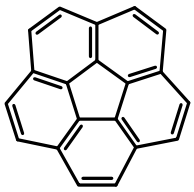
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

to *On the Stabilization of Corannulene and Coronene* by Michał A. Dobrowolski, Michał K. Cyrański and Arkadiusz Ciesielski



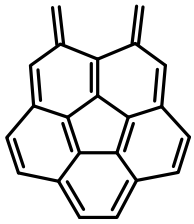
Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_{5v}	-768.3152185

C	0.00000000	1.20443300	0.62863000
C	1.14548400	0.37219000	0.62863000
C	0.70794800	-0.97440700	0.62863000
C	-0.70794800	-0.97440700	0.62863000
C	-1.14548400	0.37219000	0.62863000
C	0.00000000	2.48074900	0.09745900
C	1.30911700	2.98055400	-0.25898300
C	2.43013600	2.16608600	-0.25898300
C	2.35933300	0.76659400	0.09745900
C	3.23921400	-0.32400200	-0.25898300
C	2.81102300	-1.64183900	-0.25898300
C	1.45814800	-2.00696800	0.09745900
C	0.69282800	-3.18079800	-0.25898300
C	-0.69282800	-3.18079800	-0.25898300
C	-1.45814800	-2.00696800	0.09745900
C	-2.81102300	-1.64183900	-0.25898300
C	-3.23921400	-0.32400200	-0.25898300
C	-2.35933300	0.76659400	0.09745900
C	-2.43013600	2.16608600	-0.25898300
C	-1.30911700	2.98055400	-0.25898300
H	1.40948400	3.99768700	-0.62437000
H	3.36647100	2.57585200	-0.62437000
H	4.23758000	-0.10514600	-0.62437000
H	3.49007800	-2.40572300	-0.62437000
H	1.20948500	-4.06267000	-0.62437000
H	-1.20948500	-4.06267000	-0.62437000

H	-3.49007800	-2.40572300	-0.62437000
H	-4.23758000	-0.10514600	-0.62437000
H	-3.36647100	2.57585200	-0.62437000
H	-1.40948400	3.99768700	-0.62437000

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	D_{5h}	-768.2989305

C	0.00000000	1.18716000	0.00000000
C	1.12905600	0.36685300	0.00000000
C	0.69779500	-0.96043300	0.00000000
C	-0.69779500	-0.96043300	0.00000000
C	-1.12905600	0.36685300	0.00000000
C	0.00000000	2.55177000	0.00000000
C	1.36531600	3.07102400	0.00000000
C	2.49881200	2.24749200	0.00000000
C	2.42687800	0.78854000	0.00000000
C	3.34262300	-0.34949400	0.00000000
C	2.90966700	-1.68199800	0.00000000
C	1.49989300	-2.06442600	0.00000000
C	0.70053900	-3.28702300	0.00000000
C	-0.70053900	-3.28702300	0.00000000
C	-1.49989300	-2.06442600	0.00000000
C	-2.90966700	-1.68199800	0.00000000
C	-3.34262300	-0.34949400	0.00000000
C	-2.42687800	0.78854000	0.00000000
C	-2.49881200	2.24749200	0.00000000
C	-1.36531600	3.07102400	0.00000000
H	1.53467400	4.14303300	0.00000000
H	3.46601900	2.73982900	0.00000000
H	4.41449900	-0.17929400	0.00000000
H	3.67679100	-2.44972600	0.00000000
H	1.19363700	-4.25384300	0.00000000
H	-1.19363700	-4.25384300	0.00000000
H	-3.67679100	-2.44972600	0.00000000
H	-4.41449900	-0.17929400	0.00000000
H	-3.46601900	2.73982900	0.00000000
H	-1.53467400	4.14303300	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-845.6482967

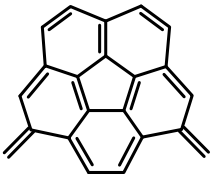
C	-1.44053200	0.61051300	-0.58681500
C	-1.33808300	-0.81279000	-0.54240100
C	-0.00521500	-1.16775600	-0.62117700
C	0.75726200	0.04859600	-0.67405600
C	-0.16872000	1.14118300	-0.66840700
C	-2.33691600	-1.61949200	0.02292900
C	-1.87340500	-2.96055100	0.35077900
C	-0.54269300	-3.31062800	0.29862700
C	0.50426100	-2.36442600	-0.08860100
C	1.87670500	-2.37521000	0.14839500
C	2.71324900	-1.18153300	-0.05116200
C	2.03600300	0.14025400	-0.23144600
C	2.45271700	1.50764800	0.19191700
C	1.50178200	2.62394200	0.09379400
C	0.16030900	2.43159000	-0.22972700
C	-1.01583600	3.25416300	0.05788500
C	-2.28519700	2.72435700	0.12857000
C	-2.55057800	1.30849700	-0.08997500
C	-3.61760300	0.48781900	0.33245200
C	-3.51237900	-0.93040100	0.38958400
H	-2.58569400	-3.69059000	0.72262100
H	-0.25511200	-4.30210000	0.63372700
H	2.38354100	-3.27095800	0.49097200
C	4.06408700	-1.31196700	-0.17407600
C	3.62364900	1.70823400	0.86588400
H	1.84768100	3.57757900	0.47783500
H	-0.87634600	4.29990000	0.31281900
H	-3.09947500	3.37437200	0.43349600
H	-4.51705500	0.94016600	0.73833000

H	-4.33761300	-1.47572300	0.83682700
H	4.53750200	-2.28242900	-0.07880800
H	4.69889600	-0.47667000	-0.43465300
H	4.26791500	0.89029600	1.15284400
H	3.91855800	2.70389600	1.17614600

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_{2v}	-845.6362874

C	0.00000000	0.70632200	-1.37161400
C	0.00000000	-0.70632200	-1.37161400
C	0.00000000	-1.14079200	-0.07983700
C	0.00000000	0.00000000	0.76728200
C	0.00000000	1.14079200	-0.07983700
C	0.00000000	-1.49893200	-2.51306300
C	0.00000000	-2.92018200	-2.14850100
C	0.00000000	-3.36761300	-0.83377700
C	0.00000000	-2.46540500	0.33316800
C	0.00000000	-2.58484700	1.72361000
C	0.00000000	-1.41452700	2.65760800
C	0.00000000	0.00000000	2.11389700
C	0.00000000	1.41452700	2.65760800
C	0.00000000	2.58484700	1.72361000
C	0.00000000	2.46540500	0.33316800
C	0.00000000	3.36761300	-0.83377700
C	0.00000000	2.92018200	-2.14850100
C	0.00000000	1.49893200	-2.51306300
C	0.00000000	0.72096100	-3.69838100
C	0.00000000	-0.72096100	-3.69838100
H	0.00000000	-3.67249700	-2.93109100
H	0.00000000	-4.44082500	-0.67197000
H	0.00000000	-3.55331100	2.21137600
C	0.00000000	-1.70381700	3.98690700
C	0.00000000	1.70381700	3.98690700
H	0.00000000	3.55331100	2.21137600
H	0.00000000	4.44082500	-0.67197000
H	0.00000000	3.67249700	-2.93109100
H	0.00000000	1.20426400	-4.67033500
H	0.00000000	-1.20426400	-4.67033500
H	0.00000000	-2.73365600	4.32369700

H	0.00000000	-0.95032500	4.75807400
H	0.00000000	0.95032500	4.75807400
H	0.00000000	2.73365600	4.32369700



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-845.6476019

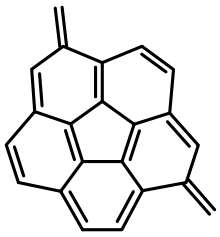
C	0.00000900	1.46779800	0.65785100
C	1.15414500	0.64602300	0.70325200
C	0.71160300	-0.68673500	0.69393100
C	-0.71158400	-0.68673500	0.69395100
C	-1.15412600	0.64602300	0.70328400
C	2.37379700	1.03197900	0.12247100
C	3.25115900	0.00088100	-0.21626200
C	2.88869900	-1.41618500	-0.10467100
C	1.46241400	-1.74829800	0.18915500
C	0.70836600	-2.86692900	-0.21797300
C	-0.70837200	-2.86692900	-0.21795300
C	-1.46240900	-1.74829800	0.18919600
C	-2.88870200	-1.41618500	-0.10459100
C	-3.25116500	0.00088100	-0.21617300
C	-2.37379300	1.03197900	0.12253600
C	-2.43208400	2.42894900	-0.29028100
C	-1.30595800	3.22011600	-0.32890500
C	0.00000100	2.70860200	0.05153400
C	1.30594800	3.22011600	-0.32894200
C	2.43207600	2.42894900	-0.29034900
H	4.22755700	0.22340300	-0.63480400
C	3.83775900	-2.37106800	-0.32073500
H	1.20428100	-3.71527600	-0.67749000
H	-4.22757400	0.22340300	-0.63468700
H	-3.36984200	2.83442900	-0.65676400
H	-1.38305100	4.22413300	-0.73329200
H	1.38303100	4.22413300	-0.73333000

H	3.36982400	2.83442900	-0.65685800
C	-3.83776800	-2.37106800	-0.32062800
H	-1.20429900	-3.71527600	-0.67745600
H	4.85468400	-2.10222300	-0.57977200
H	3.61417700	-3.42606700	-0.22709900
H	-3.61418400	-3.42606700	-0.22699800
H	-4.85470000	-2.10222300	-0.57963700

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_{2v}	-845.6291652

C	0.00000000	0.00000000	1.43782500
C	0.00000000	1.13330300	0.62240100
C	0.00000000	0.70359800	-0.69025500
C	0.00000000	-0.70359800	-0.69025500
C	0.00000000	-1.13330300	0.62240100
C	0.00000000	2.44548500	1.05858500
C	0.00000000	3.36498700	-0.00760600
C	0.00000000	2.95933800	-1.44310100
C	0.00000000	1.49736200	-1.81448800
C	0.00000000	0.71743500	-3.00501700
C	0.00000000	-0.71743500	-3.00501700
C	0.00000000	-1.49736200	-1.81448800
C	0.00000000	-2.95933800	-1.44310100
C	0.00000000	-3.36498700	-0.00760600
C	0.00000000	-2.44548500	1.05858500
C	0.00000000	-2.50274300	2.53136300
C	0.00000000	-1.36769100	3.33780900
C	0.00000000	0.00000000	2.79813900
C	0.00000000	1.36769100	3.33780900
C	0.00000000	2.50274300	2.53136300
H	0.00000000	4.43542100	0.16960000
C	0.00000000	3.94559700	-2.38715400
H	0.00000000	1.19500400	-3.97957800
H	0.00000000	-4.43542100	0.16960000
H	0.00000000	-3.46649300	3.03057100
H	0.00000000	-1.51920100	4.41231800
H	0.00000000	1.51920100	4.41231800
H	0.00000000	3.46649300	3.03057100
C	0.00000000	-3.94559700	-2.38715400

