1.95383700	0.00000000
B	-0.67919900	-3.01163600	-2.62370500	Sc	-0.29090600	1.98581900	0.00000000
B	3.31998400	-2.60545700	-0.86852900	C	-1.31097700	-0.17111100	0.73011700
B	1.93410900	-3.52984300	-1.34845300	C	-1.31097700	-0.17111100	-0.73011700

Sc₃C₂@B₈₀(C₁)

B	2.97040300	-0.84323000	3.01069800	B	-3.28182400	2.49409100	1.13927900
B	2.88915300	0.84665600	3.12283700	B	-1.93131800	3.44078900	1.71832000
B	3.72114400	1.60000300	1.75337300	B	-4.26535800	-0.29472800	0.96601000
B	3.88812600	-1.28689200	1.55512100	B	-3.74828000	1.07057200	1.91319100
B	4.33671700	0.24560400	0.83743100	B	-2.76107900	0.46426400	3.20195700
B	1.60927000	-1.71445300	3.39937500	B	-3.50380300	-1.65380200	1.70899500
B	1.11435300	-3.08991100	2.47052000	B	-2.66802700	-1.23798100	3.14978600
B	-0.59129900	-3.28720300	2.57742100	B	-1.46347100	-1.51723300	-3.63568900
B	0.16992300	-1.15541900	4.02142300	B	-0.71714500	-2.87531800	-3.00270500
B	-1.24131400	-2.06123600	3.58818100	B	1.02383300	-2.90750500	-3.08331500
B	1.42080100	1.45711300	3.58449000	B	-0.12382900	-0.53410500	-4.18617300
B	0.11586600	0.51096100	3.93485300	B	1.34598700	-1.37403900	-3.76225200
B	-1.38985600	1.34654800	3.67179000	B	-2.91050300	-2.70790500	-1.01509000
B	0.74718900	2.90473100	2.92642400	B	-2.83736000	-2.84398100	0.72041400
B	-1.00645700	2.86808700	3.02636200	B	-1.41542000	-3.69578200	1.15144300
B	3.03337000	2.92636100	1.01840200	B	-1.45875100	-3.29531200	-1.57318500
B	1.53137200	3.63234800	1.63725900	B	-0.56008500	-3.99975200	-0.27518100
B	0.59719600	4.21549000	0.29815800	B	-1.81721100	-1.23879900	-1.64686700
B	2.84755100	3.09164700	-0.64456800	B	0.17352900	-3.72383800	-1.81226900

B	1.42702700	3.93957400	-1.16476400	B	2.50881700	-2.08558600	-2.58314600
B	3.37252000	-2.56764200	0.61557500	B	1.07436200	0.32032300	-3.35643100
B	3.22382200	-2.54641300	-1.07380700	B	2.16083700	2.73850300	-2.18466600
B	1.92189700	-3.48628200	-1.75062100	B	-0.32734300	3.97535200	-1.19618600
B	1.97689300	-3.49741800	1.07482000	B	-0.15599200	3.46822400	1.65012600
B	1.13134400	-4.02793000	-0.33707200	B	2.39871400	2.37401900	2.52742800
B	4.06304000	0.33500500	-0.77721500	B	1.48970600	-0.03377500	2.36939600
B	3.26369300	1.68388800	-1.44233800	B	-1.32271700	-0.35378200	3.86681300
B	2.44981600	1.22128100	-2.89463900	B	-2.31663200	1.89975800	2.37557800
B	3.44754300	-0.99733900	-1.66095700	B	-3.96534900	1.22234500	0.17643700
B	2.57459500	-0.44629600	-3.04972300	B	-3.70367200	-1.56322700	-0.04314600
B	-2.97694900	0.93218000	-2.95666900	B	-2.19332900	-2.64673200	2.27002300
B	-3.82549700	1.27665800	-1.53393900	B	0.28928400	-3.27821000	1.01579000
B	-4.37030500	-0.17738600	-0.71066900	B	2.88444200	-0.76062600	0.14029200
B	-2.87131200	-0.82809600	-3.09943200	B	2.75430100	1.12108900	0.29971100
B	-3.68489700	-1.44201600	-1.75018600	B	-1.95659800	1.26103500	-1.45694800
B	-1.66729100	1.84932000	-3.36363400	B	-1.72378300	0.19051500	-3.86738800
B	-0.23247300	1.13863500	-4.05402500	B	2.72123900	-2.33991700	2.21188900
B	1.10643500	2.08026700	-3.46690700	Sc	-0.74461400	-0.76537500	1.43288400
B	-1.10983500	3.15442100	-2.49036900	Sc	0.42303800	1.63093500	-0.73257900
B	0.59322000	3.42866500	-2.55547900	Sc	0.68300300	-1.39342700	-1.11203000
B	-3.25485600	2.52240900	-0.60879200	C	-1.16205500	-0.00426500	-0.86381100
B	-1.89072000	3.34097200	-1.03448100	C	1.53149700	0.03850100	0.68621400
B	-1.08871000	4.00335200	0.34589700				

