

Supporting material

Theoretical exploration of noncovalent interactions in $\text{Sc}_2\text{C}_2@C_{2n}$ ($n = 40, 41, \text{ and } 42$) \subset [12]CPP, PF[12]CPP

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Table S1 Selected Interatomic Distances and Angles

Molecules	Distance(Å)	Distance(Å)	Dihedral angle(°)
	C-C	Sc-Sc	Sc-C ₂ -Sc
Sc ₂ C ₂ @C ₈₀	1.265	3.692	112.7
Sc ₂ C ₂ @C ₈₀ ⊂[12]CPP	1.265	3.698	112.3
Sc ₂ C ₂ @C ₈₀ ⊂PF[12]CPP	1.265	3.677	111.8
Sc ₂ C ₂ @C ₈₂	1.266	3.939	126.0
Sc ₂ C ₂ @C ₈₂ ⊂[12]CPP	1.266	3.937	125.6
Sc ₂ C ₂ @C ₈₂ ⊂PF[12]CPP	1.266	3.936	125.8
Sc ₂ C ₂ @C ₈₄	1.267	4.473	180.0
Sc ₂ C ₂ @C ₈₄ ⊂[12]CPP	1.267	4.477	180.0
Sc ₂ C ₂ @C ₈₄ ⊂PF[12]CPP	1.267	4.476	180.0

Table S2. Binding energies with and without (ΔE_{cp} and ΔE , kcal mol⁻¹) BSSE (kcal mol⁻¹) correction. ΔE_{def} is the deformation energy of the monomers.

Complexes	ΔE^a	BSSE ^a	ΔE_{cp}^a	ΔE_{def}	
				Full	Ring
C ₈₀ ⊂[12]CPP	-44.45	1.21	-43.24	0.91	4.74
C ₈₂ ⊂[12]CPP	-45.28	1.27	-44.01	0.80	4.96
C ₈₄ ⊂[12]CPP	-47.11	1.23	-45.88	0.74	1.94
C ₈₀ ⊂PF[12]CPP	-56.06	4.93	-51.13	0.71	1.85
C ₈₂ ⊂PF[12]CPP	-56.65	5.01	-51.65	0.66	1.64
C ₈₄ ⊂PF[12]CPP	-57.27	5.26	-52.01	0.58	1.23

^a obtained at the ω B97M-V/TZVPP level

The coordinates for optimized compounds at the theory level of M06-2X-D3/6-31G*

The coordinates of optimized of [12]CPP

C	-8.96040800	0.69365500	-0.37836500
C	-8.96015300	-0.69704100	-0.37830400
C	-8.16008700	-1.41843600	0.51786100
C	-7.46826000	-0.69432800	1.49630200
C	-7.46852000	0.69165300	1.49624500
C	-7.81850300	-2.85078900	0.32932300
C	-7.63994100	-3.35694800	-0.96449900
C	-6.94296500	-4.53809200	-1.17983400
C	-6.38434400	-5.24961200	-0.11085800
C	-6.70522200	-4.83014500	1.18615900
C	-7.41588100	-3.65664600	1.40203900
C	-5.29072700	-6.22957500	-0.32625300
C	-4.36007400	-5.96702000	-1.33873100
C	-3.15204800	-6.64242600	-1.39484200
C	-2.81956800	-7.61617800	-0.44518300
C	-3.79778200	-7.96192700	0.49686700
C	-5.00922300	-7.28022100	0.55675500
C	-1.40539700	-8.05767800	-0.35380400
C	-0.57218800	-8.05775300	-1.47991900
C	0.80895100	-8.06994800	-1.34817200
C	1.41579900	-8.11040500	-0.08617300
C	0.58051800	-8.29570600	1.02320100
C	-0.80178400	-8.25680200	0.89413600
C	2.83994000	-7.71709000	0.06548400
C	3.77832400	-7.85675800	-0.96697800
C	4.98459300	-7.16633800	-0.93809900
C	5.30574500	-6.32302400	0.13281900
C	4.43119600	-6.29563900	1.22485100
C	3.22157700	-6.97255200	1.18885600
C	6.37384600	-5.29562900	0.06176700

C	6.52712000	-4.55118100	-1.11290600
C	7.22111600	-3.34793700	-1.10888200
C	7.79273200	-2.84948200	0.06746400
C	7.77050800	-3.67215400	1.20236400
C	7.07034600	-4.87106300	1.20082200
C	7.79163400	2.85237600	0.06779400
C	7.21992400	3.35076300	-1.10853500
C	6.52547200	4.55374400	-1.11246300
C	6.37180700	5.29797600	0.06229400
C	7.06836900	4.87353000	1.20135600
C	7.76899900	3.67489000	1.20280000
C	5.30332200	6.32497200	0.13336700
C	4.98198200	7.16829600	-0.93748400
C	3.77545800	7.85826300	-0.96642400
C	2.83700200	7.71812500	0.06590900
C	3.21878700	6.97359300	1.18923800
C	4.42865200	6.29712500	1.22529200
C	1.41273000	8.11091300	-0.08589600
C	0.80604900	8.07029100	-1.34796900
C	-0.57507000	8.05758300	-1.47988600
C	-1.40842100	8.05716100	-0.35387500
C	-0.80502900	8.25648200	0.89414200
C	0.57724200	8.29587300	1.02338100
C	-2.82242600	7.61515900	-0.44542000
C	-3.15447400	6.64125600	-1.39507700
C	-4.36224800	5.96539000	-1.33903800
C	-5.29307900	6.22761800	-0.32664100
C	-5.01204200	7.27841300	0.55634300
C	-3.80085700	7.96057300	0.49653100
C	-6.38631600	5.24723300	-0.11123100
C	-6.94460400	4.53540100	-1.18017400
C	-7.64113400	3.35400600	-0.96477000
C	-7.41731800	3.65400300	1.40175100
C	-6.70710800	4.82775800	1.18580500
C	-7.81956700	2.84789000	0.32908600
C	-8.16061300	1.41542400	0.51774200
C	7.81497600	0.69482800	1.29430200
C	8.16300300	1.41764200	0.14696500
C	8.63976800	0.69666300	-0.95580500
C	8.64003100	-0.69332100	-0.95588800
C	8.16354800	-1.41461300	0.14679800
C	7.81524900	-0.69206600	1.29422200
H	-9.55592100	1.22659000	-1.11490900
H	-9.55546700	-1.23025900	-1.11480500

H	-6.82327500	-1.21954400	2.19402500
H	-6.82372700	1.21716200	2.19392400
H	-7.95663300	-2.76594000	-1.81915200
H	-6.76182700	-4.87158000	-2.19789000
H	-6.30398800	-5.37187500	2.03828800
H	-7.59163900	-3.32068300	2.42024900
H	-4.53458700	-5.14336000	-2.02402100
H	-2.41082500	-6.32752600	-2.12240300
H	-3.59592500	-8.75043200	1.21701700
H	-5.73252900	-7.54413100	1.32402100
H	-1.00862300	-7.97025400	-2.47067600
H	1.42173000	-7.94743600	-2.23642500
H	1.01539000	-8.39835600	2.01312800
H	-1.41676900	-8.28313800	1.78916800
H	3.54290700	-8.47758700	-1.82695800
H	5.67052300	-7.24931200	-1.77720500
H	4.64725200	-5.63975600	2.06322400
H	2.51586600	-6.82355700	1.99976200
H	5.99211600	-4.85379300	-2.00875600
H	7.21475100	-2.73060200	-2.00248800
H	8.26535000	-3.34304900	2.11210500
H	7.02010300	-5.46459000	2.10988100
H	7.21388200	2.73354500	-2.00222400
H	5.99043800	4.85627400	-2.00832300
H	7.01782500	5.46692200	2.11048600
H	8.26389200	3.34585500	2.11253900
H	5.66797400	7.25161800	-1.77650500
H	3.53991100	8.47910100	-1.82636200
H	2.51303500	6.82422200	2.00003600
H	4.64484900	5.64121200	2.06360500
H	1.41897700	7.94804500	-2.23615500
H	-1.01134200	7.96997600	-2.47070500
H	-1.42013000	8.28257800	1.78910100
H	1.01194800	8.39867000	2.01336500
H	-2.41307600	6.32659200	-2.12256000
H	-4.53637400	5.14163200	-2.02430700
H	-5.73550700	7.54207800	1.32354300
H	-3.59936300	8.74917900	1.21667100
H	-6.76354900	4.86886600	-2.19825000
H	-7.95754700	2.76279900	-1.81938900
H	-7.59300300	3.31806800	2.41998200
H	-6.30613000	5.36971500	2.03791000
H	7.42644500	1.22207500	2.16055700
H	8.97379500	1.23089900	-1.84135900

H	8.97426400	-1.22732300	-1.84150600
H	7.42692000	-1.21956100	2.16041600

The coordinates of optimized of PF[12]CPP

C	0.70067000	-8.66924200	-0.71307100
C	-0.69577600	-8.66970800	-0.71311500
C	-1.41753700	-7.48078900	-0.74426400
C	-0.68708400	-6.29029500	-0.73381200
C	0.69042000	-6.28983800	-0.73371500
C	-2.89011200	-7.33925100	-0.73020200
C	-3.69292800	-7.80897600	0.30564700
C	-4.97584100	-7.30740800	0.50701400
C	-5.49264500	-6.29137900	-0.29895600
C	-4.72861900	-5.91565700	-1.40757800
C	-3.47029900	-6.44436700	-1.62749700
C	-6.56062500	-5.36410500	0.13991200
C	-6.44972400	-4.78290300	1.40541500
C	-7.07853100	-3.58674100	1.70670900
C	-7.80357400	-2.88625200	0.74417300
C	-8.03354700	-3.53241200	-0.46948400
C	-7.44243300	-4.75715400	-0.75665600
C	-7.97641600	-1.42430200	0.88766600
C	-6.82977100	-0.69108700	1.20297600
C	-6.83024400	0.68763100	1.20293800
C	-7.97739200	1.42005800	0.88761200
C	-9.12478800	0.69501800	0.57616500
C	-9.12431500	-0.70005300	0.57621300
C	-7.80540600	2.88209900	0.74406200
C	-7.08080800	3.58296200	1.70666500
C	-6.45263800	4.77947600	1.40544900
C	-6.56379000	5.36065400	0.13995800
C	-7.44524900	4.75327500	-0.75665500
C	-8.03571900	3.52819600	-0.46955200
C	-5.49631000	6.28851200	-0.29887600
C	-4.98005100	7.30479100	0.50711400
C	-3.69740700	7.80706200	0.30574300
C	-2.89433400	7.33776000	-0.73009100
C	-3.47401300	6.44252300	-1.62737400
C	-4.73204600	5.91314400	-1.40745900
C	2.88989700	7.33899000	-0.73006000
C	3.69289600	7.80881600	0.30560300
C	4.97583300	7.30724300	0.50681900
C	5.49248900	6.29111000	-0.29911200

