

Supplementary Information

An atlas of endohedral Sc₂S cluster fullerenes

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S1: Isomer counts for sets of classical (C_n) and non-classical (C_n^{1h}) cages studied here.

Page 2

S2: Optimized cartesian coordinates (Å) for the favoured isomer Sc₂S@C_n for each n = 70 to 84.

Page 3

S3 Relative energies of C₄- n (energy in kcal/mol) calculated at the B3LYP/3-21G level.

Page 18

S1 Isomer counts for sets of classical (C_n) and non-classical (C_n^{1h}) cages studied here.

C_n	N_{55}				Total	C_n^{1h}	N_{55}				Total
	0	1	2	3			0	1	2	3	
C_{70}	1	1	20	124	146	C_{70}^{1h}	0	0	8	143	151
C_{72}	1	3	38	227	269	C_{72}^{1h}	0	0	33	459	492
C_{74}	1	3	72	400	476	C_{74}^{1h}	0	4	86	1267	1357
C_{76}	2	12	140	653	807	C_{76}^{1h}	0	7	242	2992	3241
C_{78}	5	18	240	1088	1351	C_{78}^{1h}	1	24	602	6729	7356
C_{80}	7	36	432	1714	2189	C_{80}^{1h}	1	71	1438	13957	15467
C_{82}	9	66	669	2704	3448	C_{82}^{1h}	6	177	3165	27088	30436
C_{84}	24	110	1059	4039	5232						

S2 Optimized cartesian coordinates (Å) for the favoured isomer Sc₂S@C_n for each n = 70 to 84

1. Sc₂S@C70-7892

C	2.03075400	-2.77665800	1.70856500
C	3.23295000	-2.18363800	1.21321300
C	3.47443600	-0.78953800	1.56302000
C	3.92606500	-0.10292900	0.35425500
C	3.52532900	1.25943500	0.07400900
C	3.06291300	1.61206500	-1.29350800
C	2.26373600	2.77620600	-1.42568600
C	1.20277000	2.86441100	-2.41090500
C	0.10223200	3.61213800	-1.84593400
C	-1.21178300	3.20118800	-2.09259600
C	-2.17122000	3.15947800	-1.00800300
C	-3.02514700	2.02040900	-1.18726600
C	-3.51192700	1.29481300	-0.07326600
C	-3.92578700	-0.06331800	-0.35399200
C	-3.97652500	-1.03623900	0.70430300
C	-3.56558000	-2.32511800	0.19092800
C	-2.57585300	-2.87616700	1.11369700
C	-1.36533600	-3.48630000	0.59989200
C	-0.18454200	-3.45187200	1.41478800
C	1.13451300	-3.50666500	0.82981100
C	1.24535300	-2.14660800	2.73033700
C	-0.10986700	-2.60796700	2.58152300
C	-1.21266900	-1.77769900	2.95664200
C	-2.44507300	-1.92741600	2.21906600
C	-3.28283400	-0.77620200	1.94212700
C	-2.84509300	0.55629100	2.28199600
C	-3.04621200	1.64207200	1.29425500
C	-2.23563400	2.79819200	1.42701800
C	-1.79710800	3.55190300	0.27460200
C	-0.44793200	4.03502300	0.51887100
C	0.48851300	4.03047000	-0.51694900
C	1.83280900	3.53378800	-0.27297900
C	2.20294700	3.13696300	1.00945100
C	3.04546200	1.98945500	1.18823200
C	2.61316300	1.31384200	2.42120500
C	2.67130400	-0.09457900	2.55640400
C	1.53762200	-0.80634700	3.18256500
C	0.43971700	-0.04576500	3.66287300
C	-0.93246300	-0.50833000	3.51081900
C	-1.76751900	0.63924700	3.21161600
C	-0.92726900	1.80183700	3.26210400

C	-1.17392200	2.87546600	2.41233000
C	-0.06587000	3.61246000	1.84776600
C	1.24394700	3.18793400	2.09406500
C	1.50403300	2.05940000	2.95332800
C	0.42910300	1.38203100	3.53961200
C	-1.48312400	2.07570000	-2.95231500
C	-2.59972400	1.34105500	-2.42048100
C	-2.67195400	-0.06664200	-2.55639800
C	-3.48161800	-0.75381600	-1.56297600
C	-3.25510400	-2.15062900	-1.21401100
C	-2.05908400	-2.75551500	-1.70988800
C	-1.17017800	-3.49429700	-0.83094100
C	0.14944400	-3.45277300	-1.41600700
C	1.32951300	-3.49921700	-0.60100800
C	2.54575900	-2.90043100	-1.11425100
C	3.54141200	-2.36036800	-0.19169800
C	3.96627000	-1.07588200	-0.70467100
C	3.27495300	-0.80825400	-1.94232900
C	2.85066800	0.52868400	-2.28173600
C	1.77389700	0.62276400	-3.21131100
C	0.94540300	1.79376800	-3.26125600
C	-0.41516500	1.38776400	-3.53892600
C	-0.44023500	-0.03982100	-3.66302300
C	-1.54581900	-0.78962200	-3.18323700
C	-1.26721300	-2.13299400	-2.73144100
C	0.08330000	-2.60801800	-2.58267000
C	1.19437900	-1.78855600	-2.95727200
C	2.42495400	-1.95047700	-2.21932400
C	0.92715400	-0.51620300	-3.51103000
Sc	1.78426700	-0.97101500	-0.07457100
Sc	-1.79244300	-0.95726300	0.07520000
S	0.00158300	0.55709800	-0.00307900

2. Sc2S@C72-10528

C	4.06035100	-0.51225100	-1.19375000
C	3.18597700	-0.90134800	-2.24870700
C	2.40105900	0.06814800	-2.96694300
C	1.22249700	-0.60332900	-3.44073700
C	-0.00015500	0.10255300	-3.63982900
C	-1.22285400	-0.60322900	-3.44062800
C	-2.40132200	0.06834400	-2.96674300
C	-3.18630900	-0.90109900	-2.24848200
C	-4.06054800	-0.51191600	-1.19343700
C	-4.19792200	-1.40925800	-0.05812700
C	-4.10972300	-0.59732500	1.13279900

