Supporting Information

Table S1. Hyperfine coupling constants of the coronene radical cation (a(H) in Gauss units, 1 G= 0.1 mT). Calculations were carried out at the CAM-B3LYP/6-311G(d,p) level. Notation "f" means a scaling factor to fit the experimental value (0.156 mT): (f=1.092)

		^2A_u (D_{2h})				$^2B_{3u}$ (D_{2h})	
		a(H)	a(H)*f			a(H)	a(H)*f
Atom				**Atom**			
17	**H(1)**	-0.567	-0.619	**17**	**H(1)**	-2.242	-2.448
18	**H(1)**	-0.567	-0.619	**18**	**H(1)**	-2.242	-2.448
19	**H(1)**	-4.712	-5.145	**19**	**H(1)**	1.848	2.018
20	**H(1)**	0.992	1.084	**20**	**H(1)**	-3.881	-4.238
21	**H(1)**	-4.712	-5.145	**21**	**H(1)**	1.848	2.018
22	**H(1)**	0.992	1.084	**22**	**H(1)**	-3.881	-4.238
26	**H(1)**	-4.712	-5.145	**26**	**H(1)**	1.848	2.018
27	**H(1)**	0.992	1.084	**27**	**H(1)**	-3.881	-4.238
31	**H(1)**	-0.567	-0.619	**31**	**H(1)**	-2.242	-2.448
32	**H(1)**	-0.567	-0.619	**32**	**H(1)**	-2.242	-2.448
34	**H(1)**	-4.712	-5.145	**34**	**H(1)**	1.848	2.018
36	**H(1)**	0.992	1.084	**36**	**H(1)**	-3.881	-4.238
<(a(H)>=		-1.429	-1.560	**<(a(H)>=**		-1.425	-1.556

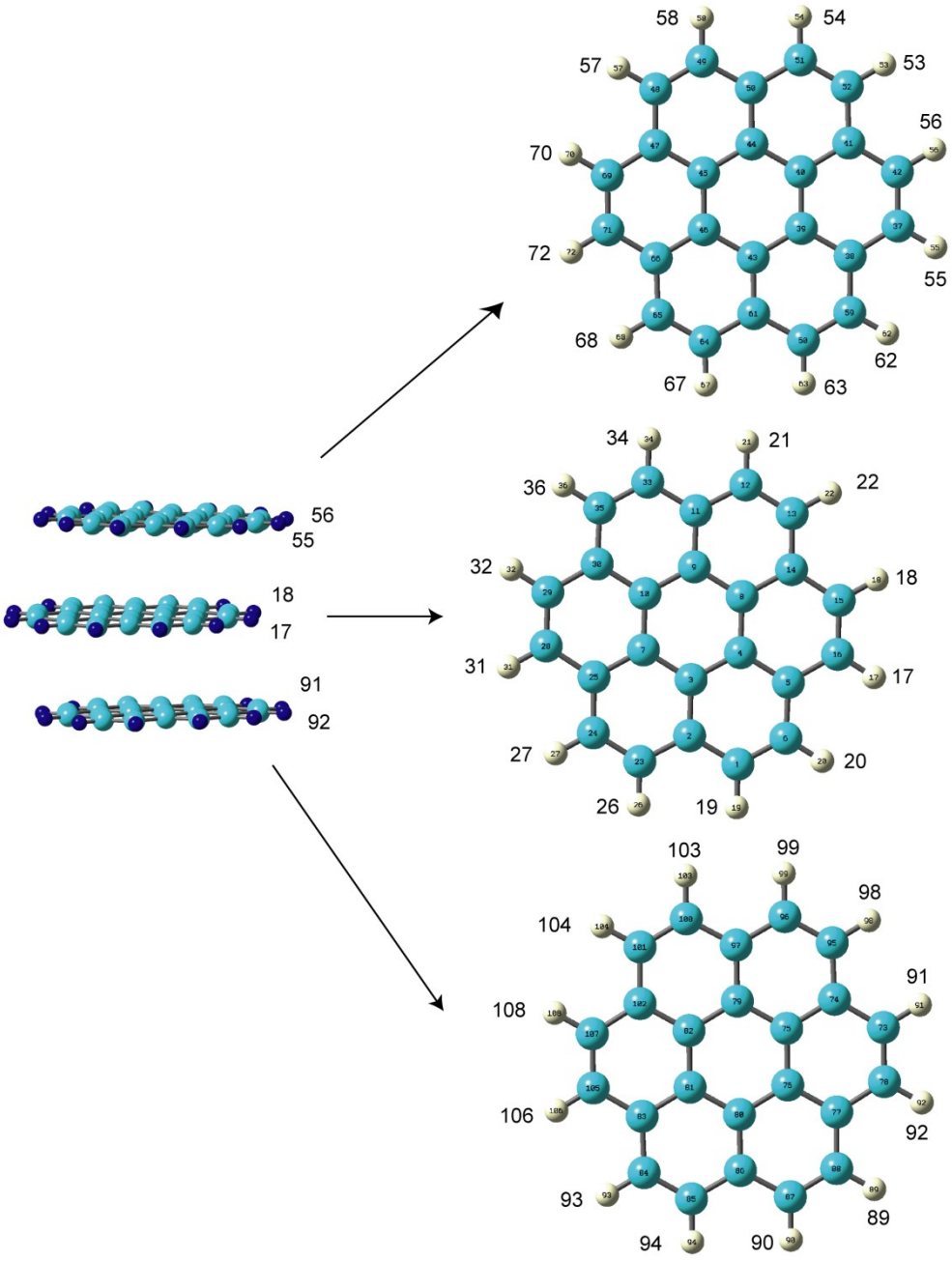

Figure S1. Numbering of the protons in the trimer cation of coronene (See Table 1).