C	4.72824800	5.91521500	-1.40751900
C	3.46992300	6.44395000	-1.62732400
C	6.56057700	5.36393500	0.13965700
C	6.45007000	4.78291300	1.40527100
C	7.07905200	3.58684600	1.70658800
C	7.80385200	2.88623000	0.74396000
C	8.03349000	3.53225500	-0.46983000
C	7.44221300	4.75692100	-0.75703200
C	7.97677900	1.42432200	0.88765300
C	6.83021900	0.69117400	1.20338200
C	6.83063100	-0.68756100	1.20345400
C	7.97762100	-1.42006500	0.88776600
C	9.12496400	-0.69507200	0.57593600
C	9.12455700	0.69997700	0.57589100
C	7.80558600	-2.88210400	0.74418500
C	7.08117200	-3.58312300	1.70679400
C	6.45290900	-4.77957800	1.40546800
C	6.56378300	-5.36052200	0.13986700
C	7.44506700	-4.75297400	-0.75683400
C	8.03561200	-3.52797600	-0.46962600
C	5.49618200	-6.28823500	-0.29896600
C	4.97999900	-7.30466300	0.50690500
C	3.69733100	-7.80688700	0.30562200
C	3.47376300	-6.44212000	-1.62728600
C	4.73180700	-5.91273700	-1.40741300
C	2.89413000	-7.33744600	-0.73005900
C	1.42165600	-7.47984500	-0.74415400
C	0.68673500	6.29022400	-0.73352800
C	1.41733900	7.48062900	-0.74405900
C	0.69573700	8.66964800	-0.71306300
C	-0.70071400	8.66937200	-0.71307800
C	-1.42183400	7.48007000	-0.74412100
C	-0.69076200	6.28995400	-0.73359300
F	1.34172900	-9.83387400	-0.70413200
F	-1.33605800	-9.83477000	-0.70420800
F	-1.31157400	-5.11542200	-0.69480500
F	1.31415300	-5.11456500	-0.69457100
F	-3.19645700	-8.67469700	1.18490800
F	-5.67151600	-7.74990700	1.54986600
F	-5.13338100	-4.93133900	-2.20613400
F	-2.76048200	-5.97485200	-2.65008200
F	-5.61523600	-5.29072200	2.30862200
F	-6.85842100	-3.04309800	2.90054700
F	-8.73091200	-2.91986600	-1.42229900

F	-7.64579100	-5.29140900	-1.95706200
F	-5.67302100	-1.30792700	1.43481300
F	-5.67391800	1.30526600	1.43473400
F	-10.24705800	1.33365000	0.25935300
F	-10.24614300	-1.33947600	0.25944100
F	-6.86044100	3.03934900	2.90047300
F	-5.61849400	5.28775900	2.30872300
F	-7.64889500	5.28747000	-1.95704000
F	-8.73275300	2.91535600	-1.42240900
F	-5.67596000	7.74686200	1.54999800
F	-3.20140200	8.67306300	1.18499700
F	-2.76388800	5.97331900	-2.64988100
F	-5.13625800	4.92856000	-2.20596800
F	3.19659800	8.67465700	1.18484900
F	5.67169900	7.74984800	1.54950400
F	5.13283300	4.93073300	-2.20596600
F	2.75995300	5.97432700	-2.64974700
F	5.61579200	5.29081400	2.30863600
F	6.85932900	3.04337800	2.90058200
F	8.73066200	2.91968400	-1.42275800
F	7.64529500	5.29099000	-1.95756700
F	5.67354100	1.30804500	1.43545300
F	5.67432400	-1.30508500	1.43569500
F	10.24708800	-1.33379300	0.25879900
F	10.24633200	1.33931300	0.25874500
F	6.86104400	-3.03976000	2.90075800
F	5.61889700	-5.28794400	2.30880700
F	7.64837600	-5.28692200	-1.95738500
F	8.73244100	-2.91493100	-1.42251200
F	5.67602500	-7.74694800	1.54961400
F	3.20144700	-8.67300100	1.18482800
F	2.76363300	-5.97288900	-2.64978500
F	5.13591400	-4.92807500	-2.20587600
F	1.31109500	5.11528500	-0.69437300
F	1.33619600	9.83461100	-0.70424100
F	-1.34163900	9.83408100	-0.70423100
F	-1.31465400	5.11476500	-0.69453800

The coordinates of optimized of $\text{Sc}_2\text{C}_2@C_{80}$

C	4.05270400	1.52397700	-0.04842700
C	3.73376600	1.73847900	1.28686400
C	4.16196600	0.19301300	-0.55560100
C	3.51548400	0.63088700	2.16694700
C	3.94877400	-0.91551700	0.28368000

C	3.62118500	-0.69786700	1.69786800
C	3.44144400	2.34332000	-1.06788400
C	2.81857700	2.79313500	1.64909400
C	3.64831000	0.19420900	-1.91939100
C	2.48941400	1.01739600	3.11019200
C	3.43965400	-2.10208300	-0.36292700
C	2.83888500	-1.68052000	2.38718300
C	3.14496700	1.52251600	-2.20355500
C	2.00257500	2.33146500	2.73092800
C	2.57742600	3.36397200	-0.72139000
C	2.25512000	3.59247200	0.67121700
C	3.10675000	-0.96045900	-2.52855800
C	1.63700600	0.06277500	3.67046300
C	3.09312200	-2.19833200	-1.76269400
C	1.85622400	-1.30179000	3.34290600
C	2.62429900	-3.02085400	0.36130600
C	2.35575200	-2.85361200	1.73088800
C	1.95957800	1.71611400	-2.94945900
C	0.63406800	2.65132000	2.79009400
C	1.39554200	3.60366900	-1.50444400
C	0.87613900	3.97894200	0.76032100
C	1.98937400	-3.16093300	-1.88187900
C	0.74255800	-2.21795400	3.25597900
C	1.68449900	-3.60587000	-0.52772100
C	1.06888000	-3.17874900	2.21849100
C	2.00227000	-0.74845400	-3.42716400
C	0.27005800	0.44404300	3.94231000
C	1.02276800	2.77717100	-2.58103200
C	0.02243100	3.48655100	1.76734800
C	0.40634100	4.12523500	-0.59617900
C	1.43958000	0.56257600	-3.60513100
C	-0.20630100	1.69478800	3.45705400
C	0.86243300	-2.91645000	-2.77265400
C	0.36806900	-3.94282900	-0.04167500
C	0.92376900	-1.71153700	-3.56828600
C	0.06318600	-3.70739000	1.36413200
C	-0.59624000	-1.85724000	3.58958500
C	-0.83968000	-0.48292000	4.03805700
C	0.05301400	0.42459700	-3.89653000
C	-1.60481100	1.57346600	3.20938800
C	-0.91470600	3.99509600	-0.87867200
C	-0.41200800	2.63378700	-2.88350700
C	-1.41357400	3.34342900	1.46336700
C	-0.26980200	-0.95913700	-3.85677500

C	-2.03182000	0.24644100	3.59041300
C	-0.67231200	-3.88107200	-0.99361300
C	-1.28197800	-3.40036800	1.72080500
C	-0.42632200	-3.29349500	-2.30904300
C	-1.60796600	-2.46891700	2.78778000
C	-1.33608100	3.33745800	-2.08831000
C	-1.85668400	3.70198400	0.17559000
C	-0.90034100	1.42857300	-3.55039400
C	-2.23491100	2.37649300	2.18989100
C	-1.99590000	-3.54789900	-0.61463500
C	-2.29304900	-3.30365700	0.73297100
C	-1.63043700	-2.58402100	-2.67214300
C	-2.80771100	-1.76016200	2.37833400
C	-1.56617500	-1.39558300	-3.44501000
C	-3.03200400	-0.39149200	2.74394700
C	-2.66805400	2.85026400	-1.84183000
C	-2.98611600	3.07684100	-0.45178200
C	-2.22651400	0.99261700	-3.34392000
C	-3.37330700	1.81269600	1.58349200
C	-2.58933800	-2.72754700	-1.62935500
C	-3.20853300	-2.26578900	1.09471500
C	-2.54658700	-0.41473200	-3.22591700
C	-3.70001800	0.40393400	1.78428800
C	-3.10798300	1.69889400	-2.46552300
C	-3.74138200	2.14768700	0.24549300
C	-3.49979500	-1.67477200	-1.30553500
C	-3.82238400	-1.43771300	0.10876200
C	-3.54025200	-0.57883800	-2.19840500
C	-4.16380900	-0.12972100	0.52832500
C	-3.90345100	0.73295000	-1.74317100
C	-4.21322100	0.95442300	-0.41148300
C	-0.60536200	0.18727600	-0.36398600
C	0.52418400	0.55171200	0.07398200
Sc	-0.80339100	-0.32486600	1.81023800
Sc	1.13332700	-1.20152500	-1.20705600

The coordinates of optimized of Sc₂C₂@C₈₂

C	-0.92886800	-2.74149400	-2.95278600
C	-2.09678000	-2.84570100	-2.16052500
C	0.34254100	-3.27012300	-2.50461200
C	-0.66215800	-1.57928500	-3.75443100
C	-3.02972000	-1.76642100	-2.22887200
C	-2.01449800	-3.56632000	-0.90553500
C	-3.80620900	-1.36124500	-1.07158900

C	-2.76386100	-0.60766700	-3.01924600
C	-0.69735000	-3.90887600	-0.43217900
C	-2.83827800	-3.20906200	0.25648400
C	0.51048500	-3.77095100	-1.20211400
C	-0.67739700	-3.78210600	0.98531800
C	1.77177300	-3.56887000	-0.49444800
C	1.36052200	-2.47800500	-3.11846100
C	-3.72105100	-2.04213600	0.19025200
C	-1.96594200	-3.33263800	1.41772400
C	-3.76393400	-1.18343900	1.33443700
C	-3.99082000	0.06368000	-1.17309300
C	-2.98949900	-1.41885500	2.53703000
C	-3.96962600	0.24027800	1.24382200
C	-2.04289400	-2.47753700	2.57968600
C	-0.87287000	-2.29142300	3.34185700
C	0.38517400	-2.87582700	2.93838600
C	-0.59491200	-1.02951700	3.96917600
C	-2.72190700	-0.16925400	3.15490400
C	2.81336400	-2.94428100	-1.21640800
C	2.57005900	-2.31636800	-2.49020700
C	3.82650900	-2.16430500	-0.56379200
C	1.78515300	-3.46273200	0.96895600
C	0.53559300	-3.55100700	1.71516700
C	2.83887500	-2.74691000	1.57811900
C	1.41705700	-2.01061400	3.41920900
C	-4.05023200	0.88822900	-0.01595900
C	-3.33443100	0.85900300	2.36391500
C	-3.53281700	2.21020600	-0.11692200
C	-3.36725500	0.51827300	-2.37734500
C	-2.87664000	2.82125400	0.99606200
C	-2.89763800	2.65772400	-1.31790500
C	-2.72381900	2.13535600	2.23737900
C	-1.53227500	2.38637200	2.97425400
C	-0.91110400	1.35721000	3.75387600
C	-0.50035700	3.22290500	2.44608100
C	-1.84662400	3.67765100	0.48904500
C	-1.48552800	0.05819800	3.83406900
C	0.82992200	-0.82932800	3.97316300
C	0.50492100	1.53944300	3.70286900
C	-2.76172100	1.80325700	-2.44937000
C	-1.85883800	3.57420300	-0.95545000
C	-1.58542300	1.94346900	-3.23643500
C	-0.54409200	2.84555200	-2.85363100
C	-0.97756700	0.81542700	-3.87636700

C	-0.66047200	3.71443400	-1.72715900
C	0.54849100	4.08919500	-1.03018000
C	0.56169400	4.19857500	0.44647500
C	1.77572900	3.42159500	-1.42360500
C	0.71430300	2.24503500	-3.24811600
C	-0.63547000	3.92828100	1.21216500
C	0.76740900	2.67858300	2.89550500
C	1.79699700	3.58952300	0.90647600
C	-1.54905300	-0.48068300	-3.75704800
C	0.43934400	1.00146700	-3.87963500
C	0.76092800	-1.38401500	-3.81775000
C	1.34045700	-0.09338000	-3.76634400
C	2.60524500	0.10467800	-3.05831100
C	3.24665800	-1.04626300	-2.54064500
C	3.77342400	1.41376600	-1.30942900
C	2.88093200	1.38847700	-2.41165900
C	4.35612600	0.21593900	-0.77871400
C	3.56468600	2.28858200	-0.19001500
C	1.88104100	2.45123400	-2.48532800
C	4.08692900	-0.98905700	-1.37998800
C	2.56548200	3.24134500	-0.24720700
C	4.36918200	0.31887600	0.67208600
C	4.11134200	-0.78895900	1.44193100
C	3.79375500	1.57933700	1.03879000
C	3.29102700	-0.68088000	2.61223700
C	3.83792700	-2.06710500	0.80390200
C	2.91993700	1.71098700	2.14745900
C	1.92005200	2.77561500	2.09091200
C	2.65551700	0.53149100	2.97270200
C	2.61498000	-1.94479600	2.75487900
C	1.40608600	0.43831800	3.72776300
C	0.12542300	-0.05311400	0.68247500
C	0.32974400	-0.17261800	-0.56070700
Sc	-1.48697600	-1.50124000	-0.07664300
Sc	0.12901500	2.08985300	-0.12549300