Sc₃CN@B₈₀(C₁)

B	1.58344100	1.81886500	3.33846700	B	2.73991500	-2.04319300	-2.78120100
B	2.33043600	0.27407000	3.50978200	B	3.15446700	-2.73443900	-1.20558500
B	1.19306800	-0.86509800	4.13279400	B	1.84919100	0.56254200	-3.73079800
B	-0.10809400	1.69095000	3.76116000	B	3.03306700	-0.42580900	-3.07734900
B	-0.23583700	0.09211300	4.25140400	B	3.76741800	0.62946800	-1.87522700
B	2.05810500	2.86942100	2.11367700	B	1.90967400	2.17966700	-3.09811200
B	0.85896400	3.84810000	1.32295000	B	3.19194000	2.26534500	-1.97291900
B	1.43385800	3.92641600	-0.23528100	B	-3.56077100	0.21090900	-2.37043000
B	3.30587800	2.44654100	0.99496700	B	-3.52007100	1.83283300	-1.74118500
B	2.94878600	3.13818000	-0.52424700	B	-4.02843100	1.77578300	-0.07805300
B	3.41167000	-0.19631900	2.29491800	B	-4.09376200	-0.88770100	-1.18692700
B	3.92924500	0.86776300	1.07990200	B	-4.27409100	0.08518000	0.23243800
B	4.05612600	-0.03970200	-0.36977100	B	-1.07019300	2.37697800	-3.32887500
B	3.23368800	-1.75275200	1.56332100	B	0.44109200	2.96510500	-2.82622300
B	3.71692700	-1.71299100	-0.03169700	B	0.18582400	3.76405700	-1.32895600
B	1.09431000	-2.42793700	3.45604000	B	-2.26994000	2.87204300	-2.18576300
B	2.17616900	-2.89479300	2.19128800	B	-1.42547100	3.77670700	-0.93728100
B	1.50987400	-3.76089900	0.91951200	B	-2.24967500	1.27280100	-2.73481400

B	-0.40104400	-3.02996200	2.85951100	B	-2.86440700	2.98341100	-0.55916800
B	-0.16494200	-3.85566000	1.37724500	B	-3.43989500	1.11915800	1.39457600
B	-1.22580800	2.70487400	3.06615600	B	-3.83233700	-1.60887800	0.37291800
B	-2.74083300	2.12327300	2.59814900	B	-1.41688100	-2.70229000	1.42686900
B	-3.30920000	2.78421100	1.07581800	B	0.32227600	-4.16976100	-0.29419400
B	-0.72137400	3.83938100	1.80179400	B	1.84525400	-2.07568600	-0.11003800
B	-1.94320900	3.81716600	0.62795000	B	2.44256000	-1.43623900	3.03563900
B	-1.64739100	-0.44408700	3.52670200	B	2.53152500	1.24365600	2.05176900
B	-1.79283400	-2.07423500	2.97324800	B	3.77398600	1.61509000	-0.47589900
B	-3.01545400	-2.10018300	1.80892700	B	3.65695400	-1.16803600	-1.65687100
B	-2.86191600	0.47414400	2.84113400	B	1.26331100	-0.99176900	-2.51425700
B	-3.69566900	-0.53736200	1.69010500	B	0.40194800	1.47744200	-3.62503800
B	-1.52195500	-1.81035500	-3.17752700	B	1.75855300	3.29144800	-1.78155700
B	0.07530800	-1.77314200	-3.75769200	B	-0.43317700	2.72489300	0.37153600
B	0.37046400	-0.14495100	-4.02685500	B	-1.21417000	1.20184400	2.07491600
B	-2.29983700	-0.26931100	-3.40779000	B	-0.39139600	-1.54203000	3.81308900
B	-1.12153600	0.79018300	-3.93053100	B	-0.08787700	-2.20502300	-1.94258200
B	-2.15784900	-2.95108400	-2.14175200	B	-2.99471500	-1.49271700	-2.43832800
B	-3.43895100	-2.45576100	-1.07431200	B	0.43815100	3.03925000	2.79569700
B	-2.86771100	-3.05734800	0.42342400	C	0.68658100	-1.17304800	-0.88156900
B	-0.91985000	-3.88557000	-1.47769500	Sc	1.31982800	1.13049500	-0.62876700
B	-1.37467400	-3.87633800	0.19707400	Sc	0.52709600	-0.70728600	1.68906700
B	1.23024600	-2.77884400	-3.17604600	Sc	-1.63989300	-0.71540400	-0.45867100
B	0.68005600	-3.85182200	-1.92981700	N	-0.58081700	1.20907900	0.68900000
B	1.94921600	-3.79901900	-0.68177400				

