Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Excited States and Excitonic Interactions in Prototypic Polycyclic Aromatic Hydrocarbon Dimers as Models for Graphitic Interaction in Carbon Dots

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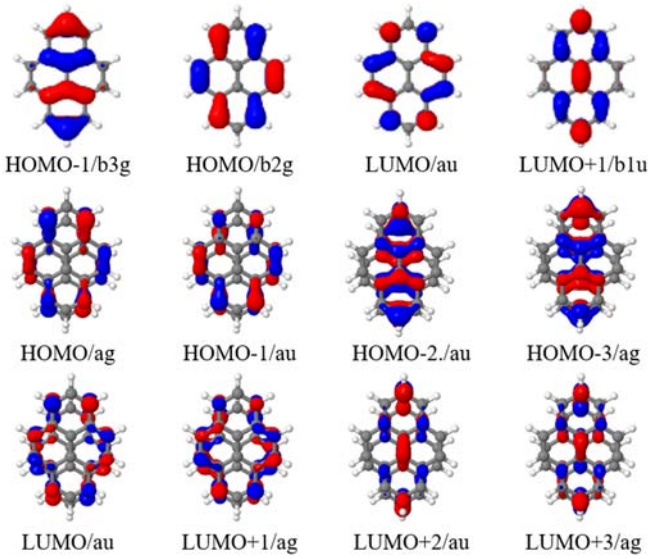

Figure S1. Natural Transition Orbitals of pyrene monomer (the first row) and dimer (the second and third row) calculated for the S_1 state at SOS-ADC(2)/def2-TZVP level using Ci symmetry labeling

Table S1. Excitation energies, oscillator strengths, CT values and PR_{NTO} for the lowest few dark and bright excited states of the pyrene dimer calculated using several computational methods and using Ci symmetry labeling

State no.	State	ΔE(eV)	*f*	CT	PR_{NTO}
DFT/MRCI[a]					
1	1^1Au	3.38	0.00	-	
2	2^1Ag	3.41	0.00	-	
3	2^1Au	3.55	0.50	-	
4	3^1Ag	3.58	0.00	-	
5	4^1Ag	3.76	0.00	-	
6	3^1Au	3.97	0.14	-	
13	6^1Au	4.56	0.11		
19	9^1Au	4.83	0.47		
27	13^1Au	5.38	1.35		
29	15^1Au	5.48	0.14		
33	17^1Au	5.58	0.32		
71	34^1Au	6.55	2.35		
SC-NEVPT2[a]					
1	2^1Ag	3.78	0.00	-	
2	1^1Au	3.78	0.00	-	
3	2^1Au	3.91	0.00	-	
4	3^1Au	4.05	0.52	-	
5	3^1Ag	4.07	0.00	-	

6	4^1Ag	4.28	0.00	-	
12	6^1Au	5.02	0.31		
13	9^1Au	5.16	0.12		
16	10^1Au	5.37	0.56		
SOS-ADC(2)[b]					
1	1^1Au	3.66	0.00	0.03	3.80
2	2^1Ag	3.66	0.00	0.04	3.74
3	3^1Ag	4.05	0.00	0.03	2.15
4	2^1Au	4.08	0.46	0.19	1.57
5	4^1Ag	4.59	0.00	0.99	1.99
6	3^1Au	4.64	0.00	0.08	2.26
11	5^1Au	4.97	0.09	0.31	3.59
12	6^1Au	5.08	0.33	0.22	3.22
18	9^1Au	5.34	0.16	0.74	2.36
24	12^1Au	5.75	1.90	0.16	2.04
30	15^1Au	6.02	0.33	0.77	1.88
TD-CAM-B3LYP[b]					
1	2^1Ag	3.94	0.00	0.26	2.30
2	1^1Au	3.96	0.38	0.33	1.32
3	3^1Ag	4.00	0.00	0.26	3.77
4	2^1Au	4.00	0.00	0.26	3.84
5	4^1Ag	4.26	0.00	0.51	2.00
6	3^1Au	4.41	0.08	0.43	1.29
10	5^1Au	4.99	0.17	0.39	2.47
15	8^1Au	5.25	0.34	0.34	2.10
24	12^1Au	5.76	1.23	0.26	2.20
26	13^1Au	5.95	0.23	-	-
55	28^1Au	6.88	0.46	-	-
57	29^1Au	6.99	1.03	-	-
86	43^1Au	7.65	0.98	-	-
88	44^1Au	7.65	0.32	-	-

[a]SV(P) basis set; [b]def2-TZVP basis set; [c]relative to DFT/MRCI results.

Table S2. Excited states properties of the lowest four states (dominant contributions and percentage using NTOs, charge transfer CT and participation ratios PR_{NTO}) of pyrene dimer calculated at several computational levels and using Ci symmetry labeling

State. no	State	Dominant contributions	%	CT	PR_{NTO}
DFT/MRCI[a]					
1	1^1Au	H/L+2	28	-	-
		H-3/L	20		
		H-2/L+1	19		
		H-1/L+3	17		

		H-2/L	28		
2	2^1Ag	H/L+3	24	-	-
		H-1/L+2	18		
		H-3/L+1	14		
3	2^1Au	H/L	79	-	-
4	3^1Ag	H/L+1	50	-	-
		H-1/L	33		
SC-NEVPT2[a]					
		H/L+3	25		
1	2^1Ag	H-2/L	25		
		H-1/L+2	19		
		H-3/L+1	15		
		H/L+3	26		
2	1^1Au	H-3/L	21		
		H-2/L+1	16		
		H-1/L+2	16		
3	2^1Au	H/L	66		
4	3^1Au	H-1/L+1	63		
5	3^1Ag	H/L+1	51		
		H-1/L	26		
SOS-ADC(2)[b]					
		H/L+2	33		
1	1^1Au	H-3/L	22	0.03	3.80
		H-2/ L+1	21		
		H-1/L+3	19		
		H-2/L	32		
2	2^1Ag	H/L+3	28	0.04	3.74
		H-1/L+2	20		
		H-3/L+1	16		
3	3^1Ag	H/L+1	51	0.03	2.15
		H-1/L	41		
4	2^1Au	H/L	77	0.19	1.57
TD-CAM-B3LYP[b]					
1	2^1Ag	H-1/L	50	0.26	2.30
		H/L+1	43		
2	1^1Au	H/L	88	0.33	1.32
		H-2/L	35		
3	3^1Ag	H/L+3	28	0.26	3.77
		H-1/L+2	21		
		H-3/L+1	14		
		H/L+2	37		
4	2^1Au	H-3/L	21	0.26	3.84
		H-2/L+1	21		
		H-1/L+3	19		

[a]SV(P) basis set; [b]def2-TZVP basis set.

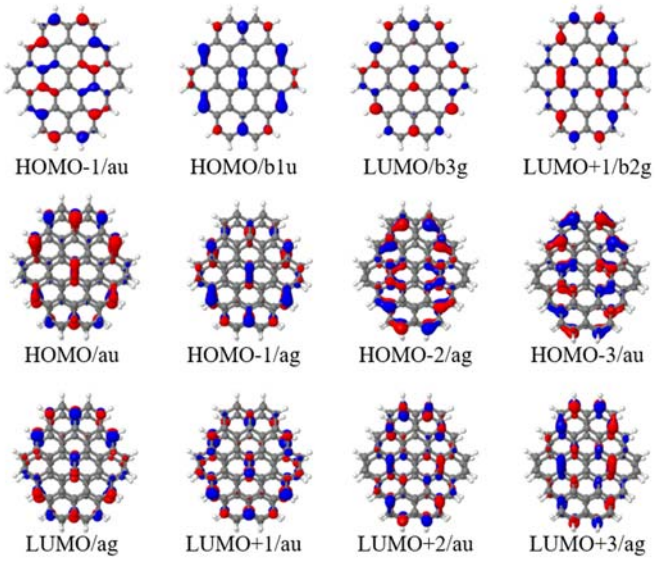

Figure S2. Natural Transition Orbitals of circum-1-pyrene monomer (the first row) and dimer (the second and third row) calculated for the S_1 state at SOS-ADC(2)/SV(P) level using C_i symmetry labeling

Table S3. Excitation energies, oscillator strengths, CT values and PR_{NTO} for the lowest few dark and bright excited states of the circum-1-pyrene dimer calculated using several computational methods and using Ci symmetry labeling

State no.	State	ΔE(eV)	f	CT	PR_{NTO}
SOS-ADC(2)[a]					
1	2^1Ag	2.50	0.00	0.29	2.76
2	1^1Au	2.54	0.55	0.37	1.06
3	2^1Au	2.57	0.00	0.26	3.88
4	3^1Ag	2.66	0.00	0.26	1.98
5	4^1Ag	2.83	0.00	0.51	1.98
7	3^1Au	3.15	0.13	0.38	1.24
TD-CAM-B3LYP [b]					
1	1^1Au	2.62	0.39	0.49	1.14
2	2^1Ag	2.66	0.00	0.22	1.81
3	3^1Ag	2.81	0.00	0.26	2.96
4	4^1Ag	2.83	0.00	0.75	1.71
5	2^1Au	2.87	0.00	0.21	4.25
6	3^1Au	3.06	0.19	0.48	1.22
17	8^1Au	3.83	0.92	0.30	3.91
20	10^1Au	3.97	0.14	0.67	3.56

[a]SV(P) basis set.;[b]SVP basis set.

Table S4. Excited states properties of the lowest four states (dominant contributions and percentage using NTOs, charge transfer CT and participation ratios PR_{NTO}) of circum-1-pyrene dimer calculated at several computational levels and using Ci symmetry labeling

State. no	State	Dominant contributions	%	CT	PR_{NTO}
SOS-ADC(2)[a]					
1	2^1Ag	H-2/L H/L+2	46 31	0.29	2.76
2	1^1Au	H/L H/L+3	93 33	0.37	1.06
3	2^1Au	H-3/L H-2/L+1 H-1/L+2	23 21 18	0.26	3.88
4	3^1Ag	H-1/L H/L+1	52 44	0.26	1.98
TD-CAM-B3LYP[b]					
1	1^1Au	H/ L	94	0.49	1.14
2	2^1Ag	H-1/ L H/ L+1	70 26	0.22	1.81
3	3^1Ag	H-2/ L H/ L+2 H-1/ L+3	50 26 12	0.26	2.96
4	4^1Ag	H/ L+1 H-1/ L H/ L+3	72 27 31	0.75	1.71
5	2^1Au	H-3/ L H-2/ L+1 H-1/ L+2	23 23 19	0.21	4.25

[a]SV(P) basis set.;[b]SVP basis set.