C	-3.20490800	-1.21055000	2.06568200
C	-2.34572300	-0.40766700	2.89604500
C	-1.17220700	-1.06151600	3.36756700
C	0.00014100	-0.31043100	3.70754200
C	1.17239600	-1.06161700	3.36747300
C	2.34593400	-0.40787200	2.89585400
C	3.20502600	-1.21083400	2.06545800
C	4.10984100	-0.59767400	1.13250100
C	4.19777800	-1.40960400	-0.05846400
C	3.90231800	0.84691000	-0.68530200
C	3.91891400	0.77670300	0.76772000
C	3.09200100	1.64045300	1.57344900
C	2.33592200	1.05757600	2.70591000
C	1.18351400	1.76329300	3.13800000
C	0.00019300	1.06980800	3.59456800
C	-1.18310600	1.76339500	3.13810300
C	-2.33560700	1.05777400	2.70610600
C	-3.09171200	1.64071300	1.57370200
C	-3.91870900	0.77701800	0.76801600
C	-3.90228700	0.84722900	-0.68499300
C	-3.10621800	1.85100900	-1.36797200
C	-2.35722600	1.45529900	-2.57358200
C	-1.17841400	2.17563000	-2.90392400
C	-0.00008300	1.50132600	-3.40181500
C	1.17834800	2.17552900	-2.90402000
C	2.35712500	1.45509600	-2.57377000
C	3.10625900	1.85074300	-1.36822200
C	2.60349900	2.89264100	-0.55183400
C	2.59326300	2.78762000	0.90445600
C	1.41883100	3.47046900	1.38087200
C	0.72850200	2.95699800	2.47247700
C	-0.72804800	2.95706300	2.47254100
C	-1.41842000	3.47059600	1.38099200
C	-2.59294500	2.78783700	0.90467000
C	-2.60330100	2.89285900	-0.55161800
C	-1.42475400	3.63768400	-0.94006000
C	-0.72477400	3.27359200	-2.09155800
C	0.72487200	3.27352800	-2.09161800
C	1.42498600	3.63756500	-0.94018000
C	0.69905300	4.01005900	0.24622000
C	-0.69869100	4.01012100	0.24627900
C	2.42310100	-2.14078300	-2.16692000
C	1.22423200	-1.95501400	-2.94829700
C	-0.00023000	-2.60186400	-2.60299600

C	-1.22466800	-1.95491200	-2.94818700
C	-2.42352000	-2.14060500	-2.16673900
C	-2.41175100	-2.93348500	-0.95665700
C	-3.30736000	-2.55297200	0.11900600
C	-2.74078000	-2.44822300	1.46828700
C	-1.44643600	-2.98600000	1.80926300
C	-0.72485800	-2.33154300	2.84132500
C	0.72488800	-2.33160400	2.84126300
C	1.44632400	-2.98612000	1.80914400
C	2.74068700	-2.44844400	1.46807000
C	3.30709900	-2.55320300	0.11873400
C	2.41135600	-2.93363200	-0.95684300
C	1.16231700	-3.55169700	-0.60457000
C	-0.00021800	-3.44158200	-1.43889500
C	-1.16269700	-3.55159600	-0.60447400
C	-0.71542600	-3.64086700	0.76589600
C	0.71516700	-3.64092900	0.76583600
Sc	-2.10014900	-0.60986400	-0.02999600
Sc	2.10019700	-0.60980300	-0.02979300
S	-0.00001000	0.41559500	0.02937200

3. Sc2S@C74-13333

C	-4.16909100	1.39102200	-0.12510100
C	-3.51225900	1.96438900	0.98992300
C	-2.46844100	2.95063600	0.82533100
C	-1.61380200	2.86297800	1.97263300
C	-0.23751100	3.23078900	1.90512300
C	0.68105200	2.53785100	2.75334800
C	2.04321800	2.34024700	2.36292900
C	2.46672700	1.05293600	2.87183900
C	3.45015900	0.25656600	2.19567600
C	3.21965000	-1.17542600	2.17867200
C	3.51251700	-1.96409400	0.99031800
C	2.46850600	-2.95023600	0.82605200
C	1.94130200	-3.27160500	-0.46964700
C	0.59843900	-3.73386600	-0.50494500
C	-0.25408900	-3.45750400	-1.63018500
C	-1.60786100	-3.29200400	-1.17625700
C	-2.48277100	-2.36314900	-1.80499400
C	-3.56473400	-1.88151900	-0.97852300
C	-4.21089200	-0.63576400	-1.26486400
C	-4.58945400	0.00481300	-0.03015700
C	-3.53784600	1.59167700	-1.43235300
C	-3.55329700	0.31559300	-2.12257400
C	-2.46435300	-0.09915900	-2.96571400

