

Carbon Rings: A DFT Study on Geometry, Aromaticity, Intermolecular Carbon-Carbon Interactions and Stability

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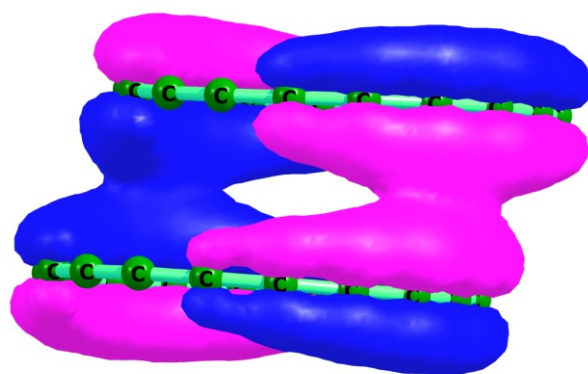
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HOMO-33
E = -0.401 eV

Figure S1. Occupied MO corresponding to C...C interactions in C₁₈

Table S1: Energy of the monomers (E_{monomer}), dimers (E_{dimer}) and the bsse energy (E_{bsse}) of C_{4N+2} and C_{4N} rings

C _{4N+2}	E_{monomer}	E_{dimer}	E_{bsse}	C _{4N}	E_{monomer}	E_{dimer}	E_{bsse}
C ₆	-228.30014	-456.60601	0.00218	C ₈	-304.44581	-608.93361	0.00484
C ₁₀	-380.72820	-761.46800	0.00331	C ₁₂	-456.85553	-913.75148	0.00568
C ₁₄	-533.10878	-1066.23282	0.00422	C ₁₆	-609.24015	-1218.51220	0.00667
C ₁₈	-685.47610	-1370.97001	0.00455	C ₂₀	-761.61614	-1523.26298	0.00616
C ₂₂	-837.83534	-1675.69220	0.00561	C ₂₄	-913.98264	-1827.99919	0.00701
C ₂₆	-990.19024	-1980.40590	0.00668	C ₂₈	-1066.34317	-2132.72321	0.00775
C ₃₀	-1142.54258	-	-	C ₃₂	-1218.69977	-	-

Table S2: Energy of the polyynes (E_{polyne}) and linear C_n molecules (E_{linearCn})

Polyne	E_{polyne}	Linear C _n	E_{linearCn}
acetylene	-77.33767	Linear C ₆	-228.26374
4yne	-305.84500	Linear C ₈	-304.44455
5yne	-382.01701	Linear C ₁₀	-380.62242
6yne	-458.18940	Linear C ₁₂	-456.79886
7yne	-534.36197	Linear C ₁₄	-532.97439
8yne	-610.53466	Linear C ₁₆	-609.14919
9yne	-686.70744	Linear C ₁₈	-685.32366
10yne	-762.88028	Linear C ₂₀	-761.49779
11yne	-839.05314	Linear C ₂₂	-837.67165
12yne	-915.22603	Linear C ₂₄	-913.84531
13yne	-991.39895	Linear C ₂₆	-990.01873
14yne	-1067.57181	Linear C ₂₈	-1066.19218
15yne	-1143.74481	Linear C ₃₀	-1142.36555
16yne	-1219.91774	Linear C ₃₂	-1218.53874
17yne	-1296.09069	-	-

Table S3: The enthalpy of the monomers (H_{monomer}), dimers (H_{dimer}) and the bsse corrected ΔH values of the C_{4N+2} rings

C_{4N+2}	H_{monomer}	H_{dimer}	ΔH (bsse corrected)
C_6	-228.26760	-456.53900	-1.01806
C_{10}	-380.67141	-761.35258	-4.05454
C_{14}	-533.02905	-1066.07139	-5.69681
C_{18}	-685.37399	-1370.76184	-5.84035
C_{22}	-837.70913	-1675.43512	-7.05367
C_{26}	-990.03981	-1980.09917	-8.07177
C_{30}	-1142.36796	-	-

Table S4: The free energy of the monomers (G_{monomer}), dimers (G_{dimer}) and the bsse corrected ΔG values of the C_{4N+2} rings

C_{4N+2}	G_{monomer}	G_{dimer}	ΔG (bsse corrected)
C_6	-228.29918	-456.58788	7.94717
C_{10}	-380.71181	-761.41721	6.09858
C_{14}	-533.07926	-1066.15300	6.11230
C_{18}	-685.43416	-1370.86158	7.08824
C_{22}	-837.77754	-1675.54809	7.90931
C_{26}	-990.11681	-1980.22640	8.72542
C_{30}	-1142.45581	-	-

Table S5: The enthalpy of the monomers (H_{monomer}), dimers (H_{dimer}) and the bsse corrected ΔH values of the C_{4N} rings

C_{4N}	H_{monomer}	H_{dimer}	ΔH (bsse corrected)
C_8	-304.401838	-608.845625	-23.28675617
C_{12}	-456.787303	-913.616422	-22.67475544
C_{16}	-609.147796	-1218.329462	-17.06824354
C_{20}	-761.499713	-1523.028087	-14.11988422
C_{24}	-913.841794	-1827.713063	-14.0995175
C_{28}	-1066.17754	-2132.386954	-15.13707585
C_{32}	-1218.51445	-	-

Table S6: The free energy of the monomers (G_{monomer}), dimers (G_{dimer}) and the bsse corrected ΔG values of the C_{4N} rings

C_{4N}	G_{monomer}	G_{dimer}	ΔG (bsse corrected)
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C ₈	-304.439544	-608.901133	-10.7968
C ₁₂	-456.833683	-913.685823	-8.016749
C ₁₆	-609.203132	-1218.414259	-0.831422
C ₂₀	-761.564138	-1523.129655	2.9998436
C ₂₄	-913.915261	-1827.827987	5.9870776
C ₂₈	-1066.259323	-2132.516741	6.0595844
C ₃₂	-1218.611992	-	-

Table S7-S59: Cartesian coordinates of all the optimized structures at M06L/6-311++g(d,p) level.
Atomic number followed by X, Y, Z coordinates in Angstrom.

Table S7: Coordinates of C₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-0.904711000	-0.522223000	0.000000000
6	0.000163000	-1.493870000	0.000000000
6	-1.294239000	0.747211000	0.000000000
6	0.904762000	-0.522279000	0.000000000
6	0.000000000	1.044429000	0.000000000
6	1.294024000	0.746731000	0.000000000

Table S8: Coordinates of C₈ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.052512000	-1.715584000	-0.001318000
6	-1.019521000	-1.060213000	-0.000055000
6	1.019501000	1.060179000	0.001071000
6	-1.972183000	-0.051209000	0.002070000
6	-0.052510000	1.715534000	-0.001764000
6	-1.169818000	0.933364000	-0.000824000
6	1.972268000	0.051192000	0.001232000
6	1.169751000	-0.933262000	-0.000412000

Table S9: Coordinates of C₁₀ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	1.467285000	-1.600175000	0.000266000
6	1.912036000	-0.388473000	0.000054000
6	-1.774965000	-0.809184000	0.000134000

6	1.975907000	0.900870000	-0.000112000
6	-2.128234000	0.432447000	0.000100000
6	0.959598000	1.696709000	-0.000291000
6	-1.068827000	-1.889639000	-0.000346000
6	0.221166000	-1.936724000	0.000014000
6	-0.246308000	2.157179000	0.000301000
6	-1.317657000	1.436990000	-0.000120000

Table S10: Coordinates of C₁₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.736132000	2.453989000	-0.001548000
6	1.686812000	1.644742000	-0.003882000
6	2.532666000	0.599359000	-0.001977000
6	-1.778024000	1.870140000	0.004486000
6	-2.285181000	0.626013000	0.001837000
6	-2.531322000	-0.599088000	-0.001928000
6	2.285698000	-0.625623000	0.002164000
6	-0.593887000	2.267794000	0.000952000
6	-1.686568000	-1.645244000	-0.003733000
6	1.776995000	-1.868877000	0.004070000
6	0.593253000	-2.267666000	0.001318000
6	-0.736574000	-2.455539000	-0.001760000

Table S11: Coordinates of C₁₄ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	2.030540000	2.073884000	-0.000614000
6	2.677807000	0.969695000	0.000265000
6	2.892385000	-0.291889000	0.000982000
6	-2.478663000	1.515943000	0.001288000
6	-2.834813000	0.286064000	0.000645000
6	-2.733434000	-0.989781000	-0.000144000
6	2.429128000	-1.484987000	-0.000234000
6	0.908978000	2.690613000	-0.001403000
6	-1.541012000	2.387124000	0.000506000
6	-1.989878000	-2.032022000	-0.001269000
6	1.572791000	-2.435901000	0.001523000
6	0.350980000	-2.818268000	-0.000947000
6	-0.927025000	-2.745281000	-0.000253000
6	-0.357783000	2.874805000	-0.000345000

