Supporting Information

Electronically Excited States of Higher Acenes up to Nonacene: A Density Functional Theory/Multireference Configuration Interaction Study

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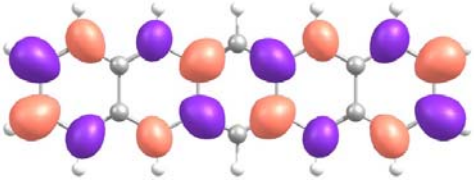
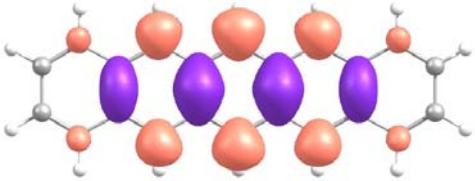
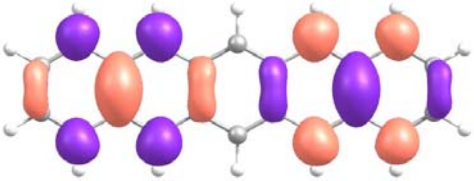


8‘, $4a_u$



7‘ $6b_{1u}$



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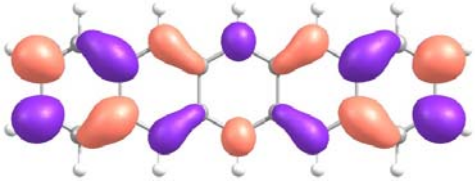

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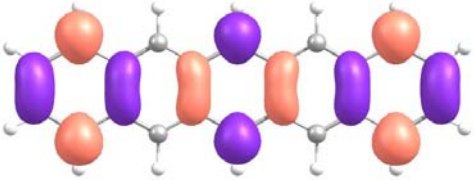

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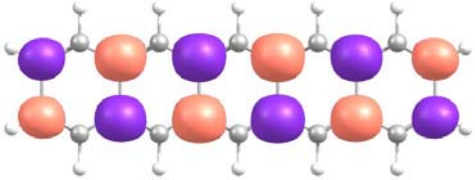

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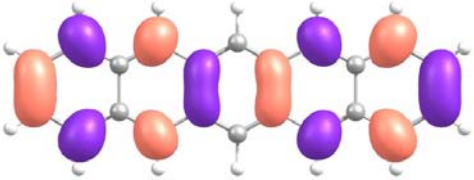

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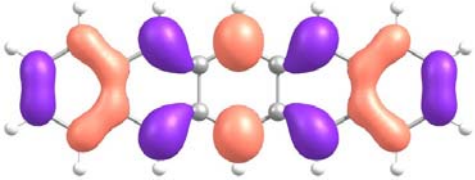

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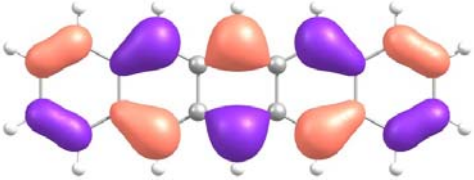

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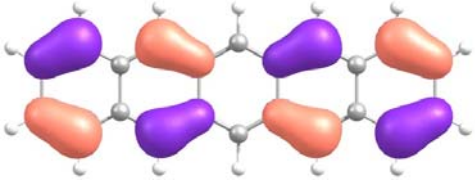

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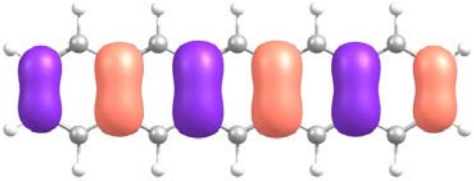

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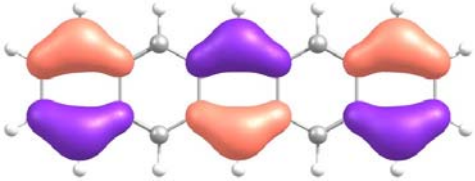

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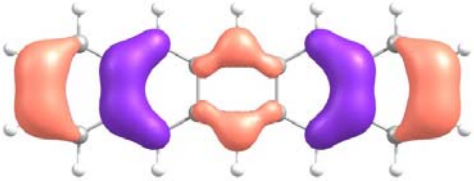

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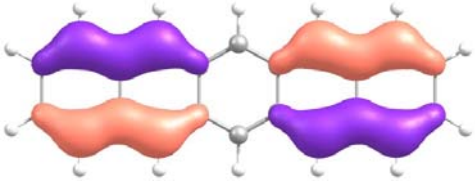

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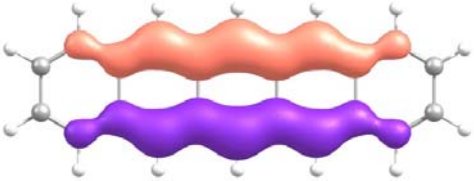

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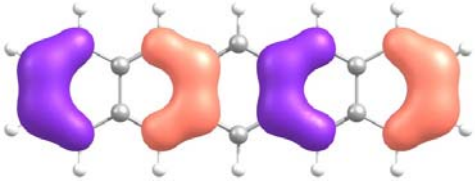
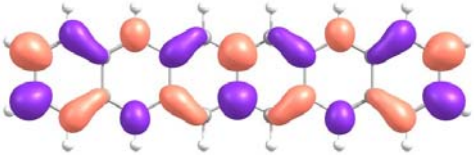


8, $2b_{2g}$

Figure S2. Molecular orbitals of hexacene as computed at the BHLYP/SV(P) level of theory and used in the DFT/MRCI computation.