H	0.00000000	-1.19500400	-3.97957800
H	0.00000000	4.99285900	-2.11069200
H	0.00000000	3.71676200	-3.44533400
H	0.00000000	-3.71676200	-3.44533400
H	0.00000000	-4.99285900	-2.11069200



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-845.6500282

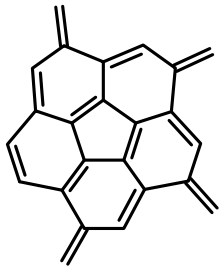
C	0.28457300	1.31274500	0.61500200
C	-1.01416400	0.82834600	0.65927900
C	-0.93277700	-0.60006000	0.68613500
C	0.43991800	-0.96910300	0.70413200
C	1.18686900	0.20933100	0.63877300
C	-2.11326800	1.52287400	0.12732200
C	-3.22269100	0.74498500	-0.20490400
C	-3.18598900	-0.71836300	-0.16689800
C	-1.90895900	-1.41033500	0.17591200
C	-1.48265700	-2.76086200	-0.15620200
C	-0.15666700	-3.13179200	-0.14840900
C	0.90510000	-2.18730400	0.17589500
C	2.25349100	-2.22486900	-0.17498700
C	3.12195500	-1.03961700	-0.12767800
C	2.47906500	0.28689900	0.11866500
C	2.86637700	1.57446200	-0.30776300
C	1.97771900	2.68297500	-0.31024000
C	0.63022400	2.56335300	0.08351300
C	-0.52115300	3.40203800	-0.22180900
C	-1.80822100	2.91684400	-0.19695500
H	-4.12552700	1.19753300	-0.59989900
C	-4.28864200	-1.45473900	-0.48057600
H	-2.21318000	-3.48450500	-0.49960200

C	4.45868500	-1.17662100	-0.35438200
H	3.83917800	1.72071000	-0.76535400
H	2.33139200	3.60926000	-0.75192900
H	-0.35828200	4.42154200	-0.55742200
H	-2.61477800	3.56978600	-0.51511800
H	0.10535000	-4.13304200	-0.47507500
H	-5.23300000	-0.97757400	-0.71451800
H	-4.27198100	-2.53660200	-0.48872300
H	2.70144600	-3.13921200	-0.55063200
H	4.89341800	-2.14390000	-0.57523400
H	5.13323200	-0.33112000	-0.30944700

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_s	-845.6358585

C	-0.78471600	-1.06697500	0.00000000
C	0.58064200	-1.14998400	0.00000000
C	1.08576400	0.17189500	0.00000000
C	0.00000000	1.05237100	0.00000000
C	-1.15206400	0.29453700	0.00000000
C	1.34042600	-2.30759700	0.00000000
C	2.72447000	-2.04896000	0.00000000
C	3.29058900	-0.67316200	0.00000000
C	2.38818100	0.52930500	0.00000000
C	2.55268900	1.98983200	0.00000000
C	1.48059300	2.87630000	0.00000000
C	0.07425300	2.43822000	0.00000000
C	-1.19160500	3.04369300	0.00000000
C	-2.47273500	2.27444500	0.00000000
C	-2.44560200	0.76557000	0.00000000
C	-3.39199900	-0.29917200	0.00000000
C	-3.02263700	-1.68756600	0.00000000
C	-1.67258400	-2.13198100	0.00000000
C	-0.93944500	-3.40259500	0.00000000
C	0.45022200	-3.48492900	0.00000000
H	3.45483500	-2.85034900	0.00000000
C	4.63985700	-0.49059600	0.00000000
H	3.54822100	2.42061200	0.00000000
C	-3.64386300	2.97165800	0.00000000
H	-4.45668400	-0.08907200	0.00000000

H	-3.83788000	-2.40428500	0.00000000
H	-1.49048400	-4.33800200	0.00000000
H	0.88687400	-4.47874900	0.00000000
H	1.71140200	3.93670700	0.00000000
H	5.32532700	-1.33007600	0.00000000
H	5.07707100	0.49984200	0.00000000
H	-1.30206800	4.12294300	0.00000000
H	-3.65593600	4.05475200	0.00000000
H	-4.60328900	2.46982800	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-923.0473433

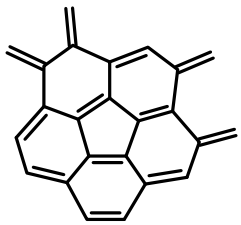
C	0.50581400	-1.31626800	0.66796900
C	-0.89207900	-1.01169400	0.67515100
C	-1.02571800	0.41323000	0.70081800
C	0.23853400	0.94897200	0.66729800
C	1.18755700	-0.12319000	0.65249900
C	-1.83198500	-1.85097700	0.16614000
C	-3.13474800	-1.21518500	-0.16792000
C	-3.21101000	0.26172100	-0.18795000
C	-2.17419200	1.07502900	0.20458400
C	-1.96063000	2.54115300	-0.02641300
C	-0.56082400	3.01745200	-0.15704700
C	0.52812400	2.24834200	0.15779600
C	1.98058900	2.47358300	-0.14096300
C	2.85856600	1.28482800	-0.25857200
C	2.49626200	0.01465800	0.12042600
C	3.19162500	-1.29523500	-0.12249500
C	2.35414500	-2.50896000	-0.23055700
C	1.01862300	-2.52179400	0.11570300
C	-0.01519400	-3.50649500	-0.20087900

C	-1.34893600	-3.18816100	-0.18450100
C	-4.20993100	-1.95871900	-0.52794500
C	-2.98402500	3.41390300	-0.15082900
C	4.53473200	-1.38916200	-0.26131600
H	2.83484400	-3.39510400	-0.63251500
H	0.28281400	-4.49586500	-0.53235600
H	-0.44068100	4.01391700	-0.56905800
C	2.48956200	3.70438100	-0.36324100
H	3.81684800	1.46217200	-0.73615600
H	-4.01515500	3.10125600	-0.04145100
H	-2.80576600	4.46424500	-0.34951400
H	1.87952100	4.59583800	-0.28790300
H	3.53501700	3.84400800	-0.61162600
H	-4.10235900	0.67911500	-0.64368100
H	-2.05807000	-3.93967400	-0.51293700
H	-4.17385700	-3.03992100	-0.56225800
H	-5.15449300	-1.49290500	-0.78249200
H	5.18026800	-0.52631100	-0.15404300
H	5.01191500	-2.33925700	-0.47053700

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_{2v}	-923. 0352843

C	0.79390700	-1.13743800	0.00000000
C	-0.61482500	-1.18151200	0.00000000
C	-1.08317700	0.15335700	0.00000000
C	0.00000000	0.97330700	0.00000000
C	1.16764200	0.16977700	0.00000000
C	-1.36532500	-2.29737600	0.00000000
C	-2.82994600	-1.99040300	0.00000000
C	-3.28912600	-0.56103600	0.00000000
C	-2.42816300	0.52541900	0.00000000
C	-2.55612300	2.03385300	0.00000000
C	-1.31291600	2.88619900	0.00000000
C	-0.03183300	2.37907300	0.00000000
C	1.36659800	2.95167300	0.00000000
C	2.55386700	2.02985200	0.00000000
C	2.48375600	0.64691300	0.00000000
C	3.47732600	-0.50019200	0.00000000
C	2.98395800	-1.91911900	0.00000000

C	1.63930000	-2.25775400	0.00000000
C	0.84866900	-3.50363500	0.00000000
C	-0.53576100	-3.52025100	0.00000000
C	-3.75108300	-2.98550800	0.00000000
C	-3.75921400	2.64966700	0.00000000
C	4.81457700	-0.28683800	0.00000000
H	3.76176700	-2.67564300	0.00000000
H	1.36244700	-4.45934200	0.00000000
H	-1.50343300	3.95442800	0.00000000
C	1.58590400	4.28505200	0.00000000
H	3.50957200	2.54461500	0.00000000
H	-4.68537500	2.08804600	0.00000000
H	-3.84163700	3.73012100	0.00000000
H	0.76805300	4.99496700	0.00000000
H	2.58925600	4.69412900	0.00000000
H	-4.36678600	-0.43625000	0.00000000
H	-1.01835800	-4.49193900	0.00000000
H	-3.45960000	-4.02838300	0.00000000
H	-4.81380000	-2.77421400	0.00000000
H	5.23245500	0.71233500	0.00000000
H	5.51736600	-1.11135200	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-923.051969

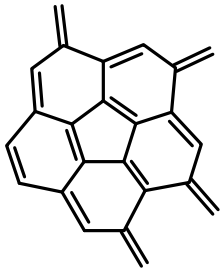
C	-0.23736300	1.63279800	-0.52300700
C	1.04513600	1.14158200	-0.59997900
C	0.96084500	-0.28700600	-0.65693100
C	-0.42978900	-0.64701800	-0.64255100
C	-1.14892100	0.53793600	-0.53476000
C	2.17582400	1.84250000	-0.15473000
C	3.28354700	1.05387000	0.13335800
C	3.20803000	-0.41558500	0.17664900

C	1.96081800	-1.11177100	-0.25616800
C	1.54665100	-2.54048600	-0.13704800
C	0.11061200	-2.83028200	0.05189100
C	-0.87840700	-1.89047900	-0.16842100
C	-2.33454000	-1.91391200	0.20244200
C	-3.17602300	-0.64637900	0.00165900
C	-2.46108700	0.66066100	-0.07209900
C	-2.82965100	1.94882900	0.32829400
C	-1.90856600	3.04914500	0.35069100
C	-0.56720200	2.90657900	-0.02647400
C	0.60509600	3.74169900	0.21336100
C	1.88770000	3.24793900	0.14773000
C	2.42634900	-3.56501700	-0.29305200
H	-2.26010800	3.98591900	0.77140200
H	0.46447100	4.77314700	0.52144900
H	-0.12449000	-3.83853300	0.37325100
C	-2.88089900	-2.99142000	0.78554600
C	-4.50470500	-0.71691600	-0.17269300
H	3.46621900	-3.39855200	-0.53657200
H	2.09087000	-4.59451000	-0.24211000
H	-2.31568000	-3.90488300	0.92422800
H	-3.89693500	-2.99048200	1.15781500
H	2.70965900	3.90705200	0.40861300
C	4.20969400	-1.09789100	0.80155500
H	4.19690400	1.49414500	0.51833600
H	-3.82015100	2.12397100	0.73502700
H	-5.03359900	-1.66073900	-0.21075300
H	-5.09440000	0.18084800	-0.31435100
H	5.10683500	-0.58423300	1.12721900
H	4.13150600	-2.14939900	1.03486500