The coordinates of optimized of Sc₂C₂@C₈₄

C	4.34997500	0.51303800	-0.51224400
C	4.34997100	-0.51304600	0.51224800
C	3.82205900	0.17627300	-1.81187800
C	3.82301000	1.81583900	-0.17638400
C	3.82300400	-1.81584500	0.17638800
C	3.82205600	-0.17628100	1.81188100

C	3.39630400	-1.15548500	-2.19246500
C	3.39705000	-2.19632700	-1.15405500
C	3.39705200	2.19632000	1.15405800
C	3.39630300	1.15547800	2.19246800
C	3.08148000	1.30826100	-2.30595000
C	3.08461600	2.31269900	-1.30665800
C	3.08461200	-2.31270800	1.30666200
C	3.08147700	-1.30826900	2.30595500
C	2.46692500	-1.23850800	-3.23807900
C	2.46545200	-3.24055100	-1.23594900
C	2.46545600	3.24054400	1.23595100
C	2.46692500	1.23850300	3.23808100
C	2.04168000	1.21620400	-3.28081400
C	2.04455200	3.28919700	-1.21571500
C	2.04454600	-3.28920200	1.21571700
C	2.04167600	-1.21620900	3.28081600
C	1.82183700	-0.06555000	-3.81146600
C	1.82300400	-3.81927200	-0.06492000
C	1.82301000	3.81926900	0.06492200
C	1.82183400	0.06554500	3.81146800
C	1.51352400	-2.31147100	-3.28200300
C	1.51214900	-3.28436700	-2.30910900
C	1.51215300	3.28436300	2.30911100
C	1.51352600	2.31146700	3.28200500
C	0.96703700	2.20286700	-3.23418700
C	0.96836600	3.24135400	-2.20005500
C	0.96835900	-3.24135700	2.20005600
C	0.96703100	-2.20286900	3.23418900
C	0.51065800	-0.46185500	-4.21437400
C	0.51099300	-4.22151200	-0.46180400
C	0.51100000	4.22151200	0.46180600
C	0.51065600	0.46185400	4.21437600
C	0.26840800	-1.81782300	-3.79431400
C	0.26783300	-3.79972600	-1.81706000
C	0.26783900	3.79972500	1.81706100
C	0.26841000	1.81782300	3.79431600
C	-0.26840600	1.81852500	-3.79397700
C	-0.26783100	3.80006100	-1.81635800
C	-0.26783900	-3.80006200	1.81636000
C	-0.26841100	-1.81852600	3.79398000
C	-0.51065500	0.46263400	-4.21428900
C	-0.51099200	4.22159700	-0.46102500
C	-0.51100000	-4.22159800	0.46102600
C	-0.51065800	-0.46263400	4.21429100

C	-0.96703500	-2.20226700	-3.23459400
C	-0.96836400	-3.24094500	-2.20065300
C	-0.96835900	3.24094700	2.20065300
C	-0.96703100	2.20226900	3.23459400
C	-1.51352200	2.31207700	-3.28157600
C	-1.51214700	3.28479300	-2.30850200
C	-1.51215400	-3.28479000	2.30850300
C	-1.51352800	-2.31207500	3.28157800
C	-1.82183400	0.06625500	-3.81145500
C	-1.82300200	3.81928300	-0.06421600
C	-1.82301000	-3.81928000	0.06421600
C	-1.82183600	-0.06625100	3.81145500
C	-2.04167900	-1.21559600	-3.28103900
C	-2.04455000	-3.28897000	-1.21632200
C	-2.04454400	3.28897500	1.21632300
C	-2.04167700	1.21560000	3.28103900
C	-2.46692400	1.23910700	-3.23785200
C	-2.46545000	3.24077700	-1.23535100
C	-2.46545700	-3.24077100	1.23535200
C	-2.46692700	-1.23910200	3.23785300
C	-3.08147900	-1.30783400	-2.30619200
C	-3.08461500	-2.31245700	-1.30708500
C	-3.08461000	2.31246500	1.30708700
C	-3.08147700	1.30784200	2.30619400
C	-3.39630300	1.15589100	-2.19225500
C	-3.39704900	2.19654000	-1.15365200
C	-3.39705500	-2.19653200	1.15365200
C	-3.39630600	-1.15588300	2.19225500
C	-3.82206000	-0.17593800	-1.81191200
C	-3.82301200	-1.81580500	-0.17672100
C	-3.82300300	1.81581200	0.17672100
C	-3.82205700	0.17594700	1.81191100
C	-4.34997800	-0.51294200	-0.51234100
C	-4.34997300	0.51295300	0.51234100
C	-0.00002500	0.63361100	-0.00002500
C	0.00002200	-0.63359500	-0.00000600
Sc	2.23718500	0.00000500	-0.00000400
Sc	-2.23718700	-0.00000800	-0.00000700

The coordinates of optimized of $\text{Sc}_2\text{C}_2@C_{80}C[12]CPP$

C	2.89761300	-6.30815800	-1.55680700
C	4.17514800	-5.78090000	-1.46485300
C	4.90745100	-5.86379400	-0.27360500
C	4.35019300	-6.58831400	0.78696700

C	3.06989200	-7.12204200	0.69176100
C	6.09330700	-4.99018800	-0.12645800
C	6.89718300	-4.66219700	-1.22702500
C	7.70768000	-3.53770500	-1.20431100
C	7.73544200	-2.69612700	-0.08327600
C	7.08486200	-3.13578500	1.07579600
C	6.27677900	-4.26556700	1.05579600
C	8.15089000	-1.27736800	-0.19054600
C	7.91964100	-0.60696700	-1.39777500
C	7.89004000	0.77818100	-1.45351800
C	8.08898700	1.54915200	-0.30340700
C	8.48144300	0.88276300	0.86646000
C	8.51069800	-0.50458600	0.92272400
C	7.60739000	2.95024200	-0.29493500
C	7.55439500	3.72543400	-1.46221800
C	6.73886500	4.84642200	-1.53845300
C	5.95818800	5.24153400	-0.44447000
C	6.13943300	4.56168900	0.76610800
C	6.94209300	3.43215000	0.83833600
C	4.78624500	6.13631100	-0.58508500
C	3.99693700	6.05723000	-1.73841700
C	2.69690800	6.54740600	-1.75007400
C	2.14013200	7.14095600	-0.61155000
C	2.99152700	7.37150800	0.48012400
C	4.28566300	6.87411600	0.49634900
C	0.67093400	7.29817300	-0.48892400
C	-0.16999400	7.39858900	-1.60441900
C	-1.54712500	7.26043500	-1.47964300
C	-2.14492100	7.04429300	-0.23159300
C	-1.31136500	7.04484400	0.89394900
C	0.06474900	7.15103000	0.76656800
C	-7.49466900	4.92842200	-0.05077500
C	-7.88356300	4.29183000	-1.23292300
C	-8.77881000	3.22930400	-1.20112900
C	-9.31992100	2.78192100	0.01017400
C	-9.08348000	3.55328400	1.15669800
C	-8.17666900	4.60269500	1.12884000
C	-9.79799900	1.38035000	0.10427700
C	-10.38234200	0.69282300	-0.96815100
C	-10.34969200	-0.69569400	-1.02574500
C	-9.72464600	-1.44398600	-0.01745400
C	-9.32111500	-0.76083700	1.13579700
C	-9.35955000	0.62257400	1.19641200
C	-9.18682700	-2.80888500	-0.24240700

C	-8.74398100	-3.16550800	-1.52271900
C	-7.82702400	-4.19067700	-1.70196700
C	-7.29740500	-4.88100700	-0.60503900
C	-7.87607600	-4.64636000	0.64846500
C	-8.81508700	-3.63896000	0.82360200
C	-6.03014400	-5.64092100	-0.72257900
C	-5.06546300	-5.19894200	-1.63826500
C	-3.78450400	-5.72834900	-1.64071200
C	-3.41160200	-6.70706500	-0.71271000
C	-4.38395900	-7.18785200	0.17069500
C	-5.67487400	-6.67112700	0.15764800
C	-1.98140500	-7.07845200	-0.62320000
C	-1.22188600	-7.30504500	-1.77752000
C	0.16112000	-7.38218900	-1.71393100
C	0.06994500	-7.08599800	0.66638000
C	-1.31796400	-7.03443900	0.60646000
C	0.83818200	-7.20690700	-0.49819000
C	2.29618300	-6.94439000	-0.46323500
C	-5.28584200	5.33917800	0.95879300
C	-6.22630600	5.69418800	-0.01604700
C	-5.83882000	6.60490700	-1.00443800
C	-4.53977500	7.10083400	-1.04518400
C	-3.57863200	6.68909200	-0.11253800
C	-3.98775900	5.81978200	0.90692700
H	2.32135300	-6.12578900	-2.45881200
H	4.56661500	-5.19798200	-2.29335400
H	4.91205900	-6.70741400	1.70935200
H	2.65425800	-7.65742100	1.54055800
H	6.83771500	-5.26152100	-2.13121600
H	8.27427500	-3.27064500	-2.09169900
H	7.08713400	-2.50998800	1.96318500
H	5.67569600	-4.50180700	1.92954300
H	7.61660000	-1.16997200	-2.27507500
H	7.56222900	1.25717700	-2.37151900
H	8.71057600	1.45622600	1.76022800
H	8.76285600	-0.99427100	1.85919900
H	8.11538500	3.41476400	-2.33902100
H	6.66821900	5.39454000	-2.47403700
H	5.53571800	4.83330100	1.62732000
H	6.94406900	2.84664900	1.75327300
H	4.34915100	5.47967700	-2.58897100
H	2.06959500	6.33754800	-2.61218700
H	2.62062000	7.90672800	1.34891000
H	4.90230300	7.01734100	1.37927700

H	0.25800300	7.54607600	-2.59163800
H	-2.16073800	7.26255600	-2.37577200
H	-1.74005100	6.92167900	1.88394600
H	0.68003300	7.05230000	1.65556400
H	-7.37410400	4.53459300	-2.16149400
H	-8.94397600	2.65116300	-2.10551600
H	-9.55163500	3.27509300	2.09685500
H	-7.93861400	5.13498900	2.04589800
H	-10.80004200	1.25156700	-1.80150400
H	-10.74784000	-1.19934600	-1.90233600
H	-8.82810200	-1.30073500	1.93738900
H	-8.89711400	1.12050100	2.04265700
H	-9.02869600	-2.56037000	-2.37797100
H	-7.45430200	-4.40027900	-2.70024700
H	-7.51173300	-5.18472100	1.51860100
H	-9.19260800	-3.43627400	1.82154600
H	-5.29486900	-4.37176200	-2.30261000
H	-3.03521900	-5.32442200	-2.31790400
H	-4.12135500	-7.96906100	0.87911700
H	-6.41217300	-7.06029100	0.85426000
H	-1.72528800	-7.39474300	-2.73629400
H	0.72619600	-7.54775300	-2.62620900
H	0.56193300	-6.93302000	1.62254600
H	-1.88826900	-6.84917000	1.51320500
H	-5.55442700	4.60643400	1.71429800
H	-6.55912600	6.91716000	-1.75601700
H	-4.26589900	7.81024400	-1.82097100
H	-3.26549800	5.45481800	1.63069000
C	3.51062400	1.98812000	-2.23349300
C	3.35755400	0.80741200	-2.95134600
C	2.41828500	2.90104600	-2.11650700
C	2.10994200	0.50047500	-3.58177200
C	1.17957000	2.62860900	-2.72429700
C	1.01350600	1.38883100	-3.49238700
C	4.21758100	1.97031700	-0.97297800
C	3.92757500	-0.42114300	-2.45125300
C	2.46372700	3.47637700	-0.77736600
C	1.92582700	-0.93326700	-3.51388300
C	0.02077800	3.19773700	-2.07099100
C	-0.29032500	0.80239700	-3.58758500
C	3.54698500	2.84650000	-0.05916900
C	3.01791300	-1.49032500	-2.73632400
C	4.77493400	0.79851700	-0.50081400
C	4.62340100	-0.42885300	-1.25607300