Table S12: Coordinates of C₁₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.775476000	1.855169000	0.001261000
6	-0.685008000	-3.170829000	-0.001144000
6	-1.758952000	2.726959000	0.001128000
6	0.650300000	-3.273090000	0.000372000
6	-0.650514000	3.274068000	0.000611000
6	0.684834000	3.171463000	-0.001303000
6	1.855064000	2.774448000	-0.000502000
6	1.758914000	-2.726396000	0.000752000
6	2.727276000	1.758403000	-0.001766000
6	3.275351000	0.650369000	0.000659000
6	2.776215000	-1.855498000	0.001248000
6	3.172582000	-0.684958000	0.000392000
6	-3.171916000	0.684752000	-0.000746000
6	-1.855847000	-2.775398000	0.000063000
6	-3.275172000	-0.650637000	0.000060000
6	-2.727648000	-1.758826000	-0.001085000

Table S13: Coordinates of C₁₈ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.482381000	-1.220102000	0.000363000
6	-3.674294000	0.043577000	-0.000412000
6	-1.881428000	-3.167514000	0.002088000
6	-2.843761000	-2.326518000	0.000982000
6	3.687521000	-0.044329000	-0.000355000
6	3.439461000	-1.298307000	-0.000806000
6	2.798151000	-2.403307000	-0.003828000
6	1.798595000	-3.200167000	-0.001881000
6	0.596728000	-3.634451000	-0.000609000
6	-0.681090000	-3.605534000	0.001848000
6	-3.450654000	1.301308000	0.000765000
6	-2.786361000	2.393214000	-0.001787000
6	-1.805475000	3.212054000	-0.000926000
6	-0.594519000	3.621693000	-0.001450000
6	0.683359000	3.621024000	-0.001456000
6	1.875041000	3.157708000	0.001180000
6	3.468079000	1.214552000	0.003658000
6	2.853027000	2.335098000	0.002625000

Table S14: Coordinates of C₂₀ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.312137000	-3.375187000	0.001899000
6	-1.112478000	-3.955301000	0.001914000

6	-3.859123000	-1.373952000	-0.000228000
6	-3.229578000	-2.548497000	0.000928000
6	-0.115448000	4.086790000	0.000947000
6	-1.427460000	3.853509000	-0.000358000
6	-2.499203000	3.239931000	-0.000330000
6	-3.424449000	2.280838000	-0.001809000
6	-3.930455000	1.154318000	-0.001830000
6	-4.113997000	-0.165578000	-0.001520000
6	0.115456000	-4.086711000	0.001740000
6	1.427484000	-3.853496000	0.000402000
6	2.499243000	-3.239957000	-0.001872000
6	3.424534000	-2.280899000	-0.002412000
6	3.859054000	1.373920000	-0.000364000
6	3.229509000	2.548471000	0.001509000
6	1.112488000	3.955397000	0.001927000
6	2.312114000	3.375209000	0.001681000
6	4.113951000	0.165553000	-0.000705000
6	3.930493000	-1.154360000	-0.001518000

Table S15: Coordinates of C₂₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.478740000	-0.439510000	-0.001333000
6	4.405963000	0.835597000	-0.000757000
6	3.528419000	-2.786517000	-0.000790000
6	4.160059000	-1.676533000	-0.001118000
6	-3.263912000	-3.091696000	0.000377000
6	-2.251303000	-3.870349000	0.000901000
6	-1.071345000	-4.358839000	0.001090000
6	0.201122000	-4.468908000	0.001034000
6	1.458678000	-4.245666000	0.000566000
6	2.589495000	-3.652216000	0.000067000
6	4.003310000	2.047647000	-0.000135000
6	3.252162000	3.080798000	0.000492000
6	2.257701000	3.882258000	0.000978000
6	1.067624000	4.345592000	0.001030000
6	-4.171687000	1.681197000	-0.001148000
6	-4.463125000	0.437539000	-0.001057000
6	-3.991915000	-2.042034000	-0.000152000
6	-4.420306000	-0.838867000	-0.000797000
6	-3.515713000	2.776988000	-0.000720000
6	-2.597755000	3.664914000	-0.000095000
6	-1.454270000	4.233581000	0.000539000
6	-0.201942000	4.485027000	0.001028000

Table S16: Coordinates of C₂₄ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.354643000	4.904663000	0.001083000
6	3.678224000	3.239779000	0.003966000
6	-2.145710000	4.423593000	-0.004091000
6	-0.968013000	4.804214000	-0.001411000
6	-4.426969000	-2.145258000	0.004284000
6	-4.808477000	-0.967886000	0.001813000
6	-4.909699000	0.354744000	-0.000993000
6	-4.649125000	1.564660000	-0.003209000
6	-4.072801000	2.759600000	-0.005315000
6	-3.241141000	3.676233000	-0.004481000
6	4.427075000	2.145301000	0.004073000
6	4.808766000	0.967979000	0.002059000
6	4.909619000	-0.354676000	-0.001242000
6	4.649223000	-1.564628000	-0.002695000
6	-0.354679000	-4.904932000	0.000998000
6	-1.564860000	-4.645541000	0.002402000
6	-3.678328000	-3.239925000	0.005244000
6	-2.760107000	-4.069810000	0.005007000
6	0.967947000	-4.804312000	-0.002395000
6	2.145636000	-4.423585000	-0.003586000
6	3.240894000	-3.675969000	-0.004976000
6	4.072780000	-2.759533000	-0.004588000
6	2.760261000	4.069938000	0.005350000
6	1.564840000	4.645349000	0.002703000

Table S17: Coordinates of C₂₆ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	3.944825000	3.549940000	0.018709000
6	0.590387000	5.241243000	0.014271000
6	5.147997000	1.316138000	-0.002886000
6	4.672845000	2.501174000	0.009445000
6	1.920034000	-4.937240000	-0.002136000
6	3.036601000	-4.318076000	-0.010174000
6	3.994175000	-3.474240000	-0.016587000
6	4.702916000	-2.411895000	-0.019514000
6	5.162858000	-1.221056000	-0.019292000
6	5.297635000	0.048572000	-0.013484000
6	-0.685876000	5.245590000	0.004924000
6	-1.921254000	4.922668000	-0.005074000
6	-3.055431000	4.337604000	-0.015902000
6	-3.998878000	3.477515000	-0.022528000
6	-2.972576000	-4.388816000	0.017551000

6	-1.833982000	-4.966323000	0.015029000
6	0.681521000	-5.247054000	0.004973000
6	-0.594992000	-5.273780000	0.011854000
6	-5.121487000	-1.307003000	0.002053000
6	-5.303948000	-0.043321000	-0.006890000
6	-5.151701000	1.223874000	-0.014990000
6	-4.724930000	2.427282000	-0.020751000
6	1.836459000	4.962201000	0.020779000
6	2.968552000	4.372893000	0.022827000
6	-4.667677000	-2.499928000	0.009755000
6	-3.924075000	-3.537960000	0.018039000

Table S18: Coordinates of C₂₈ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	3.000343000	4.868534000	0.007148000
6	5.403201000	1.903352000	0.007568000
6	0.583615000	5.677284000	-0.001559000
6	1.872321000	5.382671000	0.002896000
6	-5.441305000	1.836228000	-0.004054000
6	-4.858966000	3.023214000	-0.008167000
6	-4.096917000	4.000531000	-0.010620000
6	-3.056227000	4.815820000	-0.011023000
6	-1.945960000	5.367133000	-0.009327000
6	-0.655819000	5.654986000	-0.005849000
6	5.699410000	0.699901000	0.004194000
6	5.693478000	-0.622121000	0.001522000
6	5.435677000	-1.834544000	-0.001905000
6	4.854392000	-3.021968000	-0.003999000
6	-2.996500000	-4.865435000	0.001744000
6	-5.401762000	-1.900966000	0.016199000
6	-5.697908000	0.623551000	0.002542000
6	-5.701854000	-0.698512000	0.008996000
6	0.656913000	-5.661037000	-0.006016000
6	1.946908000	-5.372779000	-0.007835000
6	3.055619000	-4.818482000	-0.007229000
6	4.094522000	-4.001034000	-0.006487000
6	4.830034000	3.094885000	0.009706000
6	4.035705000	4.046644000	0.009201000
6	-0.582484000	-5.682673000	-0.006431000
6	-1.869887000	-5.382546000	-0.002392000
6	-4.826804000	-3.091649000	0.013952000
6	-4.029744000	-4.040988000	0.007224000

Table S19: Coordinates of C₃₀ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-6.071940000	-0.712419000	-0.010688000
6	-5.341936000	2.989137000	-0.011774000
6	-5.253622000	-3.113354000	-0.002432000
6	-5.801108000	-1.960134000	-0.006921000
6	3.648157000	-4.880975000	-0.000899000
6	2.554822000	-5.539703000	0.004011000
6	1.342075000	-5.938333000	0.007813000
6	0.075781000	-6.100021000	0.011421000
6	-3.525281000	-4.970067000	0.007833000
6	-4.495507000	-4.140805000	0.003175000
6	-4.590809000	4.021659000	-0.006103000
6	-3.655210000	4.889956000	-0.001969000
6	-2.549721000	5.528138000	0.004917000
6	-1.344350000	5.948280000	0.009231000
6	5.789838000	1.956851000	-0.004837000
6	5.848411000	-1.816513000	-0.012404000
6	4.598749000	-4.029108000	-0.007164000
6	5.331366000	-2.983311000	-0.011433000
6	3.532688000	4.980146000	0.009729000
6	2.412431000	5.591911000	0.012810000
6	1.196749000	5.981492000	0.013868000
6	-0.075365000	6.086885000	0.011641000
6	-5.838657000	1.813461000	-0.012192000
6	-6.099993000	0.563710000	-0.014031000
6	4.488127000	4.133948000	0.004639000
6	5.264714000	3.120433000	-0.000676000
6	6.087408000	-0.562385000	-0.012187000
6	6.082744000	0.714154000	-0.010223000
6	-2.416519000	-5.602592000	0.011585000
6	-1.194041000	-5.970442000	0.013259000