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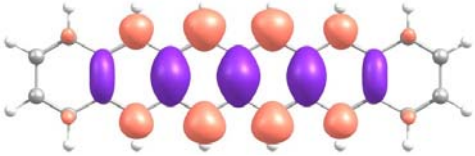

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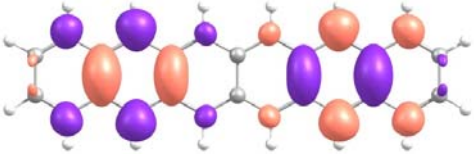

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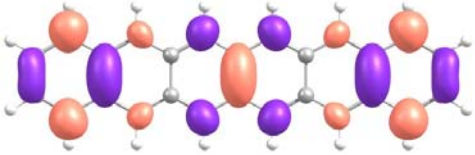

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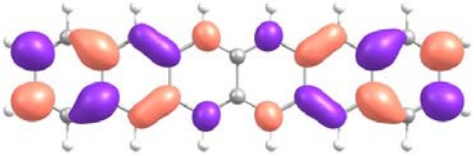

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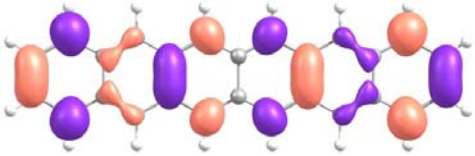

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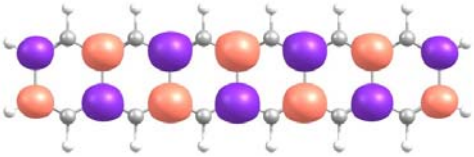

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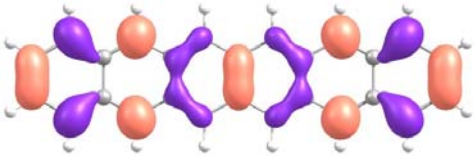

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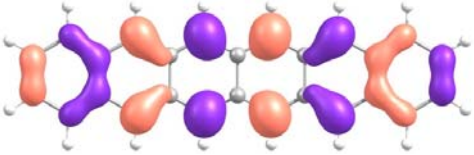

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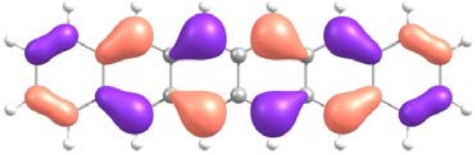

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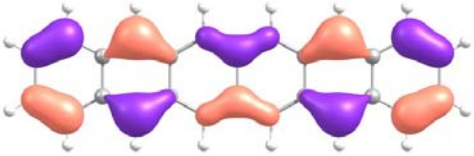

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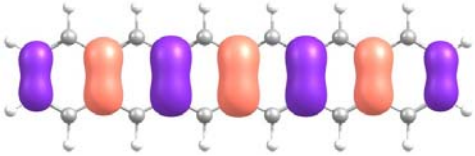

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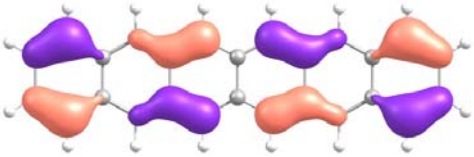

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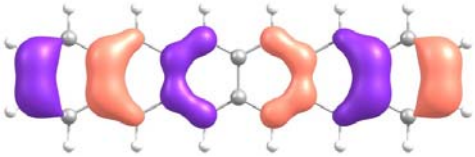

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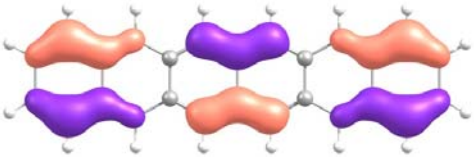
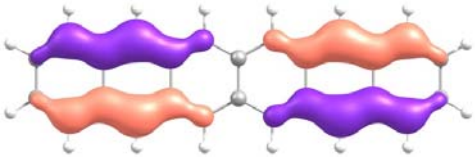
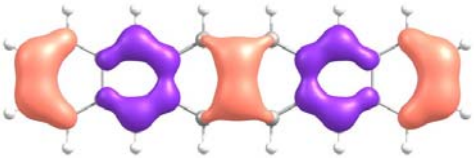


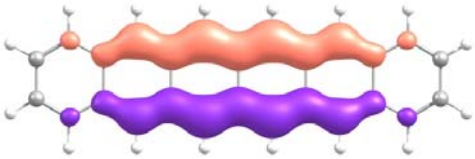
6, 2b_{3g}



7, 1a_u



8, 3b_{1u}



9, 1b_{3g}

Figure S3. Molecular orbitals of heptacene as computed at the BHLYP/SV(P) level of theory and used in the DFT/MRCI computation.

