

Electronic Supplementary Information

Paratropic Ring Currents Discovered in Six-membered Rings of Conical Nanographenes: Carboncones

Francesco F. Summa^a, Lawrence T. Scott^b, Riccardo Zanasi^{a,*} and Guglielmo
Monaco^a

^a *Dipartimento di Chimica e Biologia "A. Zambelli", Università degli studi di Salerno, via
Giovanni Paolo II 132, Fisciano 84084, SA, Italy*

^b *Department of Chemistry, University of Nevada, Reno, Nevada 89557-0216, United States*

E-mail: rzanasi@unisa.it

Contents

1	Cartesian coordinates and energies	S3
1.1	C ₇₀ H ₂₀	S3
1.2	C ₈₀ H ₂₀	S5
1.3	C ₁₇₀ H ₃₀	S7
1.4	C ₁₈₀ H ₃₀	S10
1.5	Mes ₅ -C ₇₀ H ₁₅	S13
2	σ/π Orbital separation	S20
3	Current densities	S21
3.1	C ₇₀ H ₂₀	S22
3.1.1	¹ H and ¹³ C NMR chemical shifts: a comparison with experimental data for penta-mesityl carboncone[1,2] derivative	S24
3.2	C ₈₀ H ₂₀	S26
3.3	C ₁₇₀ H ₃₀	S27
3.4	C ₁₈₀ H ₃₀	S29
4	Polansky-Derflinger indices	S30
5	Fullerene-240 of I_h symmetry	S31

1 Cartesian coordinates and energies

For all systems, the molecular geometry was optimized within the BO approximation for the (closed-shell) singlet electronic state at the B3LYP/6-31G(1d,1p) level of theory, assuming the C_{5v} symmetry point group. The stability of each found configuration was verified by means of the standard technique provided by the Gaussian package. The absence of imaginary vibrational frequencies was also verified.

Optimal Cartesian coordinates in Angstrom are given here in the following, together with some energies and lowest harmonic vibrational frequency.

1.1 $C_{70}H_{20}$

RB3LYP/6-31G(1d,1p) energy = $-2679.88834642 E_h$

Lowest excitation energies are ${}^1A \rightarrow {}^3E = 0.0458164 E_h$ and ${}^1A \rightarrow {}^1E = 0.0832821 E_h$.

Lowest harmonic vibrational frequency is 39.3615 cm^{-1} , symmetry type E_2 .

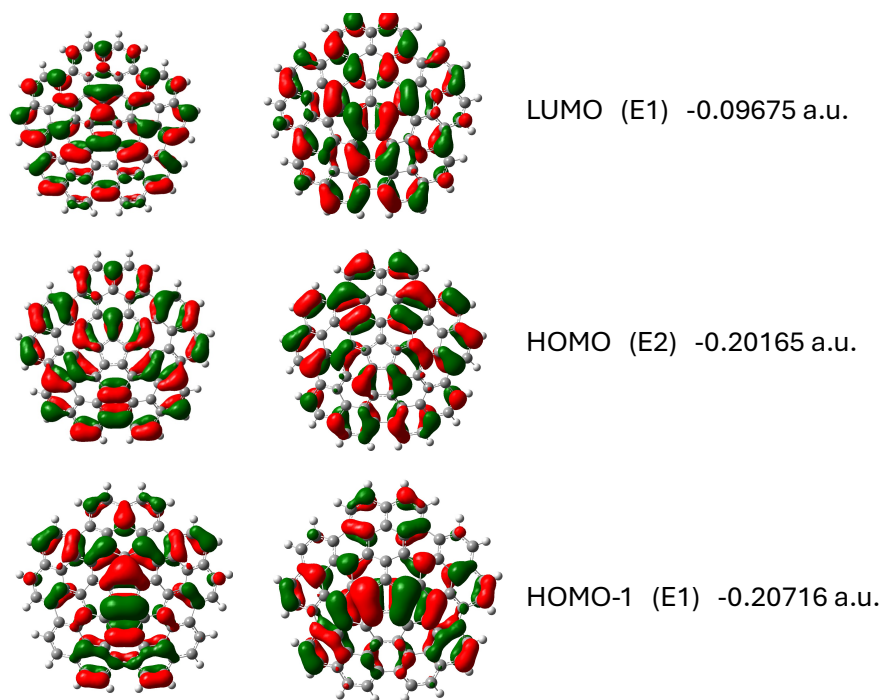


Figure S1: Frontier orbitals.

C,0,0.,4.80494092,-0.00891446	H,0,6.8059419507,3.5332428591,-1.58914039
C,0,-1.25377797,4.15104961,0.26677554	C,0,-1.4269778897,-1.964066569,1.49086949
C,0,1.25377797,4.15104961,0.26677554	C,0,1.4269778897,-1.964066569,1.49086949
C,0,0.,6.03251764,-0.71276043	C,0,-6.6655944461,0.849058344,-1.08534441
C,0,-1.2470702,2.92535108,0.99178451	C,0,-5.1852697709,-0.9187352445,-0.26689144
C,0,-2.47610562,4.6475798,-0.26689144	C,0,-3.4542534276,-2.6213174799,0.26677554
C,0,1.2470702,2.92535108,0.99178451	C,0,3.4542534276,-2.6213174799,0.26677554
C,0,2.47610562,4.6475798,-0.26689144	C,0,5.1852697709,-0.9187352445,-0.26689144
C,0,-1.25227949,6.60173049,-1.08534441	C,0,6.6655944461,0.849058344,-1.08534441
C,0,1.25227949,6.60173049,-1.08534441	C,0,-0.7105772381,-3.0996682117,0.99178451
C,0,0.,2.42771979,1.49086949	C,0,0.7105772381,-3.0996682117,0.99178451
C,0,-2.3968083228,2.0900174377,0.99178451	H,0,-7.5829107467,1.141978787,-1.58914039
C,0,-2.43540817,5.92895349,-0.89378641	C,0,-6.3913523649,-0.4840634232,-0.89378641
C,0,-3.654952338,3.7910975253,-0.26689144	C,0,-4.7349903922,-2.3045526757,-0.26689144
C,0,2.3968083228,2.0900174377,0.99178451	C,0,-2.8242734113,-3.8872788626,-0.00891446
C,0,2.43540817,5.92895349,-0.89378641	C,0,4.7349903922,-2.3045526757,-0.26689144
C,0,3.654952338,3.7910975253,-0.26689144	C,0,2.8242734113,-3.8872788626,-0.00891446
H,0,-1.25716192,7.56466753,-1.58914039	C,0,6.3913523649,-0.4840634232,-0.89378641
C,0,0.,1.20954844,2.15555346	C,0,-1.4255980578,-4.0952218807,0.26677554
C,0,-3.5604440818,2.4751585818,0.26677554	C,0,1.4255980578,-4.0952218807,0.26677554
C,0,-2.3088987267,0.7502066722,1.49086949	H,0,-7.1012863289,-1.2172769897,-1.26033039
H,0,-3.35211737,6.37756536,-1.26033039	C,0,-5.4552380211,-3.3651271279,-0.89378641
C,0,-4.8861873394,4.1483581967,-0.89378641	C,0,-3.5458249034,-4.8804092909,-0.71276043
C,0,2.3088987267,0.7502066722,1.49086949	C,0,5.4552380211,-3.3651271279,-0.89378641
C,0,3.5604440818,2.4751585818,0.26677554	C,0,3.5458249034,-4.8804092909,-0.71276043
H,0,3.35211737,6.37756536,-1.26033039	H,0,7.1012863289,-1.2172769897,-1.26033039
C,0,4.8861873394,4.1483581967,-0.89378641	C,0,-0.7285673393,-5.2153894088,-0.26689144
C,0,-1.1503489263,0.373771023,2.15555346	C,0,0.7285673393,-5.2153894088,-0.26689144
C,0,1.1503489263,0.373771023,2.15555346	H,0,-6.460558784,-3.1892336063,-1.26033039
C,0,-4.5697703731,1.4848084007,-0.00891446	C,0,-4.8935152112,-4.604840744,-1.08534441
C,0,-3.1675400928,-0.2820510423,0.99178451	C,0,-2.8672844329,-6.076983576,-1.08534441
H,0,-5.0295638599,5.1588291466,-1.26033039	C,0,4.8935152112,-4.604840744,-1.08534441
C,0,-5.8916431579,3.2310354824,-1.08534441	H,0,6.460558784,-3.1892336063,-1.26033039
C,0,3.1675400928,-0.2820510423,0.99178451	C,0,2.8672844329,-6.076983576,-1.08534441
C,0,4.5697703731,1.4848084007,-0.00891446	C,0,-1.5146648256,-6.2281211392,-0.89378641
C,0,5.8916431579,3.2310354824,-1.08534441	C,0,1.5146648256,-6.2281211392,-0.89378641
H,0,5.0295638599,5.1588291466,-1.26033039	H,0,-3.4293346551,-6.8588858262,-1.58914039
C,0,-0.7109547354,-0.9785452448,2.15555346	H,0,5.463465371,-5.3810033536,-1.58914039
C,0,0.7109547354,-0.9785452448,2.15555346	H,0,-1.0367189451,-7.1298839143,-1.26033039
C,0,-5.7372652119,1.8641504691,-0.71276043	H,0,1.0367189451,-7.1298839143,-1.26033039
C,0,-4.3353214816,0.0903311651,0.26677554	H,0,1.25716192,7.56466753,-1.58914039
C,0,-2.728379208,-1.6336492674,0.99178451	H,0,-6.8059419507,3.5332428591,-1.58914039
C,0,2.728379208,-1.6336492674,0.99178451	H,0,-5.463465371,-5.3810033536,-1.58914039
C,0,4.3353214816,0.0903311651,0.26677554	H,0,3.4293346551,-6.8588858262,-1.58914039
C,0,5.7372652119,1.8641504691,-0.71276043	H,0,7.5829107467,1.141978787,-1.58914039

1.2 C₈₀H₂₀

RB3LYP/6-31G(1d,1p) energy = $-3061.02951377 E_h$

Lowest excitation energies are $^1A \rightarrow ^3E = 0.0292749 E_h$ and $^1A \rightarrow ^1E = 0.0682531 E_h$.

Lowest harmonic vibrational frequency is 36.9080 cm^{-1} , symmetry type E₂.

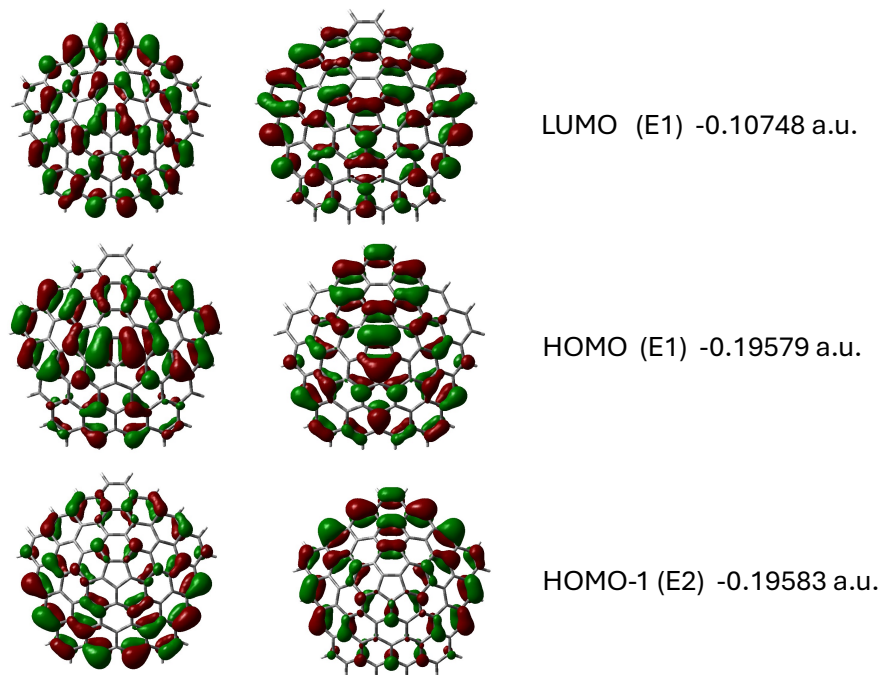


Figure S2: Frontier orbitals.

