Supplementary Information

Low-lying excited states of linear all-*trans* polyenes: The $\sigma - \pi$ electron correlation and the description of ionic states

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Contents

1 Freezing schemes and reference active spaces selection

1.1 Active space

Tests on the active space were conducted on decapentaene. All tests were performed using the optimal freezing scheme adopted in this work (Table S2). The relevant tests are presented in Table S1. For all tests involving restricted active (RAS) and/or auxiliary (AUX) spaces, one hole was allowed in the RAS (single excitations from this space), and one electron was allowed in the AUX (single excitations to this space).

Table S1. Excitation energies (eV) of decapentaene calculated using a variety of reference spaces for the MR-CISD computation. Molecular orbitals were calculated at the SA6-CASSCF(10,10) level. All calculations were performed using the cc-pVDZ basis set.

Active Space	Excitation	ΔE_{CI}	ΔE_{CI+P}	ΔE_{AQCC}
MR-CISD(CAS(10,10))	$1^1A_g^- - 2^1A_g^-$	4.562	4.472	4.462
	$1^1A_g^- - 1^1B_u^+$	5.380	4.613	4.560
	$1^1A_g^- - 2^1B_u^-$	5.657	5.559	5.541
MR-CISD(RAS(1)CAS(8,8)AUX(1))	$1^1A_g^- - 2^1A_g^-$	4.599	4.453	4.477
	$1^1A_g^- - 1^1B_u^+$	5.350	4.618	4.547
	$1^1A_g^- - 2^1B_u^-$	5.691	5.537	5.547
MR-CISD(RAS(2)CAS(6,6)AUX(2))	$1^1A_g^- - 2^1A_g^-$	4.648	4.448	4.505
	$1^1A_g^- - 1^1B_u^+$	5.311	4.622	4.536
	$1^1A_g^- - 2^1B_u^-$	5.838	5.498	5.636
MR-CISD(CAS(8,8))[a]	$1^1A_g^- - 2^1A_g^-$	4.834	4.460	–
	$1^1A_g^- - 1^1B_u^+$	5.216	4.721	–
	$1^1A_g^- - 2^1B_u^-$	6.057	5.551	–
MR-CISD(CAS(6,6))[a]	$1^1A_g^- - 2^1A_g^-$	5.019	4.547	–
	$1^1A_g^- - 1^1B_u^+$	5.146	4.752	–
	$1^1A_g^- - 2^1B_u^-$	6.485	5.690	–

[a] Important configurations are not included in the active space, and hence, many intruder states appear at the MR-AQCC level.

1.2 Freezing scheme

Freezing scheme tests were conducted on hexatriene. Table S2 present the relevant freezing schemes tested. Importantly, freezing schemes involving uneven percentage between reference doubly occupied (Docc) and virtual (Virt) orbitals were also tested, but no significant advantage was observed from using such freezing schemes, and hence, they were not listed below.

Table S2. Excitation energies (eV) of hexatriene calculated using a variety of freezing schemes of σ-orbitals at the CI/AQCC step. The frozen reference doubly occupied (Docc) and virtual (Virt) σ-orbitals were equally distributed over the irreps A_g and B_u. Molecular orbitals were calculated at the SA6-CASSCF(6,6) level. All calculations were performed using the cc-pVDZ basis set.

Freezing Scheme	Excitation	ΔE_{CI}	ΔE_{CI+P}	ΔE_{AQCC}
Docc: 30%[a]	$1^1A_g^- - 2^1A_g^-$	5.816	5.755	5.744
Virt: 0%	$1^1A_g^- - 1^1B_u^+$	6.521	5.803	5.764
	$1^1A_g^- - 2^1B_u^-$	7.005	6.915	6.880
Docc: 30%	$1^1A_g^- - 2^1A_g^-$	5.821	5.763	5.754
Virt: 30%	$1^1A_g^- - 1^1B_u^+$	6.487	5.785	5.757
	$1^1A_g^- - 2^1B_u^-$	7.008	6.918	6.888
Docc: 40%	$1^1A_g^- - 2^1A_g^-$	5.863	5.826	5.821
Virt: 40%	$1^1A_g^- - 1^1B_u^+$	6.434	5.797	5.791
	$1^1A_g^- - 2^1B_u^-$	7.057	6.989	6.969
Docc: 50%	$1^1A_g^- - 2^1A_g^-$	5.856	5.819	5.818
Virt: 50%	$1^1A_g^- - 1^1B_u^+$	6.412	5.827	5.833
	$1^1A_g^- - 2^1B_u^-$	7.044	6.976	6.964
Docc: 60%	$1^1A_g^- - 2^1A_g^-$	5.831	5.808	5.811
Virt: 60%	$1^1A_g^- - 1^1B_u^+$	6.362	5.941	5.971
	$1^1A_g^- - 2^1B_u^-$	6.997	6.942	6.944
Docc: 70%	$1^1A_g^- - 2^1A_g^-$	5.791	5.770	5.774
Virt: 70%	$1^1A_g^- - 1^1B_u^+$	6.409	6.108	6.137
	$1^1A_g^- - 2^1B_u^-$	6.945	6.896	6.902
Docc: 80%	$1^1A_g^- - 2^1A_g^-$	5.801	5.794	5.796
Virt: 80%	$1^1A_g^- - 1^1B_u^+$	6.612	6.486	6.505
	$1^1A_g^- - 2^1B_u^-$	6.918	6.894	6.899
Docc: 90%	$1^1A_g^- - 2^1A_g^-$	5.815	5.814	5.815
Virt: 90%	$1^1A_g^- - 1^1B_u^+$	6.813	6.770	6.777
	$1^1A_g^- - 2^1B_u^-$	6.926	6.915	6.919
Docc: 100%	$1^1A_g^- - 2^1A_g^-$	5.819	5.818	5.818
Virt: 100%	$1^1A_g^- - 1^1B_u^+$	6.848	6.824	6.832
	$1^1A_g^- - 2^1B_u^-$	6.933	6.924	6.930

[a] 30% of reference doubly occupied σ orbitals correspond to carbon $1s$ orbitals.