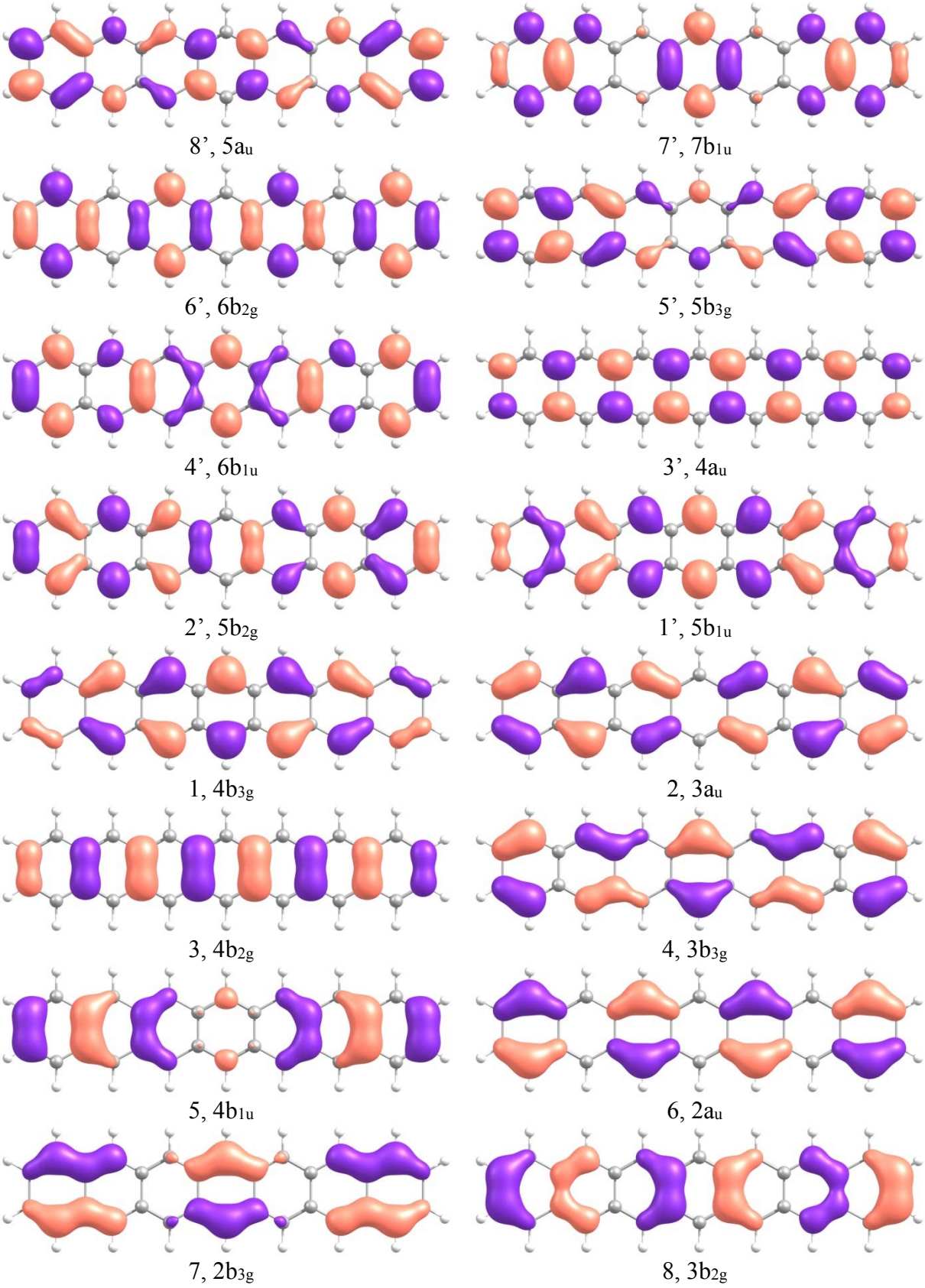


Figure S4. Molecular orbitals of octacene as computed at the BHLYP/SV(P) level of theory and used in the DFT/MRCI computation.

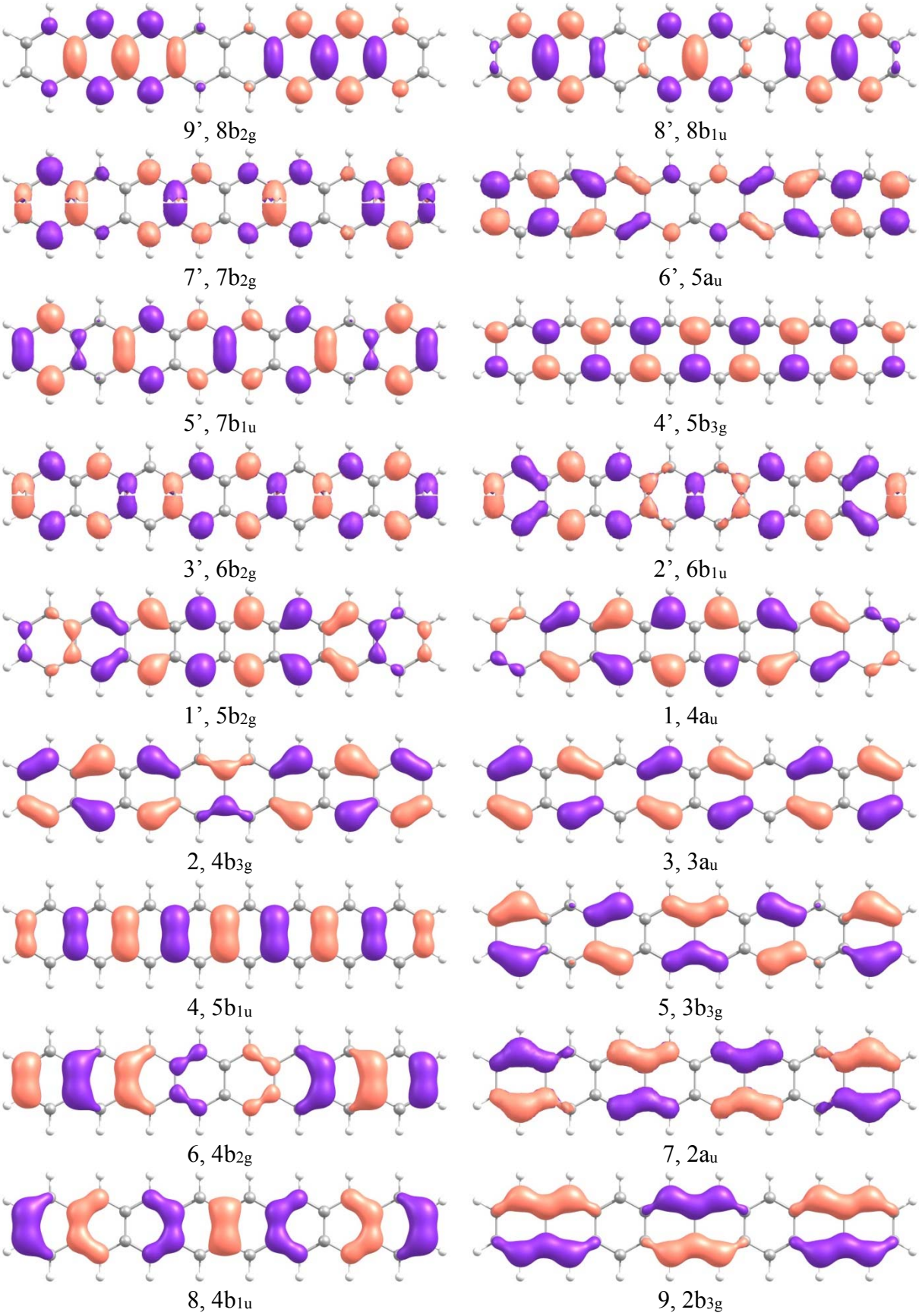


Figure S5. Molecular orbitals of nonacene as computed at the BHLYP/SV(P) level of theory and used in the DFT/MRCI computation.