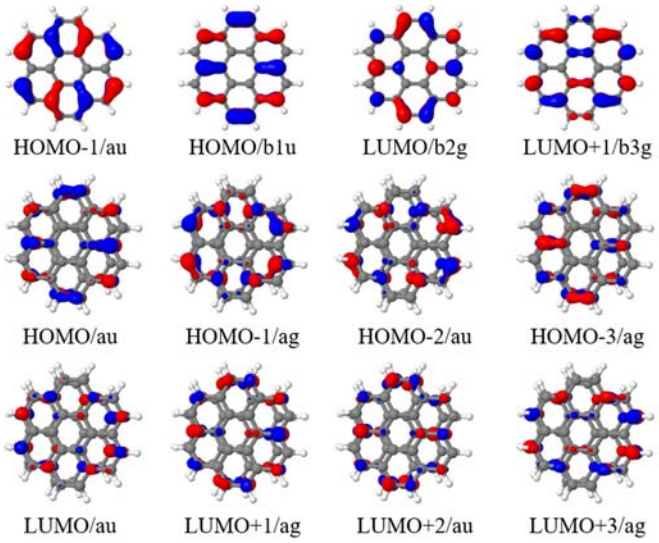

Figure S3. Natural Transition Orbitals of coronene monomer (the first row) and dimer (the second and third row) calculated for the S_1 state at SOS-ADC(2)/def2-TZVP level using Ci symmetry labeling

Table S5. Excitation energies, oscillator strengths and CT values for the lowest bright and dark excited states of the coronene dimer calculated using several computational methods and using Ci symmetry labeling

State no.	State	ΔE(eV)	f	CT	PR_{NTO}
DFT/MRCI[a]					
1	1^1Au	2.90	0.00	-	
2	2^1Ag	2.92	0.00	-	
3	2^1Au	3.32	0.01	-	
4	3^1Ag	3.43	0.00	-	
6	3^1Au	3.84	0.26	-	
12	6^1Au	3.99	0.16		
21	10^1Au	4.28	1.51	-	
22	11^1Au	4.32	1.31		
SC-NEVPT2[b]					
1	2^1Ag	3.01	0.00		
2	1^1Au	3.07	0.00		
3	2^1Au	3.58	0.02		
4	3^1Ag	3.65	0.00		
5	4^1Ag	3.71	0.00		
6	5^1Ag	3.86	0.00		
8	3^1Au	3.93	0.09		
14	10^1Au	4.24	2.40		
16	7^1Au	4.41	0.31		
17	8^1Au	4.42	0.32		
SOS-ADC(2)[c]					
1	2^1Ag	3.20	0.00	0.07	3.28

2	1^1Au	3.25	0.00	0.02	3.93
3	2^1Au	3.73	0.01	0.12	2.90
4	3^1Ag	3.80	0.00	0.05	3.62
5	4^1Ag	4.09	0.00	0.35	2.23
7	3^1Au	4.25	0.00	0.24	4.78
9	4^1Au	4.30	0.43	0.56	2.45
11	5^1Au	4.33	0.13	0.18	4.82
21	10^1Au	4.60	0.23	0.78	2.26
22	11^1Au	4.67	1.27	0.12	3.31
24	12^1Au	4.80	0.40	0.29	3.58
25	13^1Au	4.81	0.44	0.28	3.97
TD-CAM-B3LYP[c]					
1	2^1Ag	3.50	0.00	0.26	3.57
2	1^1Au	3.54	0.00	0.26	4.22
3	2^1Au	3.76	0.00	0.27	3.23
4	3^1Ag	3.81	0.00	0.26	4.05
5	4^1Ag	4.20	0.00	0.35	2.13
6	5^1Ag	4.34	0.00	0.34	2.23
7	3^1Au	4.35	0.24	0.45	2.54
9	4^1Au	4.43	0.02	0.48	3.21
10	5^1Au	4.44	0.03	0.49	3.02
21	10^1Au	4.77	1.23	0.27	3.92
22	11^1Au	4.83	1.03	0.31	2.73

[a]SV(P) basis set; [b]SVP basis set; [c]def2-TZVP basis set.

Table S6 Excited states properties of the lowest four states and selected higher states (dominant contributions and percentage using NTOs, charge transfer CT and participation ratios PR_{NTO}) of coronene dimer calculated at several computational levels and using Ci symmetry labeling

State. no	State	Dominant contributions	%	CT	PR_{NTO}
DFT/MRCI[a]					
1	1^1Au	H/L+2	24		
		H-2/ L+1	22		
		H-1/L+3	19		
		H-3/L	17		
2	2^1Ag	H/L	33		
		H-1/L+1	24		
		H-2/L+3	15		
		H-3/L+2	11		
3	2^1Au	H/L+1	39		
		H-1/ L	29		
		H-2 L+2	11		
4	3^1Ag	H/L+3	28		
		H-2/ L	26		
		H-1/L+2	18		
		H-3/L+1	14		

5	4^1Ag	H/L	42		
		H-1/L+1	39		
6	3^1Au	H-1/L	44		
		H/L+1	24		
21	10^1Au	H-3/ L	25		
		H-1/L+3	19		
		H-2/L+1	13		
		H/L+2	10		
SC-NEVPT2[b]					
1	2^1Ag	H/L+3	36		
		H-3/L	19		
		H-1/L+2	16		
		H-2/L+1	10		
2	1^1Au	H/L+2	26		
		H-2/L+1	24		
		H-1/L+3	19		
		H-3/L	19		
3	2^1Au	H-1/L	34		
		H/L+1	30		
		H-2/L+1	16		
		H-3/L+3	10		
4	3^1Ag	H-1/L+3	30		
		H/L+2	23		
		H-3/L+1	16		
		H-2/L	13		
8	3^1Au	H-1/L	43		
		H-2/L+2	36		
14	10^1Au	H-3/L	24		
		H-1/L+3	23		
		H-2/L+1	15		
		H/L+2	12		
SOS-ADC(2)[c]					
1	2^1Ag	H/L	41	0.07	3.28
		H-1/L+1	27		
		H-2/L+2	16		
		H-3/L+3	12		
2	1^1Au	H/L+3	28	0.02	3.93
		H-2/L+1	25		
		H-1/L+2	22		
		H-3/L	20		

3	2^1Au	H/L+1 H-1/L H-2/L+3	45 34 12	0.12	2.90
4	3^1Ag	H/L+2 H-2/L H-1/L+3 H-3/L+1	34 30 19 14	0.05	3.62
9	4^1Au	H-1/L H/L+1	52 30	0.56	2.45
11	5^1Au	H(H-6)/ L+1(L+5) H-1(H-4)/ L(L+7) H-2/L+4 H-3(H- 8)/L+6(L+2)	29 25 12 10	0.18	4.82
22	11^1Au	H-3(H-5)/L H-1/L+2 H-2/L+1	43 25 14	0.12	3.31
TD-CAM-B3LYP[c]					
1	2^1Ag	H/L H-1/L+1 H-2/L+3 H-3/L+2	39 30 16 12	0.26	3.57
2	1^1Au	H/L+2 H-2/L+1 H-1/L+3 H-3/L	29 25 23 20	0.26	4.22
3	2^1Au	H/L+1 H-1/L	42 33	0.27	3.23
4	3^1Ag	H/L+3 H-2/L H-1/L+2 H-3/L+1	30 28 22 18	0.26	4.05
7	3^1Au	H-1/L H/L+1	53 33	0.45	2.54
9	4^1Au	H/L+2 H-3/L H-1/L+3	40 32 21	0.48	3.21

		H-2/L+1	47		
10	5^1Au	H-1/L+3	28	0.49	3.02
		H/L+2	18		
		H-3/L	38		
		H-1/L+3	26		
21	10^1Au	H-2/L+1	19	0.27	3.92
		H/L+2	12		

[a]SV(P) basis set; [b]SVP basis set; [c]def2-TZVP basis set.

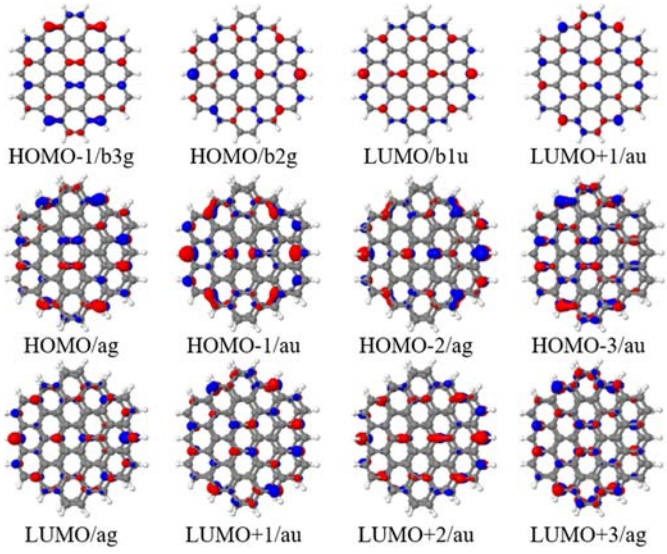

Figure S4. Natural Transition Orbitals of circum-1-coronene monomer (the first row) and dimer (the second and third row) calculated for the S_1 state at SOS-ADC(2)/SV(P) level using Ci symmetry labeling

Table S7 Excited states properties of the lowest four states (dominant contributions and percentage using NTOs, charge transfer CT and participation ratios PR_{NTO}) of circum-1-coronene dimer calculated at several computational levels and Ci symmetry labeling

State. no	State	Dominant contributions	%	CT	PR_{NTO}
SOS-ADC(2)[a]					
1	2^1Ag	H/L	52	0.21	2.43
		H-1/L+1	31		
2	1^1Au	H/L+2	29	0.06	3.94
		H-2/L+1	26		
		H-1/L+3	20		
		H-3/L	19		

3	2^1Au	H/L+1 H-1/L	52 42	0.40	2.11
4	3^1Ag	H-1/L+1 H/L	58 39	0.50	1.92
TD-CAM-B3LYP[b]					
1	2^1Ag	H/L+1 H-1/L	44 36	0.28	3.02
2	1^1Au	H/L+2 H-2/L H-3(H-1)/ L+1(L+3) H-1(H-3)/ L+3(L+1)	28 26 21 21	0.23	4.38
3	2^1Au	H/L H-1/L+1 H-2/L+1	46 40 31	0.29	2.65
4	3^1Ag	H/L+3 H-1/L+2 H-3/L	24 22 19	0.22	4.15
18	9^1Au	H-1(H-3)/ L+3(L+1, L+5) H-3/L+1 H-2/L H/L+2	30 29 19 18	0.24	4.34

[a]SV(P) basis set; [b]SVP basis set.

Table S8. Excitation energies, oscillator strengths and CT values for the lowest bright and dark excited states of the circum-1-coronene dimer calculated using several computational levels and Ci symmetry labeling

State no.	State	ΔE(eV)	f	CT	PR_{NTO}
SOS-ADC(2) [a]					
1	2^1Ag	2.17	0.00	0.21	2.43
2	1^1Au	2.30	0.00	0.06	3.94
3	2^1Au	2.50	0.03	0.40	2.11
4	3^1Ag	2.64	0.00	0.50	1.92
5	4^1Ag	2.70	0.00	0.09	3.40
6	3^1Au	2.82	0.66	0.73	2.26
TD-CAM-B3LYP [b]					
1	2^1Ag	2.52	0.00	0.28	3.02
2	1^1Au	2.60	0.00	0.23	4.38
3	2^1Au	2.69	0.01	0.29	2.65
4	3^1Ag	2.79	0.00	0.22	4.15
5	4^1Ag	2.93	0.00	0.45	2.05
6	3^1Au	3.06	0.30	0.56	2.77
18	9^1Au	3.57	1.69	0.24	4.34

[a]SV(P) basis set; [b]SVP basis set.