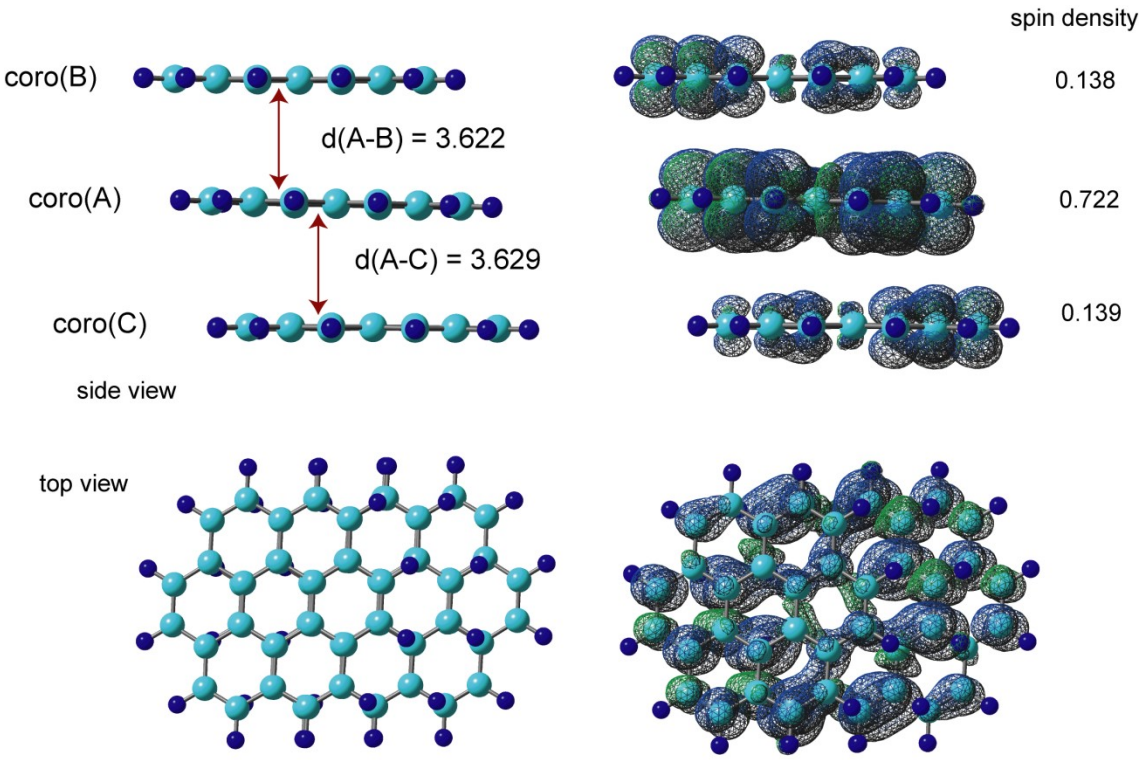

Figure S2. Optimized structures and values of the spin density in each plane of the trimer cation of coronene (*ABC* stacking form). Interplane distances, *d*(A-B) and *d*(A-C), are in Å. Calculations were carried out at the CAM-B3LYP/6-311G(d,p) level.

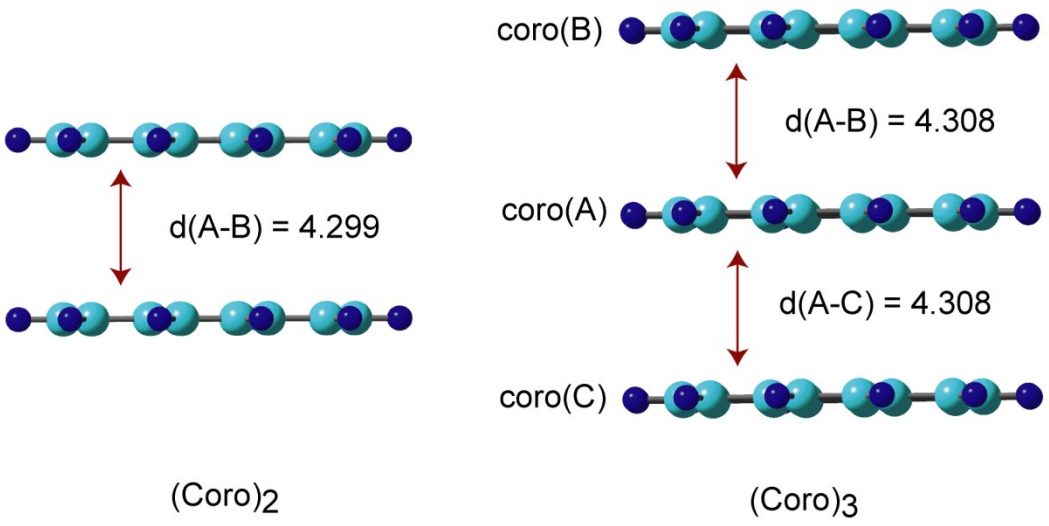

Figure S3. Optimized structures of neutral coronene dimer and trimer calculated at the CAM-B3LYP/6-311G(d,p) level. Interplane distances, *d*(A-B) and *d*(A-C), are in Å.