Table S20: Coordinates of C₃₂ optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-1.917134000	6.226122000	0.005806000
6	1.911486000	6.222129000	0.005487000
6	-4.164961000	5.023609000	0.000297000
6	-3.061753000	5.745806000	0.002475000
6	-5.046871000	-4.154335000	-0.001986000
6	-5.779153000	-3.057994000	-0.006129000
6	-6.270115000	-1.917873000	-0.007938000
6	-6.519685000	-0.622901000	-0.008928000
6	-5.786735000	3.056943000	-0.003711000
6	-5.041573000	4.144713000	-0.002493000

6	3.061924000	5.755828000	0.008106000
6	4.157688000	5.022385000	0.003239000
6	5.044602000	4.153980000	0.002854000
6	5.778838000	3.058694000	-0.006212000
6	1.917804000	-6.224249000	0.011860000
6	-1.910561000	-6.218133000	0.008561000
6	-4.158072000	-5.020987000	0.002329000
6	-3.061620000	-5.753162000	0.007798000
6	5.048086000	-4.150971000	-0.009073000
6	5.783079000	-3.056258000	-0.006780000
6	6.264272000	-1.911994000	-0.012531000
6	6.522517000	-0.618567000	-0.006142000
6	0.619122000	6.485126000	0.007626000
6	-0.622074000	6.475493000	0.006999000
6	4.164725000	-5.023100000	0.000468000
6	3.065352000	-5.750827000	-0.000583000
6	-0.618289000	-6.480882000	0.013537000
6	0.623002000	-6.473960000	0.008401000
6	-6.258491000	1.908666000	-0.006207000
6	-6.530925000	0.618329000	-0.007294000
6	6.262887000	1.915754000	-0.000268000
6	6.522626000	0.622618000	-0.009566000

Table S21: Coordinates of C₆ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-1.547924000	-0.906813000	-0.636089000
6	-2.229420000	-1.290657000	0.436793000
6	-1.017669000	-0.007349000	-1.457135000
6	-2.386671000	0.005095000	0.681249000
6	-1.542237000	0.901739000	-0.643020000
6	-2.221715000	1.297930000	0.426638000
6	1.578079000	0.906135000	0.655310000
6	1.112840000	0.005292000	1.513199000
6	2.180920000	1.291625000	-0.463190000
6	1.575873000	-0.902483000	0.661332000
6	2.320215000	-0.003674000	-0.720521000
6	2.177710000	-1.296839000	-0.454568000

Table S22: Coordinates of C₈ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
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6	1.404367000	-0.413996000	1.769592000
6	1.362094000	-1.265240000	0.779552000
6	1.363747000	1.262264000	-0.781801000
6	1.412405000	-1.809855000	-0.422366000
6	1.401681000	0.410731000	-1.771839000
6	1.351936000	-0.800069000	-1.253431000
6	1.419083000	1.806507000	0.420127000
6	1.357905000	0.797080000	1.251580000
6	-1.403217000	0.378466000	1.777488000
6	-1.354735000	-0.822116000	1.237087000
6	-1.354399000	0.825051000	-1.234767000
6	-1.416679000	-1.816292000	0.386853000
6	-1.408103000	-0.375215000	-1.775455000
6	-1.364526000	-1.247211000	-0.803500000
6	-1.411637000	1.819748000	-0.384648000
6	-1.359922000	1.250146000	0.805530000

Table S23: Coordinates of C₁₀ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.843283000	1.769548000	-1.500376000
6	1.757504000	1.950506000	-0.607026000
6	0.910917000	-1.567522000	-1.426060000
6	2.661212000	1.744880000	0.291476000
6	1.725135000	-2.170901000	-0.626449000
6	3.063257000	0.585237000	0.691783000
6	0.252690000	-0.651661000	-2.054261000
6	0.415861000	0.620599000	-1.905082000
6	3.203979000	-0.689967000	0.834315000
6	2.546927000	-1.588895000	0.181115000
6	-0.195189000	-0.156802000	2.128673000
6	-0.677304000	-1.258242000	1.657862000
6	-2.075327000	1.893626000	0.290218000
6	-1.370651000	-2.110163000	0.979519000
6	-2.915285000	1.399884000	-0.556565000
6	-2.260913000	-1.808129000	0.094658000
6	-1.164109000	2.013877000	1.196791000
6	-0.562973000	1.030011000	1.777777000
6	-3.044499000	-1.146462000	-0.689149000
6	-3.114518000	0.140575000	-0.759219000

Table S24: Coordinates of C₁₂ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-1.856666000	1.816884000	-1.478926000
6	-2.286477000	0.600980000	-1.443555000
6	-2.511205000	-0.676194000	-1.476697000
6	0.630558000	2.490051000	-1.502866000
6	1.626241000	1.659911000	-1.482595000
6	2.467710000	0.682559000	-1.526756000
6	-1.668050000	-1.653011000	-1.452535000
6	-0.637535000	2.259661000	-1.455951000
6	2.243614000	-0.594353000	-1.488874000
6	-0.673046000	-2.483304000	-1.496866000
6	0.595658000	-2.251846000	-1.476189000
6	1.814887000	-1.810960000	-1.523236000
6	-2.320620000	-1.107227000	1.522794000
6	-2.317626000	0.183324000	1.489447000
6	-2.100442000	1.461096000	1.522879000
6	-0.191276000	-2.559158000	1.501416000
6	1.023094000	-2.107920000	1.455293000
6	2.144032000	-1.468795000	1.472570000
6	-0.980754000	2.101515000	1.482064000
6	-1.313459000	-1.923695000	1.477166000
6	2.360652000	-0.190564000	1.438961000
6	0.233924000	2.553163000	1.506351000
6	1.355735000	1.918616000	1.457336000
6	2.361051000	1.099267000	1.478770000

Table S25: Coordinates of C₁₄ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.009066000	0.859276000	-0.190240000
6	-4.043955000	-0.420059000	-0.213373000
6	-3.680783000	-1.632702000	-0.024391000
6	-0.247907000	2.511040000	1.716349000
6	0.570155000	1.592904000	2.070347000
6	1.043583000	0.419389000	2.262738000
6	-2.824005000	-2.469194000	0.428919000
6	-3.406194000	1.940027000	0.135983000
6	-1.364520000	2.843303000	1.186483000
6	0.905425000	-0.851818000	2.207564000
6	-1.755113000	-2.908098000	0.979113000
6	-0.626526000	-2.665460000	1.532278000
6	0.362116000	-1.988618000	1.981301000
6	-2.500579000	2.709326000	0.612027000
6	-0.630542000	-1.601302000	-2.089963000
6	0.250261000	-2.448044000	-1.709602000

6	1.335156000	-2.900002000	-1.202278000
6	0.632448000	2.729787000	-1.529962000
6	1.777943000	2.850482000	-0.971274000
6	2.874347000	2.506094000	-0.408274000
6	2.459106000	-2.667645000	-0.635646000
6	-0.997878000	-0.383977000	-2.236616000
6	-0.306783000	1.969795000	-1.951670000
6	3.655516000	1.579079000	0.003152000
6	3.425572000	-1.999710000	-0.127589000
6	3.953737000	-0.869158000	0.157000000
6	4.096105000	0.400535000	0.237232000
6	-0.947620000	0.894750000	-2.219604000

Table S26: Coordinates of C₁₆ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-2.446375000	-2.285709000	1.539416000
6	-1.146120000	2.987616000	1.525915000
6	-1.302014000	-2.922335000	1.526501000
6	0.113418000	3.345522000	1.539671000
6	-0.113241000	-3.345473000	1.539595000
6	1.146317000	-2.987639000	1.525743000
6	2.285785000	-2.445919000	1.539652000
6	1.302151000	2.922253000	1.526578000
6	2.922867000	-1.301819000	1.527070000
6	3.346841000	-0.113307000	1.539932000
6	2.446413000	2.285474000	1.539382000
6	2.988436000	1.146133000	1.526191000
6	-2.988280000	-1.146311000	1.526281000
6	-2.285507000	2.445732000	1.539768000
6	-3.346580000	0.113156000	1.540015000
6	-2.922670000	1.301687000	1.527413000
6	3.133521000	1.178296000	-1.539269000
6	-0.081929000	-3.197417000	-1.526688000
6	2.320405000	2.204629000	-1.526484000
6	-1.382957000	-3.048807000	-1.540086000
6	1.382804000	3.049001000	-1.540028000
6	0.081757000	3.197525000	-1.526454000
6	-1.178415000	3.133027000	-1.539371000
6	-2.320629000	-2.204514000	-1.526290000
6	-2.205070000	2.320372000	-1.526288000
6	-3.049933000	1.383187000	-1.540031000
6	-3.133771000	-1.178204000	-1.539184000
6	-3.197813000	0.082029000	-1.526283000
6	3.197646000	-0.081929000	-1.526558000
6	1.178242000	-3.132891000	-1.539501000