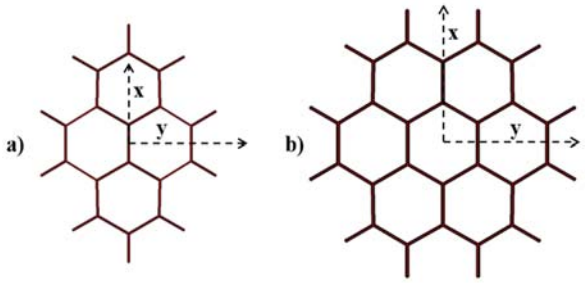

Figure S5. Definition of x and y for pyrene and coronene dimer structures of a) pyrene and b) coronene

Table S9. Adiabatic energy (in eV) comparison for different S1 optimized pyrene dimer calculated at SOS-ADC(2)/SV(P) level[a]

Symmetry	C2h[b]		Ci[c]	
Label	Ag	Bg	Ag	Au
Initial displacement x 0.0, y 0.4	3.46	3.49		
x 0.3 x 1.0	3.47	3.48	3.47	3.96
x 2.3	3.90	3.46	3.90	3.96

[a]reference energy is ground state minimum as shown in Figure 1, total energy = -1226.32229 Hartree. Definition of x and y see Figure S5; [b]Unless specified, y=0.0Å; [c]Unless specified, y=0.2Å

Table S10. Adiabatic energy (in eV) comparison for different S1 optimized coronene dimer calculated at SOS-ADC(2)/SV(P) level[a]

Symmetry	C2h[b]		Ci[c]	
Label	Ag	Bg	Ag	Au
Initial displacement x 0.0, y 0.4	3.21			
x 0.3 x 1.0	3.58	3.10	3.10	3.68
x 2.3	3.81	3.09	3.09	3.20

[a]reference energy is ground state minimum as shown in Figure 1, total energy = -1836.08180 Hartree. Definition of x and y see Figure S5; [b]Unless specified, y=0.0Å; [c]Unless specified, y=0.2Å.

Cartesian geometries (Å)

C_i symmetry: 1^1Ag

Geometry optimization of ground state at MP2/def2-TZVP level

Pyrene dimer

C	-0.0707346	-0.1301643	-1.6716092
C	-0.0791771	-1.5570498	-1.6406501
C	-1.2983654	0.5903356	-1.6483433
C	-1.3150478	-2.2608247	-1.5800969
C	-2.5330450	-0.1464258	-1.5937873
C	-2.5413817	-1.5080631	-1.5639687
C	2.3899748	-0.1796120	-1.7798880
C	2.3821489	-1.5412915	-1.7502677
C	1.1647536	0.5737165	-1.7414198
C	1.1480368	-2.2774030	-1.6733248
C	1.1508504	1.9761641	-1.7733317
C	-0.0545976	2.6760627	-1.7459703
C	-1.2680389	1.9924305	-1.6821376
C	1.1182994	-3.6792562	-1.6359147
C	-0.0954109	-4.3625115	-1.5674824
C	-1.3014261	-3.6629276	-1.5443162
H	-3.4668315	0.4094431	-1.5791686
H	-3.4824474	-2.0509610	-1.5270919
H	3.3295780	0.3636319	-1.8357426
H	3.3158775	-2.0968437	-1.7841056
H	2.0933322	2.5151199	-1.8218528
H	-0.0480255	3.7612574	-1.7648354
H	-2.2041769	2.5440338	-1.6600008
H	2.0539556	-4.2315253	-1.6641358
H	-0.1017117	-5.4479571	-1.5411455
H	-2.2439704	-4.2025312	-1.5014985
C	0.0791771	1.5570498	1.6406501
C	0.0707346	0.1301643	1.6716092
C	-1.1480368	2.2774030	1.6733248
C	-1.1647536	-0.5737165	1.7414198
C	-2.3821489	1.5412915	1.7502677
C	-2.3899748	0.1796120	1.7798880
C	2.5413817	1.5080631	1.5639687
C	2.5330450	0.1464258	1.5937873
C	1.3150478	2.2608247	1.5800969
C	1.2983654	-0.5903356	1.6483433
C	1.3014261	3.6629276	1.5443162
C	0.0954109	4.3625115	1.5674824
C	-1.1182994	3.6792562	1.6359147
C	1.2680389	-1.9924305	1.6821376
C	0.0545976	-2.6760627	1.7459703
C	-1.1508504	-1.9761641	1.7733317
H	-3.3158775	2.0968437	1.7841056
H	-3.3295780	-0.3636319	1.8357426
H	3.4824474	2.0509610	1.5270919
H	3.4668315	-0.4094431	1.5791686
H	2.2439704	4.2025312	1.5014985

H	0.1017117	5.4479571	1.5411455
H	-2.0539556	4.2315253	1.6641358
H	2.2041769	-2.5440338	1.6600008
H	0.0480255	-3.7612574	1.7648354
H	-2.0933322	-2.5151199	1.8218528

C_i symmetry: 1^1Ag

Geometry optimization of ground state at MP2/SV(P) level

Circum-1-pyrene dimer

C	-0.0363318	-0.0687697	-1.5497054
C	-0.0419790	-1.4879702	-1.5666941
C	-1.2750219	0.6514727	-1.5766120
C	-1.2842724	-2.1995263	-1.5052128
C	-2.5109603	-0.0558453	-1.5153334
C	-2.5160551	-1.4833361	-1.5440996
C	2.4376586	-0.0741572	-1.6166944
C	2.4309178	-1.5016650	-1.6455304
C	1.2054959	0.6423182	-1.6273664
C	1.1965111	-2.2087428	-1.5560853
C	1.2108351	2.0692319	-1.6185220
C	-0.0278937	2.7894440	-1.6536536
C	-1.2694170	2.0783886	-1.5678461
C	1.1898813	-3.6354229	-1.5852992
C	-0.0513394	-4.3472732	-1.5042223
C	-1.2895364	-3.6262351	-1.5344301
C	3.6657577	2.0436239	-1.7084098
C	3.6799122	0.6448153	-1.7078395
C	2.4519110	2.7759014	-1.7071826
C	4.9137308	-0.1138132	-1.7396745
C	4.9078395	-1.4826423	-1.7411916
C	3.6701731	-2.2306803	-1.6599565
C	3.6442577	-3.6292180	-1.6660324
C	2.4275840	-4.3517769	-1.5921901
C	2.3911342	-5.7852632	-1.5931515
C	1.1942093	-6.4679843	-1.5337604
C	-0.0570156	-5.7699368	-1.5199509
C	-1.3128533	-6.4586427	-1.4824552
C	-2.5317544	-4.3333527	-1.4904168
C	-2.5061123	-5.7670552	-1.4927841
C	-3.7602496	-2.2031199	-1.5075691
C	-3.7450568	-3.6017723	-1.5144180
C	-3.7505945	0.6723084	-1.5556416
C	-4.9902869	-0.0771286	-1.5366903
C	-4.9946656	-1.4459187	-1.5381256
C	-2.5078297	2.7942093	-1.6058989
C	-3.7261081	2.0709160	-1.5572293
C	-0.0231011	4.2121331	-1.6750570
C	-1.2737499	4.9087029	-1.6971694
C	-2.47H-141	4.2271621	-1.6377743
C	2.4248575	4.2091911	-1.7373865
C	1.2307513	4.8994625	-1.7479841
H	4.6181057	2.5912238	-1.7623063

```
H     5.8636200    0.4357719   -1.7947353
H     5.8549576   -2.0395969   -1.7783863
H     4.5933501   -4.1849492   -1.6984869
H     3.3405566   -6.3386656   -1.6187664
H     1.1874454   -7.5672143   -1.5341943
H    -1.3143414   -7.5579147   -1.4831495
H    -3.4599149   -6.3133271   -1.4795339
H    -4.6988131   -4.1503978   -1.5079418
H    -5.9375610    0.4795152   -1.5529711
H    -5.9466246   -1.9958363   -1.5365330
H    -4.6758226    2.6255357   -1.5721750
H    -1.2677045    6.0065990   -1.7341618
H    -3.4214113    4.7796525   -1.6482810
H     3.3775374    4.7547153   -1.7864922
H     1.2312205    5.9974453   -1.7846294
C     0.0419790    1.4879702    1.5666941
C     0.0363318    0.0687697    1.5497054
C    -1.1965111    2.2087428    1.5560853
C    -1.2054959   -0.6423182    1.6273664
C    -2.4309178    1.5016650    1.6455304
C    -2.4376586    0.0741572    1.6166944
C     2.5160551    1.4833361    1.5440996
C     2.5109603    0.0558453    1.5153334
C     1.2842724    2.1995263    1.5052128
C     1.2750219   -0.6514727    1.5766120
C     1.2895364    3.6262351    1.5344301
C     0.0513394    4.3472732    1.5042223
C    -1.1898813    3.6354229    1.5852992
C     1.2694170   -2.0783886    1.5678461
C     0.0278937   -2.7894440    1.6536536
C    -1.2108351   -2.0692319    1.6185220
C     3.7450568    3.6017723    1.5144180
C     3.7602496    2.2031199    1.5075691
C     2.5317544    4.3333527    1.4904168
C     4.9946656    1.4459187    1.5381256
C     4.9902869    0.0771286    1.5366903
C     3.7505945   -0.6723084    1.5556416
C     3.7261081   -2.0709160    1.5572293
C     2.5078297   -2.7942093    1.6058989
C     2.47H-141   -4.2271621    1.6377743
C     1.2737499   -4.9087029    1.6971694
C     0.0231011   -4.2121331    1.6750570
C    -1.2307513   -4.8994625    1.7479841
C    -2.4519110   -2.7759014    1.7071826
C    -2.4248575   -4.2091911    1.7373865
C    -3.6799122   -0.6448153    1.7078395
C    -3.6657577   -2.0436239    1.7084098
C    -3.6701731    2.2306803    1.6599565
C    -4.9078395    1.4826423    1.7411916
C    -4.9137308    0.1138132    1.7396745
C    -2.4275840    4.3517769    1.5921901
C    -3.6442577    3.6292180    1.6660324
```

C	0.0570156	5.7699368	1.5199509
C	-1.1942093	6.4679843	1.5337604
C	-2.3911342	5.7852632	1.5931515
C	2.5061123	5.7670552	1.4927841
C	1.3128533	6.4586427	1.4824552
H	4.6988131	4.1503978	1.5079418
H	5.9466246	1.9958363	1.5365330
H	5.9375610	-0.4795152	1.5529711
H	4.6758226	-2.6255357	1.5721750
H	3.4214113	-4.7796525	1.6482810
H	1.2677045	-6.0065990	1.7341618
H	-1.2312205	-5.9974453	1.7846294
H	-3.3775374	-4.7547153	1.7864922
H	-4.6181057	-2.5912238	1.7623063
H	-5.8549576	2.0395969	1.7783863
H	-5.8636200	-0.4357719	1.7947353
H	-4.5933501	4.1849492	1.6984869
H	-1.1874454	7.5672143	1.5341943
H	-3.3405566	6.3386656	1.6187664
H	3.4599149	6.3133271	1.4795339
H	1.3143414	7.5579147	1.4831495