C,0,0.,4.7768122828,0.2298049942	C,0,-3.4303545389,-2.6124418746,0.5315166545
C,0,-1.2396603122,4.1298216817,0.5315166545	C,0,3.4303545389,-2.6124418746,0.5315166545
C,0,1.2396603122,4.1298216817,0.5315166545	C,0,5.1128888246,-0.911113988,-0.0641039098
C,0,0.,5.9685533746,-0.5592669309	C,0,6.5701048359,0.8224002348,-0.9841401383
C,0,-1.2447378059,2.9266917345,1.2931654711	C,0,-0.7132522009,-3.0993818755,1.2931654711
C,0,-2.4464904327,4.5810965277,-0.0641039098	C,0,0.7132522009,-3.0993818755,1.2931654711
C,0,1.2447378059,2.9266917345,1.2931654711	H,0,-7.4462883612,1.1045658379,-1.563252227
C,0,2.4464904327,4.5810965277,-0.0641039098	C,0,-6.2919162302,-0.5288200781,-0.7936718641
C,0,-1.248124947,6.5026766658,-0.9841401383	C,0,-4.6719533149,-2.2681739473,-0.0641039098
C,0,1.248124947,6.5026766658,-0.9841401383	C,0,-2.8077398127,-3.8645223154,0.2298049942
C,0,0.,2.4316312436,1.8016351796	C,0,4.6719533149,-2.2681739473,-0.0641039098
C,0,-2.3988041096,2.0882134847,1.2931654711	C,0,2.8077398127,-3.8645223154,0.2298049942
C,0,-2.4472468237,5.8205535397,-0.7936718641	C,0,6.2919162302,-0.5288200781,-0.7936718641
C,0,-3.600874584,3.7423873481,-0.0641039098	C,0,-1.4245420192,-4.0697499734,0.5315166545

C,0,2.3988041096,2.0882134847,1.2931654711	C,0,1.4245420192,-4.0697499734,0.5315166545
C,0,2.4472468237,5.8205535397,-0.7936718641	C,0,-7.0862247994,-1.587221392,-1.3777473618
C,0,3.600874584,3.7423873481,-0.0641039098	C,0,-5.4010998006,-3.2704711384,-0.7936718641
H,0,-1.250525111,7.4231706836,-1.563252227	C,0,-3.508227651,-4.8286611116,-0.5592669309
C,0,0,1.2101215331,2.4666720213	C,0,5.4010998006,-3.2704711384,-0.7936718641
C,0,-3.5446177177,2.4551721014,0.5315166545	C,0,3.508227651,-4.8286611116,-0.5592669309
C,0,-2.3126187393,0.7514153784,1.8016351796	C,0,7.0862247994,-1.587221392,-1.3777473618
C,0,-3.6993011368,6.2489218876,-1.3777473618	C,0,-0.7134486416,-5.1441959397,-0.0641039098
C,0,-4.7794345143,4.1261199992,-0.7936718641	C,0,0.7134486416,-5.1441959397,-0.0641039098
C,0,2.3126187393,0.7514153784,1.8016351796	C,0,-6.6658216151,-2.8810893513,-1.3777473618
C,0,3.5446177177,2.4551721014,0.5315166545	C,0,-4.8319317377,-4.5271464944,-0.9841401383
C,0,3.6993011368,6.2489218876,-1.3777473618	C,0,-2.8124231513,-5.9944053681,-0.9841401383
C,0,4.7794345143,4.1261199992,-0.7936718641	C,0,4.8319317377,-4.5271464944,-0.9841401383
C,0,-1.1508939694,0.3739481191,2.4666720213	C,0,6.6658216151,-2.8810893513,-1.3777473618
C,0,1.1508939694,0.3739481191,2.4666720213	C,0,2.8124231513,-5.9944053681,-0.9841401383
C,0,-4.5430184485,1.4761161744,0.2298049942	C,0,-1.4413712609,-6.1473823217,-0.7936718641
C,0,-3.1680943807,-0.279418518,1.2931654711	C,0,1.4413712609,-6.1473823217,-0.7936718641
C,0,-4.7999309623,5.4492675118,-1.3777473618	H,0,-3.3515341863,-6.7405114527,-1.563252227
C,0,-5.7987211965,3.1964749627,-0.9841401383	H,0,5.3749263196,-5.270431017,-1.563252227
C,0,3.1680943807,-0.279418518,1.2931654711	C,0,-0.6802266412,-7.2298786553,-1.3777473618
C,0,4.5430184485,1.4761161744,0.2298049942	C,0,0.6802266412,-7.2298786553,-1.3777473618
C,0,5.7987211965,3.1964749627,-0.9841401383	H,0,1.250525111,7.4231706836,-1.563252227
C,0,4.7999309623,5.4492675118,-1.3777473618	H,0,-6.6734213388,3.483205949,-1.563252227
C,0,-0.7112915905,-0.9790088853,2.4666720213	H,0,-5.3749263196,-5.270431017,-1.563252227
C,0,0.7112915905,-0.9790088853,2.4666720213	H,0,3.3515341863,-6.7405114527,-1.563252227
C,0,-5.6764315796,1.8443844247,-0.5592669309	H,0,7.4462883612,1.1045658379,-1.563252227
C,0,-4.3107699251,0.0971980656,0.5315166545	H,0,1.2239123664,-8.0331227387,-1.8679202553
C,0,-2.7272802779,-1.6361048249,1.2931654711	H,0,-1.2239123664,-8.0331227387,-1.8679202553
C,0,2.7272802779,-1.6361048249,1.2931654711	H,0,-3.7315851717,7.2183304529,-1.8679202553
C,0,4.3107699251,0.0971980656,0.5315166545	H,0,-5.7119169798,5.7795351747,-1.8679202553
C,0,5.6764315796,1.8443844247,-0.5592669309	H,0,-7.2617440062,-3.6463812755,-1.8679202553
H,0,6.6734213388,3.483205949,-1.563252227	H,0,-8.0181634479,-1.3183616126,-1.8679202553
C,0,-1.4292769839,-1.9672309998,1.8016351796	H,0,8.0181634479,-1.3183616126,-1.8679202553
C,0,1.4292769839,-1.9672309998,1.8016351796	H,0,7.2617440062,-3.6463812755,-1.8679202553
C,0,-6.5701048359,0.8224002348,-0.9841401383	H,0,5.7119169798,5.7795351747,-1.8679202553
C,0,-5.1128888246,-0.911113988,-0.0641039098	H,0,3.7315851717,7.2183304529,-1.8679202553

1.3 C₁₇₀H₃₀

RB3LYP/6-31G(1d,1p) energy = $-6497.48389154 E_h$

Lowest excitation energies are $^1A \rightarrow ^3E = 0.0154432 E_h$ and $^1A \rightarrow ^1E = 0.0464318 E_h$.

Lowest harmonic vibrational frequency is 18.0917 cm^{-1} , symmetry type E_2 .

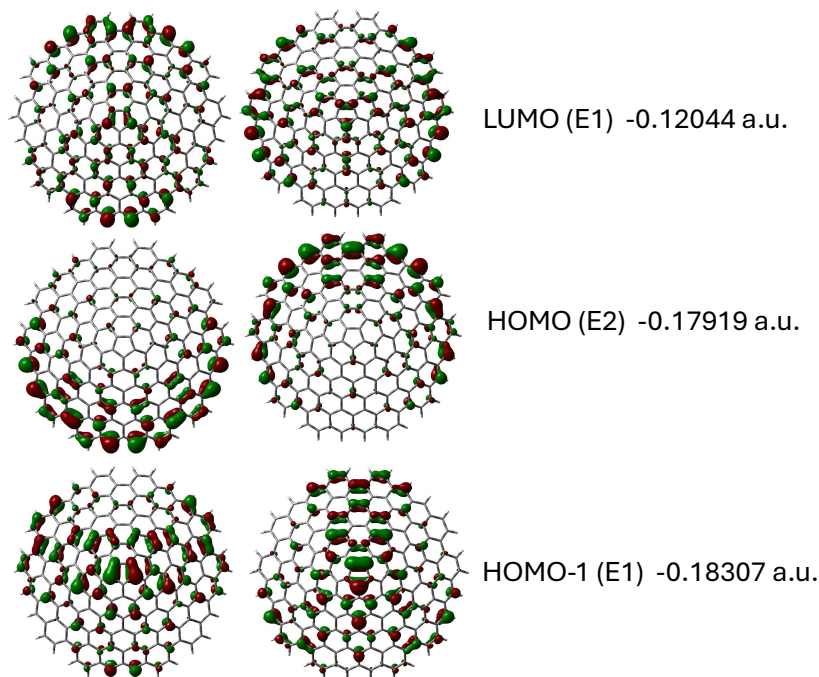


Figure S3: Frontier orbitals.

C,0,0.0000000002,4.7708778637,1.7209746013	C,0,-2.8381210286,-8.0937322333,-0.7994227268
C,0,-1.2404885826,4.1288468908,2.0307050181	C,0,-4.8900124643,-6.7305247463,-0.6428185321
C,0,1.2404885829,4.1288468907,2.0307050181	C,0,-6.8205691521,-5.2003143058,-0.7994227268
C,0,0.0000000002,5.9381480125,0.9155320757	C,0,-8.5746244116,0.1981126903,-0.7994227268
C,0,-1.2460451772,2.9322339753,2.7969575053	C,0,-7.9122063722,2.5708316913,-0.6428185321
C,0,-2.4441366181,4.5775414216,1.4226352581	C,0,-7.0534645867,4.8797612403,-0.7994227268
C,0,1.2460451774,2.9322339752,2.7969575053	C,0,-6.0477365139,7.1102647274,-1.2362737749
C,0,2.4441366184,4.5775414215,1.4226352581	C,0,-4.8934102407,7.9489318559,-1.2362737749
C,0,-1.2345070449,6.4920811526,0.4637734942	C,0,-2.4612882985,8.2161726095,-0.7994227268
C,0,1.2345070453,6.4920811525,0.4637734942	C,0,0.0000000003,8.3193861109,-0.6428185321
C,0,0.0000000001,2.4355436469,3.302540222	C,0,2.4612882991,8.2161726094,-0.7994227268
C,0,-2.4036710939,2.0911695154,2.7969575053	C,0,4.8934102412,7.9489318556,-1.2362737749
C,0,-2.4490650217,5.790680981,0.6749463279	C,0,6.0477365143,7.110264727,-1.2362737749
C,0,-3.5982208458,3.7390501494,1.4226352581	C,0,7.053464587,4.8797612399,-0.7994227268
C,0,2.403671094,2.0911695152,2.7969575053	C,0,7.9122063724,2.5708316908,-0.6428185321