6	3.049783000	-1.383089000	-1.540205000
6	2.204919000	-2.320273000	-1.526402000

Table S27: Coordinates of C₁₈ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-1.842941000	-1.846065000	-2.152368000
6	-1.023951000	-2.809470000	-1.967991000
6	-2.272255000	0.640237000	-2.242454000
6	-2.249721000	-0.637412000	-2.236319000
6	3.540194000	2.829110000	-0.739485000
6	2.469414000	3.450678000	-1.056150000
6	1.260688000	3.695806000	-1.391671000
6	0.047930000	3.447487000	-1.709740000
6	-1.038282000	2.826194000	-1.969062000
6	-1.822227000	1.832328000	-2.143490000
6	0.039253000	-3.471491000	-1.713439000
6	1.260336000	-3.671446000	-1.393669000
6	2.475415000	-3.473682000	-1.050626000
6	3.524861000	-2.811427000	-0.743835000
6	4.325528000	-1.845613000	-0.500552000
6	4.724180000	-0.637122000	-0.382438000
6	4.309227000	1.834260000	-0.510855000
6	4.744812000	0.640587000	-0.374209000
6	-1.298097000	3.696659000	1.379818000
6	-0.083006000	3.462163000	1.699448000
6	-3.568386000	2.804070000	0.730131000
6	-2.504073000	3.437944000	1.044434000
6	-2.439893000	-3.486379000	1.060811000
6	-3.496398000	-2.835881000	0.753362000
6	-4.306943000	-1.878998000	0.507527000
6	-4.718017000	-0.675019000	0.385862000
6	-4.751232000	0.602413000	0.372932000
6	-4.327440000	1.800822000	0.504955000
6	1.009045000	2.852514000	1.962016000
6	1.802948000	1.867063000	2.139293000
6	2.264780000	0.679810000	2.242290000
6	2.255585000	-0.597992000	2.238932000
6	1.861761000	-1.811083000	2.156771000
6	1.053021000	-2.783540000	1.974615000
6	-1.222738000	-3.670634000	1.403812000
6	-0.003378000	-3.456892000	1.721341000

Table S28: Coordinates of C₂₀ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	3.099595000	2.656561000	-1.605544000
6	3.816647000	1.543635000	-1.605639000
6	0.945004000	3.968530000	-1.607291000
6	2.179186000	3.489702000	-1.606395000
6	-4.070077000	-0.328632000	-1.605786000
6	-3.994644000	0.993065000	-1.606216000
6	-3.485338000	2.125234000	-1.606740000
6	-2.647599000	3.150455000	-1.607762000
6	-1.569251000	3.765616000	-1.607980000
6	-0.289152000	4.103215000	-1.607864000
6	4.070391000	0.328400000	-1.605463000
6	3.995465000	-0.993339000	-1.605852000
6	3.485231000	-2.125130000	-1.606586000
6	2.647143000	-3.149961000	-1.607597000
6	-0.944853000	-3.969267000	-1.606951000
6	-2.179283000	-3.490921000	-1.606252000
6	-3.815613000	-1.543728000	-1.605574000
6	-3.098741000	-2.656689000	-1.605671000
6	0.289300000	-4.103696000	-1.607588000
6	1.569498000	-3.766341000	-1.607462000
6	3.461383000	-2.163717000	1.606341000
6	4.003256000	-0.955779000	1.607321000
6	1.528060000	-3.784211000	1.605415000
6	2.676465000	-3.125574000	1.605842000
6	-4.072500000	-0.283472000	1.607802000
6	-3.800778000	-1.579136000	1.608229000
6	-3.127542000	-2.622227000	1.607467000
6	-2.146171000	-3.510807000	1.606772000
6	-0.988434000	-3.959033000	1.606062000
6	0.327726000	-4.101172000	1.605518000
6	4.072146000	0.283755000	1.608049000
6	3.800466000	1.579420000	1.608319000
6	3.127207000	2.622502000	1.607619000
6	2.145752000	3.510978000	1.606731000
6	-1.528335000	3.784535000	1.605046000
6	-2.676827000	3.126044000	1.605591000
6	-4.003304000	0.956043000	1.607041000
6	-3.461548000	2.164012000	1.605954000
6	-0.328051000	4.101681000	1.605333000
6	0.988118000	3.959447000	1.605760000

Table S29: Coordinates of C₂₂ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
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6	0.364555000	4.243960000	-1.747931000
6	-0.879206000	4.469221000	-1.564332000
6	2.415958000	2.773489000	-1.983902000
6	1.479699000	3.636652000	-1.885756000
6	1.122400000	-3.891792000	-1.849689000
6	2.108530000	-3.087481000	-1.956507000
6	2.869234000	-2.063994000	-2.030328000
6	3.271643000	-0.851982000	-2.058498000
6	3.358035000	0.422261000	-2.067581000
6	3.036031000	1.658147000	-2.038132000
6	-2.134691000	4.374742000	-1.350297000
6	-3.292882000	3.881649000	-1.132566000
6	-4.288509000	3.108461000	-0.927938000
6	-4.995210000	2.055508000	-0.776527000
6	-3.667970000	-3.664874000	-1.051372000
6	-2.544544000	-4.231449000	-1.272207000
6	-0.060444000	-4.346728000	-1.689654000
6	-1.313573000	-4.492662000	-1.490977000
6	-4.556331000	-2.765282000	-0.869102000
6	-5.193730000	-1.667469000	-0.728678000
6	-5.464266000	-0.420552000	-0.671808000
6	-5.422411000	0.855865000	-0.679468000
6	5.406501000	0.935700000	0.682549000
6	4.958116000	2.127424000	0.784027000
6	5.222249000	-1.591450000	0.722504000
6	5.470836000	-0.339672000	0.670284000
6	-1.052194000	-3.931568000	1.840531000
6	0.138344000	-4.364924000	1.678766000
6	1.393681000	-4.487784000	1.478845000
6	2.619828000	-4.203847000	1.260044000
6	3.732326000	-3.616605000	1.040068000
6	4.604592000	-2.700774000	0.859597000
6	4.232798000	3.166990000	0.939390000
6	3.223475000	3.921760000	1.146170000
6	2.056578000	4.393379000	1.364319000
6	0.799379000	4.464945000	1.577039000
6	-3.364584000	0.341646000	2.067423000
6	-3.255101000	-0.930816000	2.055645000
6	-2.052416000	-3.144955000	1.949615000
6	-2.831048000	-2.135334000	2.025138000
6	-3.065134000	1.583273000	2.040586000
6	-2.465404000	2.709714000	1.988995000
6	-1.544671000	3.589954000	1.893208000
6	-0.440469000	4.217254000	1.758508000

Table S30: Coordinates of C₂₄ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.984763000	4.797609000	1.659776000
6	-2.673944000	4.128590000	1.657617000
6	3.248980000	3.660232000	1.661321000
6	2.237723000	4.382023000	1.660240000
6	3.655312000	-3.249445000	1.661309000
6	4.377046000	-2.238105000	1.661490000
6	4.792968000	-0.985260000	1.661926000
6	4.910865000	0.251605000	1.661969000
6	4.643445000	1.544217000	1.662280000
6	4.126053000	2.673848000	1.661517000
6	-3.660143000	3.251254000	1.658042000
6	-4.381762000	2.239863000	1.657757000
6	-4.797895000	0.987077000	1.658579000
6	-4.915577000	-0.249791000	1.658315000
6	-0.989581000	-4.795912000	1.660179000
6	0.247357000	-4.913051000	1.659851000
6	2.669185000	-4.126841000	1.660431000
6	1.539833000	-4.644893000	1.660806000
6	-2.242473000	-4.380142000	1.659577000
6	-3.253857000	-3.658503000	1.659885000
6	-4.130825000	-2.672026000	1.658948000
6	-4.648308000	-1.542438000	1.659336000
6	-1.544616000	4.646637000	1.658432000
6	-0.252141000	4.914853000	1.658545000
6	-4.909431000	-0.291192000	-1.658549000
6	-3.276866000	-3.633287000	-1.660205000
6	-4.395373000	2.202427000	-1.660341000
6	-4.786003000	1.023032000	-1.660092000
6	2.204728000	4.394578000	-1.660473000
6	1.025322000	4.785217000	-1.662576000
6	-0.288877000	4.909460000	-1.663074000
6	-1.505585000	4.657587000	-1.663385000
6	-2.705398000	4.106749000	-1.662774000
6	-3.632009000	3.279087000	-1.662108000
6	-2.199941000	-4.396351000	-1.660644000
6	-1.020542000	-4.787095000	-1.661853000
6	0.293665000	-4.911215000	-1.661481000
6	1.510407000	-4.659401000	-1.661454000
6	4.914373000	0.289447000	-1.655791000
6	4.661562000	1.505943000	-1.656411000
6	3.281575000	3.631397000	-1.659073000
6	4.109882000	2.705362000	-1.657155000
6	4.790782000	-1.024771000	-1.656737000

6	4.400210000	-2.204194000	-1.657215000
6	3.636801000	-3.280828000	-1.659023000
6	2.710206000	-4.108535000	-1.659983000
6	-4.104987000	-2.707058000	-1.658812000
6	-4.656906000	-1.507756000	-1.658919000