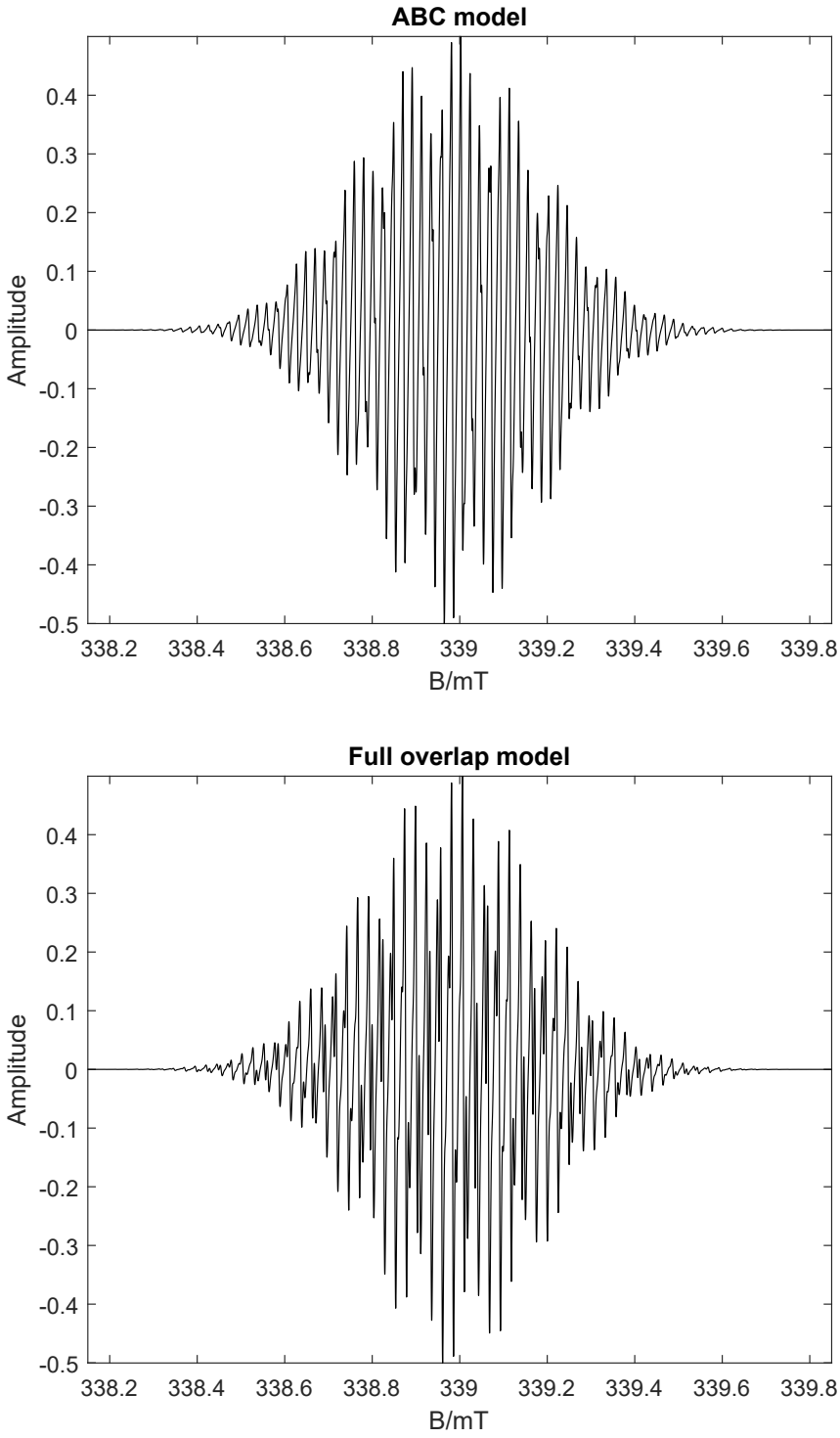

Figure S4. Simulated ESR spectra of the coronene trimer radical cation for the ABC and full overlapped forms using the hfcc's calculated at the CAM-B3LYP/6-311G(d,p) level (multiplied by f = 1.092).

Table S2. Hyperfine coupling constants of the dimer radical cation of coronene (a(H) in Gauss units, 1 G = 0.1 mT). Calculations were carried out at the CAM-B3LY P/6-311G(d,p) level. Notation "f" means a scaling factor to fit the experimental value of the coronene cation radical (0.156 mT,): (f=1.092).

	Atom	a(H)	a(H)*f
17	**H(1)**	-1.500	-1.637
18	**H(1)**	0.640	0.699
19	**H(1)**	-1.393	-1.521
20	**H(1)**	-0.749	-0.818
21	**H(1)**	-1.529	-1.670
22	**H(1)**	0.651	0.711
26	**H(1)**	-2.399	-2.620
27	**H(1)**	1.170	1.278
31	**H(1)**	1.160	1.266
32	**H(1)**	-2.371	-2.589
34	**H(1)**	-0.790	-0.863
36	**H(1)**	-1.358	-1.483
53	**H(1)**	1.170	1.277
54	**H(1)**	-2.397	-2.618
55	**H(1)**	-2.376	-2.595
56	**H(1)**	1.162	1.269
57	**H(1)**	-0.757	-0.827
58	**H(1)**	-1.391	-1.519
62	**H(1)**	-1.367	-1.493
63	**H(1)**	-0.783	-0.855
67	**H(1)**	-1.526	-1.666
68	**H(1)**	0.650	0.710
70	**H(1)**	-1.508	-1.647
72	**H(1)**	0.644	0.703
<(a(H)>=		-0.706	-0.771

Table S3. Hyperfine coupling constants of the trimer radical cation of coronene (a(H) in Gauss units, 1 G =0.1 mT). Calculations were carried out at the CAM-B3LYP/6-311G(d,p) level. Notation "f" means a scaling factor to fit the experimental value of the coronene cation radical (0.156 mT): (f=1.092). Red values indicate hyperfine coupling constants close to zero.

	Atom	a(H)	a(H)*f
17	**H(1)**	-0.363	-0.397
18	**H(1)**	-0.344	-0.376
19	**H(1)**	-3.679	-4.018
20	**H(1)**	0.850	0.929
21	**H(1)**	-3.682	-4.020
22	**H(1)**	0.862	0.941
26	**H(1)**	-3.450	-3.768
27	**H(1)**	0.741	0.810
31	**H(1)**	-0.515	-0.562
32	**H(1)**	-0.546	-0.596
34	**H(1)**	-3.439	-3.755
36	**H(1)**	0.718	0.784
53	**H(1)**	0.380	0.415
54	**H(1)**	-0.792	-0.865
55	**H(1)**	-0.672	-0.734
56	**H(1)**	0.356	0.389
57	**H(1)**	-0.115	-0.125
58	**H(1)**	-0.333	-0.364
62	**H(1)**	-0.426	-0.465
63	**H(1)**	-0.042	-0.045
67	**H(1)**	-0.157	-0.171
68	**H(1)**	0.034	0.037
70	**H(1)**	-0.309	-0.337
72	**H(1)**	0.067	0.073
89	**H(1)**	0.381	0.416
90	**H(1)**	-0.795	-0.868