C,0,2.449065022,5.7906809808,0.6749463279	C,0,8.5746244116,0.1981126897,-0.7994227268
C,0,3.5982208461,3.7390501491,1.4226352581	C,0,9.0720303639,-2.1975546663,-1.2362737749
C,0,-1.2344727051,7.6910813921,-0.3107774818	C,0,8.6311169616,-3.5545465856,-1.2362737749
C,0,0,1.210193133,3.9626466854	C,0,6.8205691517,-5.2003143063,-0.7994227268
C,0,-3.5434346868,2.4556586065,2.0307050181	C,0,4.8900124639,-6.7305247466,-0.6428185321
C,0,-2.3163396561,0.7526243775,3.302540222	C,0,2.8381210281,-8.0937322335,-0.7994227268
C,0,-3.6553825542,6.2397248605,0.0569450641	C,0,0.7134128706,-9.3070953315,-1.2362737749
C,0,-4.7504621684,4.1186180801,0.6749463279	C,0,-0.7134128712,-9.3070953315,-1.2362737749
C,0,2.3163396561,0.7526243774,3.302540222	C,0,-8.6311169618,-3.5545465851,-1.2362737749
C,0,3.5434346869,2.4556586063,2.0307050181	C,0,-9.072030364,-2.1975546657,-1.2362737749
C,0,3.6553825546,6.2397248603,0.0569450641	C,0,-9.7500783499,0.591061658,-1.5252935999
C,0,4.7504621687,4.1186180798,0.6749463279	C,0,-9.9894168113,1.9399599799,-1.7792148627
C,0,-1.1509620651,0.3739702446,3.9626466854	C,0,-9.0720947609,2.9477022743,-1.3972176437
C,0,1.1509620652,0.3739702446,3.9626466854	C,0,-9.2218878302,4.3021712892,-1.7792148627
C,0,-4.5373744806,1.4742823381,1.7209746013	C,0,-8.235396407,5.2527733373,-1.5252935999
C,0,-3.173769365,-0.2789492555,2.7969575053	C,0,-8.321255815,6.6041459222,-2.0056131256
C,0,-4.8047556579,5.4046564202,0.0569450641	C,0,-7.2839982801,7.4779627883,-1.874576094
C,0,-5.7928524277,3.1802493749,0.4637734942	C,0,-4.8610859823,9.2383116142,-1.874576094
C,0,3.173769365,-0.2789492557,2.7969575053	C,0,-3.7095065518,9.9547778902,-2.0056131256
C,0,4.5373744807,1.4742823378,1.7209746013	C,0,-2.4508068653,9.4555236461,-1.5252935999
C,0,5.7928524279,3.1802493745,0.4637734942	C,0,-1.2418879784,10.0999805546,-1.7792148627
C,0,4.8047556583,5.4046564198,0.0569450641	C,0,0.0000000003,9.5389649359,-1.3972176437
C,0,-0.7113336761,-0.9790668111,3.9626466854	C,0,1.241887979,10.0999805545,-1.7792148627
C,0,0.711333676,-0.9790668111,3.9626466854	C,0,2.4508068659,9.455523646,-1.5252935999
C,0,-5.647514362,1.8349886512,0.9155320757	C,0,3.7095065525,9.9547778899,-2.0056131256
C,0,-4.3100987936,0.0961091066,2.0307050181	C,0,4.8610859829,9.2383116139,-1.874576094
C,0,-2.7315956112,-1.6398201384,2.7969575053	C,0,-9.362844494,-4.6166764441,-1.874576094
C,0,2.7315956111,-1.6398201386,2.7969575053	C,0,-8.8523254752,-5.8731912433,-2.0056131256
C,0,4.3100987936,0.0961091063,2.0307050181	C,0,-7.5405617562,-6.2091311883,-1.5252935999
C,0,5.6475143621,1.8349886508,0.9155320757	C,0,-6.9413280985,-7.4410924723,-1.7792148627
C,0,6.9331800303,3.5507281657,-0.3107774818	C,0,-5.6068629117,-7.7171847417,-1.3972176437
C,0,-1.431576637,-1.9703962008,3.302540222	C,0,-4.9319111388,-8.9010193502,-1.7792148627
C,0,1.4315766369,-1.9703962009,3.302540222	C,0,-3.575072948,-9.090227452,-1.5252935999
C,0,-6.555819741,0.8320774356,0.4637734942	C,0,-2.8502177925,-10.2339777328,-2.0056131256
C,0,-5.1087803492,-0.9099739656,1.4226352581	C,0,-1.4974421521,-10.3312257457,-1.874576094
C,0,-3.4304516562,-2.6111664071,2.0307050181	C,0,1.4974421514,-10.3312257458,-1.874576094
C,0,3.430451656,-2.6111664073,2.0307050181	C,0,2.8502177918,-10.233977733,-2.0056131256
C,0,5.1087803492,-0.909973966,1.4226352581	C,0,3.5750729474,-9.0902274523,-1.5252935999
C,0,6.5558197411,0.8320774351,0.4637734942	C,0,4.9319111382,-8.9010193505,-1.7792148627
C,0,-0.7154521628,-3.1046340963,2.7969575053	C,0,5.6068629112,-7.7171847421,-1.3972176437
C,0,0.7154521626,-3.1046340964,2.7969575053	C,0,6.941328098,-7.4410924728,-1.7792148627
C,0,-7.6961261203,1.2026215449,-0.3107774818	C,0,7.5405617558,-6.2091311888,-1.5252935999
C,0,-6.2640675928,-0.5397804155,0.6749463279	C,0,8.8523254748,-5.8731912439,-2.0056131256
C,0,-4.6679594002,-2.2666813435,1.4226352581	C,0,9.3628444937,-4.6166764447,-1.874576094
C,0,-2.8042516489,-3.8597212697,1.7209746013	C,0,10.2883146398,-1.7683722123,-1.874576094

C,0,4.6679594,-2.2666813438,1.4226352581	C,0,10.6138569459,-0.4517548357,-2.0056131256
C,0,2.8042516486,-3.8597212699,1.7209746013	C,0,9.75007835,0.5910616574,-1.5252935999
C,0,6.2640675927,-0.5397804159,0.6749463279	C,0,9.9894168114,1.9399599792,-1.7792148627
C,0,-1.4232989668,-4.0694481963,2.0307050181	C,0,9.0720947611,2.9477022737,-1.3972176437
C,0,1.4232989665,-4.0694481964,2.0307050181	C,0,9.2218878304,4.3021712886,-1.7792148627
C,0,-7.0639063187,-1.5482943756,0.0569450641	C,0,8.2353964073,5.2527733368,-1.5252935999
C,0,-5.3850121044,-3.2452350206,0.6749463279	C,0,8.3212558154,6.6041459216,-2.0056131256
C,0,-3.4903558278,-4.8040626571,0.9155320757	C,0,7.2839982806,7.4779627878,-1.874576094
C,0,5.3850121042,-3.245235021,0.6749463279	C,0,-10.2883146399,-1.7683722116,-1.874576094
C,0,3.4903558275,-4.8040626573,0.9155320757	C,0,-10.6138569459,-0.451754835,-2.0056131256
C,0,7.0639063186,-1.548294376,0.0569450641	H,0,10.9622031399,-2.5099940291,-2.2869326888
C,0,-0.7132632788,-5.1399362613,1.4226352581	H,0,11.5309754311,-0.1683500952,-2.5148193027
C,0,0.7132632784,-5.1399362613,1.4226352581	H,0,10.8771298831,2.2239726387,-2.3390688061
C,0,-6.6248848588,-2.8994634951,0.0569450641	H,0,10.1070012443,4.5941848722,-2.3390688061
C,0,-4.8146867375,-4.5265789461,0.4637734942	H,0,9.2298013828,6.9139353904,-2.5148193027
C,0,-2.8172123792,-5.9778290161,0.4637734942	H,0,7.3932711629,8.4740491632,-2.2869326888
C,0,4.8146867372,-4.5265789464,0.4637734942	H,0,5.7746532433,9.6500439184,-2.2869326888
C,0,6.6248848586,-2.8994634955,0.0569450641	H,0,3.723377825,10.9145862826,-2.5148193027
C,0,2.8172123788,-5.9778290163,0.4637734942	H,0,1.2460943138,11.0320105943,-2.3390688061
C,0,-1.4223416585,-6.1242836242,0.6749463279	H,0,-1.2460943131,11.0320105944,-2.3390688061
C,0,1.4223416581,-6.1242836243,0.6749463279	H,0,-3.7233778243,10.9145862829,-2.5148193027
C,0,-3.5219948189,-6.9478204018,-0.3107774818	H,0,-5.7746532427,9.6500439188,-2.2869326888
C,0,5.519413614,-5.4966107009,-0.3107774818	H,0,-7.3932711623,8.4740491637,-2.2869326888
C,0,-0.7103516441,-7.1966234092,0.0569450641	H,0,-9.2298013823,6.913935391,-2.5148193027
C,0,0.7103516436,-7.1966234092,0.0569450641	H,0,-10.107001244,4.5941848729,-2.3390688061
C,0,1.2344727056,7.6910813921,-0.3107774818	H,0,-10.877129883,2.2239726394,-2.3390688061
C,0,-6.9331800301,3.5507281662,-0.3107774818	H,0,-11.5309754311,-0.1683500944,-2.5148193027
C,0,-5.5194136144,-5.4966107005,-0.3107774818	H,0,-10.9622031401,-2.5099940284,-2.2869326888
C,0,3.5219948185,-6.947820402,-0.3107774818	H,0,-10.3439461097,-4.4127935129,-2.2869326888
C,0,7.6961261204,1.2026215444,-0.3107774818	H,0,-9.4277087887,-6.6415392149,-2.5148193027
C,0,1.4229899082,-8.2136742205,-0.6433218322	H,0,-7.4925646069,-8.1926481923,-2.3390688061
C,0,-1.4229899087,-8.2136742205,-0.6433218322	H,0,-5.4763416546,-9.6575199132,-2.3390688061
C,0,-3.676653555,7.4814145131,-0.6433218322	H,0,-3.4031569156,-11.0186323632,-2.5148193027
C,0,-5.9790995925,5.8085895485,-0.6433218322	H,0,-1.0003608895,-11.2013055399,-2.2869326888
C,0,-7.3719403258,-3.8915087452,-0.6433218322	H,0,1.0003608887,-11.2013055399,-2.2869326888
C,0,-8.2513964547,-1.1848210951,-0.6433218322	H,0,3.4031569149,-11.0186323634,-2.5148193027
C,0,8.2513964546,-1.1848210956,-0.6433218322	H,0,5.476341654,-9.6575199135,-2.3390688061
C,0,7.3719403255,-3.8915087456,-0.6433218322	H,0,7.4925646064,-8.1926481927,-2.3390688061
C,0,5.9790995929,5.8085895482,-0.6433218322	H,0,9.4277087883,-6.6415392155,-2.5148193027
C,0,3.6766535555,7.4814145129,-0.6433218322	H,0,10.3439461094,-4.4127935136,-2.2869326888

1.4 C₁₈₀H₃₀

RB3LYP/6-31G(1d,1p) energy = $-6878.62489555 E_h$

Lowest excitation energies are $^1A \rightarrow ^3E = 0.0054191 E_h$ and $^1A \rightarrow ^1E = 0.0417385 E_h$.

Lowest harmonic vibrational frequency is 17.2725 cm^{-1} , symmetry type E₂.

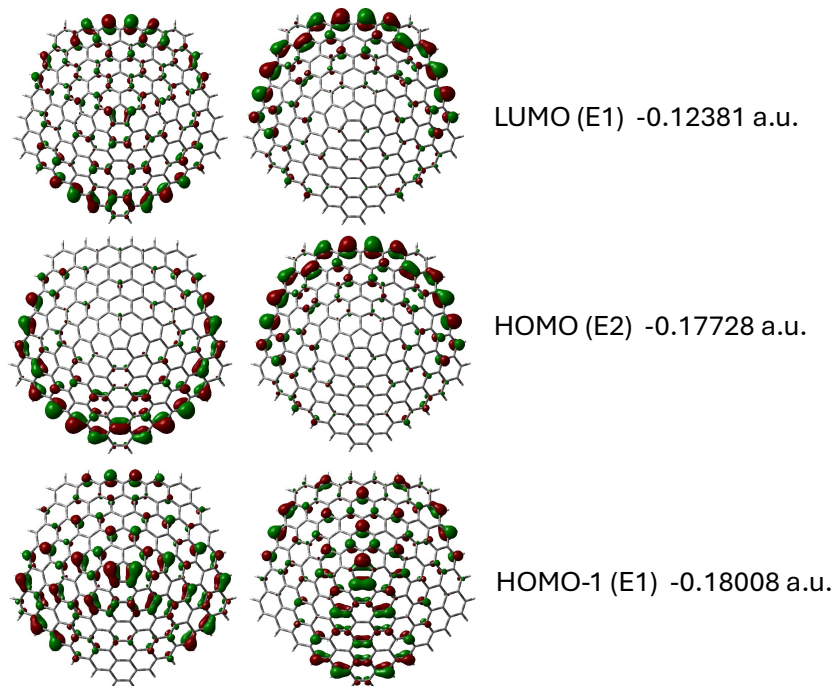


Figure S4: Frontier orbitals.