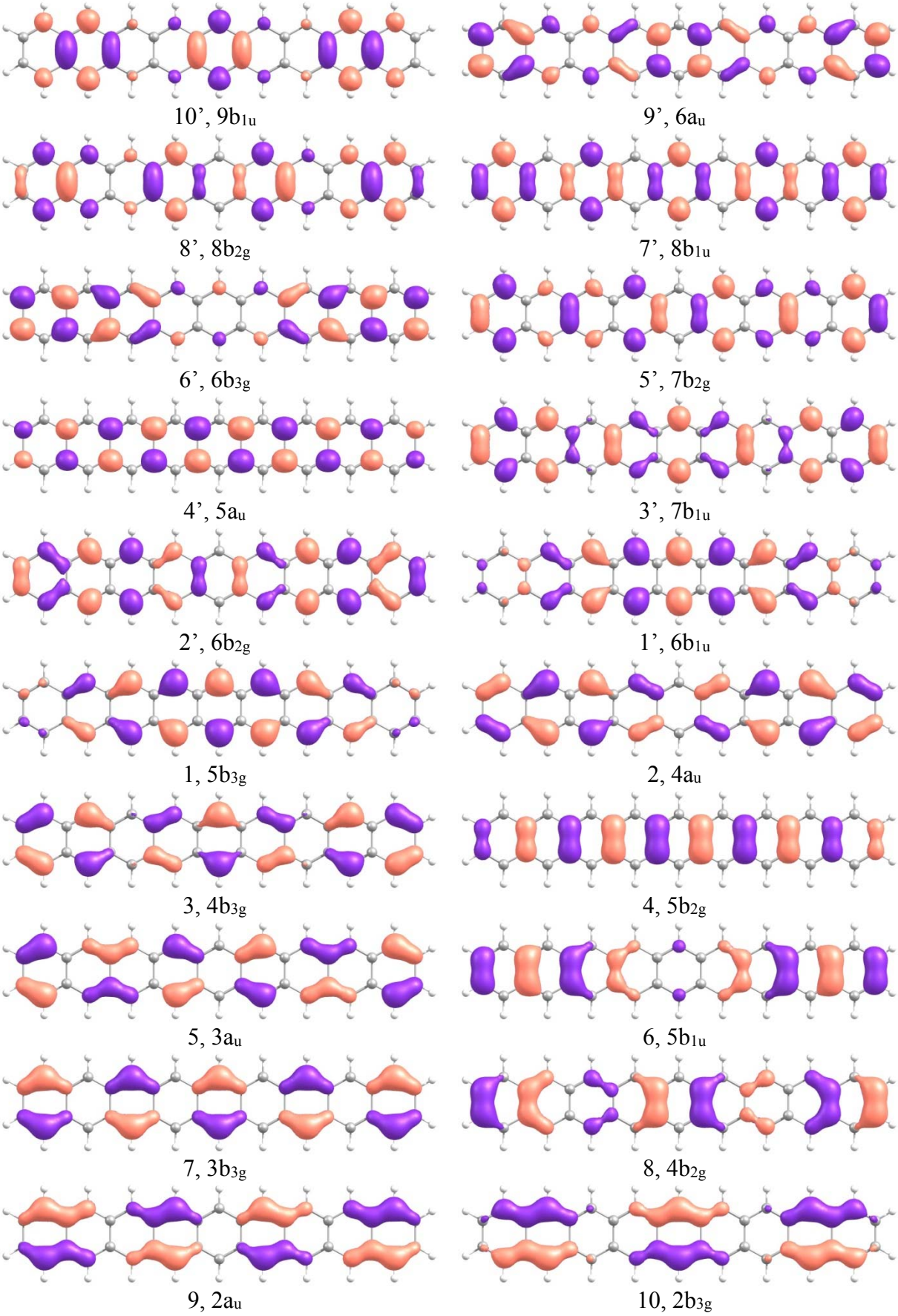


Table S1. Pentacene singlet state excitation energies (E, in eV), oscillator strengths, dominant contributions to the electronic wavefunction and their weights (above 0.1) as computed with the DFT/MRCI method.

State	E/eV	Osc. strength	Dominant contributions	Weight
GS			$(6)^2\ (5)^2\ (4)^2\ (3)^2\ (2)^2\ (1)^2$	0.87
1 $^1B_{2u}$ (^1L_a, *p*)	2.16	0.097	1 → 1'	0.86
2 $^1B_{2u}$	3.81	0.000	4 → 1' 1 → 4'	0.44 0.18
3 $^1B_{2u}$	4.38	0.049	1 → 4' 2 → 2' 4 → 1'	0.35 0.30 0.16
4 $^1B_{2u}$	4.69	0.073	2 → 2' 1 → 4' 4 → 1'	0.34 0.14 0.11
5 $^1B_{2u}$	4.84	0.000	1 → 7' 7 → 1'	0.35 0.32
6 $^1B_{2u}$	4.98	0.003	5,1 → 1',1' 4,3 → 1',1' 2,1 → 1',3'	0.18 0.13 0.11
7 $^1B_{2u}$	5.68	0.021	1 → 7' 7 → 1'	0.36 0.34
8 $^1B_{2u}$	5.71	0.212	3 → 3'	0.53
9 $^1B_{2u}$	5.85	0.024	3,1 → 1',2' 3,2 → 1',1' 1,1 → 2',3'	0.21 0.21 0.10
10 $^1B_{2u}$	6.00	0.003	6 → 2' 2 → 6' 2,1 → 1',3'	0.16 0.14 0.13
1 $^1B_{3u}$ (^1L_b, α)	2.95	0.008	3 → 1' 1 → 3'	0.43 0.36
2 $^1B_{3u}$ (D1)	3.50	0.000	2,1 → 1',1' 1,1 → 1',2'	0.36 0.29
3 $^1B_{3u}$ (^1B_b, β)	4.27	4.111	1 → 3' 3 → 1'	0.46 0.38
4 $^1B_{3u}$	4.77	0.000	6,1 → 1',1' 1,1 → 1',6' 8 → 1'	0.20 0.15 0.10
5 $^1B_{3u}$	5.27	0.000	4 → 3' 3 → 4' 5 → 2'	0.25 0.19 0.14
6 $^1B_{3u}$ (D2)	5.37	0.029	1,1 → 1',2' 2,1 → 1',1' 8 → 1'	0.23 0.10 0.14
7 $^1B_{3u}$	5.42	0.029	2,1 → 1',1' 1,1 → 1',2'	0.14 0.12
8 $^1B_{3u}$	5.77	0.001	5 → 2' 3,1 → 2',3' 3,1 → 1',3' 2 → 5'	0.17 0.10 0.10 0.11
9 $^1B_{3u}$	5.85	0.000	8 → 1'	0.15
10 $^1B_{3u}$	6.22	0.012	1 → 8' 6,1 → 1',1'	0.13 0.11