2 Singlet states

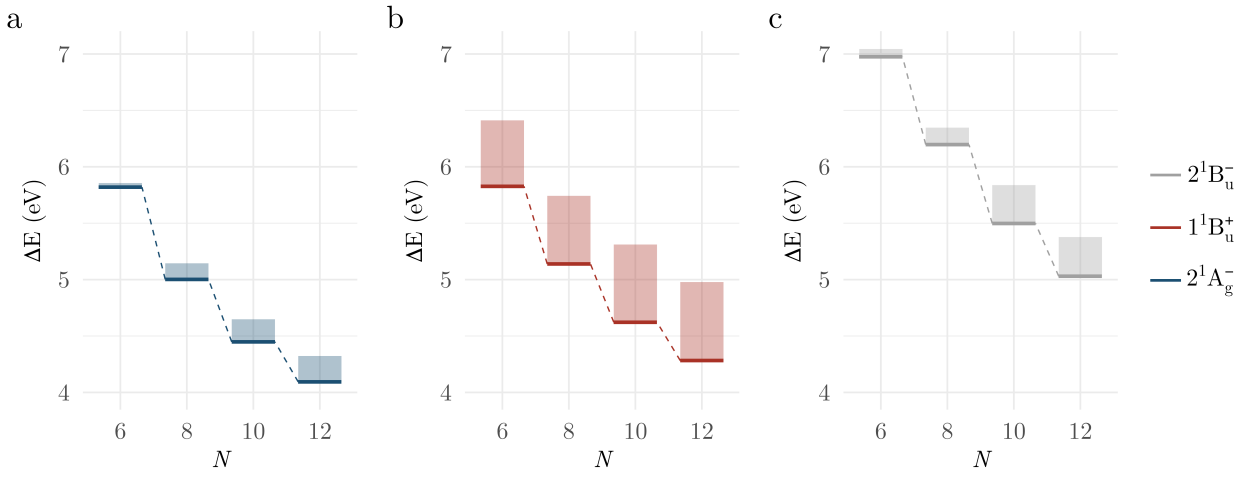

Figure S1. Vertical singlet excitation energies of polyenes with N π-electrons computed using MR-CISD and MR-CISD+P for the (a) $2A_g^-$, (b) $1B_u^+$, and (c) $2B_u^-$ states. The height of each bar indicates the difference between the MR-CISD result (top of the bar) and the MR-CISD+P result (denoted by the marker). Calculations were performed with the cc-pVDZ basis set.

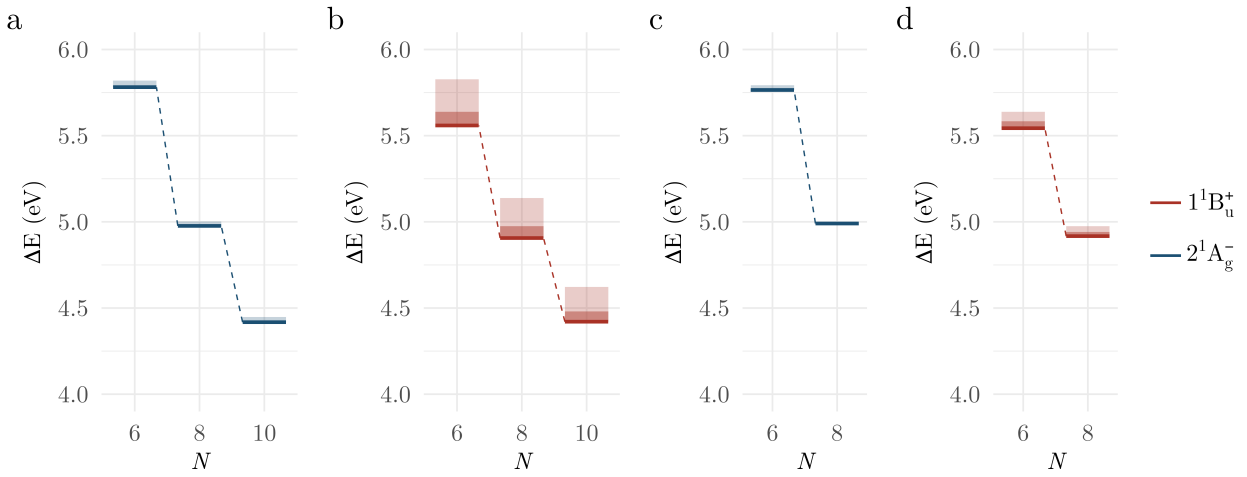

Figure S2. Vertical singlet excitation energies of polyenes with N π-electrons, obtained by extrapolating MR-CISD+P results to the complete basis set limit using (a, b) DT and (c, d) TQ extrapolations. The height of the lighter shaded bar indicates the difference between excitation energies obtained with the smaller and larger basis sets. The height of the darker shaded bar represents the difference between the larger basis set result and the extrapolated CBS value (represented by the marker).

2.1 An extrapolation for $N = 12$

An extrapolation for $N = 12$, both for the cc-pVTZ' basis set and for ΔE_{DT}^{∞} results, was performed using a 3-point power function fit. This fitting approach was chosen because it best predicts the excitation energy for dodecahexaene using the cc-pVDZ basis set, where the actual excitation energies are known (Figure S3). Additionally, it aligns with the decrease in excitation energies observed for $N = 6 - 10$ when expanding from the double- to triple-ζ basis set.