Sc₃C₂CN@B₈₀(C₁)

B	-2.98908100	0.67051900	2.91076900	B	2.70131900	3.25492000	0.83891600
B	-1.62172100	1.28250500	3.75287800	B	0.54702100	2.90775900	-3.04578400
B	-0.68580600	-0.12875600	4.27706700	B	1.15575600	3.78628400	-1.67234500
B	-2.97648600	-1.02072300	2.88488300	B	-0.22857600	4.10863700	-0.73975600
B	-1.52786800	-1.53916600	3.78179700	B	-1.20723700	2.89225900	-3.02067100
B	-3.59388300	1.52147300	1.56178600	B	-1.71167300	3.67191900	-1.58970600
B	-4.22977300	0.68619600	0.21892300	B	0.77619300	-2.64586600	-3.19590200
B	-3.80489700	1.65854500	-1.20130900	B	-0.89833000	-2.64475600	-3.14496000
B	-2.85343900	2.95933600	1.06739600	B	-1.28548900	-3.51879300	-1.67890300
B	-2.97309200	3.03884900	-0.70151700	B	1.52022300	-3.62989200	-1.88124500
B	-0.86528100	2.68269200	3.23015400	B	0.14648700	-4.10448600	-0.95438100
B	-1.49483600	3.54474100	1.87001600	B	-1.10539100	0.10978800	-4.11920000
B	-0.15182600	4.03792700	0.93713300	B	-2.02504600	1.49966600	-3.51533100
B	0.87207800	2.72839900	3.13531600	B	-3.33579000	0.88648200	-2.63457200
B	1.31102100	3.64810900	1.75071200	B	-1.82292300	-1.32126500	-3.59550500
B	1.00341300	-0.06496700	4.17585600	B	-3.17971700	-0.84649500	-2.59810000
B	1.79747500	1.39943900	3.60920800	B	-0.19342800	-0.90963200	-2.85625600

B	3.20581000	0.95890100	2.69406800	B	-2.39361500	-2.33952100	-2.34459500
B	1.97118900	-1.38055400	3.60998800	B	-1.05974400	-3.10514600	-0.01876600
B	3.35937600	-0.78385000	2.69485900	B	1.72200600	-3.85971100	-0.12848900
B	-3.58571100	-1.87518000	1.55226800	B	2.10029700	-1.58228900	1.74194600
B	-2.62663000	-3.16299000	0.93905100	B	3.97181600	0.12169700	1.38495400
B	-2.66100500	-3.09223300	-0.76226600	B	2.20412100	2.24387500	2.19541900
B	-4.28473100	-1.00636000	0.18266100	B	0.09003500	1.36448900	3.89656300
B	-3.64320200	-1.75712000	-1.24918400	B	-2.03590900	1.92234900	2.19142400
B	-0.59251200	-2.77530100	3.11811600	B	-1.67571400	3.76006200	0.14485100
B	1.15858700	-2.68180200	3.02644000	B	1.27003800	3.88015200	0.03392200
B	1.63716800	-3.40534700	1.54413700	B	2.05755200	2.49365300	-2.35423700
B	-1.14441800	-3.58280700	1.66538800	B	-0.33349800	1.61207300	-3.83773700
B	0.21843500	-4.00066200	0.73566700	B	-1.98582800	1.82510800	-1.67326100
B	2.90391200	-0.63479400	-2.83254000	B	-3.89850800	-0.04866200	-1.29334200
B	2.87248600	1.06617700	-2.83175400	B	-2.15917800	-2.48363800	2.50181300
B	1.38969600	1.56440100	-3.59161100	B	0.08538000	-1.15194000	3.00169800
B	1.48831200	-1.20185500	-3.67110100	B	3.26816000	0.17291200	-1.38311800
B	0.58140500	0.14725800	-4.16380400	B	2.36144000	-2.28507500	-2.59779300
B	3.57880700	-1.52121700	-1.54937700	B	-3.88914800	-0.19865900	1.69172700
B	2.91377200	-3.03902000	-1.09410700	C	-0.83808200	1.00253800	-1.01744700
B	3.00093300	-2.93291000	0.68393200	C	-0.28248200	-0.12080200	-1.50541400
B	4.16029400	-0.64148100	-0.17219200	Sc	1.18679300	1.34146300	-0.17399000
B	3.87009800	-1.58404800	1.27797600	Sc	0.96295200	-1.67493600	-0.64376800
B	3.47475900	1.94726400	-1.49287600	Sc	-1.84569500	-0.49104900	0.36860100
B	4.06000600	1.04899900	-0.14666000	C	0.00684300	-0.57131300	1.53956300
B	3.60189100	1.85781000	1.30470900	N	1.26421300	-0.49729000	1.06149700
B	2.61173600	3.31203900	-0.90181600				