C_i symmetry: 1^1Ag

Geometry optimization of ground state at MP2/def2-TZVP level

Coronene dimer

C	-4.3192307	-1.3284177	-1.4960407
C	-4.3311327	1.1649489	-1.5527874
C	-2.2039679	-2.5348860	-1.5453479
C	-2.2200544	-0.0728007	-1.5731830
C	-2.2273438	2.3880917	-1.6579316
C	-0.0915824	-3.7456395	-1.6041918
C	-0.0757433	-1.2989572	-1.6156133
C	-0.0875028	1.1707750	-1.6713669
C	-0.1264649	3.6150473	-1.7702473
C	2.0607822	-2.4903185	-1.6821090
C	2.0472447	-0.0557461	-1.7204212
C	2.0380211	2.3782588	-1.7888872
C	-3.6273519	-2.5145433	-1.5069734
C	-3.6362216	-0.0788436	-1.5384084
C	-3.6506224	2.3557548	-1.6181533
C	-1.4640768	-3.7517439	-1.5643663
C	-1.5017805	-1.3051930	-1.5812000
C	-1.5134556	1.1648240	-1.6375190
C	-1.4991825	3.6096673	-1.7319318
C	0.6379279	-2.5229594	-1.6335536
C	0.6311082	-0.0613284	-1.6698948
C	0.6145869	2.3994856	-1.7437005
C	2.7419998	-1.2987222	-1.7270077
C	2.7303733	1.1924518	-1.7807955
H	-4.1962030	3.2958481	-1.6383932
H	-5.4178925	1.1575239	-1.5263901
H	-5.4060015	-1.3302120	-1.4702H-1

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H    -4.1639335   -3.4597576   -1.4849699
H    -2.0059010   -4.6941461   -1.5469263
H     0.4591068   -4.6826790   -1.6183062
H     2.6055160   -3.4310452   -1.6856772
H     3.8280797   -1.2909517   -1.7630451
H     3.8165470    1.1932388   -1.8153318
H     2.5738995    3.3229961   -1.8328868
H     0.4153150    4.5556686   -1.8256878
H    -2.0499923    4.5466449   -1.7568748
C    -2.7303733   -1.1924518    1.7807955
C    -2.7419998    1.2987222    1.7270077
C    -0.6145869   -2.3994856    1.7437005
C    -0.6311082    0.0613284    1.6698948
C    -0.6379279    2.5229594    1.6335536
C     1.4991825   -3.6096673    1.7319318
C     1.5134556   -1.1648240    1.6375190
C     1.5017805    1.3051930    1.5812000
C     1.4640768    3.7517439    1.5643663
C     3.6506224   -2.3557548    1.6181533
C     3.6362216    0.0788436    1.5384084
C     3.6273519    2.5145433    1.5069734
C    -2.0380211   -2.3782588    1.7888872
C    -2.0472447    0.0557461    1.7204212
C    -2.0607822    2.4903185    1.6821090
C     0.1264649   -3.6150473    1.7702473
C     0.0875028   -1.1707750    1.6713669
C     0.0757433    1.2989572    1.6156133
C     0.0915824    3.7456395    1.6041918
C     2.2273438   -2.3880917    1.6579316
C     2.2200544    0.0728007    1.5731830
C     2.2039679    2.5348860    1.5453479
C     4.3311327   -1.1649489    1.5527874
C     4.3192307    1.3284177    1.4960407
H    -2.6055160    3.4310452    1.6856772
H    -3.8280797    1.2909517    1.7630451
H    -3.8165470   -1.1932388    1.8153318
H    -2.5738995   -3.3229961    1.8328868
H    -0.4153150   -4.5556686    1.8256878
H     2.0499923   -4.5466449    1.7568748
H     4.1962030   -3.2958481    1.6383932
H     5.4178925   -1.1575239    1.5263901
H     5.4060015    1.3302120    1.4702H-1
H     4.1639335    3.4597576    1.4849699
H     2.0059010    4.6941461    1.5469263
H    -0.4591068    4.6826790    1.6183062
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C_i symmetry: 1^1Ag

Geometry optimization of ground state at MP2/SV(P) level

Circum-1-coronene dimer

```
C    -6.4416292   -2.5418453   -1.4654876
C    -6.4422554   -0.0446122   -1.4659685
C    -6.4589447    2.4514514   -1.5405111
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C	-4.3079546	-3.7552478	-1.4926784
C	-4.3197007	-1.2727274	-1.4661863
C	-4.3282541	1.1976444	-1.5032365
C	-4.3337262	3.6782881	-1.6039815
C	-2.1744176	-4.9773438	-1.5209251
C	-2.1750620	-2.5051429	-1.4907982
C	-2.1799580	-0.0304430	-1.5073296
C	-2.1921796	2.4436188	-1.5647559
C	-2.2086290	4.9137477	-1.6685128
C	-0.0485963	-6.2038336	-1.5537452
C	-0.0268147	-3.7324656	-1.5137792
C	-0.0379309	-1.2578563	-1.5277541
C	-0.0464665	1.2106044	-1.5646407
C	-0.0524336	3.6845385	-1.6244592
C	-0.0912909	6.1533717	-1.7378409
C	2.1052611	-4.9425768	-1.5626824
C	2.1079411	-2.4904433	-1.5593443
C	2.1022583	-0.0169471	-1.5944703
C	2.0908926	2.4564748	-1.6333144
C	2.0713095	4.9073223	-1.7096716
C	4.2656147	-3.6938729	-1.6340609
C	4.2507020	-1.2399868	-1.6574177
C	4.2422388	1.2184288	-1.6942985
C	4.2402869	3.6719423	-1.7444438
C	-5.7511533	-3.7273784	-1.4972808
C	-5.7526331	-1.2723053	-1.4814166
C	-5.7611410	1.1868183	-1.5183479
C	-5.7766926	3.6402449	-1.6078379
C	-3.5821462	-4.9602963	-1.5309526
C	-3.6009648	-2.5093893	-1.5181172
C	-3.6124199	-0.0356810	-1.5258052
C	-3.6180884	2.4371680	-1.5921752
C	-3.6162434	4.8866664	-1.6780834
C	-1.4209337	-6.2077490	-1.5591405
C	-1.4579791	-3.7370359	-1.5437818
C	-1.4635617	-1.2626823	-1.5388H-1
C	-1.4720876	1.2052384	-1.5757016
C	-1.4836058	3.6783237	-1.6544652
C	-1.4636334	6.1476513	-1.7432868
C	0.6977543	-4.9681638	-1.5618275
C	0.6816700	-2.4960249	-1.5671660
C	0.6698131	-0.0218740	-1.5933729
C	0.6646156	2.4519756	-1.6410747
C	0.6636310	4.9232311	-1.7093340
C	2.8233004	-3.7318668	-1.6037982
C	2.8178076	-1.2500074	-1.6385822
C	2.8092878	1.2191277	-1.6755572
C	2.7976775	3.7009029	-1.7149222
C	4.9473521	-2.5033248	-1.6846857
C	4.9313482	-0.0091067	-1.7203772
C	4.9301536	2.4851098	-1.7595873
H	-6.3274779	4.5910931	-1.6394063

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H    -4.1698408    5.8370078   -1.7125186
H    -2.0194181    7.0954755   -1.7792255
H     0.4576752    7.1039878   -1.7872490
H     2.6175634    5.8609088   -1.7577843
H     4.7836138    4.6262002   -1.7875391
H     6.0281609    2.4859903   -1.7949674
H     6.0303092   -0.0058698   -1.7589382
H     6.0453194   -2.4977264   -1.7199015
H     4.8154735   -4.6452777   -1.6484585
H     2.6580594   -5.8933978   -1.5824218
H     0.5069721   -7.1516382   -1.5750261
H    -1.9701813   -7.1600355   -1.5668590
H    -4.1291092   -5.9150834   -1.5369746
H    -6.2952497   -4.6825543   -1.5001582
H    -7.5408716   -2.5433534   -1.4657982
H    -7.5425510   -0.0484425   -1.4678161
H    -7.5581697    2.4452726   -1.5408700
C    -4.9301536   -2.4851098    1.7595873
C    -4.9313482    0.0091067    1.7203772
C    -4.9473521    2.5033248    1.6846857
C    -2.7976775   -3.7009029    1.7149222
C    -2.8092878   -1.2191277    1.6755572
C    -2.8178076    1.2500074    1.6385822
C    -2.8233004    3.7318668    1.6037982
C    -0.6636310   -4.9232311    1.7093340
C    -0.6646156   -2.4519756    1.6410747
C    -0.6698131    0.0218740    1.5933729
C    -0.6816700    2.4960249    1.5671660
C    -0.6977543    4.9681638    1.5618275
C     1.4636334   -6.1476513    1.7432868
C     1.4836058   -3.6783237    1.6544652
C     1.4720876   -1.2052384    1.5757016
C     1.4635617    1.2626823    1.5388H-1
C     1.4579791    3.7370359    1.5437818
C     1.4209337    6.2077490    1.5591405
C     3.6162434   -4.8866664    1.6780834
C     3.6180884   -2.4371680    1.5921752
C     3.6124199    0.0356810    1.5258052
C     3.6009648    2.5093893    1.5181172
C     3.5821462    4.9602963    1.5309526
C     5.7766926   -3.6402449    1.6078379
C     5.7611410   -1.1868183    1.5183479
C     5.7526331    1.2723053    1.4814166
C     5.7511533    3.7273784    1.4972808
C    -4.2402869   -3.6719423    1.7444438
C    -4.2422388   -1.2184288    1.6942985
C    -4.2507020    1.2399868    1.6574177
C    -4.2656147    3.6938729    1.6340609
C    -2.0713095   -4.9073223    1.7096716
C    -2.0908926   -2.4564748    1.6333144
C    -2.1022583    0.0169471    1.5944703
C    -2.1079411    2.4904433    1.5593443
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C    -2.1052611    4.9425768    1.5626824
C     0.0912909   -6.1533717    1.7378409
C     0.0524336   -3.6845385    1.6244592
C     0.0464665   -1.2106044    1.5646407
C     0.0379309    1.2578563    1.5277541
C     0.0268147    3.7324656    1.5137792
C     0.0485963    6.2038336    1.5537452
C     2.2086290   -4.9137477    1.6685128
C     2.1921796   -2.4436188    1.5647559
C     2.1799580    0.0304430    1.5073296
C     2.1750620    2.5051429    1.4907982
C     2.1744176    4.9773438    1.5209251
C     4.3337262   -3.6782881    1.6039815
C     4.3282541   -1.1976444    1.5032365
C     4.3197007    1.2727274    1.4661863
C     4.3079546    3.7552478    1.4926784
C     6.4589447   -2.4514514    1.5405111
C     6.4422554    0.0446122    1.4659685
C     6.4416292    2.5418453    1.4654876
H    -4.8154735    4.6452777    1.6484585
H    -2.6580594    5.8933978    1.5824218
H    -0.5069721    7.1516382    1.5750261
H     1.9701813    7.1600355    1.5668590
H     4.1291092    5.9150834    1.5369746
H     6.2952497    4.6825543    1.5001582
H     7.5408716    2.5433534    1.4657982
H     7.5425510    0.0484425    1.4678161
H     7.5581697   -2.4452726    1.5408700
H     6.3274779   -4.5910931    1.6394063
H     4.1698408   -5.8370078    1.7125186
H     2.0194181   -7.0954755    1.7792255
H    -0.4576752   -7.1039878    1.7872490
H    -2.6175634   -5.8609088    1.7577843
H    -4.7836138   -4.6262002    1.7875391
H    -6.0281609   -2.4859903    1.7949674
H    -6.0303092    0.0058698    1.7589382
H    -6.0453194    2.4977264    1.7199015
```