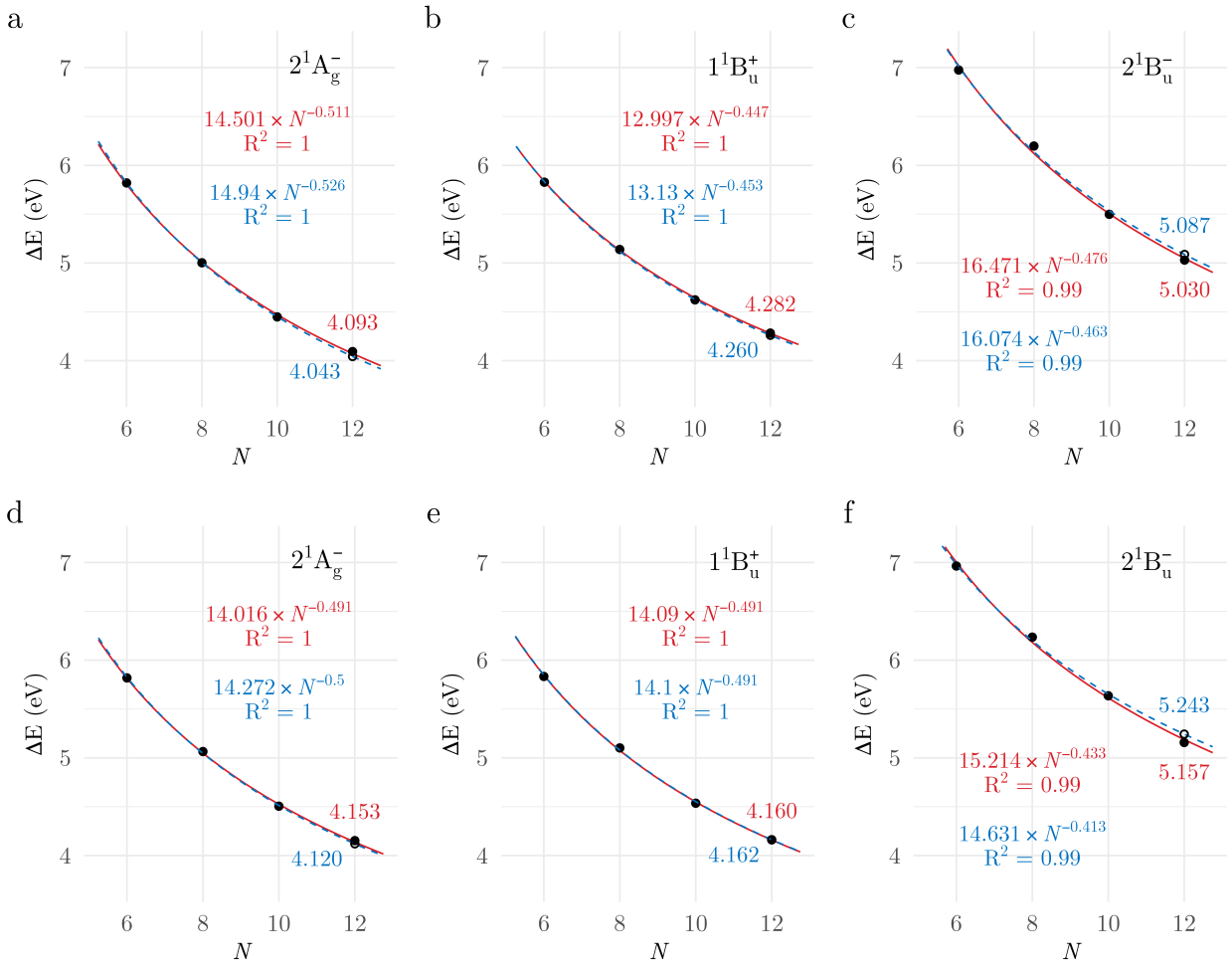

Figure S3. Vertical singlet excitation energies for the $2A_g^-$, $1B_u^+$, and $2B_u^-$ states of polyenes with N π-electrons calculated at the (a-c) MRCI+P and (d-f) MR-AQCC levels using the cc-pVDZ basis set. The dashed line represents the 3-point power function fit, while the solid line represents the 4-point power function fit. Numerical values for the actual (red) and estimated (blue) excitation energies are shown for $N = 12$. The equation and the coefficient of determination (R^2) for the 4-point (red) and 3-point (blue) power function fits are shown.

Based on the MR-CISD+P results using the cc-pVDZ basis set, this approach underestimates the excitation energy for the $2A_g^-$ and $1B_u^+$ states of dodecahexaene by 0.05 eV and 0.02 eV, respectively. For the $2B_u^-$ state, the excitation energy is overestimated by 0.06 eV. Slightly better results are also observed for the MR-AQCC estimates, where the excitation energy for the $2A_g^-$ state is underestimated by 0.03 eV, no difference between the estimated and the actual excitation energy is observed for the $1B_u^+$ state, and the excitation energy for the $2B_u^-$ state is overestimated by 0.09 eV. The estimates for $N = 12$, both for the cc-pVTZ' basis set (Figure S4) and for ΔE_{DT}^{∞} extrapolates values (Figure S5), are presented below.