C	-1.96896500	-1.48903900	-2.86970700
C	-0.64492200	-1.72859800	-3.31986100
C	0.20584600	-2.70283400	-2.69765700
C	1.57817600	-2.23166400	-2.70397000
C	2.45620900	-2.53164600	-1.63135000
C	3.53792100	-1.59216600	-1.43216100
C	4.16932900	-1.39115200	-0.12500400
C	4.58949800	-0.00478300	-0.03048000
C	4.14730200	0.84970900	1.06794700
C	3.56177400	2.05078700	0.45999000
C	2.51099700	2.80821200	1.09752300
C	1.61152400	3.50876400	0.25067700
C	0.24079100	3.72759800	0.65975000
C	-0.59849900	3.73383300	-0.50606700
C	-1.94134700	3.27157100	-0.47051400
C	-2.45629600	2.53121100	-1.63194200
C	-1.57835900	2.23092700	-2.70455700
C	-1.57976500	0.94131400	-3.35308200
C	-0.21890900	0.65381200	-3.74271500
C	0.21865400	-0.65486800	-3.74252800
C	1.57952000	-0.94224200	-3.35290300
C	2.46413400	0.09834500	-2.96588900
C	3.55312800	-0.31622400	-2.12272300
C	4.21062100	0.63537000	-1.26527400
C	3.56435800	1.88111500	-0.97928300
C	2.48261800	2.36272300	-1.80594000
C	1.60776600	3.29175500	-1.17741800
C	0.25396200	3.45715200	-1.63131300
C	-0.20603000	2.70211400	-2.69850400
C	0.64469700	1.72767400	-3.32047700
C	1.96876800	1.48824700	-2.87033700
C	-3.21944900	1.17618700	2.17854100
C	-2.05299600	1.75806800	2.79298800
C	-1.10241100	0.95190100	3.48031100
C	0.25768100	1.39154800	3.50578100
C	1.34581200	0.45973900	3.54439800
C	1.10263500	-0.95071500	3.48051200
C	2.05317400	-1.75709500	2.79334400
C	1.61392400	-2.86221700	1.97338700
C	0.23762500	-3.23008600	1.90609100
C	-0.24076800	-3.72730800	0.66093800
C	-1.61153100	-3.50863400	0.25189100
C	-2.51099400	-2.80782900	1.09857300
C	-3.56191800	-2.05070200	0.46086400

C	-4.14729600	-0.84935100	1.06851400
C	-3.44994400	-0.25577900	2.19591200
C	-2.46652500	-1.05194600	2.87231800
C	-1.34558000	-0.45854200	3.54460700
C	-0.25744500	-1.39036500	3.50620900
C	-0.68087000	-2.53688700	2.75415300
C	-2.04307000	-2.33941800	2.36375800
S	0.00002000	0.00050800	-0.00443800
Sc	-2.33636300	-0.00035900	-0.02477300
Sc	2.33642600	-0.00081500	-0.02437500

4. Sc2S@C76-19151

C	-1.42468600	2.46678100	2.85900500
C	-0.74049200	1.46012000	3.60275400
C	0.73765800	1.46404500	3.60180800
C	1.42168900	0.22338900	3.77129000
C	2.60171500	-0.07845100	3.02627200
C	2.59331500	-1.50087700	2.68359800
C	3.07810400	-1.96782100	1.44480900
C	2.34601500	-3.04320300	0.75908500
C	2.39846200	-3.07319400	-0.68322600
C	1.22633700	-3.39880000	-1.44200000
C	1.22356000	-2.60470900	-2.64989000
C	0.00331700	-2.09641300	-3.19107100
C	-0.00062800	-0.72637100	-3.74940200
C	-1.22130900	0.01453900	-3.71708200
C	-1.22491400	1.42654700	-3.40490200
C	-2.39713200	1.72202000	-2.63356900
C	-2.34604000	2.70539600	-1.57825500
C	-3.07973500	2.41381600	-0.33757300
C	-2.59609200	2.94348200	0.87646300
C	-2.60454700	2.16267400	2.11358600
C	-0.70253800	3.48758100	2.12607400
C	-1.42585700	3.78045700	0.91501100
C	-0.73036900	4.07093100	-0.26068900
C	-1.18522300	3.52178900	-1.51213300
C	-0.00997100	3.21917000	-2.29862000
C	-0.00772300	2.14149800	-3.21370500
C	1.21291800	1.43304800	-3.40686600
C	1.21611100	0.02080900	-3.71879600
C	2.45001700	-0.52711600	-3.20867300
C	2.45520800	-1.85260900	-2.67078900
C	3.20606800	-2.15595600	-1.47556500
C	3.97716600	-1.12467700	-0.82230000
C	3.80238000	-1.00840200	0.61180000

C	3.76904000	0.39171200	0.94378500
C	3.15843900	0.87812800	2.14447500
C	2.59590800	2.17612300	2.11003600
C	1.41556900	2.47425500	2.85720700
C	0.68709700	3.49124500	2.12517400
C	1.40721200	3.78787500	0.91313800
C	0.70862600	4.07462700	-0.26164500
C	1.16457700	3.52779000	-1.51369200
C	2.32965200	2.71745900	-1.58153000
C	2.38442700	1.73463900	-2.63695000
C	3.19514500	0.52708500	-2.56332300
C	3.97052300	0.24650900	-1.37873000
C	3.79509800	1.16337000	-0.27008700
C	3.06631000	2.42964400	-0.34176800
C	2.58159600	2.95679300	0.87292600
C	0.69985300	-1.01980200	3.95575600
C	1.42413900	-2.07500700	3.29486700
C	0.72944300	-3.10459200	2.65519700
C	1.18556700	-3.58429400	1.37579100
C	0.01069800	-3.91603200	0.60021400
C	0.00932800	-3.77829600	-0.80650200
C	-1.21049200	-3.40566800	-1.44056100
C	-1.21330800	-2.61125700	-2.64845900
C	-2.44851500	-1.86497400	-2.66722300
C	-2.45173000	-0.53974400	-3.20555400
C	-3.20206100	0.51060900	-2.55957100
C	-3.97442500	0.22605700	-1.37371300
C	-3.80219400	1.14382600	-0.26515700
C	-3.76994100	0.37218300	0.94877000
C	-3.16015100	0.86173100	2.14863100
C	-2.59716200	-0.09201700	3.02955900
C	-1.41779400	0.21597000	3.77316700
C	-0.68920300	-1.02344900	3.95671200
C	-1.40876700	-2.08241500	3.29675400
C	-0.70946600	-3.10828200	2.65609500
C	-1.16468600	-3.59025200	1.37724900
C	-2.32885200	-3.05536200	0.76194400
C	-2.38300900	-3.08590300	-0.68007600
C	-3.19567800	-2.17190100	-1.47090300
C	-3.97168100	-1.14503700	-0.81699900
C	-3.79584400	-1.02796600	0.61681500
C	-3.06545800	-1.98368500	1.44858800
C	-2.58155200	-1.51429200	2.68676800
S	-0.00011300	0.26423200	0.44128800