Table S2. Hexacene singlet state excitation energies (E, in eV), oscillator strengths, dominant contributions to the electronic wavefunction and their weights (above 0.1) as computed with the DFT/MRCI method.

State	E/eV	Osc. strength	Dominant contributions	Weight
GS			$(6)^2\ (5)^2\ (4)^2\ (3)^2\ (2)^2\ (1)^2$	0.82
1 $^1B_{2u}$	1.80	0.077	1 → 1'	0.85
2 $^1B_{2u}$	3.30	0.001	4 → 1' 1 → 4'	0.44 0.16
3 $^1B_{2u}$	3.76	0.077	2 → 2' 1 → 4'	0.39 0.26
4 $^1B_{2u}$	4.08	0.057	1 → 4' 2 → 2' 4 → 1'	0.22 0.20 0.16
5 $^1B_{2u}$	4.36	0.004	5,1 → 1',1' 3,2 → 1',1' 2,1 → 1',3'	0.18 0.11 0.10
6 $^1B_{2u}$	4.55	0.000	7 → 1' 1 → 7'	0.35 0.22
7 $^1B_{2u}$	5.06	0.009	2,1,1 → 1',1',2' 2 → 2'	0.54 0.11
8 $^1B_{2u}$	5.12	0.000	3,1 → 1',2' 3,2 → 1',1' 2,1 → 1',3'	0.27 0.18 0.14
9 $^1B_{2u}$	5.23	0.000	1 → 7' 7 → 1'	0.39 0.24
10 $^1B_{2u}$	5.33	0.002	2,1 → 1',3' 6 → 2' 2 → 6'	0.14 0.11 0.07
1 $^1B_{3u}$	2.63	0.003	2,1 → 1',1' 1,1 → 1',2'	0.31 0.26
2 $^1B_{3u}$	2.88	0.010	3 → 1' 1 → 3'	0.37 0.29
3 $^1B_{3u}$	3.99	4.421	1 → 3' 3 → 1'	0.37 0.30
4 $^1B_{3u}$	3.99	0.410	6,1 → 1',1' 1,1 → 1',6'	0.19 0.12
5 $^1B_{3u}$	4.48	0.004	1,1 → 1',2' 2,1 → 1',1'	0.29 0.24
6 $^1B_{3u}$	4.56	0.000	4,2 → 1',1'	0.09
7 $^1B_{3u}$	4.85	0.000	4 → 3' 3 → 4' 5 → 2'	0.18 0.14 0.13
8 $^1B_{3u}$	4.96	0.000	1,1 → 1',8' 9,1 → 1',1'	0.17 0.13
9 $^1B_{3u}$	5.09	0.000	8 → 1'	0.21
10 $^1B_{3u}$	5.38	0.026	5 → 2' 4 → 3'	0.10 0.10

Table S3. Heptacene singlet state excitation energies (E, in eV), oscillator strengths, dominant contributions to the electronic wavefunction and their weights (above 0.1) as computed with the DFT/MRCI method.

State	E/eV	Osc. strength	Dominant contributions	Weight
GS			…$(5)^2$ $(4)^2$ $(3)^2$ $(2)^2$ $(1)^2$ 1,1 → 1',1'	0.74 0.10
1 $^1B_{2u}$	1.57	0.057	1 → 1'	0.83
2 $^1B_{2u}$	2.91	0.001	4 → 1' 1 → 4'	0.43 0.15
3 $^1B_{2u}$	3.24	0.090	2 → 2' 1 → 4' 2,1,1 → 1',1',2' 4 → 1'	0.40 0.18 0.15 0.04
4 $^1B_{2u}$	3.61	0.028	1 → 4' 4 → 1' 2,1,1 → 1',1',2'	0.29 0.21 0.1
5 $^1B_{2u}$	3.94	0.003	5,1 → 1',1' 3,2 → 1',1'	0.18 0.11
6 $^1B_{2u}$	4.17	0.000	7 → 1' 1 → 7'	0.33 0.15
7 $^1B_{2u}$	4.20	0.018	2,1,1 → 1',1',2' 2 → 2'	0.44 0.22
8 $^1B_{2u}$	4.62	0.002	3,1 → 1',2' 3,2 → 1',1'	0.26 0.16
9 $^1B_{2u}$	4.72	0.000	1 → 9' 10 → 1'	0.12 0.09
10 $^1B_{2u}$	4.75	0.000	1 → 9' 10 → 1'	0.20 0.17
1 $^1B_{3u}$	2.08	0.001	2,1 → 1',1' 1,1 → 1',2'	0.35 0.30
2 $^1B_{3u}$	2.80	0.020	3 → 1' 1 → 3'	0.42 0.31
3 $^1B_{3u}$	3.36	0.000	6,1 → 1',1' 1,1 → 1',6'	0.20 0.13
4 $^1B_{3u}$	3.65	3.696	1,1 → 1',2' 2,1 → 1',1' 1 → 3' 3 → 1'	0.22 0.19 0.14 0.10
5 $^1B_{3u}$	3.87	0.000	4,2 → 1',1' 2,2 → 1',2' 4,1 → 1',2' 2,1 → 1',4'	0.10 0.09 0.09 0.08
6 $^1B_{3u}$	3.97	1.772	1 → 3' 3 → 1' 1,1 → 1',2' 2,1 → 1',1'	0.32 0.25 0.09 0.08
7 $^1B_{3u}$	4.43	0.001	9,1 → 1',1' 1,1 → 1',8'	0.14 0.12
8 $^1B_{3u}$	4.48	0.001	5 → 2' 4 → 3'	0.10 0.10
9 $^1B_{3u}$	4.58	0.001	8 → 1'	0.20
10 $^1B_{3u}$	4.69	0.013	6,1 → 1',1' 1,1 → 1',6'	0.19 0.10