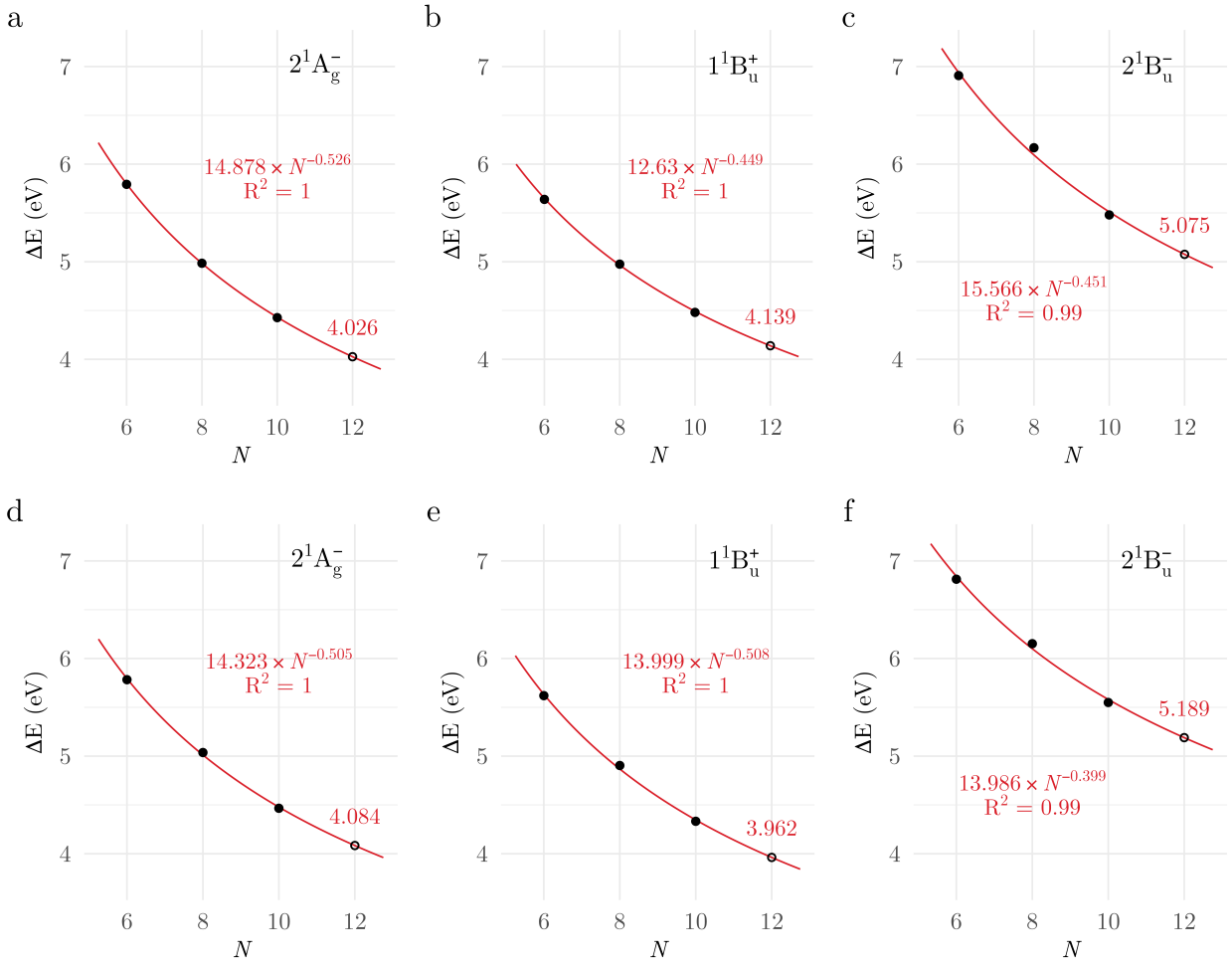

Figure S4. Vertical singlet excitation energies for the $2A_g^-$, $1B_u^+$, and $2B_u^-$ states of polyenes with N π-electrons calculated at the (a-c) MRCI+P and (d-f) MR-AQCC levels using the cc-pVTZ' basis set. The line indicates the 3-point power function fit. The estimated excitation energies for $N = 12$ are indicated. The equation and the coefficient of determination (R^2) for the 3-point power function fit are shown.

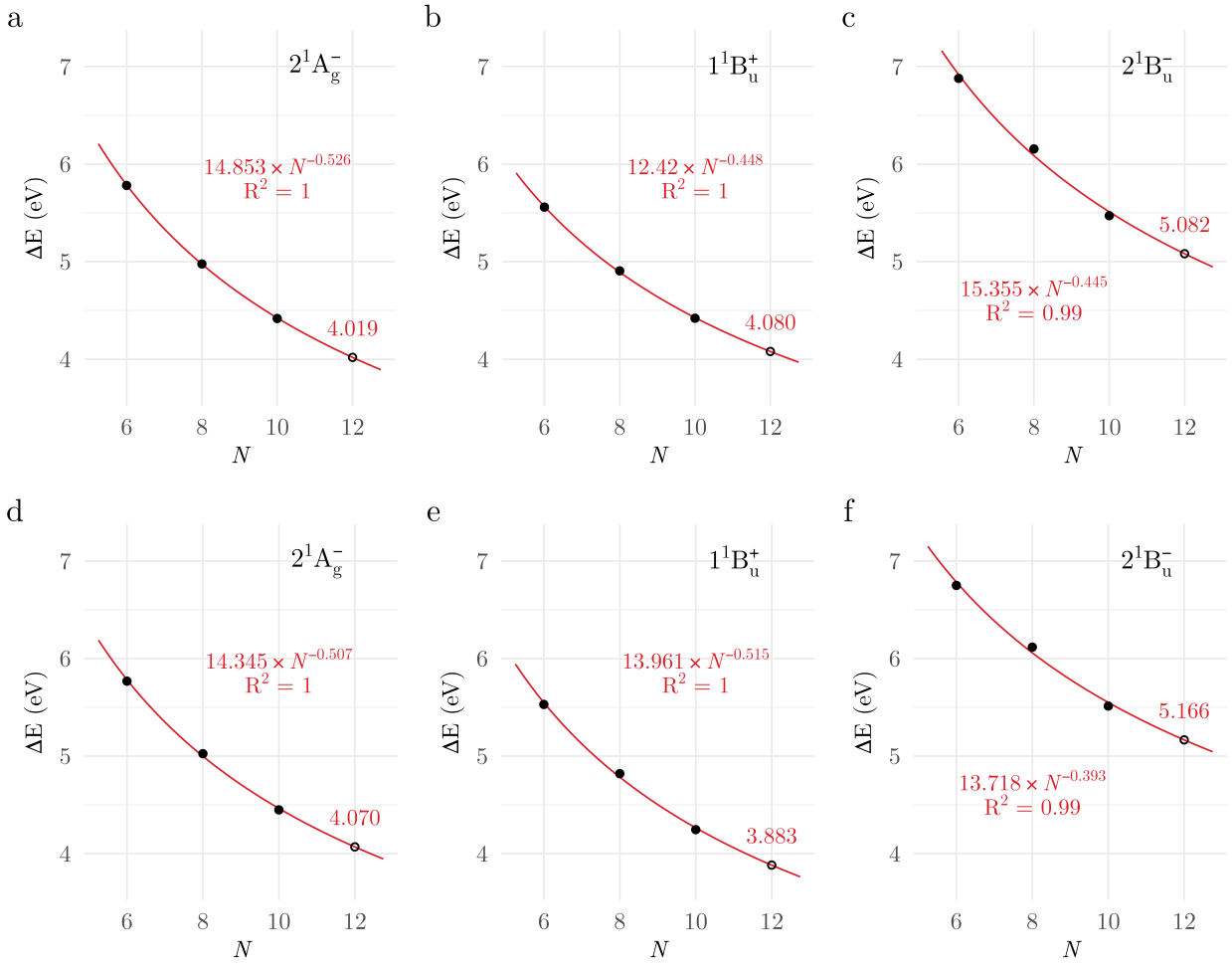

Figure S5. Vertical singlet excitation energies for the $2A_g^-$, $1B_u^+$, and $2B_u^-$ states of polyenes with N π-electrons calculated at the (a-c) MRCI+P and (d-f) MR-AQCC levels extrapolated from the double- to the triple-ζ basis set (ΔE_{DT}^{∞}). The line indicates the 3-point power function fit. The estimated excitation energies for $N = 12$ are indicated. The equation and the coefficient of determination (R^2) for the 3-point power function fit are shown.