Table S31: Coordinates of C₂₆ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	1.699520000	0.430041000	5.330528000
6	1.974191000	-2.895708000	3.607318000
6	1.368664000	2.918639000	5.023209000
6	1.541394000	1.696843000	5.350675000
6	0.827750000	6.113981000	-1.196016000
6	0.796360000	6.285428000	0.068745000
6	0.830626000	6.118081000	1.334017000
6	0.905208000	5.693109000	2.535670000
6	1.036577000	4.968320000	3.578379000
6	1.191017000	4.043078000	4.444836000
6	1.991914000	-3.611970000	2.550125000
6	1.993658000	-4.091016000	1.366832000
6	1.971595000	-4.236315000	0.098487000
6	1.950861000	-4.106077000	-1.171505000
6	1.315231000	2.886286000	-4.864789000
6	1.158736000	4.018389000	-4.295147000
6	0.897730000	5.684204000	-2.396278000
6	1.019265000	4.951584000	-3.434743000
6	1.713509000	-0.848152000	-4.866108000
6	1.798741000	-1.964464000	-4.252155000
6	1.865827000	-2.930844000	-3.420620000
6	1.909858000	-3.639609000	-2.359219000
6	1.918718000	-1.925361000	4.434968000
6	1.829181000	-0.807693000	5.045878000
6	1.600550000	0.389921000	-5.156302000
6	1.465251000	1.659272000	-5.183660000
6	-1.036577000	-4.968320000	-3.578379000
6	-0.796360000	-6.285428000	-0.068745000
6	-1.368664000	-2.918639000	-5.023209000
6	-1.191017000	-4.043078000	-4.444836000
6	-1.991914000	3.611970000	-2.550125000
6	-1.974191000	2.895708000	-3.607318000
6	-1.918718000	1.925361000	-4.434968000
6	-1.829181000	0.807693000	-5.045878000
6	-1.699520000	-0.430041000	-5.330528000
6	-1.541394000	-1.696843000	-5.350675000
6	-0.827750000	-6.113981000	1.196016000

6	-0.897730000	-5.684204000	2.396278000
6	-1.019265000	-4.951584000	3.434743000
6	-1.158736000	-4.018389000	4.295147000
6	-1.909858000	3.639609000	2.359219000
6	-1.950861000	4.106077000	1.171505000
6	-1.993658000	4.091016000	-1.366832000
6	-1.971595000	4.236315000	-0.098487000
6	-1.713509000	0.848152000	4.866108000
6	-1.600550000	-0.389921000	5.156302000
6	-1.465251000	-1.659272000	5.183660000
6	-1.315231000	-2.886286000	4.864789000
6	-0.830626000	-6.118081000	-1.334017000
6	-0.905208000	-5.693109000	-2.535670000
6	-1.798741000	1.964464000	4.252155000
6	-1.865827000	2.930844000	3.420620000

Table S32: Coordinates of C₂₈ dimer optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	4.134414000	3.966596000	-1.665777000
6	0.722744000	5.662947000	-1.663694000
6	5.448015000	1.782934000	-1.670548000
6	4.879319000	2.970069000	-1.668333000
6	2.944394000	-4.904056000	-1.668094000
6	3.976783000	-4.087790000	-1.669382000
6	4.785685000	-3.142354000	-1.670364000
6	5.360243000	-1.957844000	-1.671761000
6	5.677751000	-0.755176000	-1.672525000
6	5.682578000	0.561166000	-1.672281000
6	-0.520926000	5.703182000	-1.664019000
6	-1.803991000	5.412259000	-1.665079000
6	-2.942205000	4.909782000	-1.665936000
6	-3.974598000	4.093546000	-1.667888000
6	-4.132237000	-3.960823000	-1.669140000
6	-0.720530000	-5.657183000	-1.667429000
6	1.806194000	-5.406505000	-1.667739000
6	0.523102000	-5.697433000	-1.667215000
6	-5.680420000	-0.555440000	-1.673925000
6	-5.675545000	0.760928000	-1.673350000
6	-5.358058000	1.963583000	-1.671861000
6	-4.783482000	3.148092000	-1.669613000
6	2.004404000	5.365297000	-1.663455000
6	3.106889000	4.788640000	-1.664277000
6	-5.445838000	-1.777182000	-1.672881000
6	-4.877131000	-2.964347000	-1.671292000
6	-2.002237000	-5.359543000	-1.667248000

6	-3.104681000	-4.782897000	-1.667893000
6	4.907503000	2.938398000	1.667976000
6	1.961735000	5.354824000	1.673254000
6	5.700316000	0.516914000	1.666289000
6	5.409731000	1.800113000	1.667302000
6	1.776830000	-5.449612000	1.670633000
6	2.964299000	-4.881592000	1.669123000
6	3.961345000	-4.137439000	1.667122000
6	4.784093000	-3.110401000	1.666154000
6	5.361387000	-2.008302000	1.665576000
6	0.759160000	5.672565000	1.674459000
6	-0.557197000	5.677939000	1.674769000
6	-1.779033000	5.443883000	1.673329000
6	-2.966484000	4.875827000	1.671326000
6	-4.909665000	-2.944169000	1.665292000
6	-1.963969000	-5.360556000	1.669572000
6	0.554971000	-5.683674000	1.671753000
6	-0.761343000	-5.678313000	1.671120000
6	-5.661741000	0.720962000	1.665226000
6	-5.363572000	2.002529000	1.665658000
6	-4.786238000	3.104638000	1.666988000
6	-3.963534000	4.131677000	1.668707000
6	3.146108000	4.779958000	1.671250000
6	4.091425000	3.970947000	1.669757000
6	-5.702514000	-0.522686000	1.664829000
6	-5.411922000	-1.805821000	1.665126000
6	-3.148278000	-4.785718000	1.667733000
6	-4.093640000	-3.976651000	1.666668000
6	5.659589000	-0.726686000	1.666010000

Table S33: Coordinates of 4yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.238265000	0.000018000	-0.000203000
6	-1.893691000	-0.000550000	-0.001635000
6	-0.667734000	0.002706000	-0.000140000
6	-4.452423000	-0.000821000	0.001061000
1	-5.514866000	-0.001770000	0.002723000
6	0.667730000	-0.000650000	-0.001165000
6	1.893682000	0.001007000	0.000818000
6	3.238267000	-0.000434000	0.000636000
6	4.452434000	-0.000843000	0.000388000
1	5.514868000	-0.000838000	-0.001283000

Table S34: Coordinates of 5yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-4.517499000	0.000042000	0.000130000
6	-3.174455000	0.002153000	-0.000284000
6	-1.946514000	-0.001267000	-0.000386000
6	-5.732274000	-0.001124000	0.000675000
6	-0.615583000	0.005121000	-0.000380000
6	0.615582000	-0.004695000	-0.000621000
6	1.946514000	0.001560000	-0.000069000
6	3.174455000	-0.002037000	-0.000047000
6	4.517499000	-0.000227000	0.000338000
1	-6.794786000	-0.002666000	0.001019000
6	5.732275000	0.000615000	0.000343000
1	6.794788000	0.001824000	0.000787000

Table S35: Coordinates of 6yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	3.225243000	-0.000733000	0.000361000
6	1.896507000	0.003771000	-0.001211000
6	0.662890000	-0.003856000	0.000250000
6	4.454220000	0.001642000	-0.000080000
6	-0.662883000	0.002473000	-0.000519000
6	-1.896503000	-0.005058000	-0.000715000
6	-3.225248000	0.000204000	-0.000293000
6	-4.454213000	-0.001641000	-0.000376000
6	-5.796431000	0.000513000	0.000261000
6	-7.011517000	0.002112000	0.000954000
1	-8.074058000	0.003815000	0.001585000
6	5.796417000	0.000480000	0.000460000
6	7.011516000	-0.000352000	0.000499000
1	8.074064000	-0.001152000	0.000869000

Table S36: Coordinates of 7yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-1.941307000	-0.000874000	0.000855000
6	-0.618168000	-0.005733000	-0.004553000
6	0.618176000	-0.007700000	0.003232000
6	-3.176261000	-0.005894000	-0.003227000

6	1.941337000	-0.004216000	-0.000697000
6	3.176263000	-0.012264000	0.001768000
6	4.503744000	-0.003143000	0.001540000
6	5.733311000	-0.000280000	0.000801000
6	7.074990000	0.006801000	-0.000123000
6	8.290266000	0.012444000	-0.000947000
1	9.352833000	0.018220000	-0.001977000
6	-4.503736000	0.001714000	-0.000534000
6	-5.733318000	0.000433000	-0.000727000
6	-7.075003000	0.005265000	0.000775000
6	-8.290290000	0.008322000	0.001669000
1	-9.352861000	0.012528000	0.002980000