Table S4. Octacene singlet state excitation energies (E, in eV), oscillator strengths, dominant contributions to the electronic wavefunction and their weights (above 0.1) as computed with the DFT/MRCI method.

State	E/eV	Osc. strength	Dominant contributions	Weight
GS			$\ldots(5)^2\ (4)^2\ (3)^2\ (2)^2\ (1)^2$ 1,1 → 1',1'	0.63 0.16
1 $^1B_{2u}$	1.43	0.038	1 → 1'	0.80
2 $^1B_{2u}$	2.64	0.005	3 → 1' 1 → 3'	0.43 0.12
3 $^1B_{2u}$	2.79	0.083	2 → 2' 2,1,1 → 1',1',2' 1 → 3'	0.30 0.30 0.13
4 $^1B_{2u}$	3.22	0.005	1 → 3' 3 → 1' 2,1,1 → 1',1',2'	0.35 0.22 0.13
5 $^1B_{2u}$	3.61	0.007	2 → 2' 2,1,1 → 1',1',2'	0.13 0.12
6 $^1B_{2u}$	3.66	0.025	2 → 2' 2,1,1 → 1',1',2'	0.23 0.13
7 $^1B_{2u}$	3.84	0.002	7 → 1' 1 → 7'	0.26 0.09
8 $^1B_{2u}$	3.97	0.000	5,1,1 → 1',1',2' 3,1,1 → 1',2',2'	0.11 0.09
9 $^1B_{2u}$	4.24	0.003	4,1 → 1',2' 2,1 → 1',4'	0.20 0.12
10 $^1B_{2u}$	4.37	0.012	5 → 2' 3 → 3'	0.18 0.10
1 $^1B_{3u}$	1.64	0.001	2,1 → 1',1' 1,1 → 1',2'	0.34 0.29
2 $^1B_{3u}$	2.79	0.032	4 → 1' 1 → 4'	0.40 0.29
3 $^1B_{3u}$	2.84	0.001	5,1 → 1',1' 1,1 → 1',5'	0.18 0.11
4 $^1B_{3u}$	3.19	2.620	1,1 → 1',2' 2,1 → 1',1' 1 → 4' 4 → 1'	0.28 0.25 0.03 0.02
5 $^1B_{3u}$	3.28	0.001	2,2 → 1',2'	0.10
6 $^1B_{3u}$	3.80	3.425	1 → 4' 4 → 1' 1,1 → 1',2' 2,1 → 1',1'	0.41 0.30 0.02 0.01
7 $^1B_{3u}$	4.01	0.001	9,1 → 1',1' 1,1 → 1',8'	0.18 0.13
8 $^1B_{3u}$	4.09	0.044	3,1 → 1',2' 2,1 → 1',3'	0.17 0.10
9 $^1B_{3u}$	4.11	0.000	5,1 → 1',1' 3,2 → 1',1'	0.17 0.11
10 $^1B_{3u}$	4.12	0.032	3,1 → 1',2' 2,1 → 1',3'	0.16 0.13

Table S5. Nonacene singlet state excitation energies (E, in eV), oscillator strengths, dominant contributions to the electronic wavefunction and their weights (above 0.1) as computed with the DFT/MRCI method.

State	E/eV	Osc. strength	Dominant contributions	Weight
GS			$\ldots(5)^2\ (4)^2\ (3)^2\ (2)^2\ (1)^2$ 1,1 → 1',1'	0.50 0.23
1 $^1B_{2u}$	1.34	0.023	1 → 1'	0.77
2 $^1B_{2u}$	2.37	0.064	2,1,1 → 1',1',2' 2 → 2' 3 → 1'	0.38 0.19 0.12
3 $^1B_{2u}$	2.47	0.011	3,1 → 1' 1 → 3'	0.28 0.20
4 $^1B_{2u}$	2.91	0.000	1 → 3' 3 → 1' 2,1,1 → 1',1',2'	0.34 0.19 0.11
5 $^1B_{2u}$	3.21	0.001	5,1,1 → 1',1',2'	0.12
6 $^1B_{2u}$	3.29	0.032	2 → 2'	0.38
7 $^1B_{2u}$	3.50	0.005	6,1 → 1',1' 1,1 → 1',6'	0.18 0.06
8 $^1B_{2u}$	3.60	0.001	7 → 1' 1 → 7'	0.31 0.10
9 $^1B_{2u}$	3.90	0.012	3,1,1 → 1',1',3'	0.13
10 $^1B_{2u}$	3.97	0.012	5,1,1 → 1',1',2' 2,1,1 → 1',1',5'	0.10 0.10
1 $^1B_{3u}$	1.31	0.001	2,1 → 1',1' 1,1 → 1',2'	0.32 0.28
2 $^1B_{3u}$	2.43	0.000	5,1 → 1',1' 1,1 → 1',5'	0.16 0.11
3 $^1B_{3u}$	2.76	0.080	4 → 1' 1 → 4'	0.13 0.08
4 $^1B_{3u}$	2.81	2.849	1,1 → 1',2' 2,1 → 1',1'	0.27 0.24
5 $^1B_{3u}$	2.85	0.001	4 → 1' 1 → 4'	0.25 0.18
6 $^1B_{3u}$	3.60	0.011	9,1 → 1',1'	0.13
7 $^1B_{3u}$	3.62	0.243	3,1 → 1',2' 2,1 → 1',3'	0.27 0.20
8 $^1B_{3u}$	3.65	0.621	5,1 → 1',1' 3,2 → 1',1'	0.16 0.11
9 $^1B_{3u}$	3.68	0.097	8 → 1'	0.05
10 $^1B_{3u}$	3.76	2.920	1 → 4' 4 → 1'	0.30 0.26