3 Triplet states

Table S3. Triplet excitation energies (eV) of polyenes with N π-electrons calculated at the MR-CISD+P level using a variety of basis sets.

N	Excitation	$\Delta E_{\text{cc-pVDZ}}$[1]	$\Delta E_{\text{cc-pVTZ}}$[2]	$\Delta E_{\text{cc-pVQZ}}$[3]
6	$1^1A_g^- - 1^3A_g^-$	4.608	4.627	4.595
	$1^1A_g^- - 1^3B_u^-$	2.948	2.948	2.941
8	$1^1A_g^- - 1^3A_g^-$	3.933	3.928	3.934
	$1^1A_g^- - 1^3B_u^-$	2.581	2.578	2.581

[1] cc-pVDZ (H: (4s,1p)/[2s,1p], C: (9s,4p,1d)/[3s,2p,1d]).
[2] cc-pVTZ (H: (4s,1p)/[2s,1p], C: (10s,5p,2d)/[4s,3p,2d]).
[3] cc-pVQZ (H: (4s,1p)/[2s,1p], C: (12s,6p,3d,2f)/[5s,4p,3d,2f]).

Table S4. Triplet excitation energies (eV) of polyenes with N π-electrons calculated at the MR-AQCC level using a variety of basis sets.

N	Excitation	$\Delta E_{\text{cc-pVDZ}}$[1]	$\Delta E_{\text{cc-pVTZ}}$[2]	$\Delta E_{\text{cc-pVQZ}}$[3]
6	$1^1A_g^- - 1^3A_g^-$	4.598	4.548	4.570
	$1^1A_g^- - 1^3B_u^-$	2.945	2.942	2.935
8	$1^1A_g^- - 1^3A_g^-$	3.928	3.913	3.908
	$1^1A_g^- - 1^3B_u^-$	2.562	2.557	2.557

[1] cc-pVDZ (H: (4s,1p)/[2s,1p], C: (9s,4p,1d)/[3s,2p,1d]).
[2] cc-pVTZ (H: (4s,1p)/[2s,1p], C: (10s,5p,2d)/[4s,3p,2d]).
[3] cc-pVQZ (H: (4s,1p)/[2s,1p], C: (12s,6p,3d,2f)/[5s,4p,3d,2f]).

4 Natural transition orbitals and transition densities

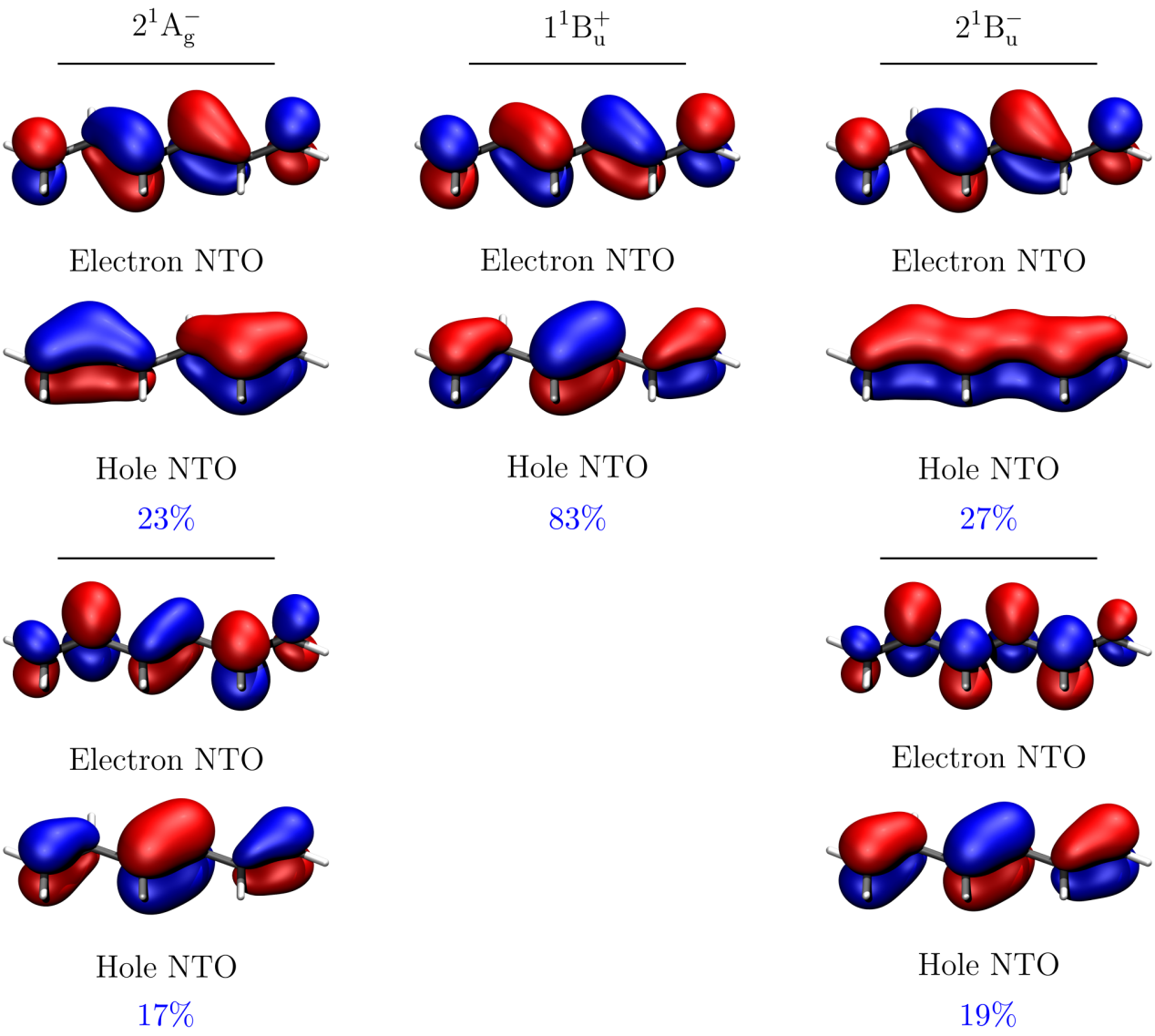

Figure S6. Natural transition orbitals (isovalue: ±0.05 a.u.). The dominant pair of natural transition orbitals and their contribution to the excitation are shown for the $2^1A_g^-$, $1^1B_u^+$, and $2^1B_u^-$ states of hexatriene.