Table S37: Coordinates of 8yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-3.219598000	-0.008235000	-0.001928000
6	-1.897956000	-0.003348000	-0.005384000
6	-0.660130000	-0.006287000	0.005426000
6	-4.455289000	0.001886000	-0.000267000
6	0.660133000	-0.009754000	-0.001098000
6	1.897949000	0.002115000	0.001963000
6	3.219597000	-0.001997000	0.005946000
6	4.455308000	0.002293000	-0.002712000
6	5.782036000	0.002996000	0.002115000
6	7.011985000	0.002801000	-0.001442000
6	-5.782034000	-0.000946000	-0.001534000
6	-7.011968000	0.003164000	0.000541000
6	-8.353359000	0.003986000	0.000456000
6	-9.568764000	0.005334000	0.000398000
1	-10.631360000	0.006033000	0.000274000
6	8.353338000	0.002594000	-0.000998000
6	9.568749000	0.002173000	-0.001319000
1	10.631366000	0.001316000	-0.001250000

Table S38: Coordinates of 9yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	1.938304000	-0.008224000	0.002164000
6	0.619736000	-0.003379000	-0.005992000
6	-0.619732000	-0.000120000	0.005947000
6	3.177052000	0.002971000	0.000619000
6	-1.938301000	-0.008422000	0.001518000

6	-3.177052000	0.002038000	-0.002472000
6	-4.497768000	-0.000301000	0.003513000
6	-5.733986000	-0.002197000	-0.004107000
6	-7.060239000	0.001281000	-0.000003000
6	-8.290416000	0.000318000	-0.001675000
6	4.497769000	-0.001788000	-0.003109000
6	5.733986000	0.000693000	0.004563000
6	7.060237000	0.001670000	-0.000533000
6	8.290415000	0.001498000	0.001573000
6	-9.631587000	0.002544000	-0.000163000
6	-10.847067000	0.004462000	0.000924000
1	-11.909685000	0.006354000	0.002169000
6	9.631584000	0.002321000	-0.000490000
6	10.847064000	0.002974000	-0.002029000
1	11.909682000	0.003604000	-0.003673000

Table S39: Coordinates of 10yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	0.658359000	0.001366000	0.003740000
6	-0.658370000	0.007106000	-0.004045000
6	-1.898848000	0.009726000	0.007710000
6	1.898833000	0.013142000	0.000524000
6	-3.216325000	0.000186000	0.003811000
6	-4.455677000	0.008078000	0.000315000
6	-5.775763000	0.003892000	0.005225000
6	-7.012288000	-0.000939000	-0.003321000
6	-8.338202000	-0.001525000	-0.000305000
6	-9.568525000	-0.006094000	-0.002455000
6	3.216312000	0.005741000	-0.006945000
6	4.455669000	0.005180000	0.001672000
6	5.775762000	0.007396000	-0.004101000
6	7.012287000	-0.002709000	-0.003583000
6	-10.909531000	-0.008212000	-0.001342000
6	-12.125050000	-0.010532000	-0.000317000
1	-13.187672000	-0.012343000	0.000953000
6	8.338212000	-0.001176000	-0.001910000
6	9.568533000	-0.006617000	-0.001537000
6	10.909546000	-0.008725000	0.001294000
6	12.125065000	-0.011087000	0.004228000
1	13.187690000	-0.012831000	0.007100000

Table S40: Coordinates of 11yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
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6	-1.936352000	-0.020027000	0.006014000
6	-0.620793000	-0.011994000	-0.000916000
6	0.620789000	-0.022802000	-0.003554000
6	-3.177508000	-0.017317000	-0.004582000
6	1.936344000	-0.015745000	0.005299000
6	3.177479000	-0.009047000	-0.005794000
6	4.494279000	-0.013207000	-0.002708000
6	5.733983000	-0.000274000	0.001530000
6	7.053648000	0.001665000	-0.003922000
6	8.290415000	0.002101000	0.003509000
6	-4.494262000	-0.007417000	0.001928000
6	-5.734034000	-0.012865000	0.002042000
6	-7.053667000	-0.003224000	-0.002933000
6	-8.290415000	0.002217000	0.004335000
6	9.616081000	0.008953000	0.000030000
6	10.846522000	0.010601000	0.001623000
6	-9.616083000	0.006685000	-0.000626000
6	-10.846499000	0.013460000	0.001312000
6	-12.187396000	0.018877000	-0.000479000
6	-13.402940000	0.024225000	-0.001650000
1	-14.465567000	0.028781000	-0.002964000
6	12.187426000	0.015830000	0.000489000
6	13.402976000	0.020402000	-0.000261000
1	14.465612000	0.024641000	-0.001158000

Table S41: Coordinates of 12yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	-0.657438000	-0.025070000	-0.003851000
6	0.657031000	-0.033757000	0.002513000
6	1.899447000	-0.022323000	0.007294000
6	-1.899788000	-0.025386000	0.007538000
6	3.214304000	-0.025805000	-0.002966000
6	4.456040000	-0.027795000	0.006301000
6	5.772372000	-0.013105000	0.003366000
6	7.012532000	-0.014997000	-0.003197000
6	8.331976000	-0.005358000	0.001705000
6	9.568920000	0.008404000	-0.006287000
6	-3.214644000	-0.027792000	-0.002171000
6	-4.456151000	-0.011268000	-0.003761000
6	-5.772525000	-0.012428000	0.001395000
6	-7.012530000	-0.007240000	-0.009591000
6	10.894501000	0.013789000	-0.004281000
6	12.125047000	0.025441000	-0.003107000
6	-8.331828000	0.005798000	-0.004149000
6	-9.568802000	0.004517000	-0.000809000

6	-10.894287000	0.015757000	-0.001186000
6	-12.124809000	0.021152000	0.003261000
6	13.465880000	0.033900000	0.000233000
6	14.681489000	0.042007000	0.004529000
1	15.744117000	0.048672000	0.008911000
6	-13.465613000	0.029334000	0.003132000
6	-14.681178000	0.036863000	0.002358000
1	-15.743795000	0.043500000	0.001475000

Table S42: Coordinates of 13yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	1.935070000	0.013542000	0.002065000
6	0.621521000	0.005016000	0.003705000
6	-0.621525000	0.011378000	-0.004352000
6	3.177855000	0.003990000	-0.006737000
6	-1.935114000	0.012618000	0.004905000
6	-3.177891000	0.002689000	-0.000818000
6	-4.492212000	0.012306000	-0.003733000
6	-5.734099000	0.007666000	0.006254000
6	-7.050075000	0.002857000	-0.002522000
6	-8.290309000	0.010256000	0.000863000
6	4.492213000	0.002234000	0.001770000
6	5.734077000	0.009863000	-0.006067000
6	7.050034000	-0.000920000	-0.006701000
6	8.290250000	0.002290000	0.003567000
6	-9.609482000	0.001515000	0.004927000
6	-10.846503000	0.001635000	-0.001896000
6	9.609474000	0.001218000	-0.001045000
6	10.846448000	-0.007476000	0.004655000
6	12.171896000	-0.005156000	0.003387000
6	13.402490000	-0.010217000	0.001317000
6	-12.171886000	-0.003066000	0.002291000
6	-13.402442000	-0.009770000	-0.001852000
6	14.743265000	-0.010657000	-0.000034000
6	15.958853000	-0.011476000	-0.001415000
1	17.021512000	-0.011771000	-0.002401000
6	-14.743184000	-0.015380000	-0.001150000
6	-15.958743000	-0.020774000	-0.000929000
1	-17.021404000	-0.025313000	-0.000316000

Table S43: Coordinates of 14yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	17.221552000	-0.349126000	-0.013404000

6	16.008297000	-0.273801000	-0.007899000
6	14.670208000	-0.192752000	-0.005106000
6	13.441227000	-0.128380000	0.000598000
6	12.118319000	-0.052780000	0.002157000
6	10.882292000	-0.000829000	0.008355000
6	9.565089000	0.061747000	0.016656000
6	8.325703000	0.108391000	0.004204000
6	7.010730000	0.139420000	0.012670000
6	5.769230000	0.180374000	0.016988000
6	4.455849000	0.192962000	0.007943000
6	3.212691000	0.194806000	0.018833000
6	1.900202000	0.197886000	0.016564000
6	0.656791000	0.185486000	0.010172000
6	-0.655350000	0.171904000	0.007585000
6	-1.898594000	0.151038000	-0.003250000
6	-3.210946000	0.135343000	-0.013954000
6	-4.453822000	0.105030000	-0.011354000
6	-5.766750000	0.072117000	-0.026800000
6	-7.008844000	0.054345000	-0.026156000
6	-8.323353000	0.012827000	-0.027584000
6	-9.563463000	-0.011885000	-0.040237000
6	-10.881837000	-0.043703000	-0.026581000
6	-12.118143000	-0.087749000	-0.020929000
6	-13.442820000	-0.119015000	-0.006698000
6	-14.672570000	-0.160322000	0.013820000
6	-16.012664000	-0.196524000	0.033288000
6	-17.227741000	-0.233241000	0.051296000
1	18.282227000	-0.416529000	-0.017873000
1	-18.289924000	-0.264891000	0.070812000

Table S44: Coordinates of 15yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	18.514139000	-0.039058000	-0.002153000
6	17.298553000	-0.032123000	-0.001862000
6	15.957859000	-0.025530000	-0.001905000
6	14.727256000	-0.015968000	-0.000792000
6	13.401998000	-0.012902000	-0.003318000
6	12.164861000	-0.002113000	0.003236000
6	10.845955000	0.004189000	-0.002056000
6	9.605481000	0.001139000	0.006017000
6	8.289971000	0.013728000	0.007599000
6	7.047661000	0.010009000	-0.002781000
6	5.734040000	0.010748000	0.006034000
6	4.490690000	0.024373000	0.000806000
6	3.178098000	0.019920000	-0.002255000