C	1.32163900	3.99505100	-0.12680500
C	0.64422700	-1.48765200	-3.46414600
C	0.05037400	3.95621200	-0.83818200
C	-0.46781900	-0.60903700	-3.55914100
C	-1.24061500	2.53672200	-2.15790000
C	-1.42395200	1.38196500	-2.94053500
C	3.42889400	2.52309300	1.31198300
C	2.80471400	-2.52589900	-1.80719700
C	4.70713800	0.47934300	0.90003900
C	4.46528300	-1.51612600	-0.33374400
C	-1.20841800	3.68946600	-0.12880900
C	-1.69525400	-0.91055400	-2.86055400
C	-1.96376200	2.75691000	-0.95527300
C	-2.27360700	0.35822700	-2.45993700
C	1.27424000	3.80960400	1.29892000
C	0.44966300	-2.68664400	-2.68115700
C	3.99986500	1.27753400	1.82215000
C	3.52902700	-2.54872700	-0.54486900
C	4.66244200	-0.95819500	0.98410000
C	2.30215700	3.07479200	1.98645500
C	1.50580800	-3.14356100	-1.84265900
C	-1.23414900	3.46427900	1.31052700
C	-2.83671900	1.71908900	-0.45612400
C	0.02614300	3.57891400	2.00430400
C	-2.97634000	0.49170900	-1.23076400
C	-1.90839700	-2.12495500	-2.14177400
C	-0.81914400	-3.10695400	-2.11962700
C	1.72227800	2.43906600	3.12178800
C	0.92834100	-3.82591900	-0.73189900
C	4.11166900	-1.56244200	2.06781800
C	3.39786200	0.62013100	2.99455900
C	2.92720600	-3.20773800	0.63046300
C	0.33041400	2.73105100	3.12748200
C	-0.50829100	-3.85145400	-0.89278200
C	-2.99223500	1.66979400	0.94559300
C	-3.24721500	-0.72265600	-0.53516800
C	-2.13688000	2.48415300	1.80627000
C	-2.69965100	-2.00167300	-0.95982700
C	3.56562700	-0.77065100	3.13866500
C	3.31808200	-2.76083900	1.90832100
C	2.23297300	1.21528300	3.64821300
C	1.61613300	-3.84916100	0.53630700
C	-3.23278700	0.44294600	1.61479800
C	-3.35375000	-0.74271200	0.87720300

C	-1.85875800	1.68898300	2.97815900
C	-2.41679100	-2.76520400	0.24317900
C	-0.61246300	1.79445600	3.64937500
C	-1.31109200	-3.67733700	0.31161600
C	2.59277900	-1.60004300	3.80093600
C	2.44414700	-2.82130800	3.04529900
C	1.31525300	0.39572000	4.34136300
C	0.79046600	-3.95093000	1.67270300
C	-2.52089800	0.43231700	2.85842500
C	-2.79979500	-1.96517900	1.37497200
C	-0.10931800	0.64786400	4.28660000
C	-0.65380500	-3.75530100	1.56249600
C	1.48810600	-1.02342700	4.39797000
C	1.19656400	-3.41666200	2.93249500
C	-1.94454600	-0.76562700	3.38173000
C	-2.09205300	-2.00940400	2.61180600
C	-0.80010900	-0.61106800	4.19886300
C	-1.09039900	-3.00578200	2.71263600
C	0.18920100	-1.64674900	4.28944200
C	0.04790700	-2.82114400	3.56829500
C	0.64100200	-0.24825900	0.98196800
C	1.31732500	0.01996600	-0.05299700
Sc	-0.27011800	-1.66409600	-0.49831000
Sc	0.17233700	1.94509500	0.17510000

The coordinates of optimized of Sc₂C₂@C₈₂C[12]CPP

C	3.10981500	7.75208100	0.32032300
C	4.38474200	7.21170200	0.25361000
C	4.75166900	6.34957200	-0.79056000
C	3.85783600	6.23024800	-1.86284800
C	2.58202100	6.77330600	-1.79984800
C	5.88546400	5.40068300	-0.65307100
C	6.37405000	5.07417000	0.62107200
C	7.17332100	3.96067200	0.82637300
C	7.49255100	3.09804500	-0.22925800
C	7.11599300	3.49313700	-1.51933500
C	6.34363400	4.62820800	-1.72866300
C	7.95835800	1.71400600	0.01780700
C	7.54818900	1.06003400	1.18501500
C	7.59778000	-0.32165400	1.28943000
C	8.05762400	-1.11183900	0.22987800
C	8.64079300	-0.44493400	-0.85908600
C	8.58947700	0.93823700	-0.96484600
C	7.67587600	-2.54430500	0.17159700

C	7.25179600	-3.24441800	1.30986600
C	6.49414600	-4.40225100	1.19836500
C	6.16560800	-4.93806200	-0.05449700
C	6.75085200	-4.34039000	-1.17870400
C	7.46937400	-3.15966900	-1.07017400
C	5.06382400	-5.91995500	-0.19480900
C	4.61042200	-6.70746200	0.87331400
C	3.37323500	-7.33778500	0.82370300
C	2.54703300	-7.21489100	-0.30089600
C	3.06509100	-6.55160500	-1.41835600
C	4.29212700	-5.91206400	-1.36394400
C	1.09941100	-7.52202000	-0.27307800
C	0.36822100	-7.27820100	0.89533000
C	-1.01836500	-7.21157800	0.86642400
C	-1.71699100	-7.37830100	-0.33342800
C	-0.99421200	-7.74541500	-1.47505100
C	0.39040900	-7.82034200	-1.44438500
C	-6.92657200	-4.97096000	-0.38340200
C	-7.24816400	-4.31591200	0.80982900
C	-8.15107100	-3.26129200	0.81844600
C	-8.76510100	-2.83116700	-0.36401600
C	-8.56290500	-3.59150200	-1.52324200
C	-7.65496800	-4.64139500	-1.53357900
C	-9.32398000	-1.45882700	-0.41212600
C	-9.93153800	-0.84636500	0.69207300
C	-10.00361800	0.53799800	0.78661700
C	-9.46247200	1.35530100	-0.21583000
C	-9.03270900	0.73593400	-1.39563300
C	-8.96725400	-0.64521700	-1.49315900
C	-9.02386200	2.74993800	0.03709000
C	-8.53130000	3.07997800	1.30652700
C	-7.67699700	4.15812300	1.48129800
C	-7.26869700	4.93270100	0.38903900
C	-7.90958200	4.71868700	-0.83737500
C	-8.78153200	3.65104700	-1.00769200
C	-6.03443800	5.74900600	0.46069200
C	-4.96587000	5.25913500	1.22340300
C	-3.70725500	5.83073100	1.14187700
C	-3.46302300	6.91247000	0.28793500
C	-4.54291300	7.44711100	-0.42474800
C	-5.80849700	6.87705500	-0.33740400
C	-2.06281600	7.34277800	0.07706000
C	-1.14045500	7.30115700	1.12870000
C	0.21763200	7.44031800	0.88846800

C	-0.22607800	7.78932100	-1.44549100
C	-1.58621700	7.63737600	-1.20620000
C	0.70450300	7.64245300	-0.41004800
C	2.15210200	7.46247300	-0.66107600
C	-4.81950800	-5.62210900	-1.51485400
C	-5.70723500	-5.80915400	-0.44836400
C	-5.31395400	-6.64635000	0.60250700
C	-4.04999300	-7.22294200	0.61758900
C	-3.13929900	-6.98002800	-0.41731200
C	-3.55636300	-6.19556500	-1.49913800
H	2.83426900	8.36344500	1.17485600
H	5.08254000	7.41916200	1.05855000
H	4.09827100	5.58729100	-2.70283700
H	1.87140300	6.53742400	-2.58734800
H	6.05698800	5.64557600	1.48670500
H	7.49548800	3.72236900	1.83562100
H	7.34715800	2.85397400	-2.36640000
H	6.03968100	4.87021200	-2.74211800
H	7.05263200	1.62079200	1.97219000
H	7.14568100	-0.78696400	2.15905200
H	9.09275400	-1.01549200	-1.66470100
H	8.99838900	1.41782900	-1.84966600
H	7.44384400	-2.84108700	2.29936700
H	6.07860600	-4.84137700	2.10038300
H	6.58476300	-4.76121000	-2.16503000
H	7.79386000	-2.66618100	-1.98053300
H	5.21072100	-6.79548500	1.77403400
H	3.02508300	-7.89813800	1.68696800
H	2.44412600	-6.41812800	-2.29902700
H	4.58906200	-5.29973100	-2.20874800
H	0.89237600	-7.02257500	1.81176000
H	-1.55769600	-6.91161800	1.76108400
H	-1.52449600	-7.93521900	-2.40410900
H	0.93351800	-8.07193900	-2.35091300
H	-6.69542100	-4.55297900	1.71465200
H	-8.28268600	-2.68313300	1.72831900
H	-9.07645800	-3.31686300	-2.44062700
H	-7.46732000	-5.18265500	-2.45695900
H	-10.28568700	-1.45843400	1.51732900
H	-10.41643800	0.98958400	1.68457700
H	-8.60310200	1.33599500	-2.19136400
H	-8.49255400	-1.08922500	-2.36287100
H	-8.71874400	2.41534200	2.14438800
H	-7.24857000	4.34592300	2.46159700

H	-7.63678000	5.32380500	-1.69745200
H	-9.20221700	3.46055900	-1.99096600
H	-5.09806000	4.36123300	1.81961300
H	-2.88200400	5.37748400	1.68569900
H	-4.38620100	8.31198300	-1.06386600
H	-6.62805500	7.30101600	-0.91143000
H	-1.48799800	7.10299300	2.13872900
H	0.91720700	7.30424000	1.70805200
H	0.12115600	7.97566400	-2.45791200
H	-2.28354100	7.67463100	-2.03850600
H	-5.08959200	-4.94560000	-2.32091800
H	-6.00082000	-6.83090200	1.42414300
H	-3.75589700	-7.85715000	1.44955800
H	-2.84907500	-5.95871200	-2.29012300
C	-2.38302100	1.31309700	2.79995400
C	-3.02635200	0.13663500	2.34604600
C	-2.23742400	2.47587200	1.94900900
C	-1.23888500	1.25857800	3.66759400
C	-2.52689600	-1.11050500	2.82996700
C	-3.61174700	0.14032200	1.02076800
C	-2.53776000	-2.30371700	2.00318900
C	-1.38686700	-1.16703000	3.68747200
C	-3.28100900	1.24961300	0.16237000
C	-3.69044700	-1.07181500	0.19558800
C	-2.58810700	2.43767300	0.58766600
C	-3.15393400	0.76713300	-1.17008600
C	-1.80298400	3.18168900	-0.39393200
C	-1.05642800	3.15900500	2.37874500
C	-3.09131900	-2.31988100	0.67714600
C	-3.37611600	-0.64836000	-1.16333100
C	-2.35012500	-3.10241600	-0.26534500
C	-1.37402300	-3.07110500	2.36833300
C	-2.17881800	-2.72263500	-1.65457300
C	-1.19896600	-3.89254900	0.09516800
C	-2.65321500	-1.46310000	-2.11334500
C	-1.92343000	-0.80572300	-3.12413100
C	-1.83619600	0.63599900	-3.17158500
C	-0.67813900	-1.34068600	-3.59990400
C	-0.94849100	-3.25919300	-2.12194300
C	-0.76028400	3.99644200	0.10594500
C	-0.33188400	3.90275400	1.47945400
C	0.41503100	4.28657300	-0.66655300
C	-1.69446300	2.68707500	-1.77048700
C	-2.36485300	1.44967900	-2.15463600