C_{2h} symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Pyrene dimer, ADC(2)-1

```
C    -0.3683322    1.5942681    0.7068274
C    -0.3683322    1.5942681   -0.7068274
C    -1.6143003    1.6780208    1.4360054
C    -1.6143003    1.6780208   -1.4360054
C    -2.8383883    1.7737213    0.6897457
C    -2.8383883    1.7737213   -0.6897457
C     2.1022771    1.4593798    0.6902125
C     2.1022771    1.4593798   -0.6902125
C     0.8795525    1.5323475    1.4344371
C     0.8795525    1.5323475   -1.4344371
C     0.8572390    1.5595115    2.8486285
```

C	-0.3611719	1.6386853	3.5454500
C	-1.5846293	1.6933235	2.8486233
C	0.8572390	1.5595115	-2.8486285
C	-0.3611719	1.6386853	-3.5454500
C	-1.5846293	1.6933235	-2.8486233
H	-3.7866452	1.8524421	1.2400800
H	-3.7866452	1.8524421	-1.2400800
H	3.0524107	1.4102414	1.2396045
H	3.0524107	1.4102414	-1.2396045
H	1.8059683	1.5268236	3.4007160
H	-0.3603648	1.6627209	4.6434817
H	-2.5302252	1.7629724	3.4042899
H	1.8059683	1.5268236	-3.4007160
H	-0.3603648	1.6627209	-4.6434817
H	-2.5302252	1.7629724	-3.4042899
C	0.3683322	-1.5942681	0.7068274
C	0.3683322	-1.5942681	-0.7068274
C	-0.8795525	-1.5323475	1.4344371
C	-0.8795525	-1.5323475	-1.4344371
C	-2.1022771	-1.4593798	0.6902125
C	-2.1022771	-1.4593798	-0.6902125
C	2.8383883	-1.7737213	0.6897457
C	2.8383883	-1.7737213	-0.6897457
C	1.6143003	-1.6780208	1.4360054
C	1.6143003	-1.6780208	-1.4360054
C	1.5846293	-1.6933235	2.8486233
C	0.3611719	-1.6386853	3.5454500
C	-0.8572390	-1.5595115	2.8486285
C	1.5846293	-1.6933235	-2.8486233
C	0.3611719	-1.6386853	-3.5454500
C	-0.8572390	-1.5595115	-2.8486285
H	-3.0524107	-1.4102414	1.2396045
H	-3.0524107	-1.4102414	-1.2396045
H	3.7866452	-1.8524421	1.2400800
H	3.7866452	-1.8524421	-1.2400800
H	2.5302252	-1.7629724	3.4042899
H	0.3603648	-1.6627209	4.6434817
H	-1.8059683	-1.5268236	3.4007160
H	2.5302252	-1.7629724	-3.4042899
H	0.3603648	-1.6627209	-4.6434817
H	-1.8059683	-1.5268236	-3.4007160

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Pyrene dimer,ADC(2)-2

C	-0.0765692	0.4576695	-1.6102389
C	-0.0753881	-0.9698515	-1.5831969
C	-1.3193789	1.1740645	-1.6630204
C	-1.3160136	-1.6845751	-1.4794223
C	-2.5333143	0.4386931	-1.5926500
C	-2.5337811	-0.9522685	-1.5310935
C	2.3812281	0.4407400	-1.6421069

```
C     2.3837584   -0.9501916   -1.5923092
C     1.1647684    1.1754337   -1.6860452
C     1.1685856   -1.6835980   -1.5160991
C     1.1390730    2.6042339   -1.7069009
C    -0.0788837    3.2917672   -1.7686816
C    -1.2930164    2.6036838   -1.6908434
C     1.1445352   -3.1103093   -1.4259760
C    -0.0703593   -3.8015637   -1.3828280
C    -1.2870970   -3.1100142   -1.3769923
H    -3.4878946    0.9832131   -1.6226789
H    -3.4871904   -1.4971743   -1.4832046
H     3.3340236    0.9868403   -1.6884174
H     3.3383406   -1.4946805   -1.5681606
H     2.0888026    3.1533169   -1.7679427
H    -0.0801457    4.3894920   -1.8099003
H    -2.2442539    3.1525075   -1.7330807
H     2.0957678   -3.6601641   -1.4257657
H    -0.0693763   -4.8983916   -1.3195202
H    -2.2373241   -3.6603530   -1.3367583
C     0.0753881    0.9698515    1.5831969
C     0.0765692   -0.4576695    1.6102389
C    -1.1685856    1.6835980    1.5160991
C    -1.1647684   -1.1754337    1.6860452
C    -2.3837584    0.9501916    1.5923092
C    -2.3812281   -0.4407400    1.6421069
C     2.5337811    0.9522685    1.5310935
C     2.5333143   -0.4386931    1.5926500
C     1.3160136    1.6845751    1.4794223
C     1.3193789   -1.1740645    1.6630204
C     1.2870970    3.1100142    1.3769923
C     0.0703593    3.8015637    1.3828280
C    -1.1445352    3.1103093    1.4259760
C     1.2930164   -2.6036838    1.6908434
C     0.0788837   -3.2917672    1.7686816
C    -1.1390730   -2.6042339    1.7069009
H    -3.3383406    1.4946805    1.5681606
H    -3.3340236   -0.9868403    1.6884174
H     3.4871904    1.4971743    1.4832046
H     3.4878946   -0.9832131    1.6226789
H     2.2373241    3.6603530    1.3367583
H     0.0693763    4.8983916    1.3195202
H    -2.0957678    3.6601641    1.4257657
H     2.2442539   -3.1525075    1.7330807
H     0.0801457   -4.3894920    1.8099003
H    -2.0888026   -3.1533169    1.7679427
```

C$_{2h}$ symmetry: 1^1Bg

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Pyrene dimer, ADC(2)-3

```
C    -0.4299885   -1.4906928    0.0000000
C    -1.8458601   -1.5229787    0.0000000
C     0.2957830   -1.5389000   -1.2507429
```

C	-2.5728598	-1.4913898	-1.2494830
C	-0.4495079	-1.5238024	-2.4786697
C	-1.8285525	-1.5200572	-2.4776145
C	-0.4495079	-1.5238024	2.4786697
C	-1.8285525	-1.5200572	2.4776145
C	0.2957830	-1.5389000	1.2507429
C	-2.5728598	-1.4913898	1.2494830
C	1.7085725	-1.5574623	1.2257920
C	2.4019142	-1.5810559	0.0000000
C	1.7085725	-1.5574623	-1.2257920
C	-3.9876262	-1.5162871	1.2231695
C	-4.6808622	-1.5113730	0.0000000
C	-3.9876262	-1.5162871	-1.2231695
H	0.1027742	-1.5520673	-3.4278497
H	-2.3812886	-1.5236523	-3.4278341
H	0.1027742	-1.5520673	3.4278497
H	-2.3812886	-1.5236523	3.4278341
H	2.2643423	-1.5889019	2.1719323
H	3.4999781	-1.5913900	0.0000000
H	2.2643423	-1.5889019	-2.1719323
H	-4.5429332	-1.5182090	2.1712214
H	-5.7793047	-1.5279289	-0.0000000
H	-4.5429332	-1.5182090	-2.1712214
C	1.8458601	1.5229787	0.0000000
C	0.4299885	1.4906928	0.0000000
C	2.5728598	1.4913898	-1.2494830
C	-0.2957830	1.5389000	-1.2507429
C	1.8285525	1.5200572	-2.4776145
C	0.4495079	1.5238024	-2.4786697
C	1.8285525	1.5200572	2.4776145
C	0.4495079	1.5238024	2.4786697
C	2.5728598	1.4913898	1.2494830
C	-0.2957830	1.5389000	1.2507429
C	3.9876262	1.5162871	1.2231695
C	4.6808622	1.5113730	-0.0000000
C	3.9876262	1.5162871	-1.2231695
C	-1.7085725	1.5574623	1.2257920
C	-2.4019142	1.5810559	0.0000000
C	-1.7085725	1.5574623	-1.2257920
H	2.3812886	1.5236523	-3.4278341
H	-0.1027742	1.5520673	-3.4278497
H	2.3812886	1.5236523	3.4278341
H	-0.1027742	1.5520673	3.4278497
H	4.5429332	1.5182090	2.1712214
H	5.7793047	1.5279289	0.0000000
H	4.5429332	1.5182090	-2.1712214
H	-2.2643423	1.5889019	2.1719323
H	-3.4999781	1.5913900	0.0000000
H	-2.2643423	1.5889019	-2.1719323

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Circum-1-pyrene dimer, ADC(2)-1

C	-0.0211331	0.2197441	-1.5458562
C	-0.0237727	-1.2161935	-1.5717568
C	-1.2556714	0.9336638	-1.5781335
C	-1.2594441	-1.9267703	-1.5257042
C	-2.4970443	0.2207300	-1.5299819
C	-2.4985988	-1.2083739	-1.5693535
C	2.4542941	0.2128184	-1.5975792
C	2.4502193	-1.2162806	-1.6366435
C	1.2143619	0.9297147	-1.6117222
C	1.2104164	-1.9307132	-1.5590485
C	1.2180431	2.3561082	-1.5878597
C	-0.0175788	3.0731392	-1.6226759
C	-1.2541059	2.3600632	-1.5544629
C	1.2084727	-3.3563950	-1.6007093
C	-0.0278753	-4.0687773	-1.5370858
C	-1.2632021	-3.3524232	-1.5677128
C	3.6722520	2.3466305	-1.6522003
C	3.6892365	0.9310470	-1.6738406
C	2.4659766	3.0689659	-1.6557781
C	4.9156524	0.1828359	-1.7104109
C	4.9137274	-1.1942343	-1.7204565
C	3.6852902	-1.9359145	-1.6431856
C	3.6614228	-3.3520446	-1.6483630
C	2.4553899	-4.0717159	-1.5990967
C	2.4171842	-5.5097670	-1.6269525
C	1.2205498	-6.1949761	-1.6060082
C	-0.0307081	-5.5006106	-1.5795433
C	-1.2844678	-6.1909442	-1.5735195
C	-2.5119030	-4.0637796	-1.5330438
C	-2.4790254	-5.5019157	-1.5627096
C	-3.7356857	-1.9240655	-1.5423674
C	-3.7164923	-3.3402377	-1.5493304
C	-3.7312978	0.9429288	-1.5722124
C	-4.9606502	0.1986362	-1.5746581
C	-4.9634210	-1.1784347	-1.5850467
C	-2.5011200	3.0769429	-1.5888562
C	-3.7091323	2.3584752	-1.5516674
C	-0.0151839	4.5055554	-1.6158175
C	-1.2656899	5.1966543	-1.6379560
C	-2.4634300	4.5146735	-1.5956694
C	2.4327397	4.5068107	-1.6605860
C	1.2365106	5.1926574	-1.6708719
H	4.6260115	2.8930994	-1.6991819
H	5.8664992	0.7319212	-1.7605980
H	5.8635161	-1.7466524	-1.7565997
H	4.6145960	-3.9009934	-1.6741978
H	3.3674433	-6.0616005	-1.6536296
H	1.2H-1804	-7.2938865	-1.6309924
H	-1.2837264	-7.2898410	-1.5993771
H	-3.4314079	-6.0506839	-1.5647368