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_s	-923.0421341

C	-1.06028300	-1.23146600	0.00000000
C	0.27321900	-1.50475800	0.00000000
C	0.97610600	-0.26927800	0.00000000
C	0.00000000	0.76621800	0.00000000
C	-1.23962200	0.17280400	0.00000000
C	0.84733300	-2.77131300	0.00000000

C	2.23856500	-2.72932800	0.00000000
C	3.02403200	-1.45770800	0.00000000
C	2.31732800	-0.11929500	0.00000000
C	2.70531200	1.33836700	0.00000000
C	1.63962500	2.39097700	0.00000000
C	0.28212400	2.12222400	0.00000000
C	-0.96846600	2.96772700	0.00000000
C	-2.37697700	2.28700100	0.00000000
C	-2.48088100	0.78935500	0.00000000
C	-3.54471800	-0.13154100	0.00000000
C	-3.36142500	-1.56747700	0.00000000
C	-2.09172500	-2.17215200	0.00000000
C	-1.55283100	-3.53489600	0.00000000
C	-0.19507600	-3.81333600	0.00000000
C	3.99004200	1.77991600	0.00000000
H	-4.26275400	-2.17229600	0.00000000
H	-2.23750500	-4.37741600	0.00000000
H	2.02003900	3.40614700	0.00000000
C	-0.84986500	4.30309100	0.00000000
C	-3.49785400	3.02604200	0.00000000
H	4.84585100	1.12448400	0.00000000
H	4.20226800	2.84246400	0.00000000
H	0.12837300	4.76759000	0.00000000
H	-1.69412700	4.97879500	0.00000000
H	0.10344500	-4.85693200	0.00000000
C	4.37820400	-1.58207500	0.00000000
H	2.83616200	-3.63412300	0.00000000
H	-4.57250200	0.21587000	0.00000000
H	-3.50113000	4.10725200	0.00000000
H	-4.47020800	2.54941400	0.00000000
H	4.83602500	-2.56420300	0.00000000
H	5.05307700	-0.74164200	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-923.0478005

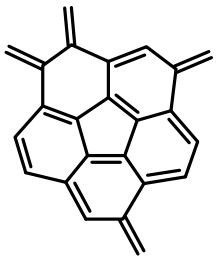
C	1.43700600	2.81234800	0.03528400
C	2.56999000	1.86434900	-0.12333900
C	2.47105800	0.52278300	0.13916700
C	1.20211100	0.08848100	0.61665500
C	0.09256900	0.88676400	0.67080600
C	0.06927200	2.23103000	0.23943200
C	0.77053800	-1.27859200	0.56234500
C	-0.59267700	-1.31694900	0.60715600
C	-1.06662600	0.04062800	0.64410500
C	-1.16487500	2.69914500	-0.13631000
C	-2.38595500	1.85699900	-0.18818700
C	-2.29028000	0.42056600	0.20606500
C	-3.24677100	-0.71798400	0.00745200
C	-2.68087400	-2.07933400	-0.17723200
C	-1.36639000	-2.38237400	0.08573300
C	-0.56095200	-3.56047800	-0.26545800
C	0.80661100	-3.52862600	-0.29513100
C	1.57313600	-2.31556000	0.01851000
C	2.86989700	-1.97138800	-0.29259500
C	3.42146200	-0.60115200	-0.16143600
C	-4.59334400	-0.57585400	0.03873000
H	-3.36339700	-2.82858200	-0.56535100
H	-1.06916200	-4.46811500	-0.57502200
H	3.54370500	-2.70836800	-0.71923400
C	4.74013600	-0.39117600	-0.36484000
H	3.49114000	2.29514300	-0.50166900
C	-3.49386100	2.39646600	-0.75815500
H	-1.27211800	3.68740000	-0.57020400
H	1.34227600	-4.41238000	-0.62711900
C	1.65742100	4.14320400	-0.03592800
H	0.85687100	4.86005700	0.09941500
H	2.64957200	4.54027800	-0.21602600
H	-4.38263900	1.82137500	-0.96643700
H	-3.50156700	3.43571100	-1.06507100
H	5.40810700	-1.20857500	-0.60946000
H	5.18082900	0.59424500	-0.28036400

H	-5.07505000	0.36892500	0.24386200
H	-5.24018600	-1.43688500	-0.08430100

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_s	-923.0387645

C	0.45304400	-1.34523100	0.00000000
C	1.06079600	-0.05960400	0.00000000
C	0.00000000	0.88801600	0.00000000
C	-1.17465200	0.21170900	0.00000000
C	-0.88790100	-1.17939200	0.00000000
C	2.37930700	0.20321600	0.00000000
C	2.64546100	1.68758000	0.00000000
C	1.48973400	2.65180800	0.00000000
C	0.16267500	2.27528300	0.00000000
C	-1.17768200	2.97562400	0.00000000
C	-2.44053200	2.15696900	0.00000000
C	-2.46194700	0.78054500	0.00000000
C	-3.53486700	-0.28522800	0.00000000
C	-3.14910300	-1.73707300	0.00000000
C	-1.84620300	-2.20451100	0.00000000
C	-1.18673200	-3.52845100	0.00000000
C	0.18271600	-3.69569500	0.00000000
C	1.13718900	-2.56514800	0.00000000
C	2.50791100	-2.40420500	0.00000000
C	3.19971800	-1.06573700	0.00000000
C	-1.28388900	4.32310300	0.00000000
H	0.56722200	-4.71064400	0.00000000
H	3.17971300	-3.25635200	0.00000000
H	-3.35453400	2.74195200	0.00000000
C	-4.84755300	0.03377100	0.00000000
H	-0.40993100	4.96292800	0.00000000
H	-2.25008000	4.81356200	0.00000000
H	-5.18236300	1.06372000	0.00000000
H	-5.61553400	-0.73062100	0.00000000
C	4.55462300	-1.09150400	0.00000000
C	3.88711400	2.23263500	0.00000000
H	-1.80338100	-4.42182200	0.00000000
H	1.78691000	3.69513100	0.00000000
H	-3.98903200	-2.42517200	0.00000000

H	5.08564800	-2.03613100	0.00000000
H	5.16417800	-0.20230600	0.00000000
H	4.79163300	1.64608800	0.00000000
H	4.01419600	3.30879400	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-923.0539374

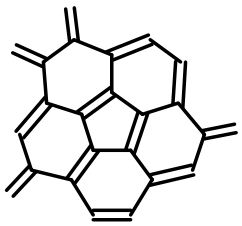
C	0.27140100	1.12028100	-0.62653900
C	-0.89384900	0.36325700	-0.67095900
C	-0.50189800	-1.01810800	-0.68991700
C	0.91618600	-1.07986600	-0.73009200
C	1.38656900	0.23491500	-0.65091500
C	-2.12825700	0.83547100	-0.19848500
C	-3.15566300	-0.24333700	-0.08007500
C	-2.65594400	-1.65388200	0.22624000
C	-1.26472000	-2.01885700	-0.14690700
C	-0.54426100	-3.23757500	0.18875500
C	0.82947800	-3.30863600	0.15693900
C	1.64704800	-2.15715100	-0.19325300
C	2.96994000	-1.90188000	0.15763800
C	3.56156400	-0.55832000	0.09846000
C	2.63642400	0.59123200	-0.13873500
C	2.72915400	1.92355800	0.30009600
C	1.61879400	2.81407300	0.30757400
C	0.33833800	2.42018000	-0.11050500
C	-2.17237000	2.16266100	0.17299600
H	1.76256900	3.77927700	0.78092700
H	1.31168400	-4.22695500	0.47708700
C	-4.45598500	-0.00391500	-0.29578900
H	3.64200800	2.27231100	0.77180300
C	-3.43496400	-2.51763200	0.90279400

C	4.89827400	-0.39796100	0.30450100
C	-0.99014400	3.04759900	0.14653300
C	-1.12845400	4.37540400	0.39968800
H	-1.09316400	-4.10481000	0.53611000
H	3.60098100	-2.69641900	0.54281800
H	-3.08700900	2.59784000	0.56137900
H	-4.80568900	0.99689300	-0.51875800
H	-5.19779800	-0.79288400	-0.28843900
H	-4.41057800	-2.23325900	1.27459500
H	-3.11071300	-3.52765600	1.11788500
H	5.53756200	-1.24521000	0.52131300
H	5.37034500	0.57453600	0.24606900
H	-2.09758700	4.80656700	0.62021300
H	-0.28258000	5.05069300	0.37673500

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_s	-923.0395828

C	-1.13085000	0.16222800	0.00000000
C	0.00000000	0.95024500	0.00000000
C	1.11810800	0.07387600	0.00000000
C	0.64542000	-1.23784200	0.00000000
C	-0.73325300	-1.18982300	0.00000000
C	0.01606900	2.33273900	0.00000000
C	1.42400600	2.87933700	0.00000000
C	2.64730900	1.90029300	0.00000000
C	2.42390400	0.42315200	0.00000000
C	3.31235000	-0.74524300	0.00000000
C	2.84686200	-2.05507800	0.00000000
C	1.41779900	-2.39135000	0.00000000
C	0.65360700	-3.56700100	0.00000000
C	-0.83748100	-3.57742100	0.00000000
C	-1.59095800	-2.27096200	0.00000000
C	-2.94863800	-1.86034000	0.00000000
C	-3.35920500	-0.48284300	0.00000000
C	-2.44381300	0.59761400	0.00000000
C	-1.25922200	2.89428500	0.00000000
H	-4.42888600	-0.30168100	0.00000000
H	3.58714500	-2.84894100	0.00000000
C	1.61931200	4.20540600	0.00000000

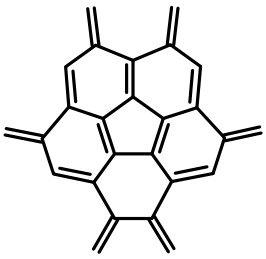
H	-3.74702200	-2.59575000	0.00000000
C	3.91111900	2.36056500	0.00000000
C	-1.47652200	-4.78232100	0.00000000
C	-2.52234800	2.09715200	0.00000000
C	-3.71641000	2.75104700	0.00000000
H	4.38709600	-0.60197800	0.00000000
H	1.12469100	-4.54434800	0.00000000
H	-1.40345600	3.96928200	0.00000000
H	0.77453600	4.88297500	0.00000000
H	2.59692400	4.66756500	0.00000000
H	4.16337200	3.41192900	0.00000000
H	4.74724400	1.67288900	0.00000000
H	-0.92324800	-5.71346500	0.00000000
H	-2.55691700	-4.85245300	0.00000000
H	-3.76763500	3.83311200	0.00000000
H	-4.65682400	2.21459100	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-923.0542772