91	**H(1)**	-0.669	-0.731
92	**H(1)**	0.355	0.387
93	**H(1)**	-0.110	-0.120
94	**H(1)**	-0.337	-0.368
98	**H(1)**	-0.424	-0.463
99	**H(1)**	-0.048	-0.052
103	**H(1)**	-0.161	-0.175
104	**H(1)**	0.037	0.040
106	**H(1)**	-0.307	-0.335
108	**H(1)**	0.067	0.074
<(a(H)>=		-0.468	-0.512

Table S4. Hyperfine coupling constants of each layer in the trimer radical cation of coronene, $(Coro)_3^+$ (in Gauss units, 1 G=0.1 mT) calculated at the CAM-B3LYP/6-311G(d,p) level. Numbering of protons is given in Figure S1.

coro(A)		**coro(B)**		**coro(C)**	
atom	a(H)	atom	a(H)	atom	a(H)
17 H(1)	-2.3233	53 H(1)	0.4262	89 H(1)	-0.4717
18 H(1)	1.0224	54 H(1)	-0.8447	90 H(1)	-0.0738
19 H(1)	-2.0183	55 H(1)	-0.8458	91 H(1)	0.4267
20 H(1)	-1.0782	56 H(1)	0.4266	92 H(1)	-0.8460
21 H(1)	-2.3271	57 H(1)	-0.0748	93 H(1)	0.0740
22 H(1)	1.0237	58 H(1)	-0.4702	94 H(1)	-0.2804
26 H(1)	-3.3493	62 H(1)	-0.4719	98 H(1)	0.4266
27 H(1)	1.6345	63 H(1)	-0.0730	99 H(1)	-0.8456
31 H(1)	1.6334	67 H(1)	-0.2796	103 H(1)	-0.4709
32 H(1)	-3.3467	68 H(1)	0.0737	104 H(1)	-0.0749
34 H(1)	-1.0819	70 H(1)	-0.2813	106 H(1)	0.0743
36 H(1)	-2.0140	72 H(1)	0.0742	108 H(1)	-0.2814
average (G)	-1.0187		-0.1951		-0.1952
average (mT)	-0.1019		-0.0195		-0.0195
scaled (mT)	-0.1112		-0.0213		-0.0213

Table S5. Optimized geometrical parameters of the benzene dimer cation calculated using several functionals. Bond lengths (R) and angles (θ) are in Å and in degrees, respectively. d(A-B) is the interplane distance of the benzene dimer cation, E_{bind} is the binding energy (in kcal/mol). Calculations were carried out using the 6-311G(d,p) basis set.

functional	R	θ	d(A-B)	E_{bind}
CAM-B3LYP	3.359	71.957	3.194	15.61
wB97XD	3.283	71.959	3.122	22.59
LC-wB97XD	3.284	71.916	3.122	22.61
M062X	3.271	70.139	3.077	21.40
wB97X	3.292	71.790	3.127	17.05
B3LYP	3.502	73.320	3.354	18.66

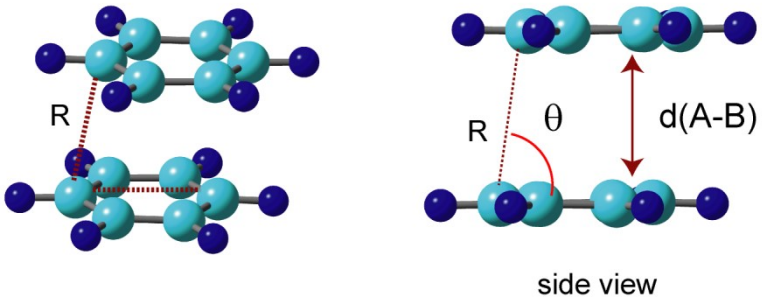

Table S6. Effects of functionals on the ionization potential of coronene (Ip in eV) and Jahn-Teller stabilization energies of the coronene radical cation from vertical ionization point to coro$^+$ (^{2}Au state) (ΔE(J-T) in kcal/mol). Total energies are in a.u.

	coro(0)	VER	coro$^+$(^{2}Au)	Ip	ΔE(J-T)
cam-B3LYP	-921.56357	-921.29527	-921.29892	7.30	-2.29
wB97XD	-921.76313	-921.49377	-921.49739	7.33	-2.27
M062X	-921.73007	-921.45419	-921.45755	7.51	-2.11
B3LYP	-922.09316	-921.83266	-921.83421	7.09	-0.97

Table S7. Effects of functionals on the relative energies (in kcal/mol) of ABA, ABC, and full overlap forms of $(Coro)_3^+$. Single point energy calculations with the wB97XD, M062X, and B3LYP functionals were performed using the optimized structure obtained at the CAM-B3LYP/6-311G(d,p) level.

	cam-B3LYP	wB97XD	M062X	B3LYP
ABA	0.00	0.73	0.43	1.24
ABC	0.10	0.00	0.00	0.00
full	2.44	14.87	17.65	0.89

Table S8. Scaled hyperfine coupling constants (a(H) in mT) of $(Coro)_3^+$ (regular structures), relative energies (ΔE in kcal/mol), and total energies (E(total) in a.u.).