Sc	1.89230600	-0.33363800	-0.80938400
Sc	-1.89195100	-0.33822400	-0.80787000
5. Sc2S@C78-24088			
C	-2.36721600	3.08002000	-1.11397900
C	-3.22283400	2.05967900	-1.64285000
C	-4.07124300	1.25428600	-0.78380100
C	-4.29852800	0.00564000	-1.46063600
C	-4.07188300	-1.24364100	-0.78433400
C	-3.22367600	-2.04923900	-1.64398700
C	-2.36671900	-3.06868000	-1.11499800
C	-1.15710300	-3.31838200	-1.82175600
C	-0.00018000	-3.81514300	-1.14640600
C	1.15678500	-3.31848000	-1.82174900
C	2.36641700	-3.06888500	-1.11498500
C	3.22342700	-2.04949000	-1.64394900
C	4.07171600	-1.24398600	-0.78431700
C	4.29853300	0.00525400	-1.46063500
C	4.07141900	1.25394500	-0.78381600
C	3.22308100	2.05942800	-1.64288200
C	2.36751400	3.07981300	-1.11398800
C	1.15709400	3.32893200	-1.82012500
C	0.00017700	3.82872200	-1.14566700
C	-1.15678200	3.32903600	-1.82012400
C	-2.40911900	3.30029600	0.28520100
C	-1.21374000	3.73246000	0.98622900
C	0.00018000	3.98717800	0.28217000
C	1.21407600	3.73234500	0.98622700
C	2.40941600	3.30007300	0.28519800
C	3.14571600	2.40847700	1.14851600
C	3.87295400	1.28438800	0.64889800
C	3.82828200	0.00484600	1.38860300
C	3.87350200	-1.27454000	0.64860900
C	3.14500000	-2.39774000	1.14744200
C	2.40823200	-3.28833800	0.28411300
C	1.21317600	-3.71954500	0.98496000
C	-0.00018400	-3.97292000	0.28066300
C	-1.21352200	-3.71943000	0.98495600
C	-2.40853700	-3.28811400	0.28410600
C	-3.14521800	-2.39744200	1.14743200
C	-3.87363400	-1.27418000	0.64859600
C	-3.82828800	0.00520000	1.38860200
C	-3.87283200	1.28474700	0.64890900
C	-3.14550800	2.40877600	1.14852200
C	-2.40798500	2.32551000	2.37866100

C	-1.20643300	3.12472300	2.27874200
C	0.00012100	2.71739000	2.91189500
C	1.20671200	3.12461000	2.27873800
C	2.40818900	2.32528400	2.37865500
C	2.41553600	1.15151300	3.10229300
C	3.14672300	0.00468200	2.64214400
C	2.41581000	-1.14239800	3.10265800
C	2.40757900	-2.31476800	2.37751000
C	1.20597600	-3.11362000	2.27766500
C	-0.00012800	-2.70830000	2.91251000
C	-1.20626700	-3.11350500	2.27765900
C	-2.40779700	-2.31454200	2.37750100
C	-2.41592000	-1.14217300	3.10265300
C	-3.14673200	0.00497300	2.64214300
C	-2.41544000	1.15173900	3.10229500
C	-1.20107400	0.71547900	3.78056200
C	0.00006400	1.47142000	3.68915500
C	1.20113100	0.71536800	3.78056400
C	1.20126300	-0.70681200	3.78152000
C	-0.00007100	-1.46282000	3.69059900
C	-1.20133500	-0.70670100	3.78151900
C	-2.81926100	1.24548900	-2.78605700
C	-3.52646700	0.00566400	-2.68237100
C	-2.81967500	-1.23491900	-2.78698900
C	-1.44462500	-1.25793200	-3.23582300
C	-0.70805000	-2.41624800	-2.86191300
C	0.70781900	-2.41631300	-2.86191400
C	1.44449200	-1.25805900	-3.23581100
C	2.81952100	-1.23514400	-2.78694500
C	3.52646700	0.00535300	-2.68236800
C	2.81941200	1.24526300	-2.78609300
C	1.44460200	1.26757500	-3.23456700
C	0.70815500	2.42587300	-2.85963200
C	-0.70792600	2.42594000	-2.85963600
C	-1.44447200	1.26770500	-3.23456200
C	-0.73430200	0.00497700	-3.49244900
C	0.73430100	0.00491200	-3.49245000
Sc	-2.08017200	-0.00205600	-0.91471500
Sc	2.08019800	-0.00187300	-0.91469500
S	0.00001600	-0.14955000	0.25946700
6. Sc2S@C80-31923			
C	0.00002300	-3.99044600	-0.97816900
C	1.16930400	-3.53427600	-1.66947600
C	2.33960300	-3.14140100	-0.95420800