C	-0.55624800	3.05302900	-2.52323400
C	-0.57912200	0.95587900	-3.77289700
C	-0.67183700	-3.85466900	1.41208200
C	-0.34401500	-3.99463200	-1.04633000
C	0.73750600	-3.98909000	1.57143900
C	-0.68240000	-2.38041000	3.41343500
C	1.59561600	-4.06641400	0.43150600
C	1.42820900	-3.28976500	2.61052700
C	1.06896000	-4.01608300	-0.89296000
C	1.86544900	-3.36094500	-1.87508100
C	1.26439800	-2.61835100	-2.94180600
C	3.09410800	-2.71486700	-1.52405200
C	2.84238400	-3.44108400	0.76564000
C	-0.15141100	-2.53629500	-3.06363000
C	0.18021800	-0.24210700	-3.95846800
C	2.10292500	-1.50271700	-3.24964700
C	0.73555800	-2.43464300	3.51605800
C	2.73360600	-2.95330400	2.12581900
C	1.41623700	-1.27101800	3.96868300
C	2.70912300	-0.92894100	3.46261800
C	0.71192500	-0.05274900	4.23790000
C	3.41795200	-1.76971600	2.55169500
C	4.32778300	-1.14754200	1.61926900
C	4.45444700	-1.64994600	0.23291600
C	4.32047600	0.30121500	1.55788500
C	2.78160700	0.51625300	3.40485300
C	3.65319600	-2.77045000	-0.20938900
C	3.22470600	-1.54890500	-2.37797700
C	4.51758100	-0.48371000	-0.63249800
C	-0.69856200	0.02020600	4.07904200
C	1.55388500	1.04771200	3.88686500
C	-0.38682800	2.37889200	3.37377900
C	1.02454600	2.26139400	3.36622600
C	1.80827800	3.00965300	2.38256600
C	1.10824800	3.90857700	1.54103700
C	3.53052100	2.84745300	0.60779800
C	3.07244500	2.45661500	1.89232700
C	2.75772100	3.71008800	-0.23655200
C	4.20633300	1.92712700	-0.26593100
C	3.52271800	1.16063000	2.39403900
C	1.56905300	4.22538800	0.22016600
C	4.55976800	0.67696400	0.20221400
C	2.86202200	3.22009500	-1.60276100
C	1.77110100	3.26947300	-2.43562700

C	3.69902600	2.05670600	-1.60444000
C	1.48046300	2.16984100	-3.30824900
C	0.51347400	3.82315900	-1.95424600
C	3.40348100	0.92130800	-2.40097900
C	3.86220600	-0.37939200	-1.91308400
C	2.24390500	0.97757500	-3.29317000
C	0.04818200	2.13401400	-3.45519800
C	1.56780000	-0.25867600	-3.68654400
C	0.49123300	-0.11504000	-0.52940600
C	0.49912100	0.42383800	0.61544700
Sc	-1.54330500	-0.62625500	0.39538600
Sc	2.38298100	-0.89563000	0.52782200

The coordinates of optimized of Sc₂C₂@C₈₄C[12]CPP

C	-9.99912100	-0.64388900	0.14319900
C	-10.00505800	0.74595100	0.13790200
C	-9.22550800	1.46416100	-0.77895900
C	-8.58624800	0.74281500	-1.79427800
C	-8.58092900	-0.64331400	-1.78948900
C	-8.79879200	2.86616500	-0.54974100
C	-8.51943800	3.27911900	0.75941000
C	-7.69775300	4.37011400	1.00141900
C	-7.11707300	5.07798200	-0.05740600
C	-7.54160500	4.77646700	-1.35711000
C	-8.37485700	3.69155100	-1.59877400
C	-5.91201600	5.91238000	0.16031900
C	-4.95536700	5.44984100	1.07248800
C	-3.69480300	6.01985900	1.13640400
C	-3.33701600	7.07525600	0.29053000
C	-4.31836300	7.59391400	-0.56405600
C	-5.58425700	7.02155900	-0.62909500
C	-1.91050000	7.46575300	0.21937400
C	-1.08158000	7.36802000	1.34278600
C	0.29910100	7.41965100	1.21728700
C	0.90398200	7.59591600	-0.03351600
C	0.06940900	7.82886600	-1.13457200
C	-1.31114600	7.75479100	-1.01264100
C	2.34983000	7.31790900	-0.19529000
C	3.25844600	7.44944900	0.86332700
C	4.51322600	6.85702500	0.80570800
C	4.90675800	6.11883000	-0.31717500
C	4.05251600	6.10590400	-1.42642500
C	2.79933500	6.69527500	-1.36631600
C	6.04185000	5.17011900	-0.28962500

C	6.27937900	4.42657700	0.87239900
C	7.03952400	3.26648600	0.82980400
C	7.58976400	2.81215900	-0.37528400
C	7.48832500	3.64450600	-1.49738100
C	6.72575800	4.80322400	-1.45565700
C	7.51166000	-2.84786200	-0.39740800
C	6.94774100	-3.30199200	0.80077300
C	6.21074700	-4.47669000	0.83868300
C	6.00358200	-5.23313900	-0.32102600
C	6.69048900	-4.85550300	-1.48196700
C	7.43237700	-3.68293400	-1.51951400
C	4.88571800	-6.20340900	-0.34937600
C	4.47446000	-6.90779400	0.79056000
C	3.21790700	-7.49276900	0.85094600
C	2.31882700	-7.38618100	-0.22061700
C	2.79336200	-6.81855100	-1.40804600
C	4.05321100	-6.24061600	-1.47263400
C	0.86702000	-7.63455500	-0.05535600
C	0.26899700	-7.46449300	1.20019600
C	-1.10932900	-7.39107300	1.33439000
C	-1.94552000	-7.45856600	0.21430000
C	-1.35675800	-7.74132500	-1.02407200
C	0.02187700	-7.83924800	-1.15404400
C	-3.36494300	-7.04554900	0.29594200
C	-3.70578900	-5.99627200	1.15679100
C	-4.95707500	-5.40438200	1.10018200
C	-5.91980000	-5.83661600	0.17930200
C	-5.61105700	-6.94305800	-0.62155500
C	-4.35553400	-7.53790500	-0.56332400
C	-7.11027700	-4.98114300	-0.03629500
C	-7.68016700	-4.26259500	1.02123100
C	-8.49628700	-3.16771200	0.77700800
C	-8.36298300	-3.59184000	-1.57985400
C	-7.53529100	-4.68025400	-1.33613800
C	-8.78107300	-2.76103100	-0.53292900
C	-9.21413900	-1.36227000	-0.76876500
C	7.58753000	-0.70485500	-1.64303400
C	7.93383000	-1.43310900	-0.49841200
C	8.44710700	-0.72819300	0.59771200
C	8.47319500	0.66006700	0.60217500
C	7.98591500	1.39035800	-0.48908000
C	7.61325300	0.68158700	-1.63831900
H	-10.55858900	-1.17750600	0.90690000
H	-10.56902900	1.28036300	0.89770800

H	-7.96651900	1.26727800	-2.51497700
H	-7.95796400	-1.16824700	-2.50711100
H	-8.85014900	2.66923400	1.59492300
H	-7.43097900	4.62313400	2.02366600
H	-7.12573200	5.32695300	-2.19649200
H	-8.62478900	3.42881400	-2.62293800
H	-5.16650800	4.56565400	1.66693100
H	-2.94414600	5.57349400	1.78250700
H	-4.08085200	8.44146200	-1.20131200
H	-6.32097000	7.42465200	-1.31895000
H	-1.52079800	7.18652500	2.31955000
H	0.91491600	7.23081300	2.09171200
H	0.50611500	8.01691900	-2.11094700
H	-1.92982700	7.84278900	-1.90116900
H	2.96438300	7.98567700	1.76094600
H	5.18172000	6.93320800	1.65892500
H	4.32311800	5.52612100	-2.30434900
H	2.11647600	6.55837700	-2.19892500
H	5.75799100	4.68564000	1.79010600
H	7.09384300	2.63853500	1.71452000
H	7.96469900	3.35077100	-2.42854800
H	6.61333000	5.40401200	-2.35384200
H	6.98066800	-2.66908400	1.68320000
H	5.67820700	-4.73639300	1.74886100
H	6.59988500	-5.46080000	-2.37960600
H	7.91730800	-3.38501900	-2.44498100
H	5.12926600	-6.95735500	1.65615100
H	2.91312100	-7.99842100	1.76231800
H	2.12549100	-6.70263200	-2.25594800
H	4.33479200	-5.69287000	-2.36733800
H	0.88981400	-7.29654600	2.07490200
H	-1.53971500	-7.21530400	2.31619400
H	-1.98071200	-7.80767100	-1.91079500
H	0.44750200	-8.02580200	-2.13536600
H	-2.94901500	-5.57459500	1.81329300
H	-5.15527600	-4.52763200	1.71009600
H	-6.35435900	-7.32578100	-1.31584700
H	-4.13273800	-8.38221500	-1.21007600
H	-7.41329900	-4.51337500	2.04400000
H	-8.82135100	-2.55227700	1.61070900
H	-8.61575000	-3.33264300	-2.60420900
H	-7.12640300	-5.23702900	-2.17472000
H	7.17411900	-1.22348700	-2.50369400
H	8.78326800	-1.27301100	1.47549800

H	8.82797100	1.18540500	1.48454400
H	7.21489400	1.21909100	-2.49394600
C	-3.56201500	-1.78057100	0.16566300
C	-3.81224200	-0.61977600	0.99814600
C	-3.20895200	-1.56237400	-1.21594800
C	-2.66681900	-2.79925700	0.66456900
C	-3.69896700	0.69154000	0.40147900
C	-3.15356800	-0.54826100	2.27943200
C	-3.19808000	-0.25886700	-1.85073600
C	-3.45554300	0.91834000	-1.00726900
C	-2.09474800	-2.79275800	1.99397100
C	-2.34818300	-1.61583500	2.83755900
C	-2.19344500	-2.51860900	-1.57871300
C	-1.86626500	-3.28075400	-0.42938200
C	-3.08644900	1.57553900	1.35794700
C	-2.75070200	0.81594300	2.50601900
C	-2.37424500	-0.11981000	-2.97651000
C	-2.86706500	2.14505300	-1.34954500
C	-0.90049700	-3.51020400	2.16377900
C	-1.39126900	-1.24320100	3.79105500
C	-1.26400300	-2.32673400	-2.64698700
C	-0.58817600	-3.90271700	-0.27309900
C	-2.37401400	2.76422800	1.00673700
C	-1.68712600	1.19692000	3.37990600
C	-1.44363100	-1.15615700	-3.40291900
C	-2.37004000	3.08817900	-0.35853200
C	-0.16886000	-4.09944600	1.05165000
C	-1.08626600	0.14791600	4.09556300
C	-1.77240800	1.14616600	-3.28804700
C	-2.01084100	2.24735100	-2.49789400
C	0.07117000	-3.08551600	3.13439500
C	-0.16862600	-1.98491200	3.92465500
C	0.05004100	-2.95257300	-2.53596300
C	0.38948300	-3.74106500	-1.34682100
C	-1.28772900	3.20018600	1.88045500
C	-0.94396100	2.41410500	3.06905400
C	-0.31951900	-0.49678200	-3.98599200
C	-1.24781300	3.75802100	-0.93794200
C	1.22081600	-4.04346900	1.38697700
C	0.29924600	0.21040500	4.43414800
C	-0.45990600	0.92710200	-3.82338500
C	-0.94880700	3.17037000	-2.21852300
C	1.38943500	-3.32262900	2.62178400
C	0.90272800	-1.08028300	4.22718100