Cartesian Coordinates

1. Pentacene

```
36
RB3LYP/6-31G*
C     0.000000    6.117773    0.716539
C     0.000000    6.117773   -0.716539
C     0.000000    4.941679    1.410493
H     0.000000    4.939589   -2.497985
C     0.000000    3.678627    0.727636
H     0.000000    4.939589    2.497985
C     0.000000    2.467610    1.407893
C     0.000000    3.678627   -0.727636
H     0.000000    2.467654   -2.496077
C     0.000000    4.941679   -1.410493
C     0.000000    1.226459    0.728546
H     0.000000    2.467654    2.496077
C     0.000000    0.000000    1.408557
C     0.000000    1.226459   -0.728546
C     0.000000    0.000000   -1.408557
C     0.000000    2.467610   -1.407893
C     0.000000   -1.226459    0.728546
H     0.000000    0.000000    2.496628
C     0.000000   -1.226459   -0.728546
H     0.000000    0.000000   -2.496628
C     0.000000   -2.467610   -1.407893
C     0.000000   -2.467610    1.407893
H     0.000000   -2.467654    2.496077
C     0.000000   -3.678627    0.727636
H     0.000000   -2.467654   -2.496077
C     0.000000   -3.678627   -0.727636
C     0.000000   -4.941679    1.410493
C     0.000000   -4.941679   -1.410493
H     0.000000   -4.939589    2.497985
C     0.000000   -6.117773    0.716539
H     0.000000   -4.939589   -2.497985
C     0.000000   -6.117773   -0.716539
H     0.000000   -7.065790    1.247585
H     0.000000   -7.065790   -1.247585
H     0.000000    7.065790    1.247585
H     0.000000    7.065790   -1.247585
```

2. Hexacene

```
42
RB3LYP/6-31G*
6 0.000000 7.346953 0.717162
1 0.000000 6.169729 2.498614
6 0.000000 6.171728 1.411129
6 0.000000 6.171728 -1.411129
6 0.000000 4.907388 0.728587
6 0.000000 7.346953 -0.717162
6 0.000000 4.907388 -0.728587
6 0.000000 3.698500 1.408768
1 0.000000 3.698611 -2.496935
1 0.000000 6.169729 -2.498614
6 0.000000 2.454391 0.729867
1 0.000000 3.698611 2.496935
6 0.000000 1.232337 1.409783
6 0.000000 2.454391 -0.729867
1 0.000000 1.232506 -2.497814
6 0.000000 3.698500 -1.408768
6 0.000000 0.000000 0.730481
1 0.000000 1.232506 2.497814
6 0.000000 -1.232337 1.409783
6 0.000000 0.000000 -0.730481
6 0.000000 -1.232337 -1.409783
6 0.000000 1.232337 -1.409783
6 0.000000 -2.454391 0.729867
1 0.000000 -1.232506 2.497814
```

```
6 0.000000 -2.454391 -0.729867
1 0.000000 -1.232506 -2.497814
6 0.000000 -3.698500 -1.408768
6 0.000000 -3.698500 1.408768
1 0.000000 -3.698611 2.496935
6 0.000000 -4.907388 0.728587
1 0.000000 -3.698611 -2.496935
6 0.000000 -4.907388 -0.728587
6 0.000000 -6.171728 1.411129
6 0.000000 -6.171728 -1.411129
1 0.000000 -6.169729 2.498614
6 0.000000 -7.346953 0.717162
1 0.000000 -6.169729 -2.498614
6 0.000000 -7.346953 -0.717162
1 0.000000 -8.295202 1.247772
1 0.000000 -8.295202 -1.247772
1 0.000000 8.295202 1.247772
1 0.000000 8.295202 -1.247772
```

3. Heptacene

```
48
RB3LYP/6-31G*
C     0.000000    8.576309    0.717500
H     0.000000    7.399636    2.498957
C     0.000000    7.401550    1.411476
C     0.000000    7.401550   -1.411476
C     0.000000    6.136513    0.729125
C     0.000000    8.576309   -0.717500
C     0.000000    6.136513   -0.729125
C     0.000000    4.928769    1.409256
H     0.000000    4.928916   -2.497416
H     0.000000    7.399636   -2.498957
C     0.000000    3.683061    0.730622
H     0.000000    4.928916    2.497416
C     0.000000    2.463339    1.410490
C     0.000000    3.683061   -0.730622
H     0.000000    2.463571   -2.498506
C     0.000000    4.928769   -1.409256
C     0.000000    1.227896    0.731581
H     0.000000    2.463571    2.498506
C     0.000000    0.000000    1.410838
C     0.000000    1.227896   -0.731581
C     0.000000    0.000000   -1.410838
C     0.000000    2.463339   -1.410490
C     0.000000   -1.227896    0.731581
H     0.000000    0.000000    2.498832
C     0.000000   -1.227896   -0.731581
H     0.000000    0.000000   -2.498832
C     0.000000   -2.463339   -1.410490
C     0.000000   -2.463339    1.410490
H     0.000000   -2.463571    2.498506
C     0.000000   -3.683061    0.730622
H     0.000000   -2.463571   -2.498506
C     0.000000   -3.683061   -0.730622
C     0.000000   -4.928769    1.409256
C     0.000000   -4.928769   -1.409256
H     0.000000   -4.928916    2.497416
C     0.000000   -6.136513    0.729125
H     0.000000   -4.928916   -2.497416
C     0.000000   -6.136513   -0.729125
C     0.000000   -7.401550    1.411476
C     0.000000   -7.401550   -1.411476
H     0.000000   -7.399636    2.498957
C     0.000000   -8.576309    0.717500
H     0.000000   -7.399636   -2.498957
C     0.000000   -8.576309   -0.717500
H     0.000000   -9.524671   -1.247892
H     0.000000   -9.524671    1.247892
H     0.000000    9.524671    1.247892
H     0.000000    9.524671   -1.247892
```