6	1.934140000	0.026510000	0.007540000
6	0.622044000	0.030402000	-0.000170000
6	-0.622093000	0.019081000	0.001446000
6	-1.934191000	0.024062000	0.003678000
6	-3.178113000	0.019958000	-0.008610000
6	-4.490666000	0.012949000	-0.002962000
6	-5.734060000	0.023463000	-0.004458000
6	-7.047681000	0.014138000	-0.010708000
6	-8.289960000	0.009605000	0.002844000
6	-9.605523000	0.011631000	-0.000876000
6	-10.845923000	-0.003585000	-0.002242000
6	-12.164824000	-0.005827000	0.003764000
6	-13.401995000	-0.010391000	-0.003423000
6	-14.727215000	-0.019307000	0.001515000
6	-15.957853000	-0.023122000	0.000809000
6	-17.298536000	-0.031379000	0.002328000
6	-18.514116000	-0.039372000	0.002876000
1	19.576797000	-0.044742000	-0.002727000
1	-19.576769000	-0.046615000	0.003209000

Table S45: Coordinates of 16yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	19.791986000	-0.022155000	0.000342000
6	18.576379000	-0.018957000	0.001196000
6	17.235702000	-0.015622000	0.002527000
6	16.005039000	-0.011807000	-0.000230000
6	14.679830000	-0.008408000	0.004115000
6	13.442608000	-0.007643000	-0.003777000
6	12.123792000	0.001158000	-0.001286000
6	10.883230000	-0.005332000	0.000689000
6	9.567833000	0.001913000	-0.007793000
6	8.325408000	0.009406000	0.003195000
6	7.011962000	0.003774000	-0.000012000
6	5.768412000	0.017013000	-0.005271000
6	4.456146000	0.017817000	0.003895000
6	3.211907000	0.012765000	-0.004567000
6	1.900270000	0.022436000	-0.002813000
6	0.655718000	0.014929000	0.004409000
6	-0.655741000	0.014724000	-0.003027000
6	-1.900275000	0.021281000	0.004123000
6	-3.211909000	0.010563000	0.005012000
6	-4.456164000	0.015176000	-0.003697000
6	-5.768428000	0.013652000	0.005113000
6	-7.011962000	0.000890000	-0.001101000
6	-8.325410000	0.006710000	-0.004072000

6	-9.567835000	-0.001339000	0.007025000
6	-10.883231000	-0.007791000	-0.001222000
6	-12.123790000	-0.000712000	0.001224000
6	-13.442608000	-0.008711000	0.003523000
6	-14.679830000	-0.008317000	-0.003962000
6	-16.005033000	-0.011147000	0.000378000
6	-17.235696000	-0.013833000	-0.002363000
6	-18.576371000	-0.016275000	-0.001123000
6	-19.791946000	-0.018580000	-0.000414000
1	20.854661000	-0.024865000	-0.000766000
1	-20.854621000	-0.020597000	0.000559000

Table S46: Coordinates of 17yne optimized at M06L/6-311++g(d,p) level

atom	x	y	z
6	21.069163000	-0.058243000	0.042263000
6	19.853509000	-0.052328000	0.031973000
6	18.512926000	-0.046532000	0.020983000
6	17.282237000	-0.036472000	0.013108000
6	15.957134000	-0.031948000	0.000307000
6	14.719876000	-0.020744000	-0.000444000
6	13.401230000	-0.009650000	-0.014439000
6	12.160551000	-0.013565000	-0.017952000
6	10.845223000	0.000835000	-0.017962000
6	9.602953000	0.006829000	-0.034908000
6	8.289570000	0.004985000	-0.031945000
6	7.045888000	0.022607000	-0.029424000
6	5.733914000	0.026785000	-0.036653000
6	4.489399000	0.026980000	-0.023913000
6	3.178231000	0.041022000	-0.018199000
6	1.933347000	0.038359000	-0.020197000
6	0.622429000	0.040260000	-0.003963000
6	-0.622485000	0.053613000	-0.001125000
6	-1.933460000	0.048464000	0.002059000
6	-3.178231000	0.052991000	0.018916000
6	-4.489519000	0.058203000	0.018359000
6	-5.733943000	0.045241000	0.024082000
6	-7.046076000	0.046554000	0.031317000
6	-8.289648000	0.039736000	0.018754000
6	-9.602880000	0.025424000	0.022352000
6	-10.845543000	0.028122000	0.019015000
6	-12.160625000	0.011376000	0.007964000
6	-13.401231000	-0.001556000	0.013344000
6	-14.719992000	-0.011088000	0.003840000
6	-15.956973000	-0.033094000	-0.000556000
6	-17.282230000	-0.043692000	-0.003913000

6	-18.512649000	-0.061848000	-0.009268000
6	-19.853235000	-0.077114000	-0.012800000
6	-21.068914000	-0.092471000	-0.016306000
1	22.131800000	-0.062798000	0.051183000
1	-22.131464000	-0.105446000	-0.019201000

Table S47: Coordinates of linear C₆

atom	x	y	z
6	3.229290000	-0.000081000	-0.000005000
6	1.924754000	0.000314000	0.000005000
6	0.636929000	0.000048000	0.000002000
6	-0.636929000	-0.000245000	0.000001000
6	-1.924754000	-0.000496000	0.000001000
6	-3.229290000	0.000460000	-0.000003000

Table S48: Coordinates of linear C₈

atom	x	y	z
6	3.200605000	-0.000577000	-0.000454000
6	1.911425000	0.003920000	-0.000284000
6	0.639784000	-0.000853000	-0.000515000
6	4.499649000	-0.004403000	0.000695000
6	-0.639789000	0.006701000	0.000672000
6	-1.911419000	-0.000660000	-0.000178000
6	-3.200606000	-0.000646000	-0.000327000
6	-4.499650000	-0.003482000	0.000391000

Table S49: Coordinates of linear C₁₀

atom	x	y	z
6	3.185832000	0.001284000	-0.002370000
6	1.915387000	0.008118000	-0.000133000
6	0.635942000	-0.001467000	0.000140000
6	4.476217000	-0.000155000	-0.000995000
6	-0.635943000	0.006648000	0.002675000
6	-1.915375000	-0.004402000	0.002894000
6	-3.185838000	-0.000756000	0.002285000
6	-4.476215000	-0.002699000	-0.000420000
6	-5.772189000	-0.000106000	-0.004188000

6	5.772183000	-0.006465000	0.000111000
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Table S50: Coordinates of linear C₁₂

atom	x	y	z
6	-3.190614000	0.004459000	0.002487000
6	-1.910887000	-0.001033000	0.000956000
6	-0.639259000	0.007443000	0.002150000
6	-4.459946000	-0.001567000	0.000925000
6	0.639258000	0.000473000	-0.002861000
6	1.910890000	0.007086000	-0.000142000
6	3.190610000	0.000916000	-0.004440000
6	4.459950000	0.001481000	-0.001165000
6	5.751110000	-0.002741000	0.000652000
6	7.044956000	-0.007851000	0.003074000
6	-5.751111000	-0.002581000	-0.000154000
6	-7.044958000	-0.006087000	-0.001481000

Table S51: Coordinates of linear C₁₄

atom	x	y	z
6	1.914322000	0.043483000	0.005525000
6	0.635952000	0.053587000	-0.003133000
6	-0.636232000	0.056851000	0.001852000
6	3.185535000	0.020002000	0.000128000
6	-1.914579000	0.061575000	-0.003968000
6	-3.185753000	0.041179000	-0.003536000
6	-4.465956000	0.024904000	0.002857000
6	-5.733963000	-0.014186000	-0.001026000
6	-7.025141000	-0.054634000	0.003193000
6	-8.316887000	-0.096291000	-0.001455000
6	4.465701000	0.007114000	0.002544000
6	5.733882000	-0.020135000	-0.001046000
6	7.025539000	-0.046364000	-0.000980000
6	8.317579000	-0.077084000	-0.000956000

Table S52: Coordinates of linear C₁₆

atom	x	y	z
6	3.189689000	-0.019143000	0.003192000
6	1.911100000	-0.019038000	-0.006306000
6	0.639078000	-0.008114000	0.002037000

6	4.460459000	-0.007126000	-0.001641000
6	-0.639037000	-0.015409000	0.001287000
6	-1.911095000	-0.003448000	-0.003678000
6	-3.189629000	0.001428000	0.006549000
6	-4.460449000	-0.002349000	0.001478000
6	-5.741015000	0.007300000	0.002384000
6	-7.009022000	0.005339000	0.000115000
6	5.741045000	-0.006384000	0.000307000
6	7.009021000	0.005948000	-0.000008000
6	-8.301385000	0.008935000	-0.001617000
6	-9.592855000	0.011473000	-0.003531000
6	8.301328000	0.014558000	-0.000081000
6	9.592767000	0.026032000	-0.000488000