C	0.06129813	1.27253001	0.64986701
C	0.96002601	0.16542591	0.65960399
C	0.18600988	-0.99564301	0.62940297
C	-1.19112408	-0.61565785	0.64528697
C	-1.26989192	0.77443615	0.68427700
C	2.27787902	0.25227477	0.19001500
C	2.95052187	-1.08280130	0.10740998
C	2.07931174	-2.31572920	-0.15708304
C	0.61501075	-2.23114905	0.12721795
C	-0.41790435	-3.09302492	-0.26241807
C	-1.79169431	-2.70644377	-0.25660107
C	-2.21449217	-1.43611573	0.15560595
C	-3.51060409	-0.73164358	-0.08292804

C	-3.48638792	0.73597042	-0.17053901
C	-2.36076184	1.48817229	0.15264800
C	-2.04839569	2.86785926	-0.19891697
C	-0.75490463	3.33736011	-0.22279296
C	0.37943427	2.49200798	0.11837203
C	2.70904216	1.50305873	-0.20277897
H	-0.58237952	4.34491610	-0.58326994
H	-2.49887738	-3.39560768	-0.70622408
C	4.26524486	-1.19586045	0.34361098
H	-2.84694461	3.52438735	-0.52966496
C	2.62390162	-3.41588825	-0.70309706
C	1.81697029	2.67435283	-0.22404496
C	2.28231443	3.89655078	-0.59247293
H	-0.18613045	-4.05618294	-0.70330908
H	3.70708218	1.65304862	-0.59861197
H	4.87117496	-0.31898653	0.53737600
H	4.76536175	-2.15525351	0.38437897
H	3.65995661	-3.45186736	-1.01273806
H	2.03843452	-4.31171819	-0.86887408
H	3.32722845	4.04822867	-0.83617893
H	1.63860353	4.76510385	-0.64099792
C	-4.68665916	-1.39480445	-0.26218806
H	-4.38470887	1.21607652	-0.54533301
H	-5.60347810	-0.86113634	-0.48173705
H	-4.75019228	-2.47243444	-0.17955608



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-1000.4511056

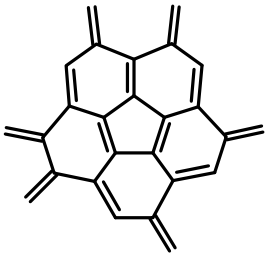
C	0.82298300	-0.81506300	-0.57965200
C	-0.51830700	-1.09488900	-0.65211800
C	-1.22541700	0.15564100	-0.63062000

C	-0.24202500	1.19652600	-0.60887100
C	0.99138200	0.60750100	-0.57656200
C	-1.10376900	-2.30078200	-0.20438500
C	-2.44629200	-2.23500200	0.07578100
C	-3.24392400	-0.99173900	-0.06608500
C	-2.50324600	0.30104900	-0.20537800
C	-2.85534200	1.68311400	0.23289500
C	-1.81325600	2.73778800	0.20344900
C	-0.50867900	2.50613900	-0.15960700
C	0.73066800	3.32341700	0.05778100
C	2.02937300	2.60363500	0.14206100
C	2.17337900	1.27617700	-0.15502400
C	3.35798200	0.36770600	-0.06707000
C	3.11700100	-1.10550900	0.27238600
C	1.79075800	-1.72509400	-0.05889800
C	-0.10035800	-3.38361300	0.05344000
C	4.06180300	-1.79115100	0.93424800
H	-2.10642100	3.68392700	0.64505500
C	4.58923500	0.81440000	-0.35317100
C	-4.59481500	-1.08479600	-0.12156800
C	1.31887400	-2.98333000	0.21250600
C	-4.03825200	1.98499000	0.82874700
C	0.69933000	4.66657100	0.19325700
C	-0.44540100	-4.68479300	0.16822300
H	-5.08408100	-2.04904900	-0.04582400
H	-5.22886700	-0.22909700	-0.30276100
H	-2.98710000	-3.09892000	0.44689800
H	-4.79534100	1.24266500	1.02976300
H	-4.24109900	2.99478500	1.16554100
H	-0.22403200	5.22627700	0.10851600
H	1.60381800	5.23426200	0.37757700
H	-1.46826600	-5.01677700	0.04014300
H	0.29569900	-5.44610100	0.38155700
H	2.87497300	3.19328000	0.48088600
H	4.98176400	-1.32517800	1.26161300
H	3.93173000	-2.83632400	1.18693000
H	4.75949200	1.85499400	-0.60204900
H	5.44850900	0.15631300	-0.37842100
H	1.97713000	-3.75841500	0.58999000

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_{2v}	-1000.4420321

C	0.00000000	0.71010800	-0.90207200
C	0.00000000	1.13972800	0.38775400
C	0.00000000	0.00000000	1.23720200
C	0.00000000	-1.13972800	0.38775400
C	0.00000000	-0.71010800	-0.90207200
C	0.00000000	2.46425900	0.83086800
C	0.00000000	2.57105100	2.20549300
C	0.00000000	1.39964300	3.14303000
C	0.00000000	0.00000000	2.58487200
C	0.00000000	-1.39964300	3.14303000
C	0.00000000	-2.57105100	2.20549300
C	0.00000000	-2.46425900	0.83086800
C	0.00000000	-3.42850100	-0.32831100
C	0.00000000	-2.88641300	-1.72615000
C	0.00000000	-1.54591100	-2.03634500
C	0.00000000	-0.78063900	-3.33486700
C	0.00000000	0.78063900	-3.33486700
C	0.00000000	1.54591100	-2.03634500
C	0.00000000	3.42850100	-0.32831100
C	0.00000000	1.46187400	-4.49050600
H	0.00000000	-3.53593300	2.70085000
C	0.00000000	-1.46187400	-4.49050600
C	0.00000000	1.68789600	4.46881000
C	0.00000000	2.88641300	-1.72615000
C	0.00000000	-1.68789600	4.46881000
C	0.00000000	-4.76839800	-0.15121800
C	0.00000000	4.76839800	-0.15121800
H	0.00000000	2.71813700	4.80478500
H	0.00000000	0.93596000	5.24088400
H	0.00000000	3.53593300	2.70085000
H	0.00000000	-0.93596000	5.24088400
H	0.00000000	-2.71813700	4.80478500
H	0.00000000	-5.21198000	0.83682200
H	0.00000000	-5.44943200	-0.99399100
H	0.00000000	5.21198000	0.83682200
H	0.00000000	5.44943200	-0.99399100
H	0.00000000	-3.64674800	-2.50011900

H	0.00000000	0.99068500	-5.46332300
H	0.00000000	2.54464400	-4.49104200
H	0.00000000	-2.54464400	-4.49104200
H	0.00000000	-0.99068500	-5.46332300
H	0.00000000	3.64674800	-2.50011900



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-1000.4548987

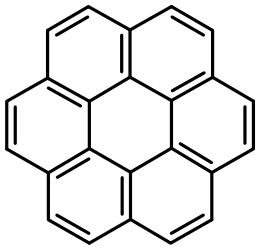
C	-1.15645000	0.57553800	-0.61871500
C	-0.82526400	-0.81787500	-0.62480500
C	0.61165100	-0.91134300	-0.60416600
C	1.10223000	0.36647800	-0.55030200
C	0.00824700	1.28891400	-0.56643300
C	-1.66289400	-1.80695400	-0.23389300
C	-0.99185700	-3.13524500	-0.08643300
C	0.48268700	-3.15120700	0.09676000
C	1.28547500	-2.06322900	-0.13370900
C	2.72604900	-1.82684500	0.21483500
C	2.39857700	0.72708500	-0.10983500
C	2.57431300	2.04267600	0.22931000
C	1.50429100	3.07368600	0.18095000
C	0.09870500	2.62894300	-0.09631000
C	-1.10146600	3.23556400	0.16956300
C	-2.41395300	2.55492700	0.01906700
C	-2.40848800	1.07055400	-0.19856700
C	-3.02522700	-1.34548600	0.16022100
C	-3.32723200	0.10710500	0.13756200
C	3.46054500	-2.77297000	0.81836200
C	-1.64925600	-4.31585500	-0.17006000
H	3.06433200	-3.76446400	1.00039400
H	4.46732600	-2.58267600	1.16645900

C	-3.55608300	3.27142100	0.10533700
C	-3.95553700	-2.17006500	0.70774300
H	-2.70729100	-4.37833200	-0.37915600
H	-1.11137200	-5.25325400	-0.08706300
C	1.81571600	4.36365700	0.42492600
H	-3.76883900	-3.21589100	0.89716800
H	-4.91928300	-1.78209000	1.01567400
H	0.89320800	-4.09285300	0.44405300
C	3.32797100	-0.44288200	-0.04133300
C	4.63893900	-0.29123400	-0.27790600
H	3.53184300	2.38720600	0.60678400
H	-1.14423400	4.25349800	0.54257300
H	-4.28974100	0.38123500	0.55567300
H	-3.53776000	4.33873600	0.29194900
H	-4.52777100	2.81064600	-0.02341300
H	2.83220600	4.66394300	0.65006400
H	1.06885700	5.14709700	0.39510300
H	5.31750900	-1.13349000	-0.32255800
H	5.06088100	0.68853900	-0.46672600

Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_s	-1000.4471026

C	0.64927900	-1.10524700	0.00000000
C	1.14158200	0.22763700	0.00000000
C	0.00000000	1.08348100	0.00000000
C	-1.11243600	0.30236200	0.00000000
C	-0.70624700	-1.06055400	0.00000000
C	2.43572300	0.60195100	0.00000000
C	2.58215400	2.09958600	0.00000000
C	1.35072800	2.96054700	0.00000000
C	0.06275000	2.47841800	0.00000000
C	-1.30129300	3.11826300	0.00000000
C	-2.44929000	0.72519500	0.00000000
C	-3.35963500	-0.31013700	0.00000000
C	-3.01116200	-1.76764100	0.00000000
C	-1.56289500	-2.18012300	0.00000000
C	-0.89415600	-3.38168300	0.00000000
C	0.60092600	-3.50729100	0.00000000
C	1.44420800	-2.25568700	0.00000000