Form	coro(A)	coro(B)	coro(C)	ΔE	E(total)
ABA	-0.11124	-0.02130	-0.02132	0.00	-2764.44724
ABC	-0.11101	-0.02108	-0.02124	0.10	-2764.44709
full	-0.10725	-0.02491	-0.02493	2.44	-2764.44336

1. Geometry of ABA

Number	atom	Type	X	Y	Z
1	6	0	0.000716	1.562058	-3.648463
2	6	0	0.000831	2.286620	-2.447164
3	6	0	0.000506	1.582020	-1.224486
4	6	0	0.000066	0.163690	-1.224735
5	6	0	0.000011	-0.541836	-2.446606
6	6	0	0.000330	0.182247	-3.648041
7	6	0	0.000696	2.287935	0.000484
8	6	0	-0.000258	-0.543894	-0.000554
9	6	0	-0.000098	0.162806	1.224148
10	6	0	0.000437	1.581131	1.224935
11	6	0	-0.000362	-0.543599	2.445495
12	6	0	-0.000883	-1.971367	2.415331
13	6	0	-0.001067	-2.652363	1.239359
14	6	0	-0.000742	-1.964826	-0.001066
15	6	0	-0.000758	-2.651479	-1.242022
16	6	0	-0.000352	-1.969648	-2.417475
17	1	0	-0.000270	-2.505725	-3.358954
18	1	0	-0.001247	-3.733932	-1.237426
19	1	0	0.000958	2.100683	-4.588968
20	1	0	0.000272	-0.356916	-4.587584
21	1	0	-0.001113	-2.508136	3.356415
22	1	0	-0.001467	-3.734812	1.233989
23	6	0	0.001309	3.715368	-2.417548
24	6	0	0.001486	4.397690	-1.240890
25	6	0	0.001205	3.710200	0.000997
26	1	0	0.001543	4.252470	-3.358981
27	1	0	0.001862	5.481102	-1.236574
28	6	0	0.001421	4.396800	1.243419
29	6	0	0.001176	3.713638	2.419559
30	6	0	0.000674	2.284842	2.448140
31	1	0	0.001804	5.480214	1.239877

32	1	0	0.001361	4.250042	3.361388
33	6	0	-0.000103	0.179608	3.647470
34	1	0	-0.000306	-0.360246	4.586615
35	6	0	0.000411	1.559419	3.648901
36	1	0	0.000603	2.097355	4.589800
37	6	0	-3.622779	-3.270300	-2.423795
38	6	0	-3.625409	-1.848058	-2.451695
39	6	0	-3.611701	-1.144938	-1.231634
40	6	0	-3.599403	-1.855917	-0.000994
41	6	0	-3.598999	-3.266859	-0.001926
42	6	0	-3.609345	-3.952098	-1.246034
43	6	0	-3.626403	0.277179	-1.230679
44	6	0	-3.611537	-1.146568	1.230587
45	6	0	-3.626314	0.275546	1.231511
46	6	0	-3.631095	0.987194	0.000885
47	6	0	-3.653364	0.978501	2.451234
48	6	0	-3.668555	0.244765	3.663647
49	6	0	-3.657038	-1.119913	3.662887
50	6	0	-3.624955	-1.851301	2.449725
51	6	0	-3.622151	-3.273514	2.419949
52	6	0	-3.608952	-3.953744	1.241289
53	1	0	-3.620445	-5.037638	1.236444
54	1	0	-3.644677	-3.812804	3.360136
55	1	0	-3.645607	-3.808347	-3.364688
56	1	0	-3.620961	-5.035996	-1.242623
57	1	0	-3.706157	0.788036	4.600946
58	1	0	-3.683810	-1.665166	4.599550
59	6	0	-3.657564	-1.115063	-3.663890
60	6	0	-3.668901	0.249614	-3.662853
61	6	0	-3.653510	0.981744	-2.449477
62	1	0	-3.684526	-1.659074	-4.601268
63	1	0	-3.706533	0.794126	-4.599431
64	6	0	-3.679799	2.402823	-2.419717
65	6	0	-3.682059	3.082748	-1.241126
66	6	0	-3.658816	2.396531	0.001813
67	1	0	-3.712106	2.941262	-3.360057

68	1	0	-3.713417	4.166088	-1.236129
69	6	0	-3.679746	2.399610	2.423346
70	1	0	-3.712048	2.936813	3.364394
71	6	0	-3.682061	3.081099	1.245648
72	1	0	-3.713456	4.164443	1.242092
73	6	0	3.605990	-3.954039	-1.245325
74	6	0	3.596342	-3.268593	-0.001327
75	6	0	3.597958	-1.857649	-0.000624
76	6	0	3.610898	-1.146888	-1.231382
77	6	0	3.624023	-1.850217	-2.451333
78	6	0	3.620028	-3.272454	-2.423200
79	6	0	3.610659	-1.148113	1.230841
80	6	0	3.626816	0.275215	-1.230653
81	6	0	3.631982	0.985427	0.000797
82	6	0	3.626589	0.273991	1.231539
83	6	0	3.660814	2.394744	0.001501
84	6	0	3.684694	3.080739	-1.241546
85	6	0	3.682023	2.400623	-2.420028
86	6	0	3.654604	0.979562	-2.449561
87	6	0	3.669506	0.247222	-3.662816
88	6	0	3.656969	-1.117447	-3.663639
89	1	0	3.683545	-1.661632	-4.600927
90	1	0	3.707717	0.791553	-4.599476
91	1	0	3.616564	-5.037947	-1.241738
92	1	0	3.642297	-3.810682	-3.364002
93	1	0	3.716890	4.164055	-1.236725
94	1	0	3.714838	2.938885	-3.360452
95	6	0	3.605771	-3.955291	1.241991
96	6	0	3.619548	-3.274881	2.420542
97	6	0	3.623492	-1.852666	2.450089
98	1	0	3.616371	-5.039195	1.237316
99	1	0	3.641654	-3.814036	3.360816
100	6	0	3.656114	-1.121112	3.663135
101	6	0	3.668700	0.243559	3.663680
102	6	0	3.654134	0.977116	2.451153
103	1	0	3.682422	-1.666235	4.599886

104	1	0	3.706683	0.786949	4.600895
105	6	0	3.684502	3.079493	1.245229
106	1	0	3.716726	4.162813	1.241501
107	6	0	3.681607	2.398201	2.423039
108	1	0	3.714267	2.935533	3.364000