Table S53: Coordinates of linear C₁₈

atom	x	y	z
6	1.914107000	-0.023848000	0.001010000
6	0.636165000	-0.016310000	-0.008108000
6	-0.636109000	-0.003578000	0.005267000
6	3.185990000	-0.011298000	-0.002365000
6	-1.914070000	-0.009957000	0.006929000
6	-3.185964000	0.001664000	0.002470000
6	-4.464763000	0.003569000	0.012023000
6	-5.735172000	0.000627000	0.004558000
6	-7.016132000	0.008823000	0.005513000
6	-8.283577000	0.004386000	-0.000239000
6	4.464799000	-0.015325000	-0.005058000
6	5.735193000	-0.006496000	0.001888000
6	7.016129000	0.001673000	-0.005848000
6	8.283559000	0.006608000	-0.000265000
6	-9.576606000	0.005687000	-0.004332000
6	-10.867280000	0.012917000	-0.014380000
6	9.576539000	0.012566000	0.000910000
6	10.867192000	0.028292000	0.000026000

Table S54: Coordinates of linear C₂₀

atom	x	y	z
6	3.189249000	0.002406000	0.007053000
6	1.911233000	0.012310000	0.001183000
6	0.638836000	0.003560000	-0.003352000
6	4.460762000	0.006348000	-0.001928000
6	-0.638954000	0.010904000	0.007894000
6	-1.911221000	0.019994000	-0.003615000

6	-3.189242000	0.012178000	-0.002868000
6	-4.460889000	0.020151000	0.000491000
6	-5.739918000	0.018072000	-0.007851000
6	-7.010105000	0.009402000	-0.001334000
6	5.739988000	0.013678000	0.005906000
6	7.009913000	0.005055000	0.004877000
6	-8.291279000	0.006548000	-0.003718000
6	-9.558244000	-0.010463000	-0.000338000
6	8.291284000	0.005377000	0.001921000
6	9.558285000	-0.009230000	0.000264000
6	10.851710000	-0.020592000	-0.004358000
6	12.141573000	-0.035473000	-0.006384000
6	-10.851530000	-0.025388000	0.001316000
6	-12.141451000	-0.044837000	0.004840000

Table S55: Coordinates of linear C₂₂

atom	x	y	z
6	-4.464353000	-0.010115000	0.007109000
6	-3.186142000	-0.023256000	0.007828000
6	-1.913881000	-0.025176000	-0.008686000
6	-5.735903000	-0.015221000	0.009257000
6	-0.636123000	-0.018421000	-0.003954000
6	0.636390000	-0.028094000	-0.006692000
6	1.914124000	-0.019195000	-0.012656000
6	3.186388000	-0.020698000	0.001514000
6	4.464588000	-0.025901000	-0.006021000
6	5.735986000	-0.009947000	-0.005260000
6	-7.015313000	-0.002661000	0.015142000
6	-8.285114000	0.006133000	0.004934000
6	7.015357000	-0.009726000	0.002263000
6	8.285113000	-0.000376000	-0.004379000
6	-9.566903000	0.008726000	0.011245000
6	-10.833559000	0.018468000	-0.000184000
6	-12.127360000	0.026491000	-0.006346000
6	-13.416811000	0.041866000	-0.017151000
6	9.566702000	0.012899000	0.003663000
6	10.833314000	0.019646000	0.002267000
6	12.127004000	0.030815000	0.003221000
6	13.416496000	0.043744000	0.002886000

Table S56: Coordinates of linear C₂₄

atom	x	y	z
6	-14.691119000	-0.027596000	-0.027545000

6	-13.402054000	-0.026859000	-0.017777000
6	-12.107975000	-0.025176000	-0.008204000
6	-10.841623000	-0.025989000	0.002549000
6	-9.559679000	-0.017545000	0.003529000
6	-8.290254000	-0.013498000	0.013926000
6	-7.010635000	-0.011946000	0.006740000
6	-5.739465000	0.003672000	0.008307000
6	-4.461049000	-0.001475000	0.017060000
6	-3.188923000	0.003603000	0.003343000
6	-1.911226000	0.023256000	0.010351000
6	-0.638638000	0.025816000	0.014223000
6	0.638860000	0.041504000	0.008476000
6	1.911396000	0.050553000	0.016822000
6	3.189196000	0.044661000	0.007616000
6	4.461326000	0.055492000	-0.000905000
6	5.739802000	0.048196000	0.001087000
6	7.010908000	0.035745000	-0.016117000
6	8.290530000	0.030896000	-0.021530000
6	9.559782000	0.006826000	-0.019839000
6	10.841620000	-0.011694000	-0.020953000
6	12.107641000	-0.041296000	-0.007457000
6	13.401355000	-0.071315000	0.005167000
6	14.690223000	-0.095828000	0.021132000

Table S57: Coordinates of linear C₂₆

atom	x	y	z
6	15.965991000	0.062681000	-0.002174000
6	14.677424000	0.043366000	-0.001628000
6	13.383225000	0.028182000	-0.000788000
6	12.117186000	0.011987000	0.002636000
6	10.835028000	0.005521000	-0.001039000
6	9.565855000	-0.009504000	0.001930000
6	8.285974000	-0.007422000	0.002143000
6	7.014991000	-0.015991000	-0.004415000
6	5.736367000	-0.017301000	0.006137000
6	4.464383000	-0.008251000	-0.000997000
6	3.186461000	-0.020806000	-0.003614000
6	1.913942000	-0.018587000	0.005368000
6	0.636306000	-0.020423000	-0.003916000
6	-0.636329000	-0.034315000	0.001141000
6	-1.913979000	-0.028004000	0.004667000
6	-3.186480000	-0.034552000	-0.003307000
6	-4.464435000	-0.037726000	0.007284000
6	-5.736401000	-0.025487000	0.000603000
6	-7.015048000	-0.029806000	-0.005979000

6	-8.286018000	-0.017696000	0.000937000
6	-9.565806000	-0.003504000	-0.006975000
6	-10.835028000	0.001651000	-0.002631000
6	-12.117071000	0.021667000	-0.001907000
6	-13.383152000	0.032933000	0.000092000
6	-14.677390000	0.051139000	0.002097000
6	-15.965997000	0.070249000	0.004334000

Table S58: Coordinates of linear C₂₈

atom	x	y	z
6	17.240764000	-0.091734000	-0.005416000
6	15.952414000	-0.074538000	-0.001652000
6	14.657970000	-0.055150000	0.000009000
6	13.392145000	-0.036965000	0.005482000
6	12.109787000	-0.021409000	0.000172000
6	10.840949000	0.001602000	0.004806000
6	9.560850000	0.006724000	0.005438000
6	8.290175000	0.022910000	-0.006202000
6	7.011423000	0.038623000	0.003163000
6	5.739584000	0.035927000	0.001510000
6	4.461542000	0.050983000	-0.006515000
6	3.189157000	0.055233000	0.004051000
6	1.911455000	0.047271000	-0.002109000
6	0.638799000	0.057442000	-0.005460000
6	-0.638772000	0.052022000	0.003964000
6	-1.911405000	0.042833000	-0.006053000
6	-3.189122000	0.049229000	-0.003719000
6	-4.461425000	0.033651000	0.004514000
6	-5.739469000	0.023644000	-0.004452000
6	-7.011278000	0.017452000	0.003918000
6	-8.289985000	-0.003556000	0.004280000
6	-9.560797000	-0.007727000	-0.000263000
6	-10.840849000	-0.018792000	0.005383000
6	-12.109815000	-0.028542000	-0.001982000
6	-13.392238000	-0.034557000	0.002827000
6	-14.658126000	-0.044608000	-0.001919000
6	-15.952664000	-0.053479000	-0.002029000
6	-17.241071000	-0.064489000	-0.001746000

Table S59: Coordinates of linear C₃₀

atom	x	y	z
6	-18.514881000	0.147219000	-0.004392000
6	-17.227080000	0.113982000	0.000346000

6	-15.932614000	0.084141000	0.000066000
6	-14.667098000	0.059061000	0.002637000
6	-13.384727000	0.030105000	-0.003525000
6	-12.116005000	0.014364000	-0.002172000
6	-10.835963000	-0.013994000	-0.001185000
6	-9.565425000	-0.027453000	-0.008233000
6	-8.286472000	-0.039263000	0.005009000
6	-7.014976000	-0.061533000	0.004352000
6	-5.736682000	-0.059748000	0.001660000
6	-4.464448000	-0.067008000	0.012828000
6	-3.186640000	-0.074510000	0.003851000
6	-1.914018000	-0.064858000	0.004585000
6	-0.636398000	-0.071961000	0.009619000
6	0.636316000	-0.070256000	-0.001475000
6	1.913931000	-0.061594000	0.003489000
6	3.186564000	-0.068415000	0.000924000
6	4.464324000	-0.056518000	-0.010139000
6	5.736574000	-0.047780000	-0.002011000
6	7.014855000	-0.046575000	-0.009083000
6	8.286325000	-0.022539000	-0.010604000
6	9.565298000	-0.011862000	0.000287000
6	10.835828000	0.001801000	-0.007472000
6	12.115918000	0.026575000	-0.004218000
6	13.384699000	0.037567000	-0.002520000
6	14.667147000	0.061374000	-0.004786000
6	15.932808000	0.075584000	0.000584000
6	18.515451000	0.116078000	0.013382000
6	17.227390000	0.098015000	0.008195000