C,0,-0.0000000007,4.7757364304,1.9257593104	C,0,-7.0358553175,4.8670176257,-0.6416293943
C,0,-1.240473151,4.1314957436,2.2345115791	C,0,-5.9989388446,7.0575846445,-1.1190553764
C,0,1.2404731499,4.131495744,2.2345115791	C,0,-4.858387816,7.8862434725,-1.1190553764
C,0,-0.0000000008,5.9439150399,1.1187266711	C,0,-2.4546099665,8.1954872053,-0.6416293943
C,0,-1.2463354075,2.933257367,2.998837327	C,0,-0.0000000011,8.3107754325,-0.4699510599
C,0,-2.4444568753,4.5790423756,1.6260128266	C,0,2.4546099643,8.195487206,-0.6416293943
C,0,1.2463354067,2.9332573673,2.998837327	C,0,4.8583878138,7.8862434738,-1.1190553764
C,0,2.444456874,4.5790423763,1.6260128266	C,0,5.9989388427,7.0575846462,-1.1190553764
C,0,-1.2335239072,6.4956577588,0.6618346869	C,0,7.0358553162,4.8670176276,-0.6416293943
C,0,1.2335239054,6.4956577592,0.6618346869	C,0,7.9040171297,2.5681708465,-0.4699510599
C,0,-0.0000000003,2.4359426285,3.503403731	C,0,8.5528877045,0.1980720227,-0.6416293943
C,0,-2.4045547113,2.0917617858,2.998837327	C,0,9.0015876441,-2.1836181335,-1.1190553764
C,0,-2.4462039546,5.7897519682,0.8738818184	C,0,8.5659359172,-3.5244162819,-1.1190553764
C,0,-3.5995493738,3.7398185514,1.6260128266	C,0,6.8030076918,-5.1875048869,-0.6416293943

C,0,2.4045547107,2.0917617865,2.998837327	C,0,4.884951235,-6.7235585598,-0.4699510599
C,0,2.446203953,5.7897519689,0.8738818184	C,0,2.8313653391,-8.0730719631,-0.6416293943
C,0,3.5995493728,3.7398185524,1.6260128266	C,0,0.704899303,-9.235793698,-1.1190553764
C,0,-1.2316679624,7.6864216482,-0.1289490203	C,0,-0.7048993004,-9.2357936982,-1.1190553764
C,0,-0.0000000002,1.2100624429,4.1625385354	C,0,-8.5659359162,-3.5244162843,-1.1190553764
C,0,-3.5459586645,2.4564624699,2.2345115791	C,0,-9.0015876435,-2.183618136,-1.1190553764
C,0,-2.3167191097,0.7527476695,3.503403731	C,0,-9.714845242,0.5740363967,-1.4060208342
C,0,-3.6466171368,6.227705812,0.2412484715	C,0,-9.9528164587,1.9284970486,-1.6604803797
C,0,-4.7504627441,4.1156099616,0.8738818184	C,0,-9.0480971764,2.9399049852,-1.2572513815
C,0,2.3167191095,0.7527476702,3.503403731	C,0,-9.1855397821,4.2899318457,-1.6604803797
C,0,3.5459586638,2.4564624709,2.2345115791	C,0,-8.1968850279,5.2458375599,-1.4060208342
C,0,3.6466171351,6.227705813,0.2412484715	C,0,-8.2553536016,6.5753696965,-1.9312315264
C,0,4.750462743,4.1156099629,0.8738818184	C,0,-7.1982985265,7.4577251355,-1.8216570859
C,0,-1.150837771,0.3739298593,4.1625385354	C,0,-4.8683215136,9.1505525252,-1.8216570859
C,0,1.1508377709,0.3739298596,4.1625385354	C,0,-3.7025036417,9.883208817,-1.9312315264
C,0,-4.541995252,1.4757837174,1.9257593104	C,0,-2.4561112223,9.4167538745,-1.4060208342
C,0,-3.174832354,-0.2789090352,2.998837327	C,0,-1.2414797434,10.0616293105,-1.6604803797
C,0,-4.7960335278,5.3926059213,0.2412484715	C,0,-0.0000000013,9.5137323823,-1.2572513815
C,0,-5.7965577893,3.1804195858,0.6618346869	C,0,1.2414797406,10.0616293108,-1.6604803797
C,0,3.1748323541,-0.2789090343,2.998837327	C,0,2.4561112197,9.4167538752,-1.4060208342
C,0,4.5419952515,1.4757837186,1.9257593104	C,0,3.702503639,9.883208818,-1.9312315264
C,0,5.7965577884,3.1804195874,0.6618346869	C,0,4.8683215111,9.1505525265,-1.8216570859
C,0,4.7960335263,5.3926059226,0.2412484715	C,0,-9.3171146617,-4.5414249133,-1.8216570859
C,0,-0.7112568579,-0.9789610798,4.1625385354	C,0,-8.8045927539,-5.8194068563,-1.9312315264
C,0,0.7112568581,-0.9789610796,4.1625385354	C,0,-7.5220647688,-6.174647963,-1.4060208342
C,0,-5.6529991307,1.83677076,1.1187266711	C,0,-6.918455531,-7.4103056201,-1.6604803797
C,0,-4.3126132333,0.0969423237,2.2345115791	C,0,-5.5920315872,-7.6967711771,-1.2572513815
C,0,-2.7324319461,-1.6404774866,2.998837327	C,0,-4.9096991119,-8.8697525865,-1.6604803797
C,0,2.7324319466,-1.6404774859,2.998837327	C,0,-3.5479933327,-9.0619798698,-1.4060208342
C,0,4.3126132333,0.0969423249,2.2345115791	C,0,-2.8138160198,-10.1719609282,-1.9312315264
C,0,5.6529991302,1.8367707616,1.1187266711	C,0,-1.4400049857,-10.264480089,-1.8216570859
C,0,6.9296150633,3.5466207571,-0.1289490203	C,0,1.4400049885,-10.2644800886,-1.8216570859
C,0,-1.4318111519,-1.970718983,3.503403731	C,0,2.8138160226,-10.1719609274,-1.9312315264
C,0,1.4318111524,-1.9707189826,3.503403731	C,0,3.5479933352,-9.0619798689,-1.4060208342
C,0,-6.558917489,0.8341176875,0.6618346869	C,0,4.9096991143,-8.8697525852,-1.6604803797
C,0,-5.1103068057,-0.9098147276,1.6260128266	C,0,5.5920315893,-7.6967711755,-1.2572513815
C,0,-3.4319961273,-2.6133184448,2.2345115791	C,0,6.918455533,-7.4103056182,-1.6604803797
C,0,3.431996128,-2.6133184438,2.2345115791	C,0,7.5220647705,-6.1746479609,-1.4060208342
C,0,5.110306806,-0.9098147262,1.6260128266	C,0,8.8045927555,-5.8194068539,-1.9312315264
C,0,6.5589174887,0.8341176893,0.6618346869	C,0,9.3171146629,-4.5414249107,-1.8216570859
C,0,-0.7158188958,-3.1056326298,2.998837327	C,0,10.2070866886,-1.8023726576,-1.8216570859
C,0,0.7158188967,-3.1056326296,2.998837327	C,0,10.543626694,-0.4672107284,-1.9312315264
C,0,-7.6908277269,1.203849074,-0.1289490203	C,0,9.7148452418,0.5740363994,-1.4060208342
C,0,-6.2622999303,-0.5373464594,0.8738818184	C,0,9.9528164581,1.9284970513,-1.6604803797
C,0,-4.6691007312,-2.2677073991,1.6260128266	C,0,9.0480971756,2.9399049877,-1.2572513815

C,0,-2.8071074418,-3.8636519323,1.9257593104
C,0,4.6691007318,-2.2677073978,1.6260128266
C,0,2.8071074429,-3.8636519315,1.9257593104
C,0,6.2622999305,-0.5373464577,0.8738818184
C,0,-1.4248684075,-4.0715820919,2.2345115791
C,0,1.4248684086,-4.0715820915,2.2345115791
C,0,-7.0497668608,-1.5436720582,0.2412484715
C,0,-5.3821513911,-3.2461651275,0.8738818184
C,0,-3.4937456004,-4.8087282799,1.1187266711
C,0,5.382151392,-3.246165126,0.8738818184
C,0,3.4937456017,-4.808728279,1.1187266711
C,0,7.0497668613,-1.5436720562,0.2412484715
C,0,-0.7138864236,-5.1413388001,1.6260128266
C,0,0.713886425,-5.1413387999,1.6260128266
C,0,-6.6107288665,-2.894892065,0.2412484715
C,0,-4.8159936369,-4.5300503559,0.6618346869
C,0,-2.8201100304,-5.9801446766,0.6618346869
C,0,4.8159936382,-4.5300503546,0.6618346869
C,0,6.6107288673,-2.8948920632,0.2412484715
C,0,2.820110032,-5.9801446758,0.6618346869
C,0,-1.4241102501,-6.1218503432,0.8738818184
C,0,1.4241102518,-6.1218503428,0.8738818184
C,0,-3.5215249744,-6.9424020025,-0.1289490203
C,0,5.5144056005,-5.4944894744,-0.1289490203
C,0,-0.710378396,-7.1817476107,0.2412484715
C,0,0.7103783979,-7.1817476105,0.2412484715
C,0,1.2316679603,7.6864216486,-0.1289490203
C,0,-6.9296150642,3.5466207552,-0.1289490203
C,0,-5.5144055989,-5.4944894759,-0.1289490203
C,0,3.5215249763,-6.9424020015,-0.1289490203
C,0,7.6908277265,1.2038490761,-0.1289490203
C,0,1.4225963802,-8.1792945795,-0.484272824
C,0,-1.422596378,-8.1792945799,-0.484272824
C,0,-3.6567640826,7.4533694889,-0.484272824
C,0,-5.958573376,5.7810071454,-0.484272824
C,0,-7.3393649513,-3.8805105842,-0.484272824
C,0,-8.2185778663,-1.1745714715,-0.484272824
C,0,8.2185778666,-1.1745714692,-0.484272824
C,0,7.3393649524,-3.8805105822,-0.484272824
C,0,5.9585733744,5.7810071471,-0.484272824
C,0,3.6567640805,7.45336949,-0.484272824
C,0,-2.8313653369,-8.0730719639,-0.6416293943
C,0,-4.8849512331,-6.7235585611,-0.4699510599
C,0,-6.8030076904,-5.1875048888,-0.6416293943
C,0,-8.5528877046,0.1980720203,-0.6416293943
C,0,9.1855397809,4.2899318482,-1.6604803797
C,0,8.1968850264,5.2458375621,-1.4060208342
C,0,8.2553535998,6.5753696988,-1.9312315264
C,0,7.1982985245,7.4577251375,-1.8216570859
C,0,-10.2070866881,-1.8023726604,-1.8216570859
C,0,-10.5436266939,-0.4672107313,-1.9312315264
H,0,11.4388111117,-0.1873175109,-2.4813611537
H,0,10.8230955876,2.2101069553,-2.2481583739
H,0,10.0551365349,4.573641888,-2.2481583739
H,0,9.1440901122,6.8751075283,-2.4813611537
H,0,3.7129365688,10.8210715526,-2.4813611537
H,0,1.2425838472,10.976336194,-2.2481583739
H,0,-1.2425838503,10.9763361937,-2.2481583739
H,0,-3.7129365718,10.8210715516,-2.4813611537
H,0,-9.1440901141,6.8751075258,-2.4813611537
H,0,-10.0551365361,4.5736418852,-2.2481583739
H,0,-10.8230955882,2.2101069523,-2.2481583739
H,0,-11.4388111117,-0.1873175141,-2.4813611537
H,0,-9.3642950555,-6.5720214246,-2.4813611537
H,0,-7.4569999881,-8.1496700559,-2.2481583739
H,0,-5.4464570867,-9.6104149777,-2.2481583739
H,0,-3.3566374861,-10.9368401412,-2.4813611537
H,0,3.3566374891,-10.9368401403,-2.4813611537
H,0,5.4464570894,-9.6104149762,-2.2481583739
H,0,7.4569999903,-8.1496700538,-2.2481583739
H,0,9.3642950573,-6.5720214221,-2.4813611537
C,0,-7.2107722365,8.7706729361,-2.4311398667
C,0,-6.1131544867,9.568138911,-2.4311398667
C,0,6.113154484,9.5681389127,-2.4311398667
C,0,7.2107722341,8.7706729381,-2.4311398667
C,0,10.9889094861,-2.8572378782,-2.4311398667
C,0,10.5696568124,-4.1475649304,-2.4311398667
C,0,0.6783650777,-11.3340090347,-2.4311398667
C,0,-0.6783650746,-11.3340090349,-2.4311398667
C,0,-10.5696568113,-4.1475649333,-2.4311398667
C,0,-10.9889094853,-2.8572378813,-2.4311398667
H,0,-8.1244408473,9.0973665233,-2.9204065874
H,0,-6.1415194239,10.5380432675,-2.9204065874
H,0,6.141519421,10.5380432692,-2.9204065874
H,0,8.1244408448,9.0973665255,-2.9204065874
H,0,11.9201085921,-2.5844976073,-2.9204065874
H,0,11.1627000056,-4.9155615459,-2.9204065874
H,0,1.2255128385,-12.1353506337,-2.9204065874
H,0,-1.2255128351,-12.135350634,-2.9204065874
H,0,-11.1627000042,-4.915561549,-2.9204065874