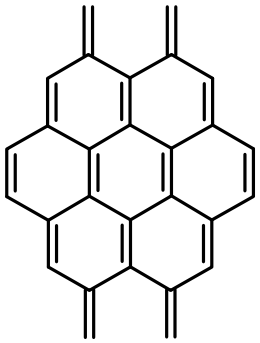
C	3.36423600	-0.58331900	0.00000000
C	2.79235200	-1.97146500	0.00000000
C	-1.39427000	4.45562900	0.00000000
C	3.77097300	2.74923800	0.00000000
H	-0.50165900	5.06869700	0.00000000
H	-2.33426000	4.99001600	0.00000000
C	1.14773300	-4.74357400	0.00000000
C	4.71776800	-0.49170300	0.00000000
H	4.72369800	2.24519300	0.00000000
H	3.80303400	3.83243200	0.00000000
C	-4.01002200	-2.67593300	0.00000000
H	5.25069000	0.44510300	0.00000000
H	5.32661700	-1.38802400	0.00000000
H	1.55784800	4.02505200	0.00000000
C	-2.57936100	2.22584500	0.00000000
C	-3.80241300	2.77668600	0.00000000
H	-4.42698300	-0.11389200	0.00000000
H	-1.42650500	-4.32715900	0.00000000
H	3.53910300	-2.75835500	0.00000000
H	0.53013000	-5.63383100	0.00000000
H	2.22058400	-4.89212500	0.00000000
H	-5.05020600	-2.37236100	0.00000000
H	-3.81131800	-3.74049900	0.00000000
H	-3.97652100	3.84374800	0.00000000
H	-4.68764700	2.15311800	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	D_{6h}	-922.0931139

C	0.00000000	0.00000000	2.84433000
C	0.00000000	0.00000000	-2.84433000
C	0.00000000	0.00000000	1.42533400
C	0.00000000	0.00000000	-1.42533400
C	0.00000000	1.24665400	3.52863600
C	0.00000000	-1.24665400	-3.52863600
C	0.00000000	-1.24665400	3.52863600
C	0.00000000	1.24665400	-3.52863600
C	0.00000000	1.23433000	0.71264500
C	0.00000000	-1.23433000	-0.71264500
C	0.00000000	-1.23433000	0.71264500
C	0.00000000	1.23433000	-0.71264500
C	0.00000000	-2.43244500	-2.84398300
C	0.00000000	2.43244500	2.84398300
C	0.00000000	-2.43244500	2.84398300
C	0.00000000	2.43244500	-2.84398300
C	0.00000000	2.46320200	-1.42221600
C	0.00000000	2.46320200	1.42221600
C	0.00000000	-2.46320200	-1.42221600
C	0.00000000	-2.46320200	1.42221600
C	0.00000000	-3.67910800	0.68461200
C	0.00000000	3.67910800	-0.68461200
C	0.00000000	3.67910800	0.68461200
C	0.00000000	-3.67910800	-0.68461200
H	0.00000000	-1.24416700	-4.61353600
H	0.00000000	1.24416700	4.61353600
H	0.00000000	1.24416700	-4.61353600
H	0.00000000	-1.24416700	4.61353600
H	0.00000000	-4.61750000	-1.22909100

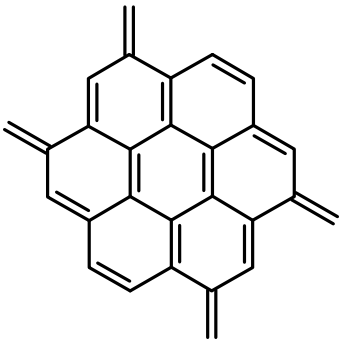
H	0.00000000	4.61750000	1.22909100
H	0.00000000	-4.61750000	1.22909100
H	0.00000000	4.61750000	-1.22909100
H	0.00000000	-3.37314100	3.38448600
H	0.00000000	3.37314100	-3.38448600
H	0.00000000	-3.37314100	-3.38448600
H	0.00000000	3.37314100	3.38448600



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	D_2	-1076.7927736

C	0.18220800	2.47899600	2.77782100
C	0.06631000	2.49294400	1.42153500
C	0.02616400	1.23729800	0.69184500
C	0.00000000	0.00000000	1.44670100
C	0.00000000	0.00000000	2.83828200
C	0.27586400	1.25933800	3.54847200
C	-0.02616400	1.23729800	-0.69184500
C	0.00000000	0.00000000	-1.44670100
C	0.02616400	-1.23729800	-0.69184500
C	-0.02616400	-1.23729800	0.69184500
C	-0.27586400	-1.25933800	3.54847200
C	-0.18220800	-2.47899600	2.77782100
C	-0.06631000	-2.49294400	1.42153500
C	-0.03038100	-3.73054600	0.67273900
C	0.03038100	-3.73054600	-0.67273900
C	0.06631000	-2.49294400	-1.42153500
C	0.18220800	-2.47899600	-2.77782100
C	0.27586400	-1.25933800	-3.54847200
C	0.00000000	0.00000000	-2.83828200
C	-0.27586400	1.25933800	-3.54847200

C	-0.18220800	2.47899600	-2.77782100
C	-0.06631000	2.49294400	-1.42153500
C	-0.03038100	3.73054600	-0.67273900
C	0.03038100	3.73054600	0.67273900
H	-0.05806900	-4.66207500	1.22795000
H	0.05806900	-4.66207500	-1.22795000
H	0.27438100	-3.41781800	-3.31431900
C	0.71689900	-1.34491700	-4.83375200
C	-0.71689900	1.34491700	-4.83375200
H	-0.27438100	3.41781800	-3.31431900
H	-0.05806900	4.66207500	-1.22795000
H	0.05806900	4.66207500	1.22795000
C	-0.71689900	-1.34491700	4.83375200
H	-0.27438100	-3.41781800	3.31431900
C	0.71689900	1.34491700	4.83375200
H	0.27438100	3.41781800	3.31431900
H	0.93474800	-2.31605600	-5.26236300
H	0.92954500	-0.48045400	-5.44291200
H	-0.92954500	0.48045400	-5.44291200
H	-0.93474800	2.31605600	-5.26236300
H	0.92954500	0.48045400	5.44291200
H	0.93474800	2.31605600	5.26236300
H	-0.92954500	-0.48045400	5.44291200
H	-0.93474800	-2.31605600	5.26236300

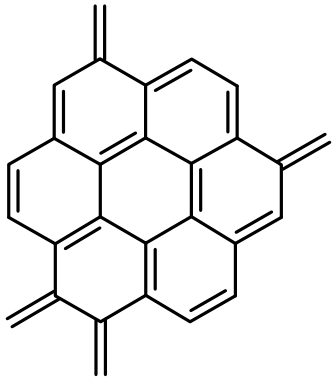


Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_{2h}	-1076.7942695

C	2.46426100	1.39477600	0.00000000
C	-2.46426100	-1.39477600	0.00000000

C	1.25141300	0.69505300	0.00000000
C	-1.25141300	-0.69505300	0.00000000
C	2.44876500	2.82942600	0.00000000
C	-2.44876500	-2.82942600	0.00000000
C	3.72788600	0.65734000	0.00000000
C	-3.72788600	-0.65734000	0.00000000
C	-0.00151100	1.41544600	0.00000000
C	0.00151100	-1.41544600	0.00000000
C	1.21836800	-0.74380400	0.00000000
C	-1.21836800	0.74380400	0.00000000
C	-1.29191900	-3.53458500	0.00000000
C	1.29191900	3.53458500	0.00000000
C	3.64599900	-0.78287000	0.00000000
C	-3.64599900	0.78287000	0.00000000
C	-2.47959300	1.48063100	0.00000000
C	0.01763400	2.87395900	0.00000000
C	-0.01763400	-2.87395900	0.00000000
C	2.47959300	-1.48063100	0.00000000
C	2.44876500	-2.96879000	0.00000000
C	-2.44876500	2.96879000	0.00000000
C	-1.15056200	3.58726400	0.00000000
C	1.15056200	-3.58726400	0.00000000
H	-3.38883300	-3.36427300	0.00000000
H	3.38883300	3.36427300	0.00000000
H	1.10748500	-4.67127800	0.00000000
H	-1.10748500	4.67127800	0.00000000
H	4.59086800	-1.31245000	0.00000000
H	-4.59086800	1.31245000	0.00000000
H	-1.30780800	-4.61893300	0.00000000
H	1.30780800	4.61893300	0.00000000
C	4.95913100	1.24242500	0.00000000
C	-4.95913100	-1.24242500	0.00000000
C	3.55586300	-3.75652700	0.00000000
C	-3.55586300	3.75652700	0.00000000
H	5.11102800	2.31192800	0.00000000
H	5.85161100	0.62917500	0.00000000
H	4.56448200	-3.36723900	0.00000000
H	3.45388600	-4.83455500	0.00000000
H	-3.45388600	4.83455500	0.00000000
H	-4.56448200	3.36723900	0.00000000

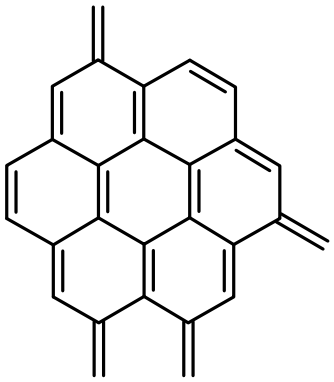
H	-5.85161100	-0.62917500	0.00000000
H	-5.11102800	-2.31192800	0.00000000



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_2	-1076.8011311

C	0.02796425	1.42360542	-0.08908699
C	0.02738221	0.71795215	-1.32467699
C	-0.02738221	-0.71795215	-1.32467699
C	-0.02796425	-1.42360542	-0.08908699
C	0.00465964	-0.72787204	1.14931501
C	-0.00465964	0.72787204	1.14931501
C	0.06283626	1.43074257	-2.56326199
C	0.02977718	0.69371666	-3.74293499
C	-0.02977718	-0.69371666	-3.74293499
C	-0.06283626	-1.43074257	-2.56326199
C	-0.12873133	-2.90830852	-2.56554499
C	-0.09339649	-3.55741666	-1.29491099
C	-0.03793893	-2.86710095	-0.09672599
C	0.00750131	-3.55069611	1.15557901
C	0.08776298	-2.86142543	2.33151001
C	0.09694207	-1.44366817	2.35902001
C	0.24628216	-0.70091818	3.61614201
C	-0.24628216	0.70091818	3.61614201
C	-0.09694207	1.44366817	2.35902001
C	0.03793893	2.86710095	-0.09672599
C	0.09339649	3.55741666	-1.29491099
C	0.12873133	2.90830852	-2.56554499
C	-0.00750131	3.55069611	1.15557901
C	-0.08776298	2.86142543	2.33151001