4. Octacene

```
54
RB3LYP/6-31G*
6 0.000000 8.631220 1.411688
6 0.000000 7.365802 0.729407
1 0.000000 6.158901 2.497686
6 0.000000 6.158688 1.409536
6 0.000000 6.158688 -1.409536
6 0.000000 4.912109 0.731032
6 0.000000 7.365802 -0.729407
6 0.000000 4.912109 -0.731032
6 0.000000 3.693661 1.410905
6 0.000000 8.631220 -1.411688
1 0.000000 3.693982 -2.498905
1 0.000000 6.158901 -2.497686
6 0.000000 2.456527 0.732203
1 0.000000 3.693982 2.498905
6 0.000000 1.231018 1.411466
6 0.000000 2.456527 -0.732203
1 0.000000 1.231110 -2.499432
6 0.000000 3.693661 -1.410905
6 0.000000 0.000000 0.732547
1 0.000000 1.231110 2.499432
6 0.000000 -1.231018 1.411466
6 0.000000 0.000000 -0.732547
6 0.000000 -1.231018 -1.411466
6 0.000000 1.231018 -1.411466
6 0.000000 9.805705 0.717695
1 0.000000 8.629331 2.499163
6 0.000000 9.805705 -0.717695
1 0.000000 8.629331 -2.499163
1 0.000000 10.754160 1.247913
1 0.000000 10.754160 -1.247913
6 0.000000 -2.456527 0.732203
1 0.000000 -1.231110 2.499432
6 0.000000 -2.456527 -0.732203
1 0.000000 -1.231110 -2.499432
6 0.000000 -3.693661 -1.410905
6 0.000000 -3.693661 1.410905
1 0.000000 -3.693982 2.498905
6 0.000000 -4.912109 0.731032
1 0.000000 -3.693982 -2.498905
6 0.000000 -4.912109 -0.731032
6 0.000000 -6.158688 1.409536
6 0.000000 -6.158688 -1.409536
1 0.000000 -6.158901 2.497686
6 0.000000 -7.365802 0.729407
1 0.000000 -6.158901 -2.497686
6 0.000000 -7.365802 -0.729407
6 0.000000 -8.631220 1.411688
6 0.000000 -8.631220 -1.411688
1 0.000000 -8.629331 2.499163
6 0.000000 -9.805705 0.717695
1 0.000000 -8.629331 -2.499163
6 0.000000 -9.805705 -0.717695
1 0.000000 -10.754160 -1.247913
1 0.000000 -10.754160 1.247913
```

5. Nonacene

```
60
RB3LYP/6-31G*
6 0.000000 11.034951 0.717743
6 0.000000 9.860578 1.411824
6 0.000000 8.595004 0.729617
6 0.000000 8.595004 -0.729617
6 0.000000 9.860578 -1.411824
6 0.000000 11.034951 -0.717743
6 0.000000 7.388248 1.409762
6 0.000000 7.388248 -1.409762
6 0.000000 6.141209 -0.731412
6 0.000000 6.141209 0.731412
6 0.000000 4.923492 1.411153
```

```
1 0.000000 4.924459 2.499186
6 0.000000 3.685415 0.732754
6 0.000000 3.685415 -0.732754
6 0.000000 4.923492 -1.411153
1 0.000000 7.389124 2.497922
1 0.000000 11.983243 1.248256
1 0.000000 9.859194 2.499293
1 0.000000 9.859194 -2.499293
1 0.000000 11.983243 -1.248256
1 0.000000 7.389124 -2.497922
1 0.000000 4.924459 -2.499186
6 0.000000 2.461281 1.411815
6 0.000000 1.228566 0.733330
6 0.000000 1.228566 -0.733330
6 0.000000 0.000000 1.412022
6 0.000000 0.000000 -1.412022
6 0.000000 -1.228566 0.733330
1 0.000000 0.000000 2.500019
6 0.000000 -1.228566 -0.733330
1 0.000000 0.000000 -2.500019
6 0.000000 -2.461281 1.411815
6 0.000000 -2.461281 -1.411815
6 0.000000 -3.685415 0.732754
1 0.000000 -2.461805 2.499821
6 0.000000 -3.685415 -0.732754
1 0.000000 -2.461805 -2.499821
6 0.000000 -4.923492 1.411153
6 0.000000 -4.923492 -1.411153
6 0.000000 -6.141209 0.731412
1 0.000000 -4.924459 2.499186
1 0.000000 -4.924459 -2.499186
6 0.000000 -6.141209 -0.731412
6 0.000000 2.461281 -1.411815
6 0.000000 -7.388248 1.409762
6 0.000000 -8.595004 0.729617
6 0.000000 -8.595004 -0.729617
6 0.000000 -9.860578 1.411824
6 0.000000 -9.860578 -1.411824
6 0.000000 -11.034951 0.717743
1 0.000000 -9.859194 2.499293
6 0.000000 -11.034951 -0.717743
1 0.000000 -9.859194 -2.499293
6 0.000000 -7.388248 -1.409762
1 0.000000 2.461805 -2.499821
1 0.000000 -7.389124 -2.497922
1 0.000000 -7.389124 2.497922
1 0.000000 2.461805 2.499821
1 0.000000 -11.983243 -1.248256
1 0.000000 -11.983243 1.248256
```