C	1.09879200	-2.35459600	-3.26457000
C	1.74752700	-3.84917500	-0.99058600
C	-0.28295200	3.99841700	1.29591900
C	0.37198400	2.49753600	3.56771900
C	0.92377600	-1.08739300	-3.92544800
C	2.16086400	-3.93216600	0.38658400
C	-0.22973400	4.21132000	-0.12791000
C	1.01099700	1.36350900	4.18328200
C	0.63483800	1.73459500	-3.45360200
C	0.37994800	2.90902600	-2.61426700
C	2.42857300	-2.38166400	2.78752200
C	2.17193100	-1.20798100	3.62677400
C	2.45467600	-2.38137000	-2.79577800
C	2.77285600	-3.11619300	-1.67681700
C	1.07855500	3.95001000	1.74979900
C	1.40024300	3.21146300	2.86632000
C	2.08169300	-0.27766600	-3.71917100
C	3.31596000	-3.11632900	0.58446700
C	1.12474900	4.11358200	-0.57034300
C	2.36240300	1.27545600	3.73189800
C	1.94549600	1.09134000	-3.43359000
C	1.43752400	3.43436400	-1.75808400
C	3.43177600	-2.31510100	1.73116900
C	2.91888800	0.02706100	3.40580000
C	3.06108500	-1.09896000	-3.02079900
C	3.72154600	-2.61536000	-0.72216600
C	1.95899700	3.97026100	0.61501000
C	2.61917600	2.45296100	2.91336300
C	2.95628000	1.64761900	-2.59176700
C	2.71263600	2.78478600	-1.78110900
C	4.15460600	-1.09136600	1.55901400
C	3.90168300	0.04353200	2.36963300
C	3.97305100	-0.56940500	-2.09551300
C	4.31869600	-1.35889000	-0.90342200
C	3.14769400	3.22518200	0.62181300
C	3.48947900	2.43477900	1.81381400
C	4.01335400	0.87638200	-1.98642500
C	3.61109000	2.73234600	-0.65857000
C	4.67373400	-0.63147100	0.29796300
C	4.26459700	1.22351100	1.62501100
C	4.47495100	1.58416500	-0.81685800
C	4.81295400	0.80590600	0.35795900
C	0.65992100	-0.59451200	0.31005400
C	0.29332000	0.58827100	0.04133900

Sc	-1.66703000	-0.61606400	0.37136500
Sc	2.62022700	0.60948100	-0.03327500

The coordinates of optimized of Sc₂C₂@C₈₀CPP[12]CPP

C	-0.50790300	7.72619400	-2.04319900
C	0.87533900	7.65633500	-2.10829400
C	1.63723500	7.43163900	-0.96516000
C	0.96875800	7.34709400	0.25587000
C	-0.41465400	7.39915300	0.31874400
C	3.05394000	7.02822100	-1.03192300
C	4.02495300	7.54123800	-0.17693300
C	5.26740900	6.93419400	-0.05166700
C	5.56795300	5.75776700	-0.73851200
C	4.61232200	5.28204200	-1.64013300
C	3.39725100	5.92266100	-1.80779000
C	6.69085700	4.87615900	-0.36435200
C	6.87591100	4.53310200	0.97623600
C	7.64278300	3.43770200	1.33826300
C	8.19001200	2.59095800	0.37556600
C	8.10656300	3.00004600	-0.95545000
C	7.39500500	4.13581900	-1.31460600
C	8.44979500	1.17150100	0.69152400
C	7.43223800	0.48796800	1.35990500
C	7.40437100	-0.88868500	1.42474500
C	8.38804100	-1.66945900	0.81390800
C	9.44628400	-0.99154900	0.21126300
C	9.47626300	0.40050000	0.15059400
C	8.05174200	-3.09020900	0.58761500
C	7.44079700	-3.84540400	1.58822000
C	6.59957200	-4.90176300	1.27525700
C	6.39947900	-5.29839100	-0.04728400
C	7.16708700	-4.66632800	-1.02605100
C	7.95288900	-3.56584200	-0.72046000
C	5.21903600	-6.10617300	-0.40723000
C	4.81196100	-7.23448100	0.30497500
C	3.54177700	-7.77245700	0.13614000
C	2.65308900	-7.24187500	-0.79391400
C	3.10125600	-6.18380200	-1.58136100
C	4.33327900	-5.59783500	-1.36033200
C	-3.02282100	-7.03400100	-0.95128200
C	-3.99167300	-7.56575000	-0.10736100
C	-5.24864100	-6.98477900	-0.00110200
C	-5.56416800	-5.81400100	-0.69150900
C	-4.60635300	-5.31740100	-1.58101400

C	-3.37423600	-5.93061500	-1.72485600
C	-6.70572200	-4.95349700	-0.32366800
C	-6.90995100	-4.62643700	1.01819300
C	-7.68812100	-3.54030800	1.38384300
C	-8.22039800	-2.68058900	0.42451800
C	-8.12427100	-3.07786500	-0.90954400
C	-7.40752900	-4.20910100	-1.27307400
C	-8.45348000	-1.25753600	0.74732800
C	-7.42109100	-0.60245000	1.42181700
C	-7.34361900	0.77370400	1.47186500
C	-8.30289300	1.58220100	0.85717000
C	-9.38385800	0.93261400	0.26113700
C	-9.45388300	-0.45767600	0.20010700
C	-7.94432200	2.99814700	0.63406600
C	-7.30907100	3.74292200	1.62822300
C	-6.49022000	4.81508100	1.30882200
C	-6.34147100	5.24631400	-0.01049100
C	-7.13292900	4.62150600	-0.97499500
C	-7.88843500	3.49997200	-0.66710900
C	-5.18339100	6.08114200	-0.38649700
C	-4.76134600	7.18957800	0.34837700
C	-3.49802500	7.73982500	0.16468700
C	-3.08292200	6.18845100	-1.59015700
C	-4.32147400	5.61099300	-1.38096200
C	-2.62106200	7.23094000	-0.78921500
C	-1.18193700	7.55119200	-0.83572900
C	-0.91603000	-7.31501900	0.30862400
C	-1.60363400	-7.42872600	-0.89779600
C	-0.86419300	-7.66981000	-2.05159700
C	0.51979300	-7.73712500	-2.01073700
C	1.21149500	-7.55192800	-0.81622300
C	0.46715700	-7.37382600	0.34894000
F	-1.19451400	7.90224200	-3.16792000
F	1.47234400	7.75582300	-3.29221500
F	1.64953500	7.09268000	1.37085800
F	-1.00837700	7.17433200	1.48735000
F	3.75025300	8.60519500	0.57110800
F	6.15558900	7.46484300	0.78249300
F	4.79785700	4.12750200	-2.27889700
F	2.50405400	5.38075600	-2.63400700
F	6.21492900	5.17611500	1.93380700
F	7.72914800	3.12357700	2.62730600
F	8.60416000	2.22975700	-1.91905200
F	7.30516400	4.44700200	-2.60393800

F	6.37656500	1.14553000	1.84021700
F	6.32645300	-1.45571500	1.96834400
F	10.42608200	-1.67394800	-0.37128600
F	10.48316800	0.98839800	-0.48607800
F	7.54053100	-3.47113000	2.86000300
F	5.88326500	-5.44480000	2.25510100
F	7.06389900	-5.03828300	-2.29828000
F	8.50522600	-2.88441200	-1.72034400
F	5.62542100	-7.78661500	1.19934900
F	3.16505900	-8.78865700	0.90572400
F	2.29168000	-5.63449900	-2.48207200
F	4.60351100	-4.46332600	-2.00668000
F	-3.70340400	-8.62339500	0.64453900
F	-6.13747800	-7.53635400	0.81845000
F	-4.81152200	-4.17241800	-2.23106400
F	-2.47237000	-5.37467700	-2.53357800
F	-6.24864800	-5.26758000	1.97754600
F	-7.79002300	-3.24270200	2.67551000
F	-8.61074600	-2.29761800	-1.87072800
F	-7.30724100	-4.50895400	-2.56434000
F	-6.39688700	-1.29288600	1.92292700
F	-6.24924900	1.30441300	2.01372000
F	-10.35082000	1.64062200	-0.31281100
F	-10.47538700	-1.01673600	-0.44000600
F	-7.37816000	3.35766500	2.89859900
F	-5.75616100	5.35254000	2.27817400
F	-7.09080900	5.02729500	-2.24033800
F	-8.46487400	2.83532800	-1.66470400
F	-5.55457000	7.71520700	1.27629500
F	-3.11762200	8.74761200	0.94355200
F	-2.28109600	5.64855100	-2.50477000
F	-4.62272500	4.52075300	-2.08345000
F	-1.58022800	-7.02142800	1.42471400
F	-1.48398400	-7.78047300	-3.22281400
F	1.19051800	-7.91895000	-3.14412100
F	1.08626400	-7.13111300	1.50146600
C	-1.94472300	-0.37996900	-3.52292800
C	-0.62184100	-0.59873200	-3.88794000
C	-2.62230600	-1.31497000	-2.68166900
C	0.07289300	-1.76290200	-3.43041600
C	-1.96371300	-2.46360500	-2.21028200
C	-0.57081000	-2.70858800	-2.60034600
C	-2.36768200	0.94828600	-3.14795000
C	0.31040500	0.50229500	-3.92276600

C	-3.50646000	-0.55999700	-1.80103600
C	1.45587600	-1.39304800	-3.22277700
C	-2.41385600	-2.96667600	-0.93315300
C	0.27221900	-3.46070500	-1.72074300
C	-3.29192700	0.84942400	-2.05800100
C	1.57892600	0.03578200	-3.45110100
C	-1.47989500	2.00547300	-3.19508300
C	-0.10572800	1.77769000	-3.58926100
C	-3.90532000	-1.03957500	-0.53252600
C	2.23284900	-2.04151500	-2.26032200
C	-3.43460500	-2.35463600	-0.11294600
C	1.63909700	-3.11211500	-1.54124300
C	-1.51794300	-3.67794200	-0.08016200
C	-0.19796800	-3.97634100	-0.47391800
C	-3.27877800	1.79754900	-1.00824500
C	2.38500200	0.84363400	-2.62868700
C	-1.49066800	2.99893000	-2.15812500
C	0.74012400	2.63407700	-2.80695600
C	-3.10106500	-2.63873100	1.29035300
C	2.01784100	-3.38093400	-0.17434400
C	-1.86662500	-3.41622000	1.27226100
C	0.83574700	-3.90159300	0.49286800
C	-4.05247700	-0.04884000	0.50077200
C	3.22924500	-1.27089100	-1.55189100
C	-2.32703400	2.90773600	-1.03088800
C	1.96033200	2.18747200	-2.26275900
C	-0.13968100	3.48585500	-2.04334100
C	-3.73205900	1.33216300	0.25878100
C	3.24579500	0.14454700	-1.71319300
C	-3.22479300	-1.61024400	2.31730300
C	-0.81997700	-3.33443200	2.26571200
C	-3.73948300	-0.33263100	1.88804700
C	0.55872100	-3.57248100	1.84994800
C	3.04775800	-2.65798500	0.50452400
C	3.75241900	-1.60802100	-0.24199400
C	-3.27980600	1.91262900	1.47835700
C	3.74253000	0.72541100	-0.50966000
C	0.28572100	4.04819200	-0.88305100
C	-1.86291800	3.51372700	0.22976000
C	2.42349900	2.78548800	-0.99723500
C	-3.26838000	0.89372800	2.47040400
C	4.09039900	-0.33485400	0.40809900
C	-1.07302900	-2.46998500	3.35240600
C	1.60006500	-2.89967600	2.55345100