H	-4.6717677	-3.8861057	-1.5499785
H	-5.9107674	0.7507530	-1.5980950
H	-5.9156202	-1.7278160	-1.5947292
H	-4.6620688	2.9079919	-1.5726622
H	-1.2615967	6.2955172	-1.6564279
H	-3.4139776	5.0665712	-1.6058076
H	3.3844361	5.0556710	-1.6955922
H	1.2355129	6.2915468	-1.6889080
C	0.0237727	1.2161935	1.5717568
C	0.0211331	-0.2197441	1.5458562
C	-1.2104164	1.9307132	1.5590485
C	-1.2143619	-0.9297147	1.6117222
C	-2.4502193	1.2162806	1.6366435
C	-2.4542941	-0.2128184	1.5975792
C	2.4985988	1.2083739	1.5693535
C	2.4970443	-0.2207300	1.5299819
C	1.2594441	1.9267703	1.5257042
C	1.2556714	-0.9336638	1.5781335
C	1.2632021	3.3524232	1.5677128
C	0.0278753	4.0687773	1.5370858
C	-1.2084727	3.3563950	1.6007093
C	1.2541059	-2.3600632	1.5544629
C	0.0175788	-3.0731392	1.6226759
C	-1.2180431	-2.3561082	1.5878597
C	3.7164923	3.3402377	1.5493304
C	3.7356857	1.9240655	1.5423674
C	2.5119030	4.0637796	1.5330438
C	4.9634210	1.1784347	1.5850467
C	4.9606502	-0.1986362	1.5746581
C	3.7312978	-0.9429288	1.5722124
C	3.7091323	-2.3584752	1.5516674
C	2.5011200	-3.0769429	1.5888562
C	2.4634300	-4.5146735	1.5956694
C	1.2656899	-5.1966543	1.6379560
C	0.0151839	-4.5055554	1.6158175
C	-1.2365106	-5.1926574	1.6708719
C	-2.4659766	-3.0689659	1.6557781
C	-2.4327397	-4.5068107	1.6605860
C	-3.6892365	-0.9310470	1.6738406
C	-3.6722520	-2.3466305	1.6522003
C	-3.6852902	1.9359145	1.6431856
C	-4.9137274	1.1942343	1.7204565
C	-4.9156524	-0.1828359	1.7104109
C	-2.4553899	4.0717159	1.5990967
C	-3.6614228	3.3520446	1.6483630
C	0.0307081	5.5006106	1.5795433
C	-1.2205498	6.1949761	1.6060082
C	-2.4171842	5.5097670	1.6269525
C	2.4790254	5.5019157	1.5627096
C	1.2844678	6.1909442	1.5735195
H	4.6717677	3.8861057	1.5499785
H	5.9156202	1.7278160	1.5947292

```
H     5.9107674   -0.7507530    1.5980950
H     4.6620688   -2.9079919    1.5726622
H     3.4139776   -5.0665712    1.6058076
H     1.2615967   -6.2955172    1.6564279
H    -1.2355129   -6.2915468    1.6889080
H    -3.3844361   -5.0556710    1.6955922
H    -4.6260115   -2.8930994    1.6991819
H    -5.8635161    1.7466524    1.7565997
H    -5.8664992   -0.7319212    1.7605980
H    -4.6145960    3.9009934    1.6741978
H    -1.2H-1804    7.2938865    1.6309924
H    -3.3674433    6.0616005    1.6536296
H     3.4314079    6.0506839    1.5647368
H     1.2837264    7.2898410    1.5993771
```

C_{2h} symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Coronene dimer, ADC(2)-1

```
C    -1.6263615   -1.7090201   -3.5505890
C     0.8715144   -1.6218075   -3.5509837
C    -2.8607379   -1.7240987   -1.4330364
C    -0.3814016   -1.6419260   -1.4272555
C     2.0994784   -1.5467625   -1.4313355
C    -4.0822038   -1.7775341    0.6930416
C    -1.6176360   -1.6504819    0.7140842
C     0.8526875   -1.5595175    0.7138013
C     3.3172486   -1.4951648    0.6947825
C    -2.8305666   -1.7357682    2.8578875
C    -0.3802071   -1.6287874    2.8646538
C     2.0711568   -1.5559076    2.8593818
C    -2.8305666   -1.7357682   -2.8578875
C    -0.3802071   -1.6287874   -2.8646538
C     2.0711568   -1.5559076   -2.8593818
C    -4.0822038   -1.7775341   -0.6930416
C    -1.6176360   -1.6504819   -0.7140842
C     0.8526875   -1.5595175   -0.7138013
C     3.3172486   -1.4951648   -0.6947825
C    -2.8607379   -1.7240987    1.4330364
C    -0.3814016   -1.6419260    1.4272555
C     2.0994784   -1.5467625    1.4313355
C    -1.6263615   -1.7090201    3.5505890
C     0.8715144   -1.6218075    3.5509837
H     3.0227239   -1.5451692   -3.4084193
H     0.8725902   -1.6342026   -4.6502189
H    -1.6276849   -1.7248563   -4.6497505
H    -3.7793295   -1.7942073   -3.4097486
H    -5.0327862   -1.8313173   -1.2422203
H    -5.0327862   -1.8313173    1.2422203
H    -3.7793295   -1.7942073    3.4097486
H    -1.6276849   -1.7248563    4.6497505
H     0.8725902   -1.6342026    4.6502189
H     3.0227239   -1.5451692    3.4084193
```

```
H     4.2691225   -1.4723297    1.2431168
H     4.2691225   -1.4723297   -1.2431168
C    -0.8715144    1.6218075   -3.5509837
C     1.6263615    1.7090201   -3.5505890
C    -2.0994784    1.5467625   -1.4313355
C     0.3814016    1.6419260   -1.4272555
C     2.8607379    1.7240987   -1.4330364
C    -3.3172486    1.4951648    0.6947825
C    -0.8526875    1.5595175    0.7138013
C     1.6176360    1.6504819    0.7140842
C     4.0822038    1.7775341    0.6930416
C    -2.0711568    1.5559076    2.8593818
C     0.3802071    1.6287874    2.8646538
C     2.8305666    1.7357682    2.8578875
C    -2.0711568    1.5559076   -2.8593818
C     0.3802071    1.6287874   -2.8646538
C     2.8305666    1.7357682   -2.8578875
C    -3.3172486    1.4951648   -0.6947825
C    -0.8526875    1.5595175   -0.7138013
C     1.6176360    1.6504819   -0.7140842
C     4.0822038    1.7775341   -0.6930416
C    -2.0994784    1.5467625    1.4313355
C     0.3814016    1.6419260    1.4272555
C     2.8607379    1.7240987    1.4330364
C    -0.8715144    1.6218075    3.5509837
C     1.6263615    1.7090201    3.5505890
H     3.7793295    1.7942073   -3.4097486
H     1.6276849    1.7248563   -4.6497505
H    -0.8725902    1.6342026   -4.6502189
H    -3.0227239    1.5451692   -3.4084193
H    -4.2691225    1.4723297   -1.2431168
H    -4.2691225    1.4723297    1.2431168
H    -3.0227239    1.5451692    3.4084193
H    -0.8725902    1.6342026    4.6502189
H     1.6276849    1.7248563    4.6497505
H     3.7793295    1.7942073    3.4097486
H     5.0327862    1.8313173    1.2422203
H     5.0327862    1.8313173   -1.2422203
```

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Coronene dimer, ADC(2)-2

```
C    -3.7830437   -1.5757086   -1.7713230
C    -3.7733279    0.9217019   -1.6594943
C    -1.6685658   -2.8160564   -1.7797054
C    -1.6549120   -0.3380266   -1.6584808
C    -1.6492277    2.1399827   -1.5322724
C     0.4539215   -4.0410712   -1.8406884
C     0.4816731   -1.5812054   -1.6934620
C     0.4896323    0.8866214   -1.5560157
C     0.4805138    3.3503037   -1.4278455
C     2.6227769   -2.8001733   -1.7635359
```

C	2.6359785	-0.3534953	-1.6036454
C	2.6386752	2.0944841	-1.4659576
C	-3.0956175	-2.7808092	-1.7985802
C	-3.0923371	-0.3314570	-1.6672415
C	-3.0754915	2.1174923	-1.5646439
C	-0.9337028	-4.0387490	-1.8345171
C	-0.9458455	-1.5773022	-1.6648719
C	-0.9381432	0.8904506	-1.5374290
C	-0.9073737	3.3536412	-1.4406065
C	1.1969886	-2.8273053	-1.7372721
C	1.1985644	-0.3527639	-1.5728191
C	1.2128211	2.1267222	-1.4568341
C	3.3200067	-1.6039464	-1.6695865
C	3.3267536	0.8900484	-1.5135509
H	-3.6212255	3.0712804	-1.5527062
H	-4.8720558	0.9293318	-1.6966831
H	-4.8818743	-1.5714832	-1.8042448
H	-3.6489720	-3.7273943	-1.8751843
H	-1.4851857	-4.9863867	-1.9120414
H	0.9993332	-4.9936803	-1.9002372
H	3.1708341	-3.7511074	-1.8269902
H	4.4188868	-1.6072159	-1.6841523
H	4.4259258	0.8871097	-1.5191183
H	3.1916056	3.0421171	-1.4132491
H	1.0325641	4.2983806	-1.3731340
H	-1.4532486	4.3073864	-1.4161876
C	-3.3267536	-0.8900484	1.5135509
C	-3.3200067	1.6039464	1.6695865
C	-1.2128211	-2.1267222	1.4568341
C	-1.1985644	0.3527639	1.5728191
C	-1.1969886	2.8273053	1.7372721
C	0.9073737	-3.3536412	1.4406065
C	0.9381432	-0.8904506	1.5374290
C	0.9458455	1.5773022	1.6648719
C	0.9337028	4.0387490	1.8345171
C	3.0754915	-2.1174923	1.5646439
C	3.0923371	0.3314570	1.6672415
C	3.0956175	2.7808092	1.7985802
C	-2.6386752	-2.0944841	1.4659576
C	-2.6359785	0.3534953	1.6036454
C	-2.6227769	2.8001733	1.7635359
C	-0.4805138	-3.3503037	1.4278455
C	-0.4896323	-0.8866214	1.5560157
C	-0.4816731	1.5812054	1.6934620
C	-0.4539215	4.0410712	1.8406884
C	1.6492277	-2.1399827	1.5322724
C	1.6549120	0.3380266	1.6584808
C	1.6685658	2.8160564	1.7797054
C	3.7733279	-0.9217019	1.6594943
C	3.7830437	1.5757086	1.7713230
H	-3.1708341	3.7511074	1.8269902
H	-4.4188868	1.6072159	1.6841523

```
H    -4.4259258   -0.8871097    1.5191183
H    -3.1916056   -3.0421171    1.4132491
H    -1.0325641   -4.2983806    1.3731340
H     1.4532486   -4.3073864    1.4161876
H     3.6212255   -3.0712804    1.5527062
H     4.8720558   -0.9293318    1.6966831
H     4.8818743    1.5714832    1.8042448
H     3.6489720    3.7273943    1.8751843
H     1.4851857    4.9863867    1.9120414
H    -0.9993332    4.9936803    1.9002372
```