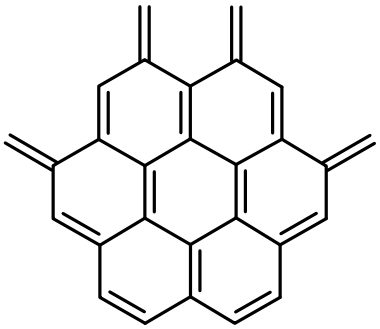
C	-0.22170682	-3.66243893	-3.70467299
C	0.86006925	-1.21498303	4.70029301
C	-0.86006925	1.21498303	4.70029301
C	0.22170682	3.66243893	-3.70467299
H	-0.26771266	-3.23819691	-4.69735799
H	-0.25958553	-4.74235685	-3.63691299
H	1.22432345	-2.23401398	4.72704201
H	1.04423624	-0.60488570	5.57530301
H	-1.04423624	0.60488570	5.57530301
H	-1.22432345	2.23401398	4.72704201
H	0.25958553	4.74235685	-3.63691299
H	0.26771266	3.23819691	-4.69735799
H	0.04687642	1.20382734	-4.69733299
H	-0.04687642	-1.20382734	-4.69733299
H	-0.11570194	-4.64189653	-1.27504099
H	-0.02333947	-4.63475597	1.15573401
H	0.11315467	-3.40446059	3.26830701
H	-0.11315467	3.40446059	3.26830701
H	0.02333947	4.63475597	1.15573401
H	0.11570194	4.64189653	-1.27504099



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-1076.7945987

C	1.64064900	0.30981607	0.01444896
C	0.59433497	1.30333203	-0.00445406
C	-0.74509002	0.93299498	-0.01357205
C	-1.13176097	-0.46005503	-0.00311901
C	-0.07583893	-1.45150799	-0.04352399
C	1.25774206	-1.08008894	-0.01299200

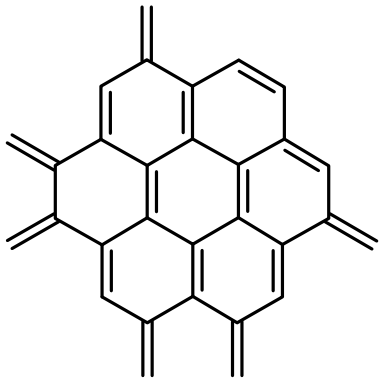
C	0.95641391	2.71606905	0.00256990
C	-0.00876513	3.68475901	-0.08016312
C	-1.40637711	3.37072495	-0.21151711
C	-1.78499606	1.94858694	-0.02114807
C	-3.06689604	1.56471490	0.21545694
C	-3.47190699	0.18480389	0.36865097
C	-2.47284595	-0.83964808	0.05223800
C	-2.82839990	-2.24565310	-0.18918197
C	-1.75333486	-3.21117906	-0.13524595
C	-0.44048287	-2.85709701	-0.06533096
C	0.61693916	-3.84504197	-0.04994193
C	1.91451515	-3.48259792	-0.01835394
C	2.30515510	-2.08988590	0.00324702
C	2.98286599	0.69078613	0.05833395
C	3.30776794	2.09020914	0.09139592
C	2.35221690	3.05079610	0.06503789
C	4.03914803	-0.33192083	0.06951598
C	3.61404608	-1.71236885	0.04221501
C	-2.29589615	4.34141191	-0.54486213
C	-4.70810298	-0.06200415	0.88827898
C	-4.06570688	-2.68034316	-0.55702696
C	5.36946402	-0.04778778	0.10270497
H	-1.97463419	5.37185992	-0.63630916
H	-3.33600614	4.13205286	-0.75598513
H	-5.36734701	0.76523883	1.12322196
H	-5.05218994	-1.05261415	1.14212000
H	-4.89593091	-2.01371119	-0.73174397
H	-4.22909284	-3.73356917	-0.75282093
H	5.76409198	0.95767123	0.12216994
H	6.09632805	-0.85072975	0.10928399
H	4.34661192	2.38851418	0.13441291
H	2.62824586	4.09963011	0.08189187
H	0.28594383	4.72864402	-0.10956814
H	-3.83534907	2.31509587	0.36104192
H	-2.01970482	-4.26076807	-0.20858992
H	0.33405520	-4.89220598	-0.06810791
H	2.69935718	-4.23143689	-0.00793893
H	4.38647611	-2.47462382	0.05495403



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_2	-1076.789535

C	0.00000000	0.00000000	-0.97217599
C	-0.01662618	1.24013991	-0.22942299
C	-0.01690642	1.23640462	1.16030901
C	0.00000000	0.00000000	1.88643901
C	0.01690642	-1.23640462	1.16030901
C	0.01662618	-1.24013991	-0.22942299
C	-0.03357308	2.49889850	-0.95568799
C	0.10400888	3.77079451	-0.20038899
C	-0.00370953	3.68861613	1.23339801
C	-0.04016266	2.49449687	1.90186001
C	-0.06473044	2.43560113	3.34019701
C	-0.04026322	1.24812014	3.99600301
C	0.00000000	0.00000000	3.28761101
C	0.04026322	-1.24812014	3.99600301
C	0.06473044	-2.43560113	3.34019701
C	0.04016266	-2.49449687	1.90186001
C	0.00370953	-3.68861613	1.23339801
C	-0.10400888	-3.77079451	-0.20038899
C	0.03357308	-2.49889850	-0.95568799
C	0.00000000	0.00000000	-2.37157699
C	-0.31392164	1.24740493	-3.07008699
C	-0.23258772	2.46860534	-2.29986099
C	0.31392164	-1.24740493	-3.07008699
C	0.23258772	-2.46860534	-2.29986099
C	0.37495589	4.96414859	-0.78921299
C	-0.37495589	-4.96414859	-0.78921299
C	0.75866841	-1.33346970	-4.35724399
C	-0.75866841	1.33346970	-4.35724399

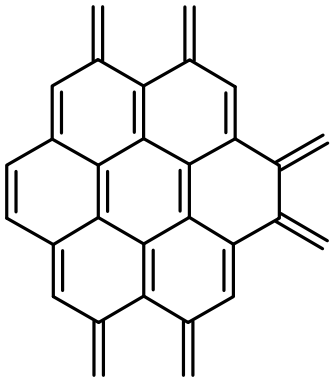
H	0.56430143	5.06414106	-1.84948699
H	0.43481951	5.86743625	-0.19441599
H	-0.43481951	-5.86743625	-0.19441599
H	-0.56430143	-5.06414106	-1.84948699
H	0.94688738	-0.46725498	-4.97267699
H	0.99887531	-2.30175362	-4.77988199
H	-0.94688738	0.46725498	-4.97267699
H	-0.99887531	2.30175362	-4.77988199
H	-0.38686933	3.39388965	-2.84284199
H	0.38686933	-3.39388965	-2.84284199
H	-0.00693658	-4.61525331	1.79800301
H	0.08933898	-3.36982786	3.89057401
H	0.04813278	-1.22282521	5.08066301
H	-0.04813278	1.22282521	5.08066301
H	-0.08933898	3.36982786	3.89057401
H	0.00693658	4.61525331	1.79800301



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-1154.1927809

C	-0.01203955	3.42299097	0.07380512
C	0.89269731	2.42313484	-0.05255288
C	0.44844410	1.04003790	0.01568206
C	-0.97816293	0.77575211	0.00197802
C	-1.90370478	1.81916725	-0.02370698
C	-1.43483559	3.18842517	0.21854308
C	1.36842295	0.00016777	0.02522606
C	0.93052276	-1.37364616	-0.03351999
C	-0.48793528	-1.64115196	-0.01336204
C	-1.41086913	-0.60383283	0.01719696

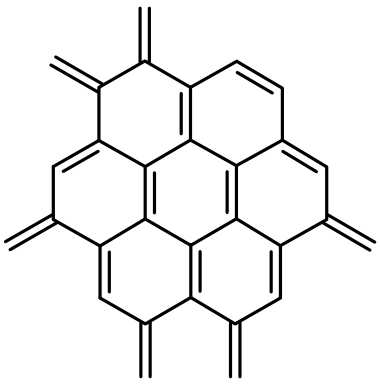
C	-3.30751082	1.50572446	-0.30238303
C	-3.71087702	0.12484151	-0.16290508
C	-2.83563618	-0.89334762	0.04538791
C	-3.28621938	-2.29523156	0.22802886
C	-2.28655153	-3.31539570	0.06061685
C	-0.95186348	-3.02413889	-0.03842010
C	0.03501937	-4.06346703	-0.13353010
C	1.35816341	-3.77537622	-0.17250706
C	1.84567061	-2.42537029	-0.11485500
C	3.28542965	-2.14313250	-0.14524995
C	3.68249385	-0.75795256	-0.00070690
C	2.79894299	0.26379656	0.10810311
C	3.24169219	1.66016049	0.32088016
C	2.33638135	2.69245264	-0.23940483
H	4.74588588	-0.54786372	0.00710214
C	-4.22608468	2.39619960	-0.77377203
C	-2.21754946	4.21286027	0.65098508
H	0.32720859	4.45132592	0.12389816
H	-3.26544148	4.09493841	0.88080005
H	-1.77681832	5.18478020	0.83952713
H	-3.98380152	3.42128558	-1.00802499
H	-5.23579972	2.06535576	-0.98625407
C	2.79945752	3.75503559	-0.91200379
C	4.34037021	1.98115431	1.01817220
H	3.86204155	3.90021444	-1.06259575
H	2.13161964	4.48337070	-1.35556878
H	4.97381509	1.22410621	1.46399220
H	4.61119636	3.01592427	1.18738224
H	-0.30463478	-5.09318298	-0.16172114
H	-2.60538468	-4.35243366	0.07742281
H	-4.76585705	-0.08914433	-0.28963512
H	2.06930030	-4.58801732	-0.23430706
C	4.24536252	-3.09289463	-0.29527595
C	-4.55221144	-2.63157539	0.58646881
H	4.02982037	-4.14505160	-0.41385899
H	5.29121056	-2.81139879	-0.30638691
H	-5.30652034	-1.89407929	0.82573681
H	-4.83995760	-3.67245835	0.67097977



Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-1154.1908905

C	-0.67661182	-4.07408708	-0.17616084
C	-1.42515989	-2.83839112	-0.10041288
C	-0.69340795	-1.58431408	-0.03462290
C	0.68983405	-1.58472701	-0.01046187
C	1.41811011	-2.84266398	-0.03537583
C	0.66945318	-4.07597502	-0.14347181
C	-1.44513401	-0.34530712	-0.02695094
C	-0.69077908	0.89284692	0.01590504
C	0.69649793	0.89643499	-0.03100393
C	1.44639199	-0.34658597	-0.01284189
C	2.77285811	-2.83910890	0.09237919
C	3.53905105	-1.62609486	0.26561517
C	2.83802199	-0.35711990	0.00998713
C	3.56047493	0.89998213	-0.22080789
C	2.78774387	2.12265909	-0.14266593
C	1.43541486	2.14937702	-0.08307795
C	0.67832580	3.42336899	-0.12545100
C	-0.67517621	3.36767293	0.47621198
C	-1.43173814	2.13462889	0.17055000
C	-2.77599514	2.13590682	0.01201998
C	-3.53382807	0.93223577	-0.27114600
C	-2.83589101	-0.34536919	-0.06842896
C	-3.55924995	-1.61655422	0.08763806
C	-2.78520589	-2.82931619	-0.04878790
C	4.86008193	0.99422218	-0.61020987
C	-1.15191327	4.33611993	1.26967495
H	-3.32476484	-3.77098621	-0.04486889