2. Geometry of ABC

Number	Number	Type	X	Y	Z
1	6	0	0.392477	3.650008	0.554877
2	6	0	0.807534	2.450837	1.153069
3	6	0	0.404365	1.226354	0.579242
4	6	0	-0.406316	1.221938	-0.584424
5	6	0	-0.814589	2.442108	-1.164001
6	6	0	-0.404418	3.645737	-0.571562
7	6	0	0.808286	0.003882	1.163835
8	6	0	-0.806146	-0.004875	-1.162597
9	6	0	-0.402137	-1.227357	-0.578045
10	6	0	0.408498	-1.222952	0.585634
11	6	0	-0.805998	-2.451822	-1.151400
12	6	0	-1.626637	-2.426787	-2.320475
13	6	0	-2.015804	-1.252766	-2.885071
14	6	0	-1.622241	-0.009301	-2.326468
15	6	0	-2.020565	1.230053	-2.891214
16	6	0	-1.635469	2.408212	-2.332793
17	1	0	-1.951593	3.347970	-2.769929
18	1	0	-2.650631	1.222043	-3.771914
19	1	0	0.701780	4.591637	0.992752
20	1	0	-0.717751	4.584016	-1.013724
21	1	0	-1.939361	-3.369871	-2.752882
22	1	0	-2.645373	-1.251511	-3.766170
23	6	0	1.627818	2.425810	2.322388
24	6	0	2.017017	1.251792	2.886942
25	6	0	1.623690	0.008297	2.328195
26	1	0	1.940063	3.368890	2.755148

27	1	0	2.646150	1.250555	3.768357
28	6	0	2.021202	-1.231044	2.893519
29	6	0	1.636284	-2.409208	2.334963
30	6	0	0.816062	-2.443103	1.165706
31	1	0	2.650279	-1.223032	3.774937
32	1	0	1.951863	-3.348982	2.772464
33	6	0	-0.391480	-3.651003	-0.552845
34	1	0	-0.701331	-4.592626	-0.990345
35	6	0	0.405355	-3.646739	0.573635
36	1	0	0.718091	-4.585026	1.016208
37	6	0	-5.343319	2.415583	-1.374514
38	6	0	-4.540444	2.447827	-0.200561
39	6	0	-4.127234	1.229805	0.373061
40	6	0	-4.517108	-0.003061	-0.217254
41	6	0	-5.315595	-0.006365	-1.380518
42	6	0	-5.714856	1.235762	-1.942188
43	6	0	-3.332609	1.233077	1.552520
44	6	0	-4.123439	-1.232638	0.377447
45	6	0	-3.328784	-1.229263	1.556880
46	6	0	-2.930427	0.003566	2.142143
47	6	0	-2.950482	-2.446841	2.154425
48	6	0	-3.379130	-3.661507	1.563060
49	6	0	-4.144246	-3.664947	0.433065
50	6	0	-4.532961	-2.453950	-0.191764
51	6	0	-5.335907	-2.428352	-1.365811
52	6	0	-5.711013	-1.251695	-1.937732
53	1	0	-6.334516	-1.250124	-2.824438
54	1	0	-5.659192	-3.370132	-1.794563
55	1	0	-5.669464	3.354841	-1.806618
56	1	0	-6.338396	1.229113	-2.828841
57	1	0	-3.101189	-4.597037	2.034888
58	1	0	-4.475490	-4.603198	0.002567
59	6	0	-4.155359	3.662208	0.419879
60	6	0	-3.390320	3.665139	1.549957
61	6	0	-2.958100	2.453922	2.145761
62	1	0	-4.489366	4.597917	-0.013999

63	1	0	-3.115206	4.603207	2.018397
64	6	0	-2.171488	2.428415	3.329631
65	6	0	-1.783434	1.251825	3.892160
66	6	0	-2.152165	0.006848	3.317222
67	1	0	-1.893449	3.370308	3.788573
68	1	0	-1.191985	1.249921	4.800313
69	6	0	-2.163922	-2.414707	3.338167
70	1	0	-1.882980	-3.354108	3.800433
71	6	0	-1.779543	-1.234942	3.896541
72	1	0	-1.188100	-1.227979	4.804671
73	6	0	1.778227	1.229115	-3.899700
74	6	0	2.151804	-0.011442	-3.318309
75	6	0	2.930042	-0.005605	-2.143209
76	6	0	3.327494	1.228476	-1.560052
77	6	0	2.948443	2.444783	-2.159731
78	6	0	2.161895	2.410086	-3.343437
79	6	0	3.332813	-1.233819	-1.551322
80	6	0	4.122042	1.234413	-0.380547
81	6	0	4.516360	0.006149	0.216366
82	6	0	4.127268	-1.227995	-0.371769
83	6	0	5.314772	0.011972	1.379709
84	6	0	5.709511	1.258472	1.934669
85	6	0	5.333729	2.433911	1.360628
86	6	0	4.530806	2.456965	0.186527
87	6	0	4.141336	3.666612	-0.440415
88	6	0	3.376233	3.660722	-1.570437
89	1	0	3.097638	4.595259	-2.043841
90	1	0	4.471911	4.605829	-0.011517
91	1	0	1.186718	1.220174	-4.807769
92	1	0	1.880272	3.348497	-3.807290
93	1	0	6.332978	1.258863	2.821399
94	1	0	5.656513	3.376631	1.787685
95	6	0	1.783938	-1.257627	-3.891117
96	6	0	2.172609	-2.432996	-3.326429
97	6	0	2.959039	-2.455934	-2.142392
98	1	0	1.192627	-1.257696	-4.799360

99	1	0	1.895177	-3.375863	-3.783734
100	6	0	3.391783	-3.665842	-1.544321
101	6	0	4.156656	-3.660459	-0.414123
102	6	0	4.540999	-2.444766	0.204143
103	1	0	3.117217	-4.604894	-2.011103
104	1	0	4.491081	-4.595196	0.021522
105	6	0	5.714635	-1.228955	1.943670
106	1	0	6.338050	-1.220349	2.830394
107	6	0	5.343764	-2.409978	1.378137
108	1	0	5.670330	-3.348282	1.811987