C,0,-7.9040171304,2.5681708443,-0.4699510599 H,0,-11.9201085914,-2.5844976106,-2.9204065874

1.5 Mes₅-C₇₀H₁₅

6 -4.619813 -1.330223 -1.001663

6 -4.334691 0.056008 -1.278057

6 -3.641164 -2.349096 -1.280681

6 -5.803692 -1.670654 -0.301477

6 -3.155089 0.388445 -2.004749

6 -5.147375 1.096349 -0.747227

6 -2.464845 -2.005793 -2.005489

6 -3.781252 -3.658733 -0.748418

6 -6.693357 -0.617386 0.065520

6 -6.022274 -3.042498 0.073842

6 -2.331984 -0.670896 -2.506116

6 -2.669301 1.724383 -2.005489

6 -6.368223 0.705013 -0.124313

6 -4.648133 2.465573 -0.748418

6 -1.344410 -2.880631 -2.004749

6 -5.024965 -3.975792 -0.129429

6 -2.633316 -4.556653 -0.747227

1 -7.622627 -0.874445 0.563033

6 -1.162457 -0.334167 -3.173147

6 -3.359305 2.737042 -1.280681

6 -1.358683 2.010530 -2.506116

1 -7.053204 1.462391 0.240733

6 -5.334002 3.550438 -0.129429

6 -0.082563 -2.425167 -2.506116

6 -1.392761 -4.105229 -1.278057
 1 -5.202445 -4.984675 0.227654
 6 -2.638396 -5.838679 -0.124313
 6 -0.677031 1.002299 -3.173147
 6 -0.041407 -1.208825 -3.173147
 6 -2.692719 3.982642 -1.001663
 6 -0.605542 3.120704 -2.004749
 1 -6.348352 3.407471 0.227654
 6 -4.754573 4.787340 0.073842
 6 1.145943 -2.964031 -2.005489
 6 -0.162484 -4.804766 -1.001663
 6 -1.481192 -6.556544 0.065520
 1 -3.570377 -6.256092 0.240733
 6 0.744029 0.953621 -3.173147
 6 1.136866 -0.412929 -3.173147
 6 -3.382326 5.003379 -0.301477
 6 -1.286226 4.139844 -1.278057
 6 0.815126 3.071520 -2.005489
 6 2.324197 -2.168773 -2.004749
 6 1.108942 -4.188863 -1.280681
 6 -0.204553 -6.035900 -0.301477
 1 -1.523874 -7.519767 0.563033
 6 1.492272 1.913472 -2.506116
 6 2.280958 -0.827939 -2.506116
 6 -2.655530 6.174978 0.065520
 6 -0.547936 5.234234 -0.747227
 6 1.564999 4.040681 -1.280681

6 3.473918 -2.593179 -1.278057
 6 2.311191 -4.726795 -0.748418
 6 1.032603 -6.667707 0.073842
 6 2.780843 1.540255 -2.004749
 6 3.173078 0.173921 -2.005489
 1 -3.187168 6.979330 0.563033
 6 -1.297382 6.274401 -0.124313
 6 0.908548 5.182541 -0.748418
 6 2.955622 3.791631 -1.001663
 6 3.519896 -3.912516 -0.747227
 6 4.519393 -1.639285 -1.001663
 6 2.228403 -6.007613 -0.129429
 6 3.539760 2.502557 -1.278057
 6 4.326528 -0.239764 -1.280681
 1 -0.788743 7.159899 0.240733
 6 1.728370 6.170083 -0.129429
 6 3.713301 4.762912 -0.301477
 6 4.737605 -4.313515 -0.124313
 6 5.677271 -2.059738 -0.301477
 1 3.133064 -6.488169 0.227654
 6 4.808732 2.138586 -0.747227
 6 5.209647 0.737413 -0.748418
 1 1.278948 7.090608 0.227654
 6 3.083787 6.001237 0.073842
 6 5.052149 4.433732 0.065520
 6 5.777930 -3.434780 0.065520
 1 4.846590 -5.328869 0.240733

6 6.660458 -1.078372 0.073842
 6 5.566397 3.172781 -0.124313
 6 6.402193 0.262883 -0.129429
 1 5.652849 5.187909 0.563033
 1 6.680821 -3.773026 0.563033
 1 6.565734 2.962670 0.240733
 1 7.138785 0.974766 0.227654
 6 7.939152 -1.490856 0.741389
 6 8.028907 -1.523769 2.148896
 6 9.059506 -1.839001 -0.042587
 6 9.237952 -1.898292 2.744822
 6 10.248864 -2.206049 0.594894
 6 10.361553 -2.238810 1.987429
 1 9.300575 -1.926080 3.830556
 1 11.109087 -2.474355 -0.014656
 6 1.035445 -8.011283 0.741389
 6 1.031879 -8.106815 2.148896
 6 1.050547 -9.184385 -0.042587
 6 1.049301 -9.372419 2.744822
 6 1.068995 -10.428955 0.594894
 6 1.072661 -10.546252 1.987429
 1 1.042225 -9.440564 3.830556
 1 1.079645 -11.329987 -0.014656
 6 -7.299213 -3.460389 0.741389
 6 -7.391172 -3.486518 2.148896
 6 -8.410233 -3.837261 -0.042587
 6 -8.589448 -3.894181 2.744822

6 -9.588188 -4.239400 0.594894
 6 -9.698611 -4.279133 1.987429
 1 -8.656444 -3.908509 3.830556
 1 -10.441830 -4.527963 -0.014656
 6 -5.546606 5.872645 0.741389
 6 -6.248357 6.812827 -0.042587
 6 -5.599874 5.952028 2.148896
 6 -6.994822 7.808863 0.594894
 6 -6.357872 6.965682 2.744822
 6 -7.066732 7.901602 1.987429
 1 -7.533051 8.531553 -0.014656
 1 -6.392201 7.024972 3.830556
 6 3.871222 7.089883 0.741389
 6 4.548536 8.047820 -0.042587
 6 3.930259 7.165075 2.148896
 6 5.265151 9.065541 0.594894
 6 4.660067 8.199210 2.744822
 6 5.331130 9.162592 1.987429
 1 5.786148 9.800752 -0.014656
 1 4.705847 8.250181 3.830556
 6 1.125542 -11.901142 2.653241
 1 0.626257 -12.664394 2.048702
 1 2.161733 -12.230884 2.800441
 1 0.648603 -11.882590 3.637749
 6 1.047268 -9.112944 -1.553037
 1 0.160782 -8.591396 -1.929961
 1 1.916969 -8.565517 -1.931799

1 1.060694 -10.114332 -1.991034
 6 1.001972 -6.868989 3.017421
 1 1.896434 -6.253049 2.875810
 1 0.143029 -6.231944 2.780963
 1 0.942736 -7.137435 4.075424
 6 11.666471 -2.607201 2.653241
 1 12.238079 -3.317907 2.048702
 1 12.300274 -1.723620 2.800441
 1 11.501443 -3.055065 3.637749
 6 8.990548 -1.820044 -1.553037
 1 8.220587 -2.501976 -1.929961
 1 8.738666 -0.823744 -1.931799
 1 9.947074 -2.116721 -1.991034
 6 6.842424 -1.169703 3.017421
 1 6.533033 -0.128682 2.875810
 1 5.971129 -1.789748 2.780963
 1 7.079426 -1.308993 4.075424
 6 6.084733 10.289804 2.653241
 1 6.937292 10.613815 2.048702
 1 5.440253 11.165628 2.800441
 1 6.459680 9.994456 3.637749
 6 4.509196 7.988095 -1.553037
 1 4.919821 7.045090 -1.929961
 1 3.483824 8.056414 -1.931799
 1 5.086936 8.806127 -1.991034
 6 3.226879 6.146073 3.017421
 1 2.141202 6.173518 2.875810

1 3.547332 5.125819 2.780963
1 3.432590 6.328432 4.075424
6 -6.203711 6.756958 -1.553037
1 -5.179970 6.856080 -1.929961
1 -6.585545 5.802882 -1.931799
1 -6.803174 7.559206 -1.991034
6 -4.848102 4.968185 3.017421
1 -5.209697 3.944127 2.875810
1 -3.778757 4.957678 2.780963
1 -4.957969 5.220179 4.075424
6 -7.905899 8.966650 2.653241
1 -7.950597 9.877605 2.048702
1 -8.938012 8.624358 2.800441
1 -7.509141 9.231978 3.637749
6 -8.343301 -3.812066 -1.553037
1 -8.121218 -2.807799 -1.929961
1 -7.553914 -4.470036 -1.931799
1 -9.291529 -4.134280 -1.991034
6 -6.223171 -3.075565 3.017421
1 -5.360972 -3.735915 2.875810
1 -5.882732 -2.061805 2.780963
1 -6.496782 -3.102184 4.075424
6 -10.970847 -4.748109 2.653241
1 -11.851031 -4.509120 2.048702
1 -10.964250 -5.835482 2.800441
1 -11.100586 -4.288780 3.637749

2 σ/π Orbital separation

In carboncones σ/π orbital separation is not strictly possible. However, descendants of p orbitals can be easily detected by using a combination of symmetry arguments and analysis of the contributions to the electron density given by each individual orbital.

The doubly occupied molecular orbitals of the four carboncones considered here can be initially divided into

Carbon-cone	number of 1s cores n_c	number of σ -orbitals n_s	number of π -orbitals n_p
C ₇₀ H ₂₀	70	115	35
C ₈₀ H ₂₀	80	130	40
C ₁₇₀ H ₃₀	170	270	85
C ₁₈₀ H ₃₀	180	285	90

As can be established by inspecting the results of the geometry optimization, these orbitals span the symmetries

Carbon-cone	$\Gamma_{\text{core}+\sigma}$	Γ_{π}
C ₇₀ H ₂₀	$23A_1 \oplus 14A_2 \oplus 37E_1 \oplus 37E_2$	$5A_1 \oplus 2A_2 \oplus 7E_1 \oplus 7E_2$
C ₈₀ H ₂₀	$26A_1 \oplus 16A_2 \oplus 42E_1 \oplus 42E_2$	$6A_1 \oplus 2A_2 \oplus 8E_1 \oplus 8E_2$
C ₁₇₀ H ₃₀	$51A_1 \oplus 37A_2 \oplus 88E_1 \oplus 88E_2$	$11A_1 \oplus 6A_2 \oplus 17E_1 \oplus 17E_2$
C ₁₈₀ H ₃₀	$54A_1 \oplus 39A_2 \oplus 93E_1 \oplus 93E_2$	$12A_1 \oplus 6A_2 \oplus 18E_1 \oplus 18E_2$

For each orbital ϕ_i the partial electron density $2\phi_i\phi_i$ at the center of each pair of bonded atoms was calculated, storing in two separate lists the largest value across all atom pairs and the total sum over all pairs. The two lists are sorted from lowest to highest value and orbitals are selected as π -orbitals only if they are present in the first n_p positions in both lists. Obviously, the total number of selected π -orbitals can be only lower than (or at maximum equal to) n_p . By counting how many of them are for each symmetry species, one can further verify the goodness of the selection, since each counter cannot exceed the tabulated value

obtained during the preliminary symmetry analysis. According to this scheme, π -orbitals were determined and adopted in the magnetic response calculations.