C	3.17564300	-2.11974500	-1.56605200
C	4.03142500	-1.22576100	-0.80626000
C	3.89527600	0.09653800	-1.40591000
C	3.81565500	1.32721300	-0.64243400
C	3.13247500	2.42136500	-1.25414200
C	2.41342200	3.38396300	-0.45392000
C	1.20602900	3.79624100	-1.15695900
C	-0.00007200	4.08318800	-0.45248700
C	-1.20621000	3.79620400	-1.15687600
C	-2.41354600	3.38389300	-0.45375600
C	-3.13262500	2.42127400	-1.25392900
C	-3.81574400	1.32710700	-0.64217700
C	-3.89539800	0.09642500	-1.40565400
C	-4.03147700	-1.22588400	-0.80600200
C	-3.17570500	-2.11984300	-1.56584200
C	-2.33958200	-3.14147000	-0.95405300
C	-1.16931800	-3.53430800	-1.66939800
C	0.00007200	-4.08520200	0.41273000
C	-1.16952200	-3.72905300	1.16106300
C	-2.34473800	-3.24636100	0.50888200
C	-3.19279600	-2.32745100	1.26003400
C	-4.05113500	-1.33255100	0.63268400
C	-3.91096000	-0.10102100	1.40656100
C	-3.82002900	1.22549700	0.81720100
C	-3.13284200	2.22253400	1.57293900
C	-2.41368100	3.28866900	0.91402300
C	-1.20657400	3.59898600	1.66631100
C	-0.00002100	3.98145200	1.00873500
C	1.20658500	3.59901800	1.66622800
C	2.41365100	3.28873600	0.91385800
C	3.13288500	2.22262000	1.57272600
C	3.82005100	1.22560400	0.81694400
C	3.91107000	-0.10091300	1.40630200
C	4.05123600	-1.33244600	0.63242100
C	3.19297400	-2.32738400	1.25983200
C	2.34487300	-3.24630100	0.50872700
C	1.16970500	-3.72901500	1.16098200
C	0.71358600	-3.20494400	2.43368100
C	-0.71333800	-3.20496600	2.43372800
C	-1.43618700	-2.16526600	3.08632400
C	-2.67159700	-1.75492500	2.48442600
C	-3.11247700	-0.39742500	2.57130200
C	-2.34296700	0.59323200	3.27216000
C	-2.39006200	1.90999600	2.75721600

C	-1.21162300	2.76997900	2.81918400
C	0.00008300	2.29811700	3.39935700
C	1.21173500	2.77001400	2.81910300
C	2.39019200	1.91006400	2.75705500
C	2.34316800	0.59329900	3.27200100
C	3.11265600	-0.39733800	2.57108500
C	2.67181100	-1.75485300	2.48424100
C	1.43644900	-2.16522600	3.08622800
C	0.71655600	-1.20555200	3.84767600
C	-0.71626400	-1.20557200	3.84772300
C	-1.15668600	0.16355000	3.93520900
C	0.00012100	1.00613900	4.00727600
C	1.15694700	0.16358400	3.93513400
C	2.67502300	-1.39308600	-2.71485800
C	3.11611000	-0.03803900	-2.61182400
C	2.34283600	1.03953400	-3.16091200
C	2.38887600	2.27271800	-2.46879300
C	1.21116400	3.13539200	-2.41373200
C	-0.00014000	2.75041500	-3.05540700
C	-1.21141200	3.13535900	-2.41365100
C	-2.38910300	2.27265300	-2.46863400
C	-2.34307200	1.03947100	-3.16075500
C	-3.11627400	-0.03812500	-2.61160200
C	-2.67515400	-1.39315800	-2.71466400
C	-1.43886500	-1.71462700	-3.36212600
C	-0.71271400	-2.83132300	-2.85217100
C	0.71260700	-2.83130300	-2.85221800
C	1.43869600	-1.71458800	-3.36222600
C	0.71609800	-0.66115500	-3.98429700
C	1.15520100	0.70763100	-3.87539300
C	-0.00014900	1.55294100	-3.83316800
C	-1.15547800	0.70760100	-3.87531800
C	-0.71634300	-0.66117500	-3.98424900
Sc	2.03172300	-0.66492600	0.01758100
Sc	-2.03172200	-0.66492300	0.01752600
S	0.00000300	0.52490100	-0.08192400
7. Sc2S@C82-39715			
C	1.53207100	-0.28144900	3.88627100
C	0.98450800	1.04008600	3.85492800
C	-0.41653100	1.24192600	3.73580400
C	-0.82089700	2.42670100	3.04613900
C	-2.06449200	2.51198700	2.35763000
C	-1.92611100	3.46155600	1.27674100
C	-2.64537100	3.23760400	0.04715500

C	-1.93687400	3.50561500	-1.18311600
C	-2.07377000	2.56957700	-2.27727000
C	-0.83217400	2.49693200	-2.96984400
C	-0.43236600	1.33192300	-3.69677000
C	0.96741500	1.13476400	-3.82790700
C	1.51513000	-0.18523000	-3.89558300
C	2.74094600	-0.23206700	-3.14745900
C	3.08159600	-1.37861200	-2.38562600
C	3.88791000	-1.16509200	-1.19041500
C	3.86727000	-2.04825700	-0.03233200
C	3.89464800	-1.19434400	1.14769500
C	3.09215200	-1.43731600	2.34027100
C	2.75452600	-0.30997600	3.13203300
C	0.68179600	-1.37785300	3.90015000
C	1.00663400	-2.54860300	3.13029400
C	2.17435300	-2.58740200	2.33010200
C	2.09665300	-3.38205000	1.11894300
C	2.93865700	-3.15910800	-0.04397500
C	2.09119200	-3.35236200	-1.20805600
C	2.16369000	-2.52874700	-2.39982400
C	0.99311300	-2.47127900	-3.19413300
C	0.66444800	-1.28087100	-3.93242400
C	-0.75977000	-1.08948300	-3.91589200
C	-1.34416000	0.19069100	-3.71743300
C	-2.63706400	0.26571500	-3.01895000
C	-2.99989300	1.47382500	-2.28017800
C	-3.85618600	1.39336600	-1.14998700
C	-3.60318300	2.19246800	0.03663900
C	-3.84876400	1.36484700	1.20360000
C	-2.98851100	1.41752100	2.33356200
C	-2.62378200	0.19066500	3.04024800
C	-1.32761600	0.09885900	3.73046900
C	-0.74283000	-1.18583600	3.89483300
C	-1.30161000	-2.34766400	3.25332300
C	-0.24754500	-3.14802300	2.70070400
C	-0.39353500	-3.72061200	1.41931400
C	0.81065600	-3.86446600	0.66365400
C	0.80747800	-3.84688900	-0.75937500
C	-0.39978900	-3.68487200	-1.50606900
C	-0.25919600	-3.08107100	-2.77378300
C	-1.31570100	-2.26699200	-3.30102100
C	-2.52629500	-2.19986000	-2.65483800
C	-3.23935300	-0.95218100	-2.59313400
C	-4.07663500	-1.01594000	-1.42323600