C	-2.22389800	-1.56943000	3.32328400
C	2.80332700	-2.42020600	1.89032600
C	-0.61256900	4.16444500	0.23875100
C	1.61909500	3.77570500	-0.39599300
C	-2.34808600	2.99343200	1.50768600
C	3.32555100	2.05042800	-0.11325300
C	-0.01912300	-1.79550700	4.01825600
C	1.30464600	-2.00685600	3.61368000
C	-1.80357800	-0.34343300	3.95855800
C	3.17781500	-1.17621100	2.54135500
C	-2.31509000	0.91012300	3.53162700
C	3.79186600	-0.10662100	1.81474500
C	0.21610200	4.22072600	1.41722200
C	1.58662800	3.98517400	1.02289300
C	-1.54667100	3.10388600	2.66497300
C	3.32234100	2.30294200	1.27219400
C	-0.44851600	-0.47496400	4.37543200
C	2.23226800	-0.91711600	3.58943700
C	-1.48236800	2.03557700	3.64139400
C	3.44896300	1.20161000	2.22320500
C	-0.24795600	3.70207600	2.61109200
C	2.43309100	3.26048200	1.84864300
C	0.44642500	0.63829900	4.35361300
C	1.83876300	0.40600500	3.94747000
C	-0.12623200	1.90729600	4.10090400
C	2.55628300	1.45416500	3.32229600
C	0.63438000	2.95359000	3.47786300
C	1.94921300	2.73711500	3.10198100
C	0.00915500	0.57445700	0.82100300
C	-0.15789200	0.24890500	-0.39011700
Sc	1.87032900	-0.61834300	0.43391200
Sc	-1.79132300	-0.96598100	0.57777900

The coordinates of optimized of Sc₂C₂@C₈₂-PF[12]CPP

C	1.98574700	-7.32739700	-2.15340500
C	0.61359600	-7.52185400	-2.10507500
C	-0.08465500	-7.42747600	-0.90390900
C	0.64900700	-7.19827300	0.25984200
C	2.01957000	-7.00048300	0.21097600
C	-1.55281400	-7.30119600	-0.87005100
C	-2.35671200	-7.94993400	0.06393200
C	-3.68784300	-7.59329800	0.24090000
C	-4.26066900	-6.55252100	-0.49012800
C	-3.46816700	-5.95038300	-1.46878800

C	-2.15129100	-6.32503200	-1.66286800
C	-5.52826500	-5.89815200	-0.11212100
C	-5.73326800	-5.50156400	1.21027300
C	-6.71528500	-4.58145200	1.54169500
C	-7.47933800	-3.95428000	0.55727800
C	-7.34607000	-4.42683400	-0.74871000
C	-6.41237500	-5.40140000	-1.07005000
C	-8.08611500	-2.63014900	0.80299600
C	-7.27951800	-1.66988600	1.41506800
C	-7.61156100	-0.33286600	1.41247300
C	-8.76332400	0.13618500	0.77669100
C	-9.60919900	-0.82353800	0.22481400
C	-9.28132700	-2.17850900	0.24428900
C	-8.78263400	1.58153200	0.46651200
C	-8.37268800	2.50915400	1.42289000
C	-7.74732000	3.68948300	1.05296600
C	-7.57599800	4.02552900	-0.29091100
C	-8.18657300	3.19921500	-1.23585700
C	-8.75319900	1.98795200	-0.86802500
C	-6.51117300	4.97439900	-0.67289100
C	-6.29183700	6.18678400	-0.01938200
C	-5.08944300	6.86868800	-0.15724500
C	-4.08250200	6.39654400	-0.99340600
C	-4.33818200	5.23699200	-1.71968700
C	-5.51074900	4.52613200	-1.54055900
C	1.52837100	7.43217400	-0.97159600
C	2.32242200	8.02781500	0.00725800
C	3.63924100	7.63494800	0.20565300
C	4.20509000	6.59302600	-0.53230300
C	3.43376400	6.06071600	-1.56741700
C	2.14352900	6.50264100	-1.80894300
C	5.43933000	5.89599600	-0.12055800
C	5.61958800	5.51102600	1.21004600
C	6.60608800	4.60789600	1.57737100
C	7.38462100	3.95613000	0.61901200
C	7.26063800	4.40241900	-0.69884800
C	6.34145700	5.38006100	-1.05146300
C	8.00657800	2.64164400	0.88868700
C	7.23193100	1.68372900	1.54640300
C	7.53621600	0.33916800	1.49119400
C	8.65061100	-0.13648700	0.79682500
C	9.49258400	0.82489000	0.23924500
C	9.17931100	2.18190100	0.28618200
C	8.65155900	-1.57491800	0.45682700

C	8.24557400	-2.52285100	1.39570500
C	7.63824400	-3.70507000	1.00374200
C	7.50302200	-4.04129500	-0.34541700
C	8.11457500	-3.19246000	-1.27023900
C	8.64156200	-1.96865300	-0.88226000
C	6.48488300	-5.03299200	-0.74808600
C	6.28069900	-6.23222200	-0.06320200
C	5.09227200	-6.93932800	-0.19004700
C	4.34643100	-5.39212000	-1.83846200
C	5.50089700	-4.64818800	-1.66495300
C	4.08776000	-6.51343600	-1.05365900
C	2.70903400	-7.03327200	-1.00136700
C	-0.63323200	7.23513700	0.20871800
C	0.05442400	7.51381600	-0.97517800
C	-0.68909600	7.57527300	-2.15291000
C	-2.04391200	7.27575700	-2.16004100
C	-2.71542500	6.94898000	-0.98665300
C	-1.99229300	6.96628300	0.20405800
F	2.60337500	-7.37875900	-3.32983600
F	-0.04381900	-7.75300100	-3.23792200
F	0.02175500	-7.05973500	1.42435300
F	2.66091200	-6.67857600	1.33152900
F	-1.84032900	-8.90367300	0.83209700
F	-4.40418100	-8.23517500	1.15810900
F	-3.92264300	-4.90274200	-2.15629700
F	-1.42180500	-5.63326700	-2.53694500
F	-4.90855300	-5.91134000	2.16948000
F	-6.83172100	-4.21196400	2.81350800
F	-8.03607300	-3.86121700	-1.73515600
F	-6.30376800	-5.78061100	-2.33962000
F	-6.08234400	-1.99338300	1.90496000
F	-6.71201000	0.51543300	1.91063000
F	-10.72816600	-0.44913400	-0.38567200
F	-10.11056000	-3.03969400	-0.33528500
F	-8.41967900	2.19590600	2.71414800
F	-7.18046500	4.42057800	2.00734700
F	-8.11604300	3.49913700	-2.52921600
F	-9.12970100	1.14546500	-1.82654000
F	-7.22040800	6.68608600	0.78995800
F	-4.89099000	7.97509400	0.55281700
F	-3.40460400	4.72865700	-2.52217200
F	-5.61169600	3.33952400	-2.13916000
F	1.80824000	8.96202200	0.80109900
F	4.34528800	8.23938500	1.15614800

F	3.86874000	5.01676100	-2.27067600
F	1.44663700	5.90986000	-2.77460400
F	4.78245100	5.93291900	2.15332900
F	6.72296500	4.29561100	2.86436500
F	7.95626700	3.81948800	-1.67138500
F	6.27750800	5.75235300	-2.32591900
F	6.08390500	2.01752600	2.13332200
F	6.64201500	-0.50434500	2.00683400
F	10.59336600	0.45139100	-0.40410600
F	10.00228300	3.03832800	-0.30920500
F	8.29517600	-2.24049200	2.69401200
F	7.06689100	-4.44761500	1.94716600
F	8.09820000	-3.48978400	-2.56570800
F	9.01753200	-1.11418000	-1.82996800
F	7.20675200	-6.69147400	0.77236100
F	4.90229000	-8.01861100	0.56286700
F	3.42081600	-4.94611300	-2.68531800
F	5.59479400	-3.49083800	-2.31601500
F	0.03103100	7.11559500	1.35497000
F	-0.09576100	7.87732300	-3.30366600
F	-2.69897800	7.26997100	-3.31787300
F	-2.58605300	6.63045900	1.34609300
C	3.28445200	-2.41518900	1.29409300
C	3.24512300	-1.60888900	2.45784800
C	3.71448200	-1.88001400	0.01887400
C	2.28359700	-3.41502300	1.03632100
C	2.20220400	-1.86928000	3.39693700
C	3.72008100	-0.24333400	2.36728900
C	1.59912500	-0.80082800	4.17267500
C	1.20503200	-2.85905100	3.14160400
C	3.96109600	0.27899500	1.04796800
C	3.16984900	0.83720100	3.19273900
C	3.96802300	-0.50646300	-0.15555600
C	3.58002700	1.64872700	1.02694600
C	3.63443500	0.14972500	-1.41608800
C	3.03395900	-2.62353800	-0.99170400
C	2.04033500	0.56331000	4.08325700
C	3.07461900	2.00008200	2.31896700
C	0.98954000	1.53467300	4.13048800
C	0.21797600	-1.15805400	4.36735400
C	0.99909900	2.76011500	3.35502900
C	-0.39247000	1.18862300	4.34368300
C	2.02716800	2.99130900	2.40299900
C	1.70066700	3.70921200	1.23431400

C	2.33804300	3.40530900	-0.02632400
C	0.34314100	4.09650500	0.96325700
C	-0.34385300	3.14251500	3.09417000
C	3.14337300	-0.67585100	-2.45272000
C	2.75650900	-2.03996200	-2.20281500
C	2.25151800	-0.17679500	-3.46181400
C	3.26552500	1.57046400	-1.43072700
C	3.22490200	2.32471000	-0.18376600
C	2.44334500	2.03617200	-2.47968500
C	1.38951400	3.70399000	-1.04918200
C	-0.80095400	-0.16788700	4.43055400
C	-1.20748200	2.17811100	3.71174100
C	-2.08518500	-0.50672300	3.92201000
C	-0.01467100	-2.42785200	3.75033100
C	-2.89043200	0.47667000	3.26742800
C	-2.31018500	-1.77031500	3.29049100
C	-2.44366200	1.82200400	3.10954900
C	-2.83301200	2.50125700	1.92015500
C	-1.96629400	3.45484600	1.29312100
C	-3.56859800	1.82925600	0.89349800
C	-3.64440100	-0.17898600	2.24321500
C	-0.69908500	3.77162500	1.86073200
C	0.13485400	4.05579100	-0.46159500
C	-2.14788400	3.37115900	-0.12330100
C	-1.26875000	-2.73201000	3.15310100
C	-3.27969600	-1.58001000	2.25542500
C	-1.27277500	-3.53757500	1.98001800
C	-2.23678600	-3.32544700	0.94417900
C	-0.05089700	-3.96496100	1.36590900
C	-3.29433100	-2.37169700	1.06354100
C	-3.79975100	-1.75709700	-0.14398100
C	-4.17175500	-0.32124900	-0.15740400
C	-3.07558700	-2.02193300	-1.37405000
C	-1.58042300	-3.60104000	-0.31746600
C	-4.02894800	0.48404700	1.03490300
C	-3.12542600	2.36840000	-0.37833300
C	-3.66248500	0.24055200	-1.39731800
C	1.20722200	-3.61407300	1.93012300
C	-0.24210600	-4.00566400	-0.05182900
C	2.09220900	-3.51508200	-0.38673600
C	0.80983200	-3.70122200	-0.96162100
C	0.47867800	-3.03881000	-2.22406500
C	1.51301800	-2.32221000	-2.87210500
C	-1.13262600	-1.55287400	-3.38251800