3. Geometry of full overlap

Number	Number	Type	X	Y	Z
1	6	0	0.000163	-0.705716	-1.224919
2	6	0	0.000041	0.712908	-1.224920
3	6	0	-0.000001	1.420029	-0.000001
4	6	0	0.000041	0.712908	1.224919
5	6	0	0.000163	-0.705716	1.224920
6	6	0	0.000253	-1.412842	0.000000
7	6	0	0.000085	-0.685784	-3.648993
8	6	0	-0.000058	0.693003	-3.648994
9	6	0	-0.000089	1.418116	-2.447157
10	6	0	-0.000246	2.845812	-2.418113
11	6	0	-0.000292	3.527192	-1.241629
12	6	0	-0.000190	2.840508	-0.000001
13	6	0	-0.000292	3.527193	1.241627
14	6	0	-0.000246	2.845813	2.418112
15	6	0	-0.000089	1.418117	2.447156
16	6	0	-0.000058	0.693005	3.648994
17	6	0	0.000085	-0.685782	3.648994
18	6	0	0.000191	-1.410901	2.447160
19	6	0	0.000309	-2.838596	2.418113
20	6	0	0.000384	-3.519976	1.241633
21	6	0	0.000345	-2.833307	0.000001

22	6	0	0.000384	-3.519977	-1.241632
23	6	0	0.000309	-2.838597	-2.418112
24	6	0	0.000191	-1.410903	-2.447159
25	1	0	0.000105	-1.224346	-4.589232
26	1	0	-0.000155	1.231570	-4.589233
27	1	0	-0.000344	3.382575	-3.359461
28	1	0	-0.000427	4.610323	-1.236910
29	1	0	-0.000427	4.610324	1.236907
30	1	0	-0.000344	3.382577	3.359459
31	1	0	-0.000155	1.231572	4.589232
32	1	0	0.000105	-1.224344	4.589232
33	1	0	0.000332	-3.375353	3.359462
34	1	0	0.000464	-4.603104	1.236919
35	1	0	0.000464	-4.603105	-1.236917
36	1	0	0.000332	-3.375355	-3.359461
37	6	0	-3.898401	-0.713075	-1.230807
38	6	0	-3.898933	0.709192	-1.230808
39	6	0	-3.901393	1.419841	0.000000
40	6	0	-3.898933	0.709192	1.230808
41	6	0	-3.898401	-0.713075	1.230808
42	6	0	-3.900243	-1.423721	0.000000
43	6	0	-3.919902	-0.684556	-3.662881
44	6	0	-3.920415	0.680628	-3.662883
45	6	0	-3.912688	1.413287	-2.450417
46	6	0	-3.933752	2.835077	-2.421797
47	6	0	-3.940637	3.515732	-1.243526
48	6	0	-3.922276	2.830219	-0.000001
49	6	0	-3.940637	3.515733	1.243525
50	6	0	-3.933752	2.835079	2.421795
51	6	0	-3.912688	1.413289	2.450417
52	6	0	-3.920415	0.680630	3.662882
53	6	0	-3.919902	-0.684555	3.662881
54	6	0	-3.911596	-1.417195	2.450414
55	6	0	-3.931570	-2.839006	2.421789
56	6	0	-3.937896	-3.519663	1.243520
57	6	0	-3.920015	-2.834129	0.000001

58	6	0	-3.937896	-3.519664	-1.243518
59	6	0	-3.931570	-2.839007	-2.421787
60	6	0	-3.911596	-1.417197	-2.450413
61	1	0	-3.941304	-1.228415	-4.600409
62	1	0	-3.942228	1.224466	-4.600413
63	1	0	-3.958803	3.373124	-3.362579
64	1	0	-3.969492	4.599261	-1.239285
65	1	0	-3.969492	4.599261	1.239283
66	1	0	-3.958803	3.373126	3.362577
67	1	0	-3.942228	1.224468	4.600413
68	1	0	-3.941304	-1.228413	4.600410
69	1	0	-3.956246	-3.377073	3.362570
70	1	0	-3.965927	-4.603214	1.239274
71	1	0	-3.965927	-4.603214	-1.239271
72	1	0	-3.956246	-3.377075	-3.362568
73	6	0	3.898494	-0.712766	-1.230802
74	6	0	3.898864	0.709497	-1.230803
75	6	0	3.901241	1.420146	0.000000
76	6	0	3.898864	0.709497	1.230803
77	6	0	3.898494	-0.712765	1.230803
78	6	0	3.900451	-1.423413	0.000000
79	6	0	3.919883	-0.684251	-3.662875
80	6	0	3.920215	0.680941	-3.662876
81	6	0	3.912445	1.413595	-2.450417
82	6	0	3.933291	2.835390	-2.421796
83	6	0	3.940102	3.516047	-1.243526
84	6	0	3.921874	2.830531	-0.000001
85	6	0	3.940102	3.516047	1.243525
86	6	0	3.933291	2.835392	2.421794
87	6	0	3.912445	1.413597	2.450417
88	6	0	3.920215	0.680943	3.662876
89	6	0	3.919883	-0.684249	3.662875
90	6	0	3.911724	-1.416886	2.450414
91	6	0	3.931876	-2.838696	2.421788
92	6	0	3.938318	-3.519353	1.243519
93	6	0	3.920375	-2.833822	0.000001

94	6	0	3.938318	-3.519354	-1.243517
95	6	0	3.931876	-2.838697	-2.421786
96	6	0	3.911724	-1.416887	-2.450413
97	1	0	3.941313	-1.228099	-4.600408
98	1	0	3.941906	1.224774	-4.600412
99	1	0	3.958224	3.373440	-3.362579
100	1	0	3.968777	4.599580	-1.239287
101	1	0	3.968777	4.599580	1.239284
102	1	0	3.958224	3.373442	3.362577
103	1	0	3.941906	1.224777	4.600411
104	1	0	3.941313	-1.228097	4.600409
105	1	0	3.956588	-3.376759	3.362570
106	1	0	3.966477	-4.602900	1.239275
107	1	0	3.966477	-4.602901	-1.239273
108	1	0	3.956588	-3.376761	-3.362568

4. Harmonic vibrational frequency (in cm^{-1}) of $Coro^{+}$ at the $^{2}A_{u}$ state calculated at the CAM-B3LYP/6-311G(d,p) level.