3 Current densities

The first-order perturbed molecular orbitals, required for the calculation of origin-independent current densities and molecular magnetic response properties using the CTOCD-DZ2 method, were determined performing G16 calculations with the CSGT keyword and the B3LYP/6-311+G(2d,1p) combination of functional and basis set. Optimized geometries determined with the smaller 6-31G(1d,1p) basis set reported in the previous section were employed.

3.1 $C_{70}H_{20}$

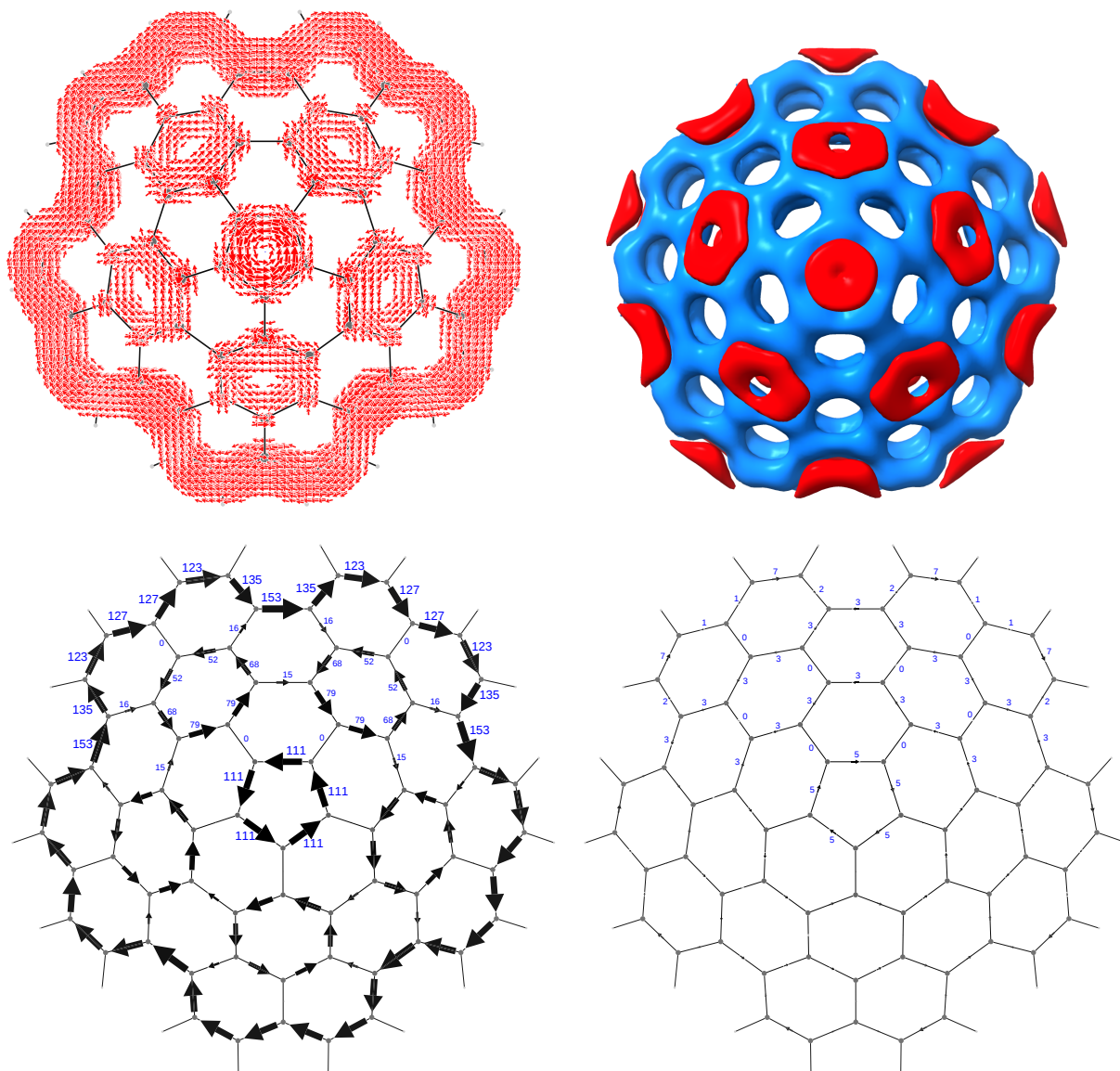


Figure S5: Top left: map of the current density induced in the π -electrons of $C_{70}H_{20}$ by a magnetic field parallel to the main symmetry axis. Top right: ChimeraX map of π -DIAL. Red/Blue isosurface value is $+0.003/-0.003$ a.u.. Bottom left: π -orbital contribution to BCSs. Bottom right: contribution to BCSs from all orbitals but π .

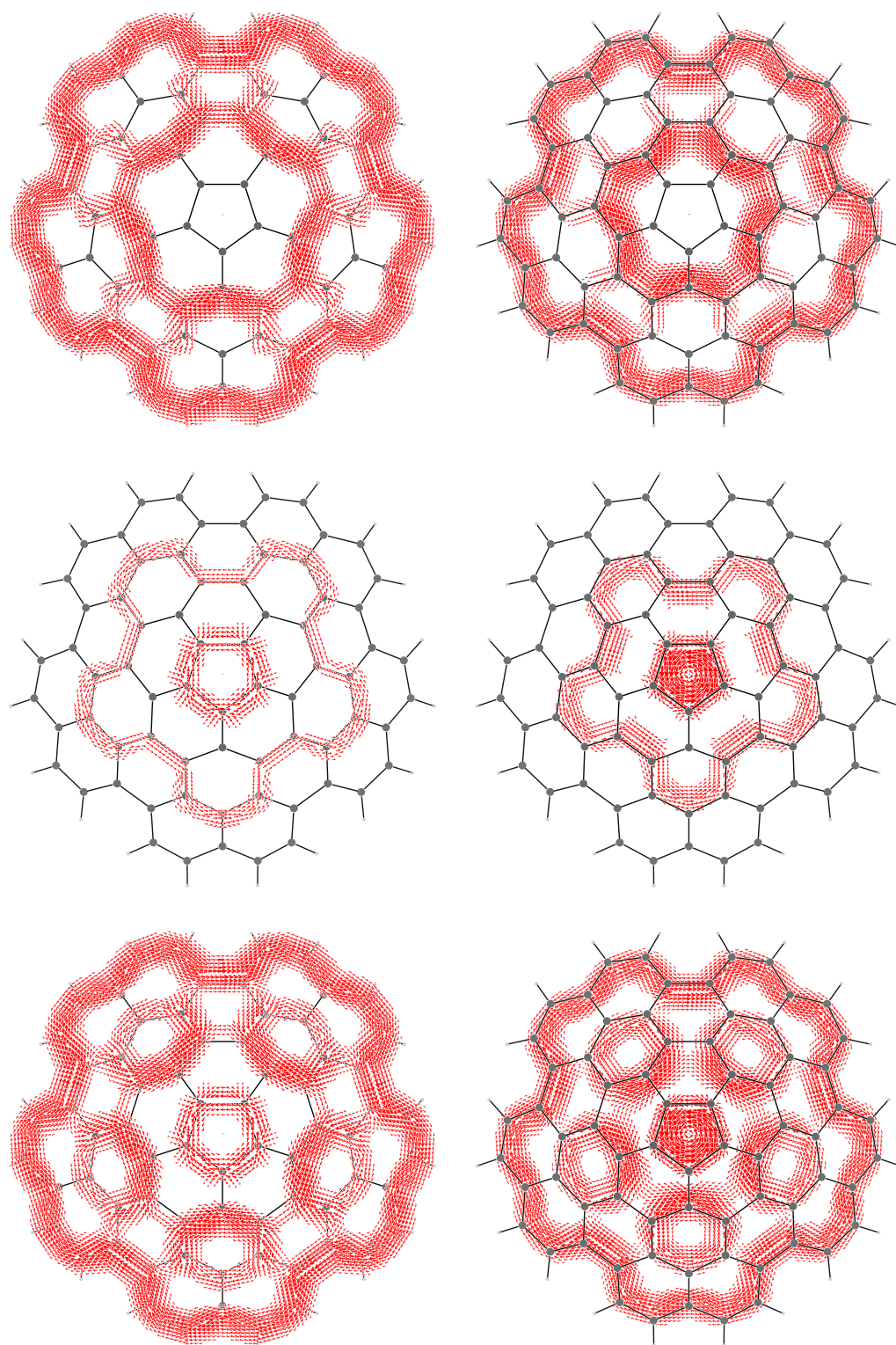


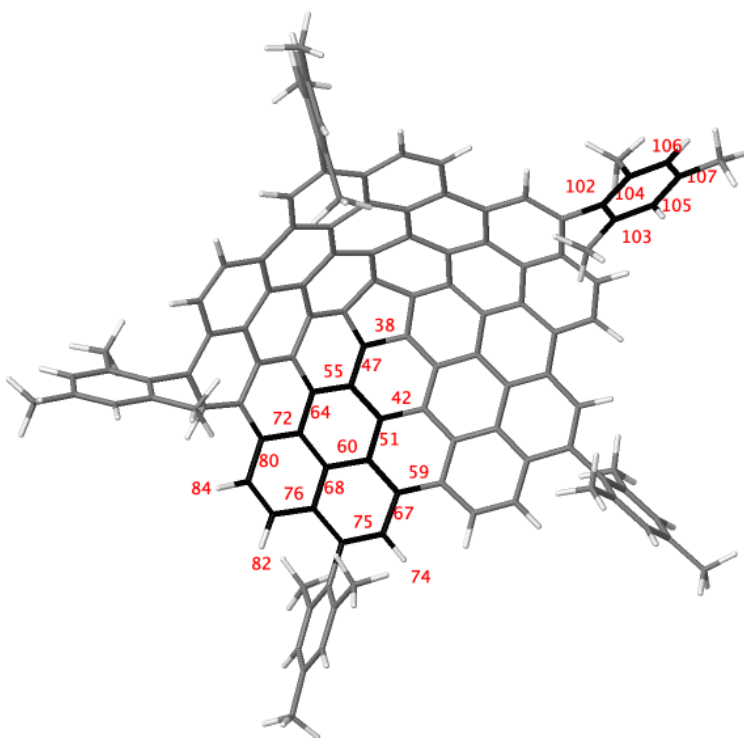
Figure S6: Frontier orbital contributions to the MICD of $C_{70}H_{20}$. Top HOMO; center HOMO-1; bottom the sum of the two. Left: at 1 a.u. outside the cone; right: at 1 a.u. inside the cone.

3.1.1 ^1H and ^{13}C NMR chemical shifts: a comparison with experimental data for penta-mesityl carboncone[1,2] derivative

Due to the poor solubility of C₇₀H₂₀, NMR data have been reported for the penta-mesityl derivative (see Ref.7, Zhu et al., *Sci. Adv.* **2019**, 5). Here, Fig.S7 shows the predicted and the experimental ¹H and ¹³C NMR chemical shifts of the penta-mesityl derivative of C₇₀H₂₀.