C	4.80709604	-1.72872879	0.74891520
H	-1.23290578	-5.00282911	-0.24527382
H	5.47846898	0.13420621	-0.81447884
H	5.29580388	1.96934920	-0.79387989
H	-0.55723831	5.21028696	1.50462294
H	-2.13042827	4.26227289	1.72852794
H	5.23016809	-2.70766576	0.94170923
H	5.40516800	-0.87308875	1.02086218
C	-4.86723095	-1.72456128	0.45008604
H	-5.48636300	-0.87221430	0.68255201
H	-5.30931690	-2.70569430	0.57798606
H	-3.31870718	3.07421879	0.02782895
H	1.22570922	-5.00641099	-0.18484078
H	3.30774916	-3.78222788	0.13908422
C	-4.78301807	1.06280570	-0.78865803
H	-5.20387312	2.05067767	-0.93566506
H	-5.36963302	0.22286366	-1.12758402
H	3.34123182	3.05334012	-0.19005494
C	1.13430375	4.53443199	-0.72109602
H	0.52832671	5.43078996	-0.76233305
H	2.10068376	4.57038003	-1.20829600



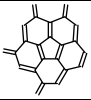
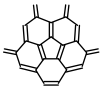
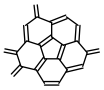
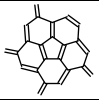
Level of theory	Point group	Total energy [Hartree]
B3LYP/6-311G**	C_1	-1154.1872941

C	-2.66087584	2.45803624	-0.03984587
C	-2.56672391	1.11699723	0.12106212
C	-1.26969795	0.45122516	0.00589407
C	-0.11103091	1.20567610	-0.07808498
C	-0.17859984	2.65798910	-0.16767797

C	-1.51043981	3.30613217	-0.27513592
C	-1.21792903	-0.98988484	0.01132906
C	0.07446094	-1.62935691	-0.01151900
C	1.24029598	-0.87573298	-0.00368605
C	1.19179706	0.57030103	-0.00308904
C	0.97794220	3.36749104	-0.18562002
C	2.29375917	2.76891197	-0.16134308
C	2.36087510	1.32580696	0.08547691
C	3.60800008	0.64374189	0.44458586
C	3.63960599	-0.79182511	0.27763385
C	2.53582694	-1.53580205	0.00694990
C	2.60318685	-3.00381305	-0.19832311
C	1.36160082	-3.72207098	-0.10475606
C	0.14924285	-3.08663892	-0.03390201
C	-1.08098119	-3.82503285	-0.01561096
C	-2.28111115	-3.19100578	-0.02067890
C	-2.38233807	-1.76176678	-0.02432189
C	-3.70099704	-1.11436971	-0.07828484
C	-3.74866894	0.28246930	0.42422317
H	-3.19222818	-3.77499373	0.00527313
C	3.35817120	3.56287691	-0.46650012
C	-1.70186175	4.60742819	-0.59150090
H	-3.63521182	2.93283529	-0.03108183
H	-0.89213172	5.28605514	-0.82337694
H	-2.70376773	5.01702124	-0.63343486
H	3.20180125	4.61577892	-0.66926911
H	4.36106118	3.18390685	-0.58624717
C	-4.76962889	0.72591635	1.17289422
C	-4.79865209	-1.71641064	-0.57230079
H	-5.60700991	0.08394539	1.41593625
H	-4.77473081	1.72517835	1.59039422
H	-4.78079917	-2.72940464	-0.95256379
H	-5.73844607	-1.18438559	-0.64443075
H	-1.03126024	-4.90837285	-0.00200596
H	4.59277697	-1.28096116	0.44234381
H	0.94751426	4.44750804	-0.26733102
H	1.39208875	-4.80553699	-0.15546406
C	4.69331714	1.24339883	1.01037881
C	3.74941180	-3.66061111	-0.51465816
H	4.68350982	-3.14766016	-0.70031720

H	3.75293374	-4.73889511	-0.61794716
H	4.71669621	2.28946683	1.27384082
H	5.55945712	0.64805378	1.27415178

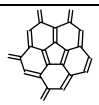
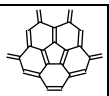
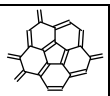
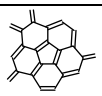
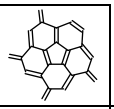
Table 1. Aromatic Stabilization Energies for bowl-shaped corannulene (ZPE included).

I											
E→	-768.084104	-845.387211	-845.387058	-845.389337	-922.758763	-922.754541	-922.751467	-922.761123	-922.761395	-922.754625	**ASE↓ kcal/mol**
(7)	**-1**	**-1/4**	**4**	**-7/4**	**0**	**1/4**	**0**	**0**	**0**	**-5/4**	**43.08**
(8)	**-1**	**0**	**4**	**-2**	**1**	**-1**	**0**	**0**	**-1**	**0**	**45.00**
(9)	**-1**	**17/32**	**133/32**	**-43/16**	**15/32**	**-1**	**0**	**-15/32**	**0**	**0**	**44.98**
(10)	**-1**	**1**	**19/5**	**-14/5**	**0**	**-8/5**	**3/5**	**0**	**0**	**0**	**45.56**
(11)	**-1**	**1/2**	**9/2**	**-3**	**1/2**	**0**	**-1**	**-1/2**	**0**	**0**	**43.55**
(12)	**-1**	**-1/6**	**13/3**	**-13/6**	**7/6**	**0**	**-1**	**0**	**-7/6**	**0**	**43.61**
(13)	**-1**	**-27/44**	**167/44**	**-13/11**	**0**	**0**	**27/44**	**0**	**0**	**-71/44**	**43.51**
(14)	**-1**	**0**	**4**	**-2**	**0**	**0**	**0**	**0**	**0**	**-1**	**43.41**
(15)	**-1**	**-1/2**	**4**	**-3/2**	**1/2**	**0**	**0**	**0**	**-1/2**	**-1**	**43.56**
(16)	**-1**	**1**	**73/20**	**-53/20**	**0**	**-1**	**0**	**21/20**	**-21/20**	**0**	**44.37**
(17)	**-1**	**1**	**79/20**	**-59/20**	**0**	**0**	**-1**	**23/20**	**-23/20**	**0**	**42.88**
(18)	**-1**	**0**	**37/10**	**-17/10**	**0**	**0**	**0**	**9/10**	**-9/10**	**-1**	**43.13**
(19)	**-1**	**-39/28**	**95/28**	**0**	**0**	**-3/7**	**51/28**	**0**	**0**	**-67/28**	**44.27**
(20)	**-1**	**0**	**83/20**	**-43/20**	**1**	**-31/20**	**11/20**	**-1**	**0**	**0**	**46.11**
(21)	**-1**	**0**	**37/10**	**-17/10**	**0**	**-9/10**	**9/10**	**0**	**0**	**-1**	**46.67**
(22)	**-1**	**0**	**149/38**	**-73/38**	**-9/38**	**9/38**	**0**	**9/38**	**0**	**-47/38**	**44.83**
(23)	**-1**	**0**	**79/22**	**-35/22**	**-27/44**	**0**	**27/44**	**27/44**	**0**	**-71/44**	**44.99**
(24)	**-1**	**0**	**2**	**0**	**-17/8**	**-7/4**	**31/8**	**17/8**	**0**	**-25/8**	**46.85**

$$ASE(kcal/mole) = 627.5095 \cdot \sum_{i=1}^{n} c_i E_i$$

mean value: 44.47 kcal/mol
standard deviation: 1.24 kcal/mol

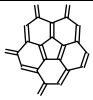
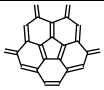
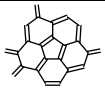
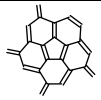
Table 2. Aromatic Stabilization Energies for planar corannulene (ZPE not included).

											
E →	-768.298931	-845.636287	-845.629165	-845.635859	-923.042134	-923.038765	-923.035096	-923.039583	-923.041658	-923.035284	**ASE↓ kcal/mol**
(7)	**-1**	**-1/4**	**4**	**-7/4**	**0**	**1/4**	**0**	**0**	**0**	**-5/4**	**55.54**
(8)	**-1**	**0**	**4**	**-2**	**1**	**-1**	**0**	**0**	**-1**	**0**	**57.91**
(9)	**-1**	**17/32**	**133/32**	**-43/16**	**15/32**	**-1**	**0**	**-15/32**	**0**	**0**	**57.97**
(10)	**-1**	**1**	**19/5**	**-14/5**	**0**	**-8/5**	**3/5**	**0**	**0**	**0**	**58.48**
(11)	**-1**	**1/2**	**9/2**	**-3**	**1/2**	**0**	**-1**	**-1/2**	**0**	**0**	**57.07**
(12)	**-1**	**-1/6**	**13/3**	**-13/6**	**7/6**	**0**	**-1**	**0**	**-7/6**	**0**	**57.00**
(13)	**-1**	**-27/44**	**167/44**	**-13/11**	**0**	**0**	**27/44**	**0**	**0**	**-71/44**	**55.40**
(14)	**-1**	**0**	**4**	**-2**	**0**	**0**	**0**	**0**	**0**	**-1**	**56.02**
(15)	**-1**	**-1/2**	**4**	**-3/2**	**1/2**	**0**	**0**	**0**	**-1/2**	**-1**	**56.00**
(16)	**-1**	**1**	**73/20**	**-53/20**	**0**	**-1**	**0**	**21/20**	**-21/20**	**0**	**57.83**
(17)	**-1**	**1**	**79/20**	**-59/20**	**0**	**0**	**-1**	**23/20**	**-23/20**	**0**	**56.92**
(18)	**-1**	**0**	**37/10**	**-17/10**	**0**	**0**	**0**	**9/10**	**-9/10**	**-1**	**55.93**
(19)	**-1**	**-39/28**	**95/28**	**0**	**0**	**-3/7**	**51/28**	**0**	**0**	**-67/28**	**54.99**
(20)	**-1**	**0**	**83/20**	**-43/20**	**1**	**-31/20**	**11/20**	**-1**	**0**	**0**	**58.50**
(21)	**-1**	**0**	**37/10**	**-17/10**	**0**	**-9/10**	**9/10**	**0**	**0**	**-1**	**56.83**
(22)	**-1**	**0**	**149/38**	**-73/38**	**-9/38**	**9/38**	**0**	**9/38**	**0**	**-47/38**	**55.55**
(23)	**-1**	**0**	**79/22**	**-35/22**	**-27/44**	**0**	**27/44**	**27/44**	**0**	**-71/44**	**55.36**
(24)	**-1**	**0**	**2**	**0**	**-17/8**	**-7/4**	**31/8**	**17/8**	**0**	**-25/8**	**55.30**

$$ASE(kcal/mole) = 627.5095 \cdot \sum_{i=1}^{n} c_i E_i$$

mean value: 56.59 kcal/mole
standard deviation: 1.17 kcal/mole

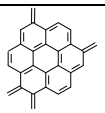
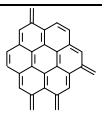
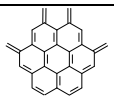
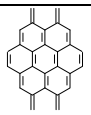
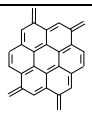
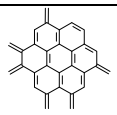
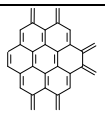
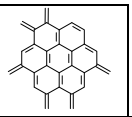
Table 3. Aromatic Stabilization Energies for bowl-shaped corannulene (ZPE not included).