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Coronene dimer, ADC(2)-3

```
C    -4.0490640   -1.2905499   -1.5432657
C    -4.0553553    1.2101124   -1.5877575
C    -1.9242746   -2.5161687   -1.5414591
C    -1.9253061   -0.0345178   -1.5474286
C    -1.9366202    2.4457301   -1.6259261
C     0.2049319   -3.7301902   -1.5694840
C     0.2173331   -1.2655647   -1.5520476
C     0.2112408    1.2063238   -1.5941969
C     0.1866806    3.6687938   -1.6950959
C     2.3653696   -2.4743617   -1.5896634
C     2.3664754   -0.0246976   -1.6104104
C     2.3534139    2.4241895   -1.6731850
C    -3.3508833   -2.4896086   -1.5554258
C    -3.3638998   -0.0385496   -1.5718276
C    -3.3629985    2.4115938   -1.6401285
C    -1.1828693   -3.7340374   -1.5759430
C    -1.2097257   -1.2695581   -1.5823713
C    -1.2158595    1.2020881   -1.6246574
C    -1.2010414    3.6653583   -1.7009480
C     0.9403435   -2.5076878   -1.5894088
C     0.9275100   -0.0285829   -1.6192658
C     0.9282810    2.4500347   -1.6740650
C     3.0579445   -1.2720890   -1.6227666
C     3.0519288    1.2248435   -1.6652492
H    -3.9160149    3.3612239   -1.6675137
H    -5.1545193    1.2079947   -1.5968787
H    -5.1482176   -1.2941562   -1.5504698
H    -3.8991500   -3.4423493   -1.5503109
H    -1.7287936   -4.6883101   -1.5740508
H     0.7558757   -4.6809010   -1.5880742
H     2.9172866   -3.4248646   -1.5997404
H     4.1562443   -1.2702152   -1.6381864
H     4.1503019    1.2278273   -1.6797014
H     2.9005252    3.3766217   -1.7151651
H     0.7327912    4.6210953   -1.7462663
H    -1.7517509    4.6163424   -1.7304145
C    -3.0519288   -1.2248435    1.6652492
C    -3.0579445    1.2720890    1.6227666
```

```
C    -0.9282810   -2.4500347    1.6740650
C    -0.9275100    0.0285829    1.6192658
C    -0.9403435    2.5076878    1.5894088
C     1.2010414   -3.6653583    1.7009480
C     1.2158595   -1.2020881    1.6246574
C     1.2097257    1.2695581    1.5823713
C     1.1828693    3.7340374    1.5759430
C     3.3629985   -2.4115938    1.6401285
C     3.3638998    0.0385496    1.5718276
C     3.3508833    2.4896086    1.5554258
C    -2.3534139   -2.4241895    1.6731850
C    -2.3664754    0.0246976    1.6104104
C    -2.3653696    2.4743617    1.5896634
C    -0.1866806   -3.6687938    1.6950959
C    -0.2112408   -1.2063238    1.5941969
C    -0.2173331    1.2655647    1.5520476
C    -0.2049319    3.7301902    1.5694840
C     1.9366202   -2.4457301    1.6259261
C     1.9253061    0.0345178    1.5474286
C     1.9242746    2.5161687    1.5414591
C     4.0553553   -1.2101124    1.5877575
C     4.0490640    1.2905499    1.5432657
H    -2.9172866    3.4248646    1.5997404
H    -4.1562443    1.2702152    1.6381864
H    -4.1503019   -1.2278273    1.6797014
H    -2.9005252   -3.3766217    1.7151651
H    -0.7327912   -4.6210953    1.7462663
H     1.7517509   -4.6163424    1.7304145
H     3.9160149   -3.3612239    1.6675137
H     5.1545193   -1.2079947    1.5968787
H     5.1482176    1.2941562    1.5504698
H     3.8991500    3.4423493    1.5503109
H     1.7287936    4.6883101    1.5740508
H    -0.7558757    4.6809010    1.5880742
```

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Coronene dimer, ADC(2)-4

```
C    -4.6286916   -1.2996429   -1.4440821
C    -4.6425410    1.2018457   -1.4836941
C    -2.5022405   -2.5183720   -1.4620988
C    -2.5119803   -0.0375285   -1.4890106
C    -2.5297177    2.4428790   -1.5407961
C    -0.3718206   -3.7295666   -1.4928943
C    -0.3640370   -1.2619170   -1.5119495
C    -0.3777181    1.2092219   -1.5511648
C    -0.4128226    3.6759923   -1.6103851
C     1.7854488   -2.4687086   -1.5676682
C     1.7779327   -0.0154771   -1.5961273
C     1.7582911    2.4373585   -1.6455444
C    -3.9312285   -2.4978524   -1.4556190
C    -3.9486419   -0.0455138   -1.4904409
```

C	-3.9583941	2.4067429	-1.5333841
C	-1.7589079	-3.7364663	-1.4780612
C	-1.7925718	-1.2701292	-1.5260985
C	-1.8062549	1.2011681	-1.5653013
C	-1.7999060	3.6680092	-1.5954998
C	0.3599288	-2.5038793	-1.5428455
C	0.3407058	-0.0233691	-1.5920743
C	0.3324634	2.4575151	-1.6215831
C	2.4710987	-1.2610236	-1.6188553
C	2.4572756	1.2363181	-1.6584952
H	-4.5139769	3.3550566	-1.5397748
H	-5.7418970	1.1968396	-1.4736036
H	-5.7280405	-1.3065150	-1.4340834
H	-4.4762661	-3.4519904	-1.4318456
H	-2.3040436	-4.6907731	-1.4545270
H	0.1839169	-4.6772287	-1.5048584
H	2.3412507	-3.4158895	-1.5824457
H	3.5698545	-1.2565909	-1.6380650
H	3.5560156	1.2434304	-1.6777607
H	2.3035704	3.3896983	-1.6904452
H	0.1324020	4.6288858	-1.6525255
H	-2.3555695	4.6164938	-1.6020981
C	-2.4572756	-1.2363181	1.6584952
C	-2.4710987	1.2610236	1.6188553
C	-0.3324634	-2.4575151	1.6215831
C	-0.3407058	0.0233691	1.5920743
C	-0.3599288	2.5038793	1.5428455
C	1.7999060	-3.6680092	1.5954998
C	1.8062549	-1.2011681	1.5653013
C	1.7925718	1.2701292	1.5260985
C	1.7589079	3.7364663	1.4780612
C	3.9583941	-2.4067429	1.5333841
C	3.9486419	0.0455138	1.4904409
C	3.9312285	2.4978524	1.4556190
C	-1.7582911	-2.4373585	1.6455444
C	-1.7779327	0.0154771	1.5961273
C	-1.7854488	2.4687086	1.5676682
C	0.4128226	-3.6759923	1.6103851
C	0.3777181	-1.2092219	1.5511648
C	0.3640370	1.2619170	1.5119495
C	0.3718206	3.7295666	1.4928943
C	2.5297177	-2.4428790	1.5407961
C	2.5119803	0.0375285	1.4890106
C	2.5022405	2.5183720	1.4620988
C	4.6425410	-1.2018457	1.4836941
C	4.6286916	1.2996429	1.4440821
H	-2.3412507	3.4158895	1.5824457
H	-3.5698545	1.2565909	1.6380650
H	-3.5560156	-1.2434304	1.6777607
H	-2.3035704	-3.3896983	1.6904452
H	-0.1324020	-4.6288858	1.6525255
H	2.3555695	-4.6164938	1.6020981

```
H     4.5139769   -3.3550566    1.5397748
H     5.7418970   -1.1968396    1.4736036
H     5.7280405    1.3065150    1.4340834
H     4.4762661    3.4519904    1.4318456
H     2.3040436    4.6907731    1.4545270
H    -0.1839169    4.6772287    1.5048584
```

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level

Circum-1-coronene dimer, ADC(2)-1

```
C    -6.3517865   -2.5314216   -1.6539542
C    -6.3515326   -0.0351723   -1.6217483
C    -6.3612183    2.4602508   -1.6964563
C    -4.2215874   -3.7505796   -1.6297483
C    -4.2272442   -1.2694853   -1.5777185
C    -4.2320440    1.2083849   -1.5995390
C    -4.2358585    3.6881199   -1.6966189
C    -2.0849223   -4.9766271   -1.6010011
C    -2.0837434   -2.4992081   -1.5532473
C    -2.0919478   -0.0261122   -1.5503551
C    -2.0931216    2.4466360   -1.5982039
C    -2.1037395    4.9228100   -1.6930571
C     0.0396782   -6.2031909   -1.5797235
C     0.0586077   -3.7325704   -1.5177505
C     0.0557331   -1.2600588   -1.5160729
C     0.0510002    1.2164067   -1.5386193
C     0.0445574    3.6883589   -1.5861516
C     0.0164483    6.1573702   -1.6957745
C     2.1932583   -4.9463819   -1.5020162
C     2.2005317   -2.4900140   -1.4923960
C     2.1929009   -0.0177969   -1.5144700
C     2.1911890    2.4545041   -1.5362085
C     2.1744951    4.9103025   -1.5907049
C     4.3538898   -3.6981592   -1.5046123
C     4.3469196   -1.2447632   -1.5218597
C     4.3422100    1.2168157   -1.5421296
C     4.3397667    3.6700722   -1.5667651
C    -5.6606324   -3.7200170   -1.6814204
C    -5.6629698   -1.2654404   -1.6334589
C    -5.6675855    1.1977156   -1.6546999
C    -5.6746135    3.6510082   -1.7459152
C    -3.4942163   -4.9559042   -1.6605115
C    -3.5122928   -2.5016082   -1.6226645
C    -3.5156442   -0.0293999   -1.6088430
C    -3.5218338    2.4422754   -1.6668807
C    -3.5127547    4.8955825   -1.7510219
C    -1.3344421   -6.2049995   -1.6326337
C    -1.3652575   -3.7349938   -1.5929534
C    -1.3738942   -1.2628163   -1.5705301
C    -1.3785622    1.2128674   -1.5930682
C    -1.3793016    3.6840842   -1.6613425
C    -1.3575741    6.1530971   -1.7492517
```

C	0.7858138	-4.9708600	-1.5523943
C	0.7709517	-2.4933412	-1.5426181
C	0.7686992	-0.0207742	-1.5547612
C	0.7615762	2.4516163	-1.5875858
C	0.7672530	4.9285060	-1.6438056
C	2.9161250	-3.7344586	-1.5184969
C	2.9108888	-1.2544382	-1.5456053
C	2.9062521	1.2207889	-1.5669669
C	2.9020602	3.7008378	-1.5838075
C	5.0401331	-2.5052406	-1.5340670
C	5.0320588	-0.0130208	-1.5580725
C	5.0305720	2.4793368	-1.5746382
H	-6.2249832	4.6014690	-1.7938718
H	-4.0637332	5.8467564	-1.8034444
H	-1.9097718	7.1022045	-1.8044055
H	0.5669420	7.1078641	-1.7299633
H	2.7232787	5.8633623	-1.6178163
H	4.8865609	4.6233660	-1.5846736
H	6.1291607	2.4800492	-1.5782566
H	6.1314783	-0.0111716	-1.5684738
H	6.1387352	-2.5018977	-1.5395315
H	4.9041149	-4.6497255	-1.5070950
H	2.7456455	-5.8977694	-1.5120148
H	0.5935598	-7.1522186	-1.5950230
H	-1.8832342	-7.1570066	-1.6682693
H	-4.0415691	-5.9099455	-1.6953638
H	-6.2070190	-4.6734374	-1.7134530
H	-7.4505559	-2.5318400	-1.6875377
H	-7.4513778	-0.0376055	-1.6531225
H	-7.4600215	2.4558477	-1.7282979
C	-5.0305720	-2.4793368	1.5746382
C	-5.0320588	0.0130208	1.5580725
C	-5.0401331	2.5052406	1.5340670
C	-2.9020602	-3.7008378	1.5838075
C	-2.9062521	-1.2207889	1.5669669
C	-2.9108888	1.2544382	1.5456053
C	-2.9161250	3.7344586	1.5184969
C	-0.7672530	-4.9285060	1.6438056
C	-0.7615762	-2.4516163	1.5875858
C	-0.7686992	0.0207742	1.5547612
C	-0.7709517	2.4933412	1.5426181
C	-0.7858138	4.9708600	1.5523943
C	1.3575741	-6.1530971	1.7492517
C	1.3793016	-3.6840842	1.6613425
C	1.3785622	-1.2128674	1.5930682
C	1.3738942	1.2628163	1.5705301
C	1.3652575	3.7349938	1.5929534
C	1.3344421	6.2049995	1.6326337
C	3.5127547	-4.8955825	1.7510219
C	3.5218338	-2.4422754	1.6668807
C	3.5156442	0.0293999	1.6088430
C	3.5122928	2.5016082	1.6226645