C	-4.38136900	0.13485600	-0.71308300
C	-4.37696800	0.11714900	0.73832300
C	-4.07075700	-1.05067500	1.41866300
C	-3.22796200	-1.01585000	2.58640100
C	-2.51479800	-2.26436100	2.61375400
C	-2.73930400	-2.97604300	1.37259200
C	-1.66581400	-3.60471700	0.69499200
C	-1.66904300	-3.58688700	-0.77363200
C	-2.74559500	-2.94197100	-1.43081400
C	-3.77431100	-2.24519100	-0.71002600
C	-3.77116800	-2.26195800	0.67372500
C	0.11364700	3.29624100	2.38948300
C	-0.55405400	3.96743000	1.28924400
C	0.16843300	4.24144100	0.05339300
C	-0.56337200	4.01548700	-1.19070400
C	0.10299000	3.35677500	-2.30084300
C	1.50205300	3.04495700	-2.31221600
C	1.92592200	1.95725400	-3.11660900
C	3.01349600	1.12119900	-2.69355100
C	3.65522200	1.34894200	-1.45431200
C	4.07862900	0.18826300	-0.72044000
C	4.08174800	0.17043000	0.71055600
C	3.66079400	1.31250300	1.47472800
C	3.02518800	1.05427100	2.71125700
C	1.93988200	1.87936100	3.16040800
C	1.51106000	2.98674300	2.38506600
C	2.23656100	3.31697500	1.20301700
C	1.55123800	3.86524900	0.04607500
C	2.23379200	3.34700800	-1.12709800
C	3.30205800	2.50902500	-0.69644100
C	3.30375700	2.49045100	0.74749000
Sc	-0.50623000	2.04554700	-0.01658800
Sc	1.80498600	-1.24477100	-0.01204100
S	-0.37666100	-0.29969600	-0.01164900

8. Sc2S@C84-51591

C	1.83186100	3.41859700	1.71223800
C	2.47789800	2.39254400	2.52060500
C	3.42114400	1.48432000	1.99292600
C	3.42104000	0.09155400	2.48297000
C	3.85854500	-0.94796800	1.56722400
C	3.10983500	-2.18903700	1.52407400
C	3.10979800	-2.66098200	0.18294100
C	2.06070900	-3.49693600	-0.32009800
C	1.83220800	-3.41828400	-1.71237000

C	0.51515900	-3.60704400	-2.24151400
C	0.27109200	-2.64128800	-3.28395200
C	-0.97668700	-1.97118600	-3.39211500
C	-0.97724300	-0.58805700	-3.87980700
C	-2.06062900	0.31988600	-3.49698200
C	-1.83231100	1.71216200	-3.41829400
C	-2.47829000	2.52054600	-2.39223000
C	-1.51867800	3.50670900	-1.96643500
C	-1.51832400	3.96484200	-0.66317300
C	-0.27099800	4.21527600	0.00215900
C	-0.51460500	4.00549200	1.40774000
C	0.51484600	3.60714100	2.24148100
C	0.27099000	2.64138300	3.28397200
C	1.51832100	1.96664000	3.50674300
C	1.51811400	0.66336600	3.96484200
C	2.47798400	-0.28617500	3.46326100
C	1.83182100	-1.59227400	3.47556300
C	2.06063400	-2.52575600	2.43975500
C	0.97700800	-3.39210000	1.97110400
C	0.97742400	-3.87977600	0.58797500
C	-0.27041600	-4.21523200	-0.00214200
C	-0.51418800	-4.00552900	-1.40769600
C	-1.83141000	-3.47572600	-1.59234700
C	-2.06026300	-2.43990600	-2.52576100
C	-3.10958600	-1.52437400	-2.18911300
C	-3.10967600	-0.18326700	-2.66107000
C	-3.85847200	0.62763600	-1.72062500
C	-3.42142600	1.99282900	-1.48389400
C	-3.42112400	2.48283700	-0.09112400
C	-2.47804000	3.46317100	0.28646900
C	-1.83174600	3.47550200	1.59248700
C	2.06023600	3.49732700	0.31994300
C	0.97681000	3.87998000	-0.58804500
C	0.97633600	3.39227200	-1.97118000
C	-0.27142800	3.28395300	-2.64131500
C	-0.51535200	2.24145800	-3.60703700
C	0.51409600	1.40777400	-4.00551900
C	0.27051100	0.00219300	-4.21522000
C	1.51788000	-0.66308600	-3.96497600
C	1.51831400	-1.96637300	-3.50686700
C	2.47802900	-2.39215200	-2.52078500
C	3.42120500	-1.48379500	-1.99320300
C	3.85847700	-1.72053100	-0.62804400
C	4.40127100	-0.68897500	0.24246500