102	101	100	99	98	97
AG	B2U	B1U	AG	B3G	B2U
3220.532	3220.343	3218.445	3217.93	3217.633	3217.265
96	95	94	93	92	91
B1U	B3G	AG	B1U	B2U	B3G
3205.533	3205.017	3204.797	3203.874	3203.135	3202.694
90	89	88	87	86	85
AG	B2U	AG	B1U	B3G	B1U
1718.473	1667.632	1650.459	1637.635	1601.473	1597.099
84	83	82	81	80	79
B2U	B3G	B1U	AG	B2U	AG
1580.729	1568.385	1533.51	1530.787	1524.144	1520.104
78	77	76	75	74	73
B3G	B1U	AG	B3G	B2U	B2U

1479.733	1459.808	1457.378	1456.266	1440.076	1404.944
72	71	70	69	68	67
AG	B1U	B1U	B2U	B3G	AG
1404.075	1397.655	1360.398	1354.633	1342.21	1283.268
66	65	64	63	62	61
B3G	B2U	AG	B1U	B2U	B3G
1271.467	1258.828	1255.111	1249.76	1237.781	1209.797
60	59	58	57	56	55
AG	B1U	B2U	B2U	B1U	AG
1199.117	1197.556	1178.543	1166.842	1165.258	1072.197
54	53	52	51	50	49
B3G	B2G	AU	AG	B3U	B2G
1037.114	1031.861	1029.171	1026.858	1022.339	1017.081
48	47	46	45	44	43
B1G	AU	B3G	B3U	B2G	B1G
1009.509	1004.074	951.698	910.9592	891.9427	886.4415
42	41	40	39	38	37
AU	B1U	B3U	B2U	B1G	B1U
851.1703	841.3075	832.0702	813.5258	805.6066	785.8767
36	35	34	33	32	31
B2U	AU	B3U	B3G	B2G	AG
780.0052	774.4076	758.061	747.7511	711.7529	694.7491
30	29	28	27	26	25
B1U	B3G	B1G	B2G	B3G	B2G
683.4067	681.8647	675.3881	673.3925	644.5558	587.3786
24	23	22	21	20	19
B3U	B1U	AU	B3U	AU	AG
575.0503	566.4083	561.2933	533.5966	509.3985	502.1834
18	17	16	15	14	13
AG	B3G	B2U	B1G	B2G	B2U
493.9482	480.3549	469.8108	450.8933	443.3776	388.4935
12	11	10	9	8	7
B1U	AG	B1G	AU	B3U	B2G
384.6571	374.9324	302.8381	301.4874	296.9332	284.0111
6	5	4	3	2	1
B2G	B1G	B3G	B3U	AU	B3U

222.7102	161.7655	142.9997	123.938	90.5171	85.5568

5. Harmonic vibrational frequency (in cm^{-1}) of $Coro^{+}$ at the $^{2}B_{3u}$ state calculated at the CAM-B3LYP/6-311G(d,p) level.

102	101	100	99	98	97
AG	B1U	B2U	B3G	AG	B2U
3220.566	3220.346	3219.009	3218.859	3216.572	3216.409
96	95	94	93	92	91
B1U	AG	B3G	B2U	B1U	B3G
3205.446	3204.947	3204.815	3203.967	3202.844	3202.498
90	89	88	87	86	85
AG	B1U	AG	B2U	B1U	B3G
1695.483	1664.297	1648.231	1632.536	1611.49	1604.772
84	83	82	81	80	79
B3G	B2U	B1U	B3G	B2U	AG
1587.74	1554.958	1550.71	1521.197	1517.971	1504.94
78	77	76	75	74	73
AG	B3G	B1U	AG	B1U	B2U
1477.022	1464.914	1462.22	1450.684	1443.702	1409.649
72	71	70	69	68	67
AG	B2U	B2U	B3G	B1U	AG
1404.321	1396.225	1364.611	1356.139	1351.999	1282.702
66	65	64	63	62	61
B3G	B1U	AG	B2U	B2U	B3G
1271.705	1259.694	1252.549	1250.402	1233.163	1221.651
60	59	58	57	56	55
B1U	AG	B1U	B2U	B2U	AG
1197.868	1186.1	1178.013	1172.59	1160.002	1072.071
54	53	52	51	50	49
B3G	B2G	B3U	AU	AG	B1G
1045.512	1031.15	1026.632	1024.469	1019.113	1016.609
48	47	46	45	44	43
B2G	AU	B3G	B3U	B1G	B2G

1011.28	1005.077	951.5347	911.4998	893.9711	884.5146
42	41	40	39	38	37
B3U	B2U	AU	B1U	B1G	B2U
849.3861	840.6476	833.4122	813.8101	805.6619	785.0379
36	35	34	33	32	31
B1U	B3U	AU	B3G	B2G	AG
781.2322	773.3202	759.6083	726.8092	711.7898	695.312
30	29	28	27	26	25
B1U	B2G	B1G	B3G	B3G	B2G
683.2118	678.3546	670.7837	645.3329	640.3599	587.0483
24	23	22	21	20	19
B3U	B1U	B3U	AU	AU	AG
575.9968	566.4135	558.5582	536.5529	507.8517	502.9048
18	17	16	15	14	13
AG	B3G	B2U	B2G	B1G	B1U
493.8505	478.5496	469.9093	450.8497	442.8187	388.283
12	11	10	9	8	7
B2U	AG	B2G	B3U	AU	B1G
385.1019	375.7207	302.3938	301.6468	296.4206	284.5979
6	5	4	3	2	1
B2G	B1G	B3U	B3U	AU	B3G
222.4613	161.8966	124.008	90.5462	85.6181	-157.08