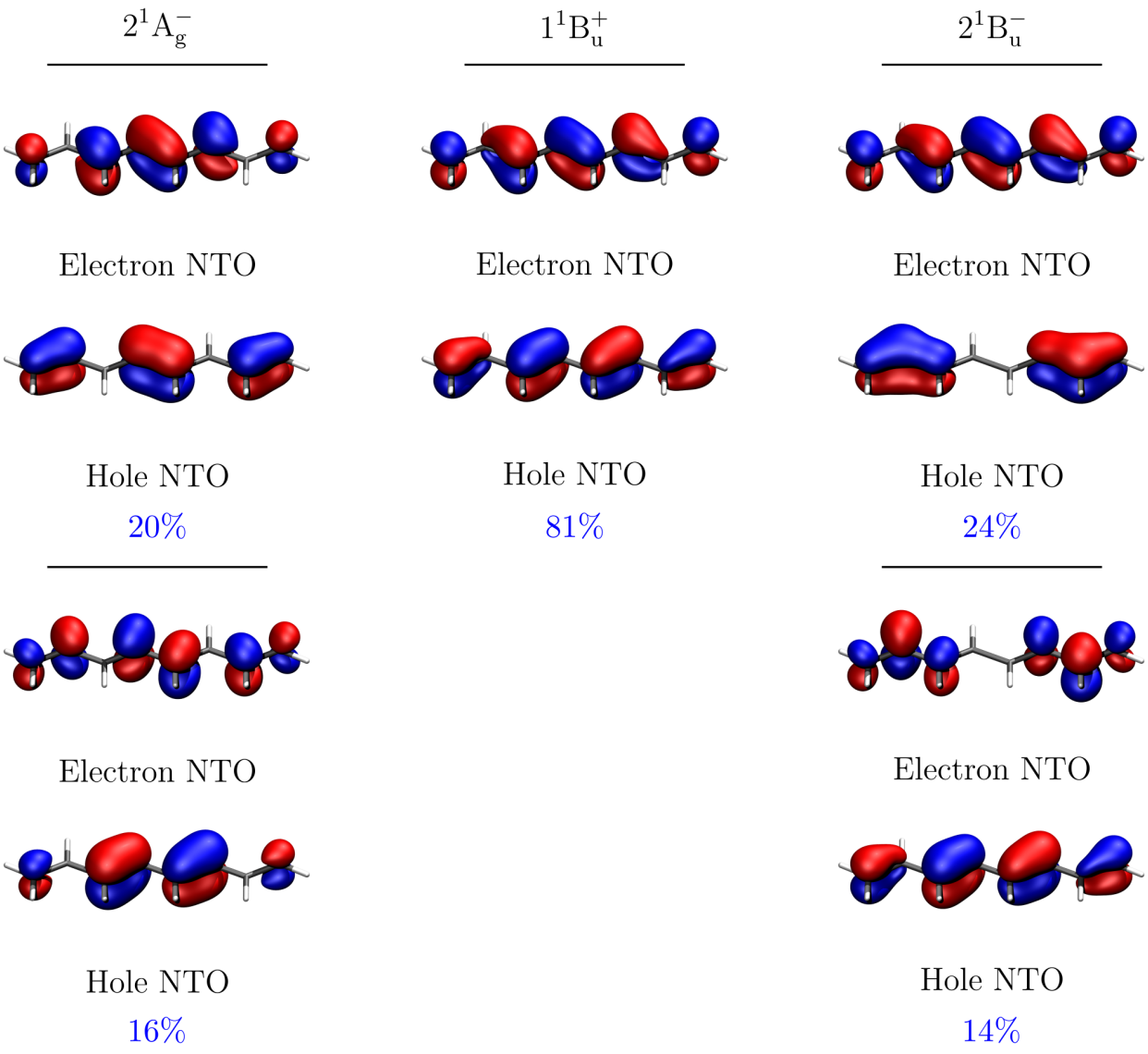

Figure S7. Natural transition orbitals (isovalue: ±0.05 a.u.). The dominant pair of natural transition orbitals and their contribution to the excitation are shown for the $2^1A_g^-$, $1^1B_u^+$, and $2^1B_u^-$ states of octatetraene.