C	4.40103800	0.68960800	-0.24279400
C	3.85816000	1.72106700	0.62772700
C	3.10934000	2.66145900	-0.18318600
C	3.10935600	2.18950200	-1.52429800
C	2.06006300	2.52605900	-2.43989300
C	1.83130600	1.59258500	-3.47571200
C	2.47760500	0.28657700	-3.46342200
C	3.42073500	-0.09101800	-2.48318100
C	3.85815600	0.94852800	-1.56749700
C	-2.06042400	2.43967800	2.52596900
C	-0.97669700	1.97109400	3.39222700
C	-0.97701000	0.58795300	3.87989800
C	0.27086400	-0.00210800	4.21522600
C	0.51464900	-1.40765600	4.00549100
C	-0.51470000	-2.24150700	3.60709300
C	-0.27070800	-3.28396200	2.64132900
C	-1.51800000	-3.50691800	1.96656700
C	-1.51771800	-3.96501700	0.66328000
C	-2.47761000	-3.46349600	-0.28626800
C	-3.42073300	-2.48326500	0.09144900
C	-3.85830300	-1.56759900	-0.94805600
C	-4.40114100	-0.24291100	-0.68906800
C	-4.40107200	0.24233300	0.68947200
C	-3.85843100	1.56709400	0.94843200
C	-3.10967300	1.52401300	2.18945000
C	-3.10954500	0.18288600	2.66143200
C	-2.06034400	-0.32015000	3.49724000
C	-1.83179400	-1.71242100	3.41852100
C	-2.47770800	-2.52086100	2.39246800
C	-3.42098800	-1.99325900	1.48422300
C	-3.85818200	-0.62811700	1.72096700
S	0.00007400	-0.00037300	-0.00022700
Sc	2.31554000	-0.00006700	-0.00004300
Sc	-2.31536500	-0.00015100	-0.00009400

S3 Relative energies of C4- n (energy in kcal/mol) calculated at the B3LYP/3-21G level

Molecule	N_{55}	ΔE	Gap	Molecule	N_{55}	ΔE	Gap
C ₇₀ :8149	0	0.0	0.99	C ₇₆ :19151	0	0.0	1.77
C ₇₀ :7852	3	2.0	2.03	C ₇₆ :19138	1	16.6	0.91
C ₇₀ :7957	2	2.1	1.25	C ₇₆ :17490	2	20.1	1.33
C ₇₀ :7851	3	2.3	1.57	C ₇₆ :17459	1	25.0	0.97
C ₇₀ :7892	2	2.6	1.14	C ₇₆ :17465	2	28.6	1.07
C ₇₀ :7887	3	3.5	1.75	C ₇₆ :17491	2	28.9	1.50
C ₇₀ :7893	3	5.7	1.58	C ₇₆ :19142	1	30.4	1.05
C ₇₀ :7854	3	6.6	1.03	C ₇₆ :17508	2	30.9	1.65
C ₇₀ :7886	3	7.5	1.60	C ₇₆ :17899	2	31.7	1.31
C ₇₀ :7924	2	8.6	1.24	C ₇₆ :17418	1	31.9	1.06
C ₇₀ :7846	3	8.6	1.97	C ₇₆ :17588	2	32.2	1.08
C ₇₀ :7850	3	10.9	1.58	C ₇₆ :17894	1	32.3	0.86
C ₇₀ :7853	3	11.5	2.17	C ₇₆ :17464	2	32.8	1.52
C ₇₀ :7921	3	11.6	1.56	C ₇₆ :18161	2	32.9	0.97
C ₇₀ :7922	3	11.6	1.25	C ₇₆ :17750	1	33.4	1.03
C ₇₀ :7847	3	11.7	1.36	C ₇₆ :17492	2	34.0	1.36
C ₇₀ :7960	2	11.9	0.93	C ₇₆ :17519	2	34.0	1.77
C ₇₀ :8008	2	13.6	1.31	C ₇₆ :17425	2	34.7	1.45
C ₇₀ :7848	3	14.1	1.58	C ₇₆ :17512	2	34.9	1.05
C ₇₀ :7888	3	15.4	1.43	C ₇₆ :18638	2	35.1	1.19
C ₇₀ :8005	2	15.5	0.98	C1h 76:136015	2	37.3	1.36
C ₇₀ :7849	3	15.5	1.03	C1h 76:54549	2	37.7	1.26
C ₇₀ :7889	3	15.7	1.39	C1h 76:59553	2	37.8	1.09
C ₇₀ :8064	2	15.7	1.06	C1h 76:726505	2	39.9	1.44
C ₇₀ :7911	3	15.9	1.42	C1h 76:63537	2	42.3	0.97
C ₇₂ :10528	2	0.0	1.50	C ₇₈ :24109	0	0.0	0.83
C ₇₂ :10611	2	1.7	1.29	C ₇₈ :24107	0	8.5	1.09
C ₇₂ :10616	2	3.7	1.68	C ₇₈ :24099	1	14.4	1.53
C ₇₂ :10610	2	8.3	1.36	C ₇₈ :22595	1	19.0	1.14
C ₇₂ :11188	1	9.3	0.95	C ₇₈ :21981	2	22.7	1.40
C ₇₂ :10626	2	14.5	1.53	C ₇₈ :23349	1	23.6	0.99
C ₇₂ :10538	2	15.1	1.25	C ₇₈ :22010	2	25.2	0.87
C ₇₂ :10482	3	15.7	1.36	C ₇₈ :22135	2	25.4	1.50
C ₇₂ :10518	3	16.2	1.53	C ₇₈ :24088	2	26.0	1.05
C ₇₂ :10557	2	17.0	1.29	C1h 78:83318	2	26.3	1.02