											
E→	-768.315218	-845.648297	-845.647602	-845.650028	-923.051969	-923.047800	-923.044584	-923.053937	-923.054277	-923.047343	**ASE↓ kcal/mol**
(7)	**-1**	**-1/4**	**4**	**-7/4**	**0**	**1/4**	**0**	**0**	**0**	**-5/4**	**44.97**
(8)	**-1**	**0**	**4**	**-2**	**1**	**-1**	**0**	**0**	**-1**	**0**	**47.05**
(9)	**-1**	**17/32**	**133/32**	**-43/16**	**15/32**	**-1**	**0**	**-15/32**	**0**	**0**	**46.99**
(10)	**-1**	**1**	**19/5**	**-14/5**	**0**	**-8/5**	**3/5**	**0**	**0**	**0**	**47.59**
(11)	**-1**	**1/2**	**9/2**	**-3**	**1/2**	**0**	**-1**	**-1/2**	**0**	**0**	**45.50**
(12)	**-1**	**-1/6**	**13/3**	**-13/6**	**7/6**	**0**	**-1**	**0**	**-7/6**	**0**	**45.60**
(13)	**-1**	**-27/44**	**167/44**	**-13/11**	**0**	**0**	**27/44**	**0**	**0**	**-71/44**	**45.40**
(14)	**-1**	**0**	**4**	**-2**	**0**	**0**	**0**	**0**	**0**	**-1**	**45.31**
(15)	**-1**	**-1/2**	**4**	**-3/2**	**1/2**	**0**	**0**	**0**	**-1/2**	**-1**	**45.49**
(16)	**-1**	**1**	**73/20**	**-53/20**	**0**	**-1**	**0**	**21/20**	**-21/20**	**0**	**46.38**
(17)	**-1**	**1**	**79/20**	**-59/20**	**0**	**0**	**-1**	**23/20**	**-23/20**	**0**	**44.84**
(18)	**-1**	**0**	**37/10**	**-17/10**	**0**	**0**	**0**	**9/10**	**-9/10**	**-1**	**45.05**
(19)	**-1**	**-39/28**	**95/28**	**0**	**0**	**-3/7**	**51/28**	**0**	**0**	**-67/28**	**46.15**
(20)	**-1**	**0**	**83/20**	**-43/20**	**1**	**-31/20**	**11/20**	**-1**	**0**	**0**	**48.17**
(21)	**-1**	**0**	**37/10**	**-17/10**	**0**	**-9/10**	**9/10**	**0**	**0**	**-1**	**46.67**
(22)	**-1**	**0**	**149/38**	**-73/38**	**-9/38**	**9/38**	**0**	**9/38**	**0**	**-47/38**	**44.83**
(23)	**-1**	**0**	**79/22**	**-35/22**	**-27/44**	**0**	**27/44**	**27/44**	**0**	**-71/44**	**44.99**
(24)	**-1**	**0**	**2**	**0**	**-17/8**	**-7/4**	**31/8**	**17/8**	**0**	**-25/8**	**46.85**

$$ASE(kcal/mole) = 627.5095 \cdot \sum_{i=1}^{n} c_i E_i$$

mean value: 45.99 kcal/mol
standard deviation: 1.03 kcal/mol

Table 4. Aromatic Stabilization Energies for coronene (ZPE included).

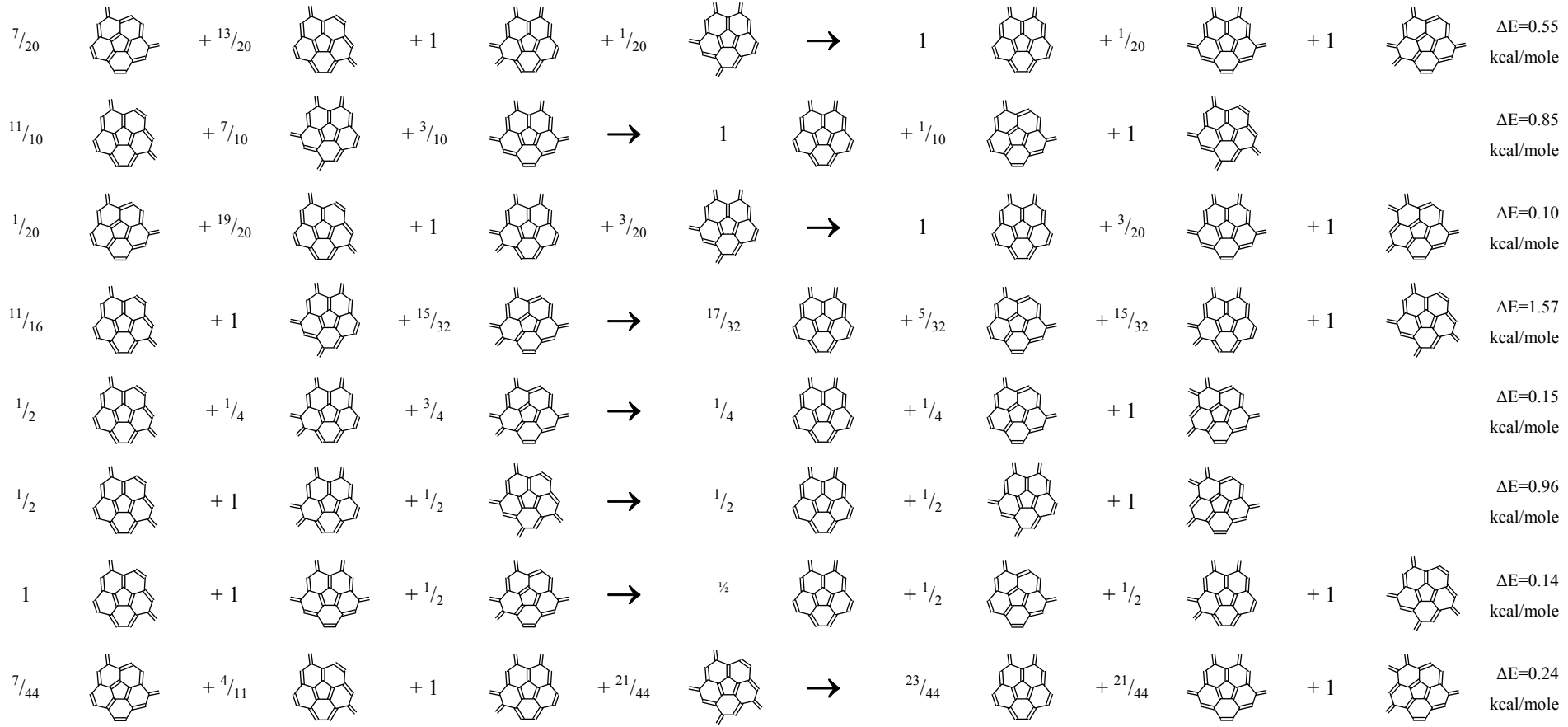
										
E→	**-921.814507 [Hartree]**	**-1076.460988**	**-1076.454117**	**-1076.449422**	**-1076.451809**	**-1076.454803**	**-1153.819901**	**-1153.818224**	**-1153.81562**	**ASE↓ kcal/mol**
(25)	**-1**	**2**	**-7/3**	**10/3**	**-5/18**	**-23/18**	**-2**	**0**	**0**	**59.05**
(26)	**-1**	**2**	**-7/3**	**10/3**	**13/18**	**-41/18**	**0**	**-2**	**0**	**58.82**
(27)	**-1**	**2**	**-1**	**4**	**-1/2**	**-3/2**	**0**	**0**	**-2**	**55.41**
(28)	**-1**	**2**	**-11/4**	**10/3**	**5/12**	**0**	**-31/12**	**7/12**	**0**	**60.12**
(29)	**-1**	**2**	**-33/10**	**33/10**	**1**	**0**	**-21/10**	**0**	**1/10**	**60.52**
(30)	**-1**	**2**	**-63/16**	**192/32**	**29/32**	**0**	**0**	**3/32**	**-67/32**	**56.74**
(31)	**-1**	**2**	**-3/4**	**10/3**	**0**	**-19/21**	**-17/12**	**-7/12**	**0**	**58.97**
(32)	**-1**	**2**	**-7/5**	**17/5**	**0**	**-1**	**-9/5**	**0**	**-1/5**	**58.99**
(33)	**-1**	**2**	**-7/11**	**161/44**	**0**	**-89/44**	**0**	**-45/44**	**-43/44**	**57.03**
(34)	**-1**	**2**	**0**	**10/3**	**-11/30**	**-59/30**	**-7/5**	**-3/5**	**0**	**58.59**
(35)	**-1**	**2**	**0**	**133/39**	**-55/78**	**-133/78**	**-23/13**	**0**	**-3/13**	**58.22**
(36)	**-1**	**2**	**0**	**43/12**	**-1/6**	**-29/12**	**0**	**-5/4**	**-3/4**	**57.11**
(37)	**-1**	**2**	**-5/2**	**7/2**	**0**	**0**	**-5/2**	**1**	**-1/2**	**59.10**
(38)	**-1**	**2**	**0**	**55/16**	**-39/16**	**0**	**-41/8**	**55/16**	**-5/16**	**58.46**
(39)	**-1**	**2**	**0**	**89/28**	**0**	**-61/28**	**-9/7**	**-33/28**	**13/28**	**59.39**

$$ASE(kcal/mole) = 627.5095 \cdot \sum_{i=1}^{n} c_i E_i$$

mean value: 58.43 kcal/mol
std deviation: 1.35 kcal/mol

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Corannulene: Additivity of energies of reference compounds.



Coronene: Additivity of energies of reference compounds.