C	-0.90214000	-2.62901100	-2.48912900
C	-0.05398600	-0.81728800	-3.97437700
C	-2.19420400	-0.60853900	-3.17006800
C	-1.92703200	-2.88631200	-1.48222000
C	1.24107900	-1.19221400	-3.71314500
C	-3.11627700	-0.83375400	-2.16592900
C	-0.41799500	0.59113300	-3.98896500
C	0.53416400	1.54779000	-3.73991700
C	-1.72105100	0.72731700	-3.40574300
C	0.22058800	2.68033900	-2.91841300
C	1.90851900	1.15045400	-3.47440500
C	-2.04835400	1.79819900	-2.53523600
C	-3.08080100	1.55462600	-1.52978000
C	-1.03360300	2.82165500	-2.27819900
C	1.44119300	3.04296200	-2.24818000
C	-1.07227500	3.58726400	-1.03147000
C	-0.04036100	0.67644200	0.24055300
C	0.32557500	-0.51912500	0.04471300
Sc	1.53641500	0.20935600	1.85345400
Sc	-1.98628200	-0.51772000	0.25285000

The coordinates of optimized of Sc₂C₂@C₈₄CPP[12]CPP

C	9.32187800	-0.43764100	-0.51807200
C	9.14870900	-1.81661200	-0.55562200
C	7.98378700	-2.38568700	-1.06737500
C	7.04052300	-1.51936300	-1.62656600
C	7.22195100	-0.14909100	-1.60465500
C	7.57693900	-3.77930100	-0.79669300
C	7.58413400	-4.24836800	0.51800800
C	6.84334000	-5.35976600	0.88911600
C	6.03019200	-6.02133100	-0.02854700
C	6.12033800	-5.62862600	-1.36473400
C	6.89211800	-4.54020200	-1.74335600
C	4.85534900	-6.79942600	0.41334500
C	3.99678900	-6.19143600	1.32817800
C	2.70364100	-6.64073500	1.51936100
C	2.18538800	-7.71744600	0.79594300
C	3.09325500	-8.41480900	-0.00869900
C	4.38932100	-7.95315600	-0.21241500
C	0.71873300	-7.87591200	0.68916000
C	-0.14950200	-7.64710400	1.76044600
C	-1.49618200	-7.37761600	1.55480900
C	-2.08011100	-7.47206100	0.28893100
C	-1.24106100	-7.86337500	-0.75495400

C	0.12732100	-7.99233200	-0.57293900
C	-3.44794800	-6.97625400	0.04052700
C	-4.50426600	-7.17178500	0.93506300
C	-5.67324400	-6.42579600	0.84696400
C	-5.87056900	-5.51115400	-0.18308200
C	-4.87824000	-5.42307400	-1.15598000
C	-3.68186500	-6.10520700	-1.02591500
C	-6.86143600	-4.41796200	-0.13324800
C	-6.81311400	-3.54964200	0.95557500
C	-7.35289600	-2.27718300	0.88139100
C	-7.99524400	-1.82759200	-0.27409000
C	-8.15053300	-2.74219900	-1.31546500
C	-7.58077200	-4.00657200	-1.25187500
C	-7.08165500	3.74318500	-0.32214300
C	-6.32360000	4.00088300	0.82210000
C	-5.44708000	5.07106800	0.87432500
C	-5.28001200	5.91952800	-0.21904900
C	-6.08474700	5.70566500	-1.33382500
C	-6.98042200	4.64645100	-1.37898600
C	-4.09949700	6.80253300	-0.24889700
C	-3.77757300	7.67268000	0.78839600
C	-2.51164400	8.23279000	0.89047400
C	-1.49567800	7.89204900	-0.00586100
C	-1.84858000	7.08076100	-1.08698200
C	-3.12835100	6.57166800	-1.21867100
C	-0.06609000	8.11638500	0.28252400
C	0.44489800	7.80952500	1.54583500
C	1.80782500	7.69075400	1.76631800
C	2.71786900	7.74403900	0.70972600
C	2.21636300	8.13153000	-0.53446200
C	0.86278600	8.36408800	-0.72914700
C	4.04236100	7.09852500	0.80804300
C	4.10591500	5.82996400	1.39122100
C	5.21472100	5.02029900	1.24727700
C	6.31664600	5.42545000	0.49437500
C	6.28890300	6.71284900	-0.03233200
C	5.18325000	7.54114200	0.13752400
C	7.27949400	4.37929700	0.09692000
C	7.79943400	3.49064900	1.03425100
C	8.29201900	2.25399200	0.64868500
C	7.89137800	2.80569000	-1.63743400
C	7.39411900	4.04112500	-1.25100300
C	8.28807900	1.86449500	-0.69055300
C	8.34722100	0.42448600	-1.01092400

C	-7.35632900	1.61790300	-1.55402100
C	-7.71207000	2.41793100	-0.46961200
C	-8.42793400	1.81184200	0.56293600
C	-8.66194600	0.44489700	0.56886400
C	-8.18569400	-0.37546100	-0.45427800
C	-7.58596300	0.25168400	-1.54613900
F	10.41605200	0.05718700	0.05145600
F	10.09482100	-2.59284400	-0.03737600
F	5.88035100	-1.98697300	-2.08705000
F	6.23329700	0.62449900	-2.05191300
F	8.20341300	-3.55771900	1.47118400
F	6.82323700	-5.71156700	2.17095000
F	5.36067900	-6.21972300	-2.28260600
F	6.88155300	-4.16395800	-3.01846600
F	4.35300400	-5.06754700	1.94746200
F	1.93205400	-5.91976900	2.32688100
F	2.71607900	-9.51920300	-0.64428800
F	5.17249300	-8.60669900	-1.06460900
F	0.30376400	-7.61909800	3.00898200
F	-2.21036400	-6.96990400	2.59969200
F	-1.72767500	-8.05817900	-1.97651100
F	0.87411900	-8.16903500	-1.65889000
F	-4.38897800	-8.04813800	1.92719800
F	-6.59378200	-6.55883800	1.79671900
F	-4.99741500	-4.54146100	-2.14708600
F	-2.70603900	-5.78667000	-1.87464200
F	-6.08943500	-3.86961200	2.02662700
F	-7.10234800	-1.43618800	1.88446000
F	-8.78848100	-2.38401700	-2.42494100
F	-7.66002600	-4.80097100	-2.31470500
F	-6.33152800	3.14444400	1.84164300
F	-4.67265600	5.20985300	1.94842300
F	-5.96251200	6.49323400	-2.39784800
F	-7.70645600	4.46851800	-2.47810500
F	-4.67765000	7.93746500	1.73057100
F	-2.26478500	9.06327800	1.89828900
F	-0.93167800	6.66321700	-1.95574300
F	-3.37394700	5.73364600	-2.22283300
F	-0.37116500	7.52482000	2.55614800
F	2.22209500	7.41683500	2.99924600
F	3.01914400	8.19199300	-1.59298000
F	0.45710500	8.74083600	-1.93744400
F	3.04633400	5.31301000	2.01083600
F	5.15459600	3.78352800	1.74409900

F	7.31545400	7.15368000	-0.75220500
F	5.21583900	8.75701700	-0.39676100
F	7.71370900	3.77093100	2.33131500
F	8.64404000	1.38456400	1.59176000
F	7.87658600	2.48244300	-2.92710800
F	6.89900300	4.85340200	-2.18069300
F	-6.63461200	2.12040400	-2.55321500
F	-8.84280500	2.53655800	1.59712400
F	-9.29091400	-0.09126600	1.61017400
F	-7.05796100	-0.46961900	-2.53286700
C	3.94913200	0.66834000	0.38006400
C	3.65455700	0.36378300	1.76751500
C	3.76797500	-0.38009600	-0.59583900
C	3.37875600	1.86801000	-0.19202600
C	3.20581000	-0.96978300	2.09719900
C	2.81126200	1.27547300	2.50237800
C	3.42874400	-1.74911500	-0.26273400
C	3.13378100	-2.05625800	1.14338200
C	2.62055300	2.84127900	0.56654100
C	2.32542200	2.53137600	1.97256900
C	3.20557700	0.20227500	-1.78641000
C	2.96927600	1.57769400	-1.54090400
C	2.18847400	-0.87114900	3.10933600
C	1.94476300	0.50289800	3.35482900
C	2.80705000	-2.50146600	-1.26938900
C	2.23253500	-3.08788500	1.44095100
C	1.72517700	3.64308600	-0.15575400
C	1.15832900	3.04614000	2.55311900
C	2.45570900	-0.53142000	-2.75567500
C	1.95967300	2.30757700	-2.24349200
C	1.18751800	-1.86610200	3.33602300
C	0.68811000	0.97009900	3.84580100
C	2.35732800	-1.91363000	-2.52417300
C	1.29626500	-3.02418500	2.55133000
C	1.42052100	3.40953700	-1.55996500
C	0.36260000	2.29536700	3.51181700
C	1.87475400	-3.54019800	-0.92977800
C	1.59669800	-3.82768100	0.38708500
C	0.52540800	4.14045800	0.46397600
C	0.25034800	3.84958200	1.78184300
C	1.42549000	0.17941200	-3.50749100
C	1.17662400	1.60097600	-3.25110100
C	-0.10710500	-1.43555200	3.85333400
C	-0.35702700	-0.01426400	4.10759000

C	1.18758900	-2.62696000	-2.92778800
C	0.12581800	-3.74205900	2.15679400
C	0.05887900	3.78963300	-1.76264800
C	-0.99985400	2.67689800	3.31883700
C	0.81602600	-3.56336100	-1.89820100
C	0.25527700	-4.15469100	0.78207800
C	-0.53795500	4.13826100	-0.49906400
C	-1.09653000	3.55398900	2.18011000
C	0.37104300	-0.59899300	-4.02626700
C	-0.10598500	2.11462600	-3.53323100
C	-1.21092200	-2.26652600	3.57301300
C	-1.68733900	0.44984100	4.06252100
C	0.22059400	-1.98599400	-3.67089400
C	-0.68710600	3.16297700	-2.73507300
C	-1.10081400	-3.38116300	2.66667100
C	-2.00388200	1.77530400	3.59572200
C	-0.52958100	-3.73962600	-1.51903300
C	-0.82486300	-4.05541700	-0.11699400
C	-1.84631400	3.72355800	-0.16534800
C	-2.13690700	3.41517900	1.23778600
C	-0.95511800	-0.07145400	-4.17185900
C	-1.18876700	1.26200800	-3.92866600
C	-2.52952100	-1.73091800	3.39856200
C	-2.76513400	-0.39653600	3.64097800
C	-1.15849000	-2.26632600	-3.42716800
C	-2.06527100	2.87217800	-2.49467700
C	-2.25655800	-3.42923900	1.82728700
C	-3.15811800	1.72193000	2.75637600
C	-1.53262300	-3.07561600	-2.34413300
C	-2.12055900	-3.70062400	0.45705000
C	-2.62645600	3.09175600	-1.22679200
C	-3.20808600	2.47937400	1.57439800
C	-1.90914300	-1.06406900	-3.76301300
C	-2.39051400	1.68009000	-3.26153400
C	-3.16945700	-2.39390900	2.29757300
C	-3.65359900	0.35294800	2.79767300
C	-2.78826500	-2.75450200	-1.74522800
C	-3.07509500	-3.05822100	-0.39214500
C	-3.67737100	2.19769700	-0.85312100
C	-3.95527500	1.89745500	0.50453900
C	-3.08120100	-0.69064600	-3.09212300
C	-3.33162800	0.73402300	-2.83308600
C	-4.02639600	-1.68619000	1.44421700
C	-4.27504700	-0.25984400	1.70164800

C	-3.61715800	-1.65035400	-2.14732000
C	-4.08479800	-2.14236300	0.06875700
C	-4.09112300	1.07405700	-1.65033800
C	-4.56184400	0.59161700	0.56584500
C	-4.48056600	-1.30647600	-1.04272900
C	-4.71307300	0.10213000	-0.78268700
C	-0.39095600	0.46353900	-0.29040700
C	-0.40534000	-0.56340000	0.45186600
Sc	1.76350700	0.25059300	0.58517000
Sc	-2.55729700	-0.35666200	-0.41923500