Figure S7: In light blue, magnetic shielding constants and chemical shifts of the pentamesityl derivative of $C_{70}H_{20}$. Only symmetry unique atoms are shown. In light green, the experimental values.

benzene	48.54	128.00		
C nucleus	σ	δ	expt.	
75	35.71	140.83	138.8	
102	36.00	140.54	138.71	
104	36.29	140.25	137.84	
103	37.41	139.13	137.47	
107	37.56	138.98	137.28	
38	38.99	137.55	136.97	
47	46.51	130.03	130.05	
68	47.92	128.62	129.02	
106	48.77	127.77	128.93	
59	48.88	127.66	128.65	
72	49.08	127.46	127.98	
105	49.11	127.43	127.91	
60	51.66	124.88	125.18	
59	52.03	124.51	125.08	
42	52.62	123.92	124.73	
55	52.78	123.76	124.68	
67	52.99	123.55	124.57	
64	53.07	123.47	123.72	
76	53.43	123.11	123.66	
80	54.55	121.99	123.53	
benzene	24.16	7.26		
H nucleus	σ	δ	expt.	
84	21.36	10.06	9.9	doublet
74	21.42	10.00	9.83	singlet
82	22.64	8.78	8.72	doublet



Calculated chemical shifts relative to TMS have been obtained converting the computed

shielding constants according to:

$$\delta_I = \sigma_{\text{ref}} - \sigma_I + \delta_{\text{ref}} \quad (1)$$

In this equation, the chemical shift relative to TMS for each nucleus in the molecule of interest (δ_I) is determined from the computed shielding constants for the same nucleus type in the reference compound (σ_{ref}), the computed shielding constants for each nucleus in the molecule of interest (σ_I), and the known experimental chemical shift for the reference compound (δ_{ref}). We took benzene as the reference compound, for which calculated σ_{C} and σ_{H} values (same functional, basis set, etc.) are 48.54 and 24.16 ppm, while standard δ_{C} and δ_{H} relative to TMS are 128.00 and 7.26 ppm, respectively.

Shielding constants have been computed with the CSGT method, using Gaussian 16. The C_{5v} symmetry of the pristine incomplete [1,2]carboncone reduces to C_5 in the pentamesityl derivative. Consequently, the number of aromatic carbon signals increases from 9 to 14, plus an additional 6 from the mesityl carbons for a total of 20 signals in the aromatic region.

As can be seen from Fig. S7, the δ_I of the aromatic carbon are very well described. Now, let us consider the ^1H NMR chemical shifts. The very intense diatropic current flowing on the carboncone rim, which is 27% and 53% larger than in benzene (see Fig.S5), provides the large downfield shift calculated in the pure carboncone and measured in the spectrum of penta-mesityl derivative. Assuming the mesityl-substituents attached to carbon 75, the two doublets, observed at 9.90 and 8.72 ppm, have to be assigned to the protons 84 and 82, respectively, while the singlet at 9.83 ppm to proton 74. Due to the orientation of mesityl groups, which are found to be almost perpendicular to the carboncone surface, protons 82 and 74 undergo an additional shielding effect by the ring current in mesityl-moiety. Since proton 82 faces the benzene ring centre, the shielding effect is larger. The quantitative agreement is very good.

3.2 $C_{80}H_{20}$

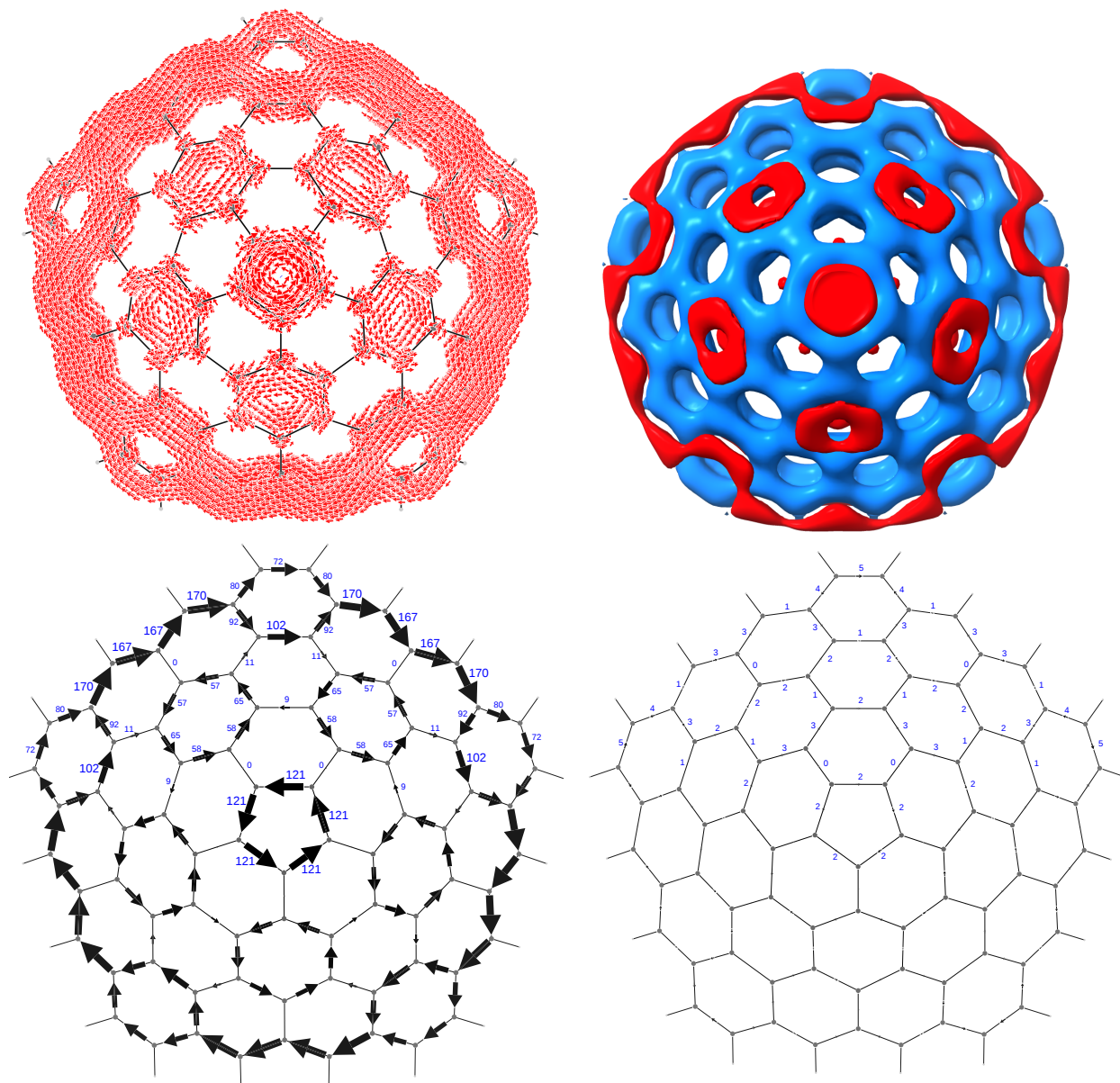


Figure S8: Top left: map of the current density induced in the π -electrons of $C_{80}H_{20}$ by a magnetic field parallel to the main symmetry axis. Top right: ChimeraX map of π -DIAL. Red/Blue isosurface value is $+0.003/-0.003$ a.u.. Bottom left: π -orbital contribution to BCSs. Bottom right: contribution to BCSs from all orbitals but π .

3.3 $C_{170}H_{30}$

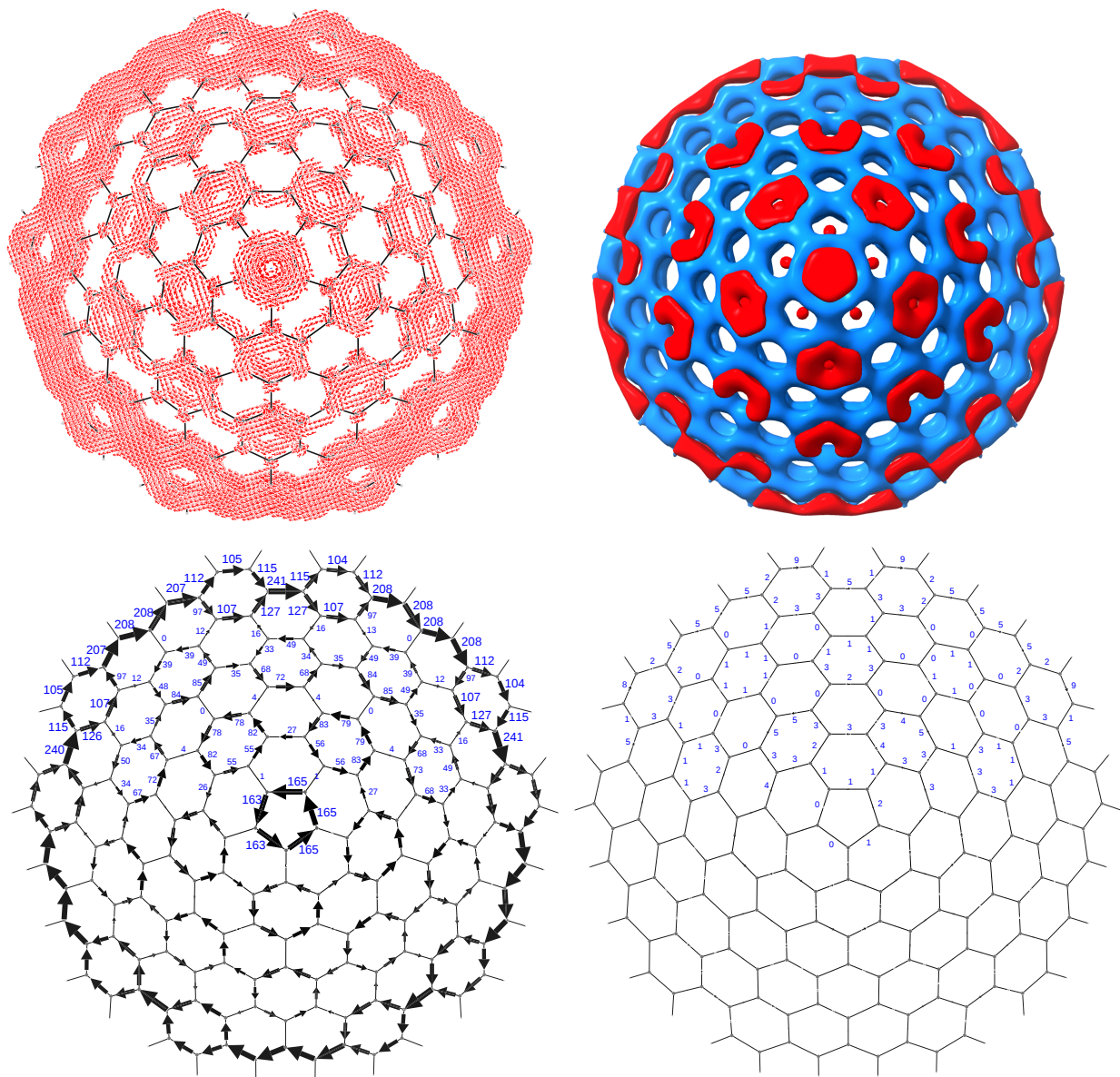


Figure S9: Top left: map of the current density induced in the π -electrons of $C_{170}H_{30}$ by a magnetic field parallel to the main symmetry axis. Top right: ChimeraX map of π -DIAL. Red/Blue isosurface value is $+0.003/-0.003$ a.u.. Bottom left: π -orbital contribution to BCSs. Bottom right: contribution to BCSs from all orbitals but π .