C	3.4942163	4.9559042	1.6605115
C	5.6746135	-3.6510082	1.7459152
C	5.6675855	-1.1977156	1.6546999
C	5.6629698	1.2654404	1.6334589
C	5.6606324	3.7200170	1.6814204
C	-4.3397667	-3.6700722	1.5667651
C	-4.3422100	-1.2168157	1.5421296
C	-4.3469196	1.2447632	1.5218597
C	-4.3538898	3.6981592	1.5046123
C	-2.1744951	-4.9103025	1.5907049
C	-2.1911890	-2.4545041	1.5362085
C	-2.1929009	0.0177969	1.5144700
C	-2.2005317	2.4900140	1.4923960
C	-2.1932583	4.9463819	1.5020162
C	-0.0164483	-6.1573702	1.6957745
C	-0.0445574	-3.6883589	1.5861516
C	-0.0510002	-1.2164067	1.5386193
C	-0.0557331	1.2600588	1.5160729
C	-0.0586077	3.7325704	1.5177505
C	-0.0396782	6.2031909	1.5797235
C	2.1037395	-4.9228100	1.6930571
C	2.0931216	-2.4466360	1.5982039
C	2.0919478	0.0261122	1.5503551
C	2.0837434	2.4992081	1.5532473
C	2.0849223	4.9766271	1.6010011
C	4.2358585	-3.6881199	1.6966189
C	4.2320440	-1.2083849	1.5995390
C	4.2272442	1.2694853	1.5777185
C	4.2215874	3.7505796	1.6297483
C	6.3612183	-2.4602508	1.6964563
C	6.3515326	0.0351723	1.6217483
C	6.3517865	2.5314216	1.6539542
H	-4.9041149	4.6497255	1.5070950
H	-2.7456455	5.8977694	1.5120148
H	-0.5935598	7.1522186	1.5950230
H	1.8832342	7.1570066	1.6682693
H	4.0415691	5.9099455	1.6953638
H	6.2070190	4.6734374	1.7134530
H	7.4505559	2.5318400	1.6875377
H	7.4513778	0.0376055	1.6531225
H	7.4600215	-2.4558477	1.7282979
H	6.2249832	-4.6014690	1.7938718
H	4.0637332	-5.8467564	1.8034444
H	1.9097718	-7.1022045	1.8044055
H	-0.5669420	-7.1078641	1.7299633
H	-2.7232787	-5.8633623	1.6178163
H	-4.8865609	-4.6233660	1.5846736
H	-6.1291607	-2.4800492	1.5782566
H	-6.1314783	0.0111716	1.5684738
H	-6.1387352	2.5018977	1.5395315

C_i symmetry: 2^1Ag

Geometry optimization of S_1 state at SOS-ADC(2)/SV(P) level
Circum-1-coronene dimer, ADC(2)-2

C	-6.8502743	-2.5341970	-1.4938792
C	-6.8498711	-0.0365214	-1.4869822
C	-6.8665717	2.4604530	-1.5412680
C	-4.7186471	-3.7482554	-1.5950546
C	-4.7302467	-1.2656560	-1.5883509
C	-4.7382984	1.2043077	-1.6118771
C	-4.7429475	3.6863576	-1.6651485
C	-2.5852581	-4.9711766	-1.6165157
C	-2.5861338	-2.4989726	-1.6106920
C	-2.5907675	-0.0238805	-1.6201873
C	-2.6023276	2.4508870	-1.6577867
C	-2.6174951	4.9224498	-1.7085554
C	-0.4580194	-6.1974907	-1.5989023
C	-0.4381183	-3.7260245	-1.6039639
C	-0.4499429	-1.2512800	-1.6020725
C	-0.4579975	1.2175204	-1.6256565
C	-0.4623177	3.6917654	-1.6739884
C	-0.4983022	6.1626640	-1.7131377
C	1.6943293	-4.9356669	-1.5800531
C	1.6958308	-2.4836682	-1.5995041
C	1.6903200	-0.0098979	-1.6118404
C	1.6796852	2.4636314	-1.6476190
C	1.6621626	4.9154793	-1.6742583
C	3.8548628	-3.6866250	-1.5949665
C	3.8397177	-1.2325101	-1.6131858
C	3.8316971	1.2263737	-1.6383351
C	3.8307694	3.6804592	-1.6694773
C	-6.1609105	-3.7204841	-1.5337229
C	-6.1602034	-1.2646448	-1.4992459
C	-6.1681949	1.1955H-1	-1.5226012
C	-6.1850053	3.6502852	-1.6034992
C	-3.9928984	-4.9545485	-1.5963120
C	-4.0109869	-2.5031500	-1.5640048
C	-4.0219777	-0.0281196	-1.5727487
C	-4.0271181	2.4466777	-1.6108216
C	-4.0249478	4.8970939	-1.6883090
C	-1.8303894	-6.2025351	-1.6067569
C	-1.8691807	-3.7309386	-1.5712978
C	-1.8748895	-1.2556722	-1.5744962
C	-1.8829390	1.2131739	-1.5982208
C	-1.8933335	3.6879806	-1.6411767
C	-1.8706577	6.1586326	-1.7205455
C	0.2872858	-4.9611326	-1.5698328
C	0.2698823	-2.4890838	-1.5592052
C	0.2582328	-0.0141814	-1.5746972
C	0.2537633	2.4605539	-1.6065762
C	0.2550405	4.9319487	-1.6626951
C	2.4125763	-3.7241102	-1.5686805
C	2.4068216	-1.2419926	-1.5661423

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C     2.3987858    1.2275263   -1.5904135
C     2.3883341    3.7090756   -1.6410153
C     4.5377447   -2.4952720   -1.6003801
C     4.5221088   -0.0006787   -1.6145130
C     4.5214183    2.4937126   -1.6522107
H    -6.7365140    4.6008272   -1.6241605
H    -4.5784743    5.8475231   -1.7197703
H    -2.4250165    7.1070713   -1.7610078
H     0.0515930    7.1139562   -1.7282088
H     2.2092956    5.8693466   -1.6852095
H     4.3750107    4.6347469   -1.6843720
H     5.6201867    2.4941265   -1.6656631
H     5.6219747    0.0027527   -1.6300523
H     5.6365318   -2.4885641   -1.6112002
H     4.4052847   -4.6374789   -1.5893133
H     2.2477685   -5.8859352   -1.5726673
H     0.0982211   -7.1452554   -1.5971605
H    -2.3786809   -7.H-11140   -1.6309455
H    -4.5404003   -5.9089043   -1.6105435
H    -6.7059944   -4.6749330   -1.5364702
H    -7.9484512   -2.5355738   -1.4482048
H    -7.9488014   -0.0395861   -1.4358557
H    -7.9647233    2.4554821   -1.4958895
C    -4.5214183   -2.4937126    1.6522107
C    -4.5221088    0.0006787    1.6145130
C    -4.5377447    2.4952720    1.6003801
C    -2.3883341   -3.7090756    1.6410153
C    -2.3987858   -1.2275263    1.5904135
C    -2.4068216    1.2419926    1.5661423
C    -2.4125763    3.7241102    1.5686805
C    -0.2550405   -4.9319487    1.6626951
C    -0.2537633   -2.4605539    1.6065762
C    -0.2582328    0.0141814    1.5746972
C    -0.2698823    2.4890838    1.5592052
C    -0.2872858    4.9611326    1.5698328
C     1.8706577   -6.1586326    1.7205455
C     1.8933335   -3.6879806    1.6411767
C     1.8829390   -1.2131739    1.5982208
C     1.8748895    1.2556722    1.5744962
C     1.8691807    3.7309386    1.5712978
C     1.8303894    6.2025351    1.6067569
C     4.0249478   -4.8970939    1.6883090
C     4.0271181   -2.4466777    1.6108216
C     4.0219777    0.0281196    1.5727487
C     4.0109869    2.5031500    1.5640048
C     3.9928984    4.9545485    1.5963120
C     6.1850053   -3.6502852    1.6034992
C     6.1681949   -1.1955H-1    1.5226012
C     6.1602034    1.2646448    1.4992459
C     6.1609105    3.7204841    1.5337229
C    -3.8307694   -3.6804592    1.6694773
C    -3.8316971   -1.2263737    1.6383351
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C    -3.8397177    1.2325101    1.6131858
C    -3.8548628    3.6866250    1.5949665
C    -1.6621626   -4.9154793    1.6742583
C    -1.6796852   -2.4636314    1.6476190
C    -1.6903200    0.0098979    1.6118404
C    -1.6958308    2.4836682    1.5995041
C    -1.6943293    4.9356669    1.5800531
C     0.4983022   -6.1626640    1.7131377
C     0.4623177   -3.6917654    1.6739884
C     0.4579975   -1.2175204    1.6256565
C     0.4499429    1.2512800    1.6020725
C     0.4381183    3.7260245    1.6039639
C     0.4580194    6.1974907    1.5989023
C     2.6174951   -4.9224498    1.7085554
C     2.6023276   -2.4508870    1.6577867
C     2.5907675    0.0238805    1.6201873
C     2.5861338    2.4989726    1.6106920
C     2.5852581    4.9711766    1.6165157
C     4.7429475   -3.6863576    1.6651485
C     4.7382984   -1.2043077    1.6118771
C     4.7302467    1.2656560    1.5883509
C     4.7186471    3.7482554    1.5950546
C     6.8665717   -2.4604530    1.5412680
C     6.8498711    0.0365214    1.4869822
C     6.8502743    2.5341970    1.4938792
H    -4.4052847    4.6374789    1.5893133
H    -2.2477685    5.8859352    1.5726673
H    -0.0982211    7.1452554    1.5971605
H     2.3786809    7.H-11140    1.6309455
H     4.5404003    5.9089043    1.6105435
H     6.7059944    4.6749330    1.5364702
H     7.9484512    2.5355738    1.4482048
H     7.9488014    0.0395861    1.4358557
H     7.9647233   -2.4554821    1.4958895
H     6.7365140   -4.6008272    1.6241605
H     4.5784743   -5.8475231    1.7197703
H     2.4250165   -7.1070713    1.7610078
H    -0.0515930   -7.1139562    1.7282088
H    -2.2092956   -5.8693466    1.6852095
H    -4.3750107   -4.6347469    1.6843720
H    -5.6201867   -2.4941265    1.6656631
H    -5.6219747   -0.0027527    1.6300523
H    -5.6365318    2.4885641    1.6112002
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