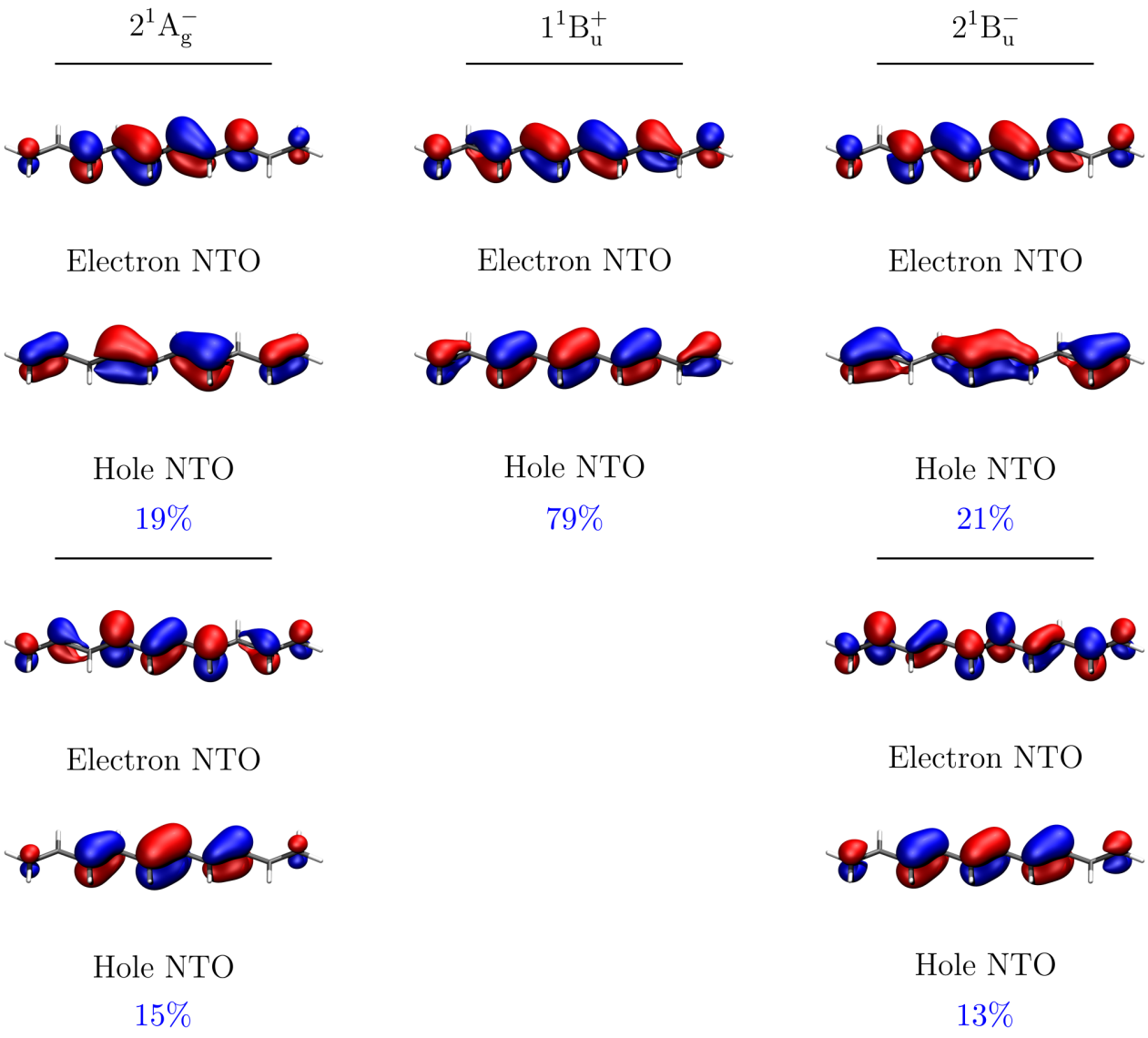

Figure S8. Natural transition orbitals (isovalue: ±0.05 a.u.). The dominant pair of natural transition orbitals and their contribution to the excitation are shown for the $2^1A_g^-$, $1^1B_u^+$, and $2^1B_u^-$ states of decapentaene.

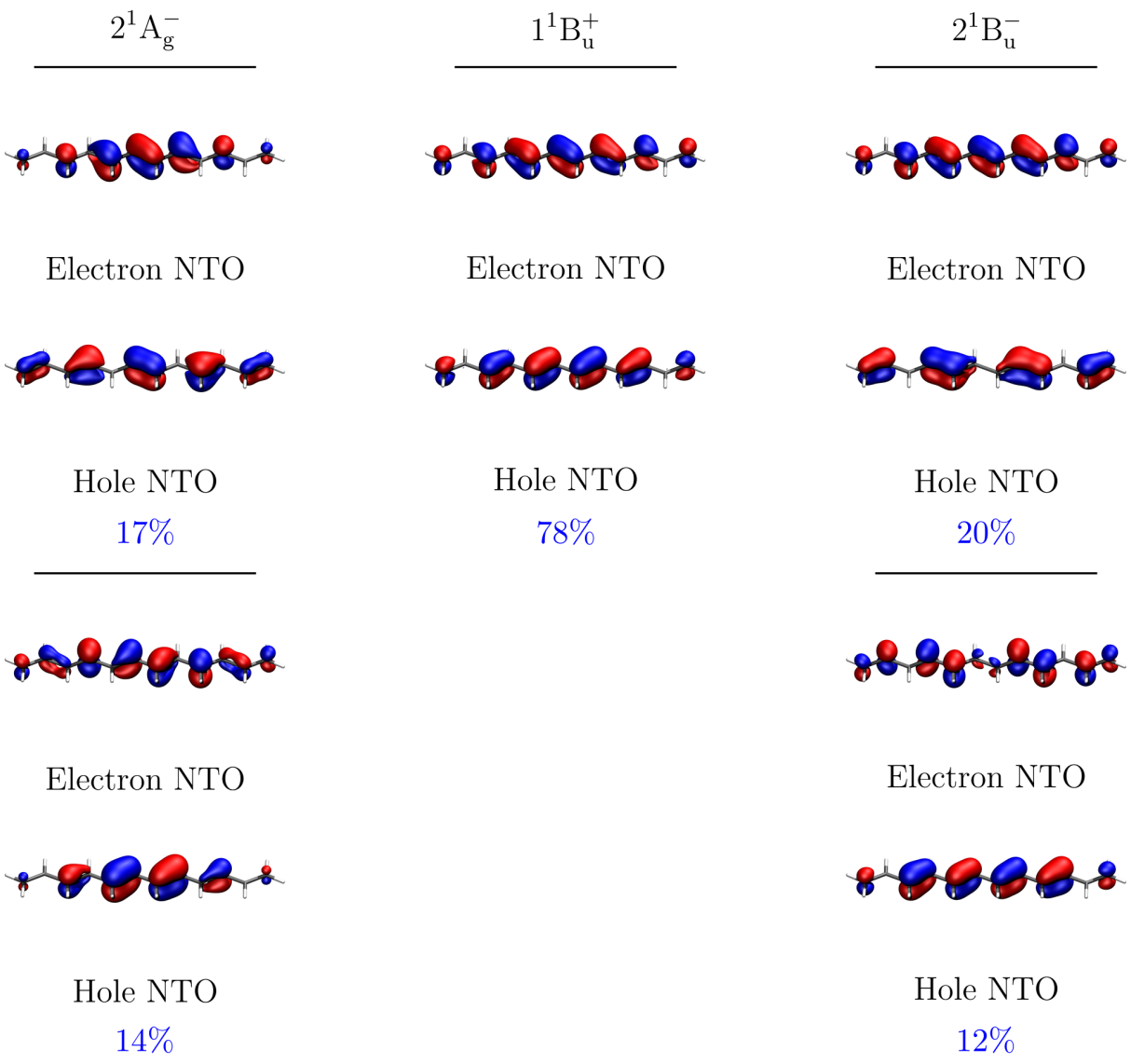

Figure S9. Natural transition orbitals (isovalue: ±0.05 a.u.). The dominant pair of natural transition orbitals and their contribution to the excitation are shown for the $2^1A_g^-$, $1^1B_u^+$, and $2^1B_u^-$ states of dodecahexaene.