C ₇₂ :10612	1	17.7	0.74	C ₇₈ :21982	2	26.4	1.41
C ₇₂ :10554	2	18.4	1.17	C ₇₈ :22096	2	27.5	1.73
C ₇₂ :10693	2	18.6	0.98	C1h 78:83323	1	27.7	1.20
C ₇₂ :10615	2	19.2	1.14	C1h 78:185827	2	28.3	1.20
C1h 72:408641	3	19.5	1.41	C ₇₈ :23295	1	28.3	1.13
C ₇₂ :10530	2	19.5	1.10	C ₇₈ :21791	2	29.2	1.40
C ₇₂ :10688	3	19.8	1.40	C ₇₈ :21971	2	29.8	1.29
C ₇₂ :10526	3	20.7	1.49	C ₇₈ :21983	2	29.9	1.59
C ₇₂ :10689	2	20.9	1.05	C ₇₈ :22395	2	30.2	1.48
C ₇₂ :11029	2	21.5	1.15	C ₇₈ :22646	2	30.5	0.77
C ₇₂ :10849	2	21.8	1.07	C ₇₈ :21769	2	32.2	1.49
C1h 72:413844	3	22.3	1.46	C1h 78:185820	2	32.5	1.18
C ₇₂ :10533	3	22.3	1.35	C1h 78:579517	2	32.8	1.42
C ₇₂ :10784	2	22.5	1.03	C ₇₈ :22598	2	33.0	1.02
C ₇₂ :10779	3	22.6	1.56	C ₇₈ :23318	1	33.0	1.00
C ₇₄ :13333	2	0.0	1.58	C ₈₀ :31924	0	0.0	0.78
C ₇₄ :14246	0	4.4	0.62	C ₈₀ :31923	0	6.1	0.52
C ₇₄ :13290	2	6.1	1.53	C ₈₀ :31922	0	7.3	1.12
C ₇₄ :13295	2	9.0	1.21	C1h 80:112912	2	28.6	1.12
C ₇₄ :13384	2	10.7	1.75	C ₈₀ :31891	1	29.0	1.01
C ₇₄ :13291	2	13.5	1.22	C ₈₀ :28324	1	29.4	1.31
C ₇₄ :13334	2	14.5	1.45	C ₈₀ :31876	1	29.4	1.20
C ₇₄ :13336	2	16.3	1.20	C ₈₀ :31911	1	31.8	1.31
C ₇₄ :13408	2	16.4	1.13	C ₈₀ :31920	0	33.1	1.12
C ₇₄ :13549	2	17.6	1.46	C1h 80:112926	1	33.3	1.20
C ₇₄ :13771	2	17.8	1.27	C ₈₀ :28319	1	34.8	0.91
C ₇₄ :13391	2	18.1	1.15	C1h 80:112916	2	36.1	1.33
C ₇₄ :13335	2	20.0	1.22	C1h 80:112913	2	37.4	0.85
C ₇₄ :13292	2	20.5	0.89	C ₈₀ :28334	2	37.5	1.71
C ₇₄ :14239	2	20.9	1.01	C ₈₀ :28863	1	37.8	1.06
C ₇₄ :14239	2	20.9	1.01	C ₈₀ :29558	2	38.0	1.55
C ₇₄ :14049	1	21.1	0.93	C ₈₀ :31607	1	38.4	1.47
C ₇₄ :13492	3	23.5	1.36	C1h	2	38.5	1.28

				80:249134			
C ₇₄ :13393	1	23.5	0.86	C ₈₀ :28316	1	39.0	1.13
C1h 74:100259	2	24.0	1.08	C ₈₀ :28285	2	40.0	1.47
C ₇₄ :13293	2	24.2	1.20	C ₈₀ :29097	1	40.3	1.21
C ₇₄ :13410	2	25.3	1.18	C ₈₀ :28335	2	40.4	1.37
C ₇₄ :13565	2	27.4	1.21	C ₈₀ :30291	1	40.7	1.01
C ₇₄ :13406	2	27.9	1.30	C ₈₀ :28871	1	40.8	1.12
C ₇₄ :13825	2	28.2	1.01	C ₈₀ :29162	2	41.2	1.59
C ₈₂ :39717	0	0.0	1.73	C ₈₄ :51589	0	0	1.03
C ₈₂ :39718	0	4.2	1.06	C ₈₄ :51591	0	1.25	1.21
C ₈₂ :39715	0	9.0	1.21	C ₈₄ :51590	0	3.1	1.14
C ₈₂ :39705	1	20.5	1.24	C ₈₄ :51580	0	3.99	1.17
C ₈₂ :39714	0	24.3	0.81	C ₈₄ :51578	0	4.38	0.95
C1h 82:155199	1	27.1	1.44	C ₈₄ :51575	0	7.6	1.13
C ₈₂ :39704	1	28.6	1.05	C ₈₄ :51581	0	9.21	0.95
C1h 82:155195	1	31.5	1.11	C ₈₄ :51383	1	10.19	1.59
C ₈₂ :39686	1	31.8	1.20	C ₈₄ :51483	1	12.75	1.49
C ₈₂ :39656	1	31.9	1.36	C ₈₄ :51583	0	13.78	1.08
C ₈₂ :39663	1	33.4	0.85	C ₈₄ :51573	0	13.84	1.35
C ₈₂ :39712	0	35.0	1.04	C ₈₄ :51579	0	14.54	1.05
C ₈₂ :39662	1	36.8	1.18	C ₈₄ :51482	1	14.91	1.06
C1h 82:155255	1	37.2	1.33	C ₈₄ :51577	0	14.91	0.89
C ₈₂ :38471	1	37.3	1.30	C ₈₄ :51550	1	15.1	1.44
C1h 82:155219	1	37.3	1.24	C ₈₄ :51499	1	15.15	1.16
C1h 82:155196	1	37.8	1.28	C ₈₄ :51365	1	15.71	0.98
C ₈₂ :39716	0	38.3	0.90	C ₈₄ :51576	0	16.80	0.70
C1h 82:155250	2	38.9	1.17	C ₈₄ :51539	1	16.94	1.14
C ₈₂ :37359	1	39.0	1.26	C ₈₄ :45206	1	17.72	1.35
C1h 82:155182	2	39.3	1.34	C ₈₄ :51353	1	18.54	1.42
C ₈₂ :35776	1	39.3	1.31	C ₈₄ :43990	1	19.09	1.33
C1h 82:331996	2	40.7	1.50	C ₈₄ :51397	1	19.43	1.05
C ₈₂ :36531	2	41.0	1.51	C ₈₄ :51425	1	19.66	1.04

C ₈₂ :36652	2	41.3	1.18	C ₈₄ :51481	1	19.82	1.17
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