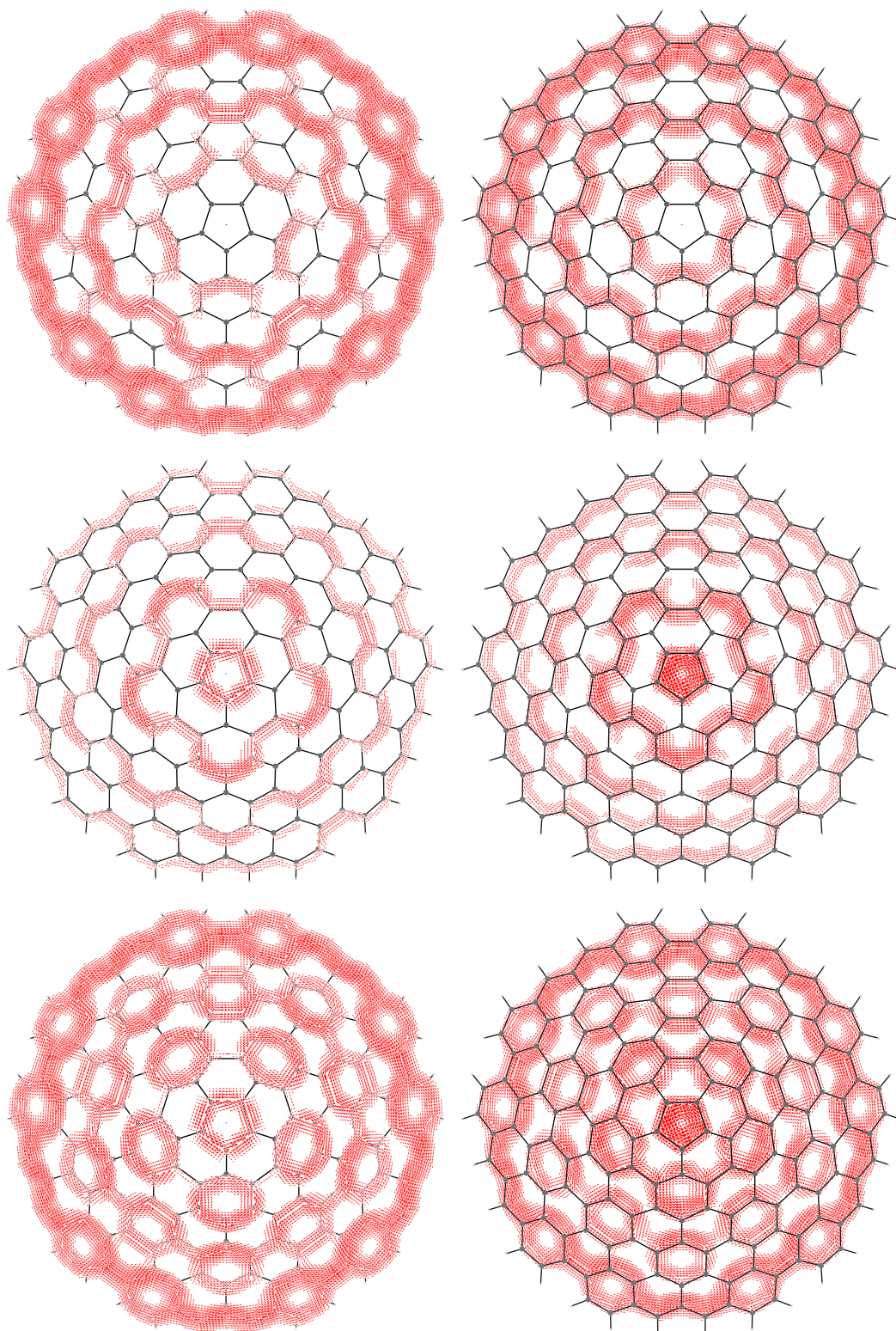


Figure S10: Frontier orbital contributions to the MICD of C₁₇₀H₃₀. Top HOMO; center HOMO-1; bottom the sum of the two. Left: at 1 a.u. outside the cone; right: at 1 a.u. inside the cone.

3.4 $C_{180}H_{30}$

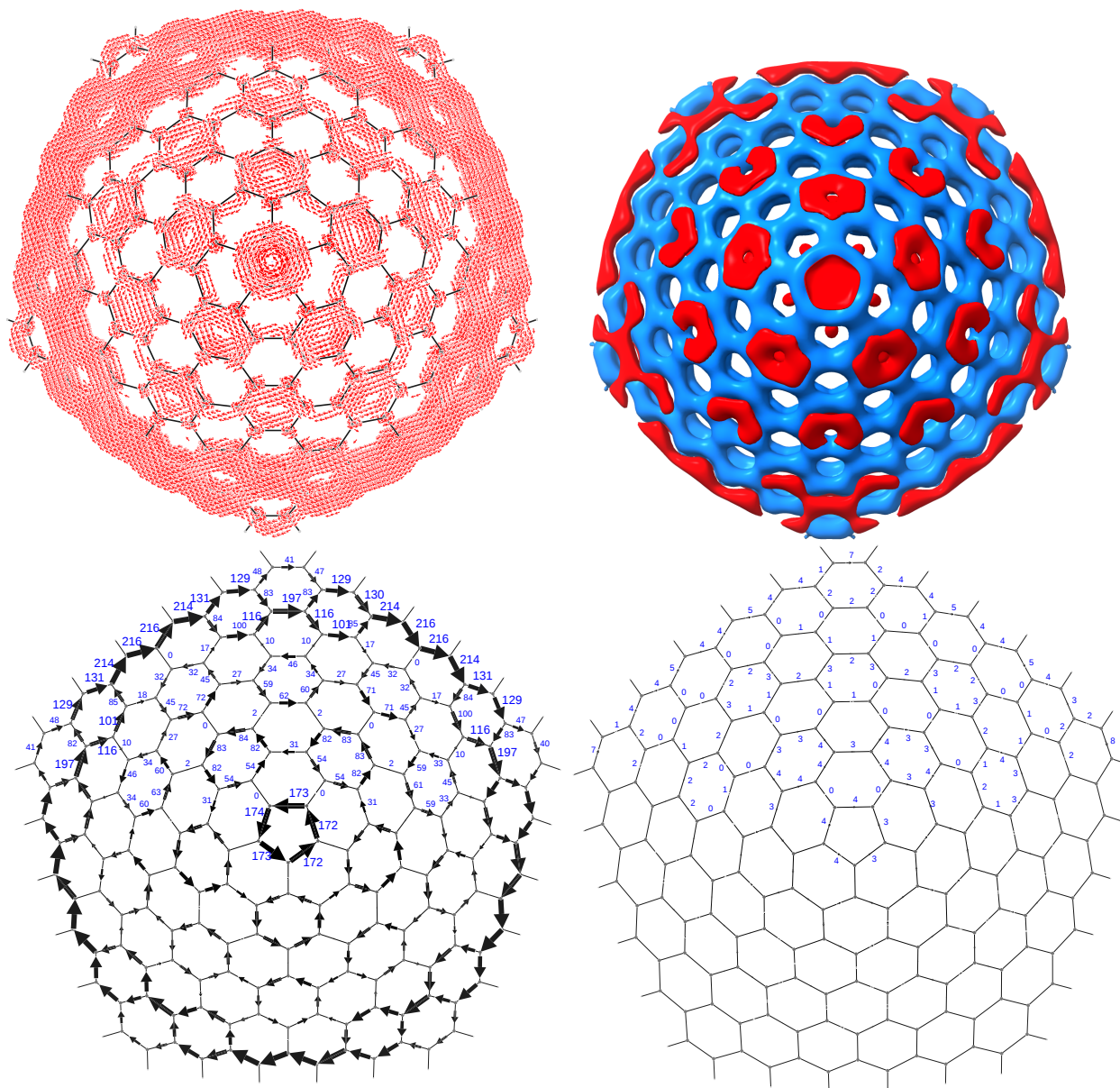


Figure S11: Top left: map of the current density induced in the π -electrons of $C_{180}H_{30}$ by a magnetic field parallel to the main symmetry axis. Top right: ChimeraX map of π -DIAL. Red/Blue isosurface value is $+0.003/-0.003$ a.u.. Bottom left: π -orbital contribution to BCSs. Bottom right: contribution to BCSs from all orbitals but π .

4 Polansky-Derflinger indices

Out of the Hückel density matrix of the polycyclic system, indication of the submatrix containing only the AOs of ring L as $\mathbf{P} = \mathbf{C}\mathbf{n}\mathbf{C}^T$, where the columns of matrix $\mathbf{C}$ are the eigenvectors of the Hückel problem, and the diagonal matrix $\mathbf{n}$ contains the orbital occupation numbers, and indication of the density matrix of benzene as $\mathbf{P}_B = \mathbf{C}_B\mathbf{n}_B\mathbf{C}_B^T$, allows writing the index as

$$\rho_L = \frac{1}{n_L} \sum_{i,j \in L} P_{ij} P_{B,ij} = \frac{1}{n_L} \text{Tr} [(\mathbf{P} - \text{diag } \mathbf{P})(\mathbf{P}_B - \text{diag } \mathbf{P}_B)], \quad (2)$$

where n_L is the number of atoms in the ring, i.e. 6 in the case of benzene. If $\mathbf{P} = \mathbf{P}_B$ the quasi-idempotency of the density matrix for closed-shell systems, $\mathbf{P}_B^2 = 2\mathbf{P}_B$, and the fact that $\text{diag } \mathbf{P}_B = \mathbf{1}$ gives for the similarity index $\rho_6 = \frac{\text{Tr } \mathbf{P}_B}{6} = 1$.

5 Fullerene-240 of I_h symmetry

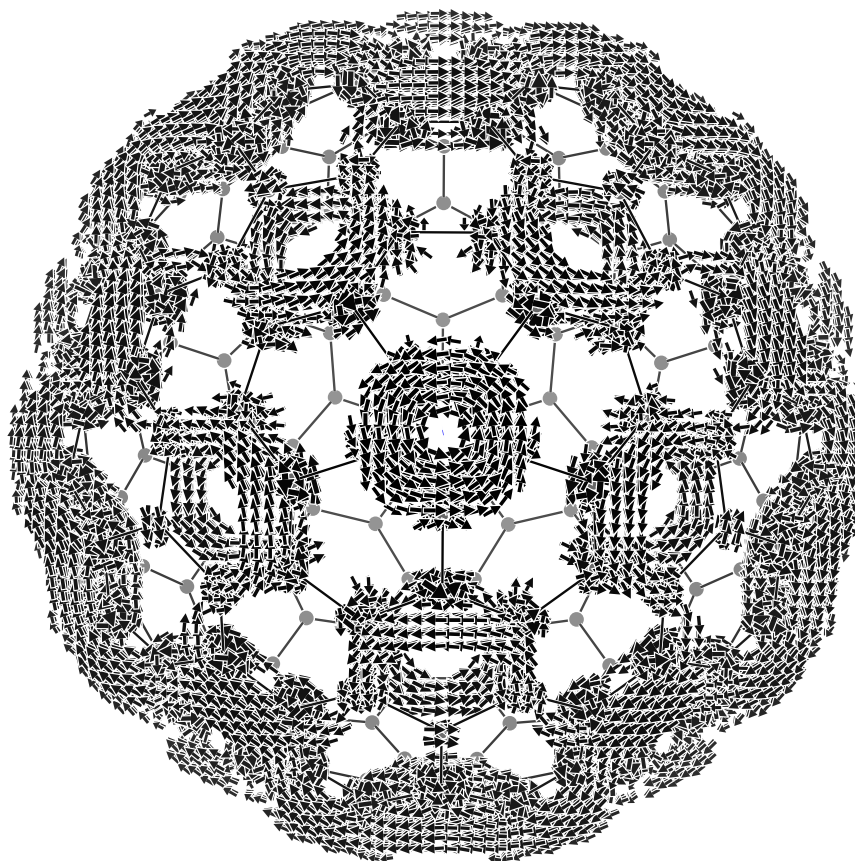


Figure S12: B3LYP/6-311+G(2d) map of the current density induced in the π -electron cloud of fullerene-240 by a magnetic field perpendicular to a pentagonal face. Current of magnitude lower than 0.033 a.u. is not shown.