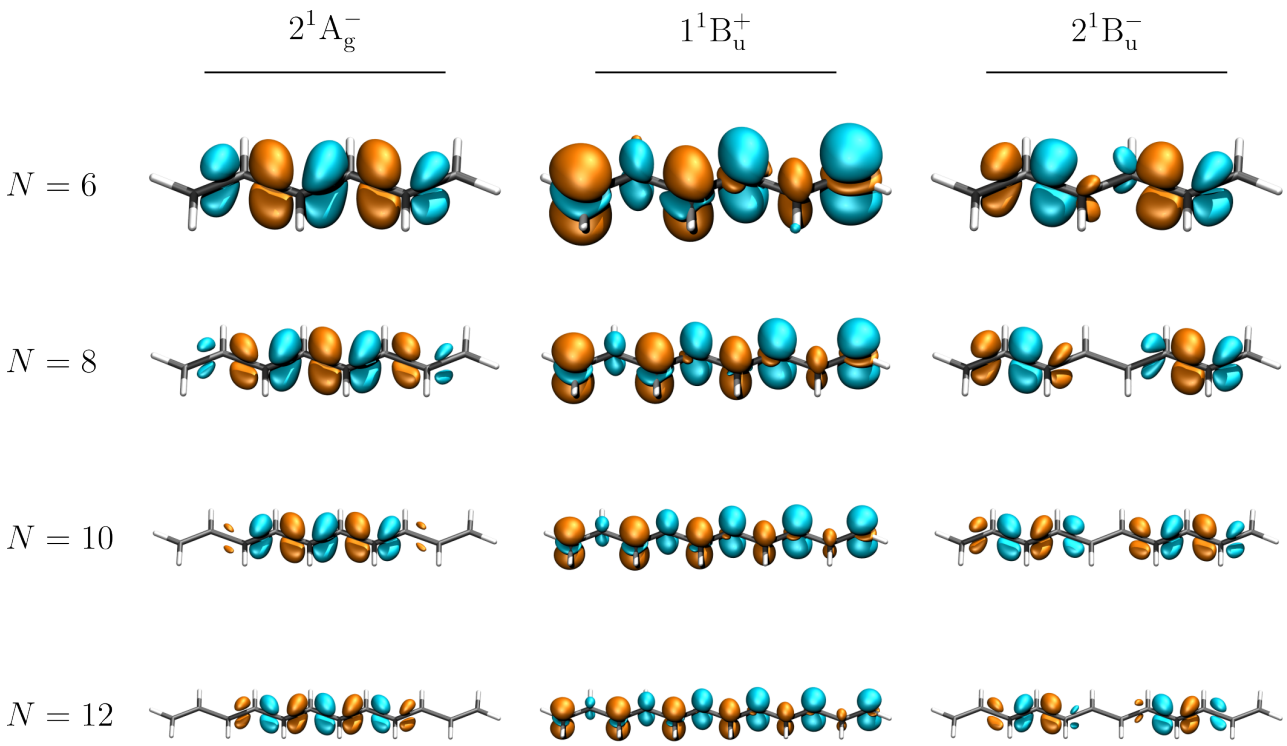

Figure S10. Transition densities (isovalue: ±0.002 a.u.) of the excited states $2^1A_g^-$, $1^1B_u^+$, and $2^1B_u^-$ of polyenes with N π-electrons calculated with respect to the ground state at the MR-CISD level of theory.

Table S5. Transition dipole moment, $\vec{\mu}_{0I}$, (e·bohr) and oscillator strength, f, for the transition from $1A_g^-$ to $2^1A_g^-$, $1^1B_u^+$, and $2^1B_u^-$ calculated using CASSCF and MR-CISD.

N	CASSCF		MR-CISD	
	$\vec{\mu}_{0I}$	f	$\vec{\mu}_{0I}$	f
		$2^1A_g^-$		
6	0.000000	0.000000	0.000000	0.000000
8	0.000000	0.000000	0.000000	0.000000
10	0.000000	0.000000	0.000000	0.000000
12	0.000000	0.000000	0.000000	0.000000
		$1^1B_u^+$		
6	2.788669	1.449741	2.851668	1.277410
8	3.310041	1.856344	3.489630	1.713239
10	3.766966	2.241605	4.072724	2.158272
12	4.171382	2.610051	4.605338	2.586742
		$2^1B_u^-$		
6	0.014323	0.000035	0.110412	0.002104
8	0.019647	0.000059	0.095771	0.001426
10	0.034695	0.000167	0.092181	0.001215
12	0.035388	0.000160	0.047863	0.000302

5 Transition charges

Transition charge (q_M^{t}) on each atom, calculated as the sum over the diagonal elements of the one-electron transition density matrix (1TDM) between the states of interest and the ground state for hexatriene, octatetraene, decapentaene, and dodecahexaene. Results were obtained at the MR-CISD/cc-pVDZ level of theory.

Hexatriene			
	$2A_g^-$	$1B_u^+$	$2B_u^-$
C	-0.02166	0.20236	-0.02192
C	-0.02166	-0.20236	0.02192
C	0.01845	-0.04893	0.01487
C	0.01845	0.04893	-0.01487
C	0.00327	0.14398	0.01994
C	0.00327	-0.14398	-0.01994
H	0.00051	0.01467	0.00023
H	0.00051	-0.01467	-0.00023
H	-0.00048	0.01403	-0.00047
H	-0.00048	-0.01403	0.00047
H	0.00009	0.00556	-0.00043
H	0.00009	-0.00556	0.00043
H	-0.00019	0.00628	-0.00068
H	-0.00019	-0.00628	0.00068

Octatetraene			
	$2A_g^-$	$1B_u^+$	$2B_u^-$
C	0.01004	-0.08974	-0.01294
C	0.01004	0.08974	0.01294
C	-0.00566	0.13612	0.01807
C	-0.00566	-0.13612	-0.01807
C	0.01223	-0.02572	0.01748
C	0.01223	0.02572	-0.01748
C	-0.01624	0.15206	-0.02435
C	-0.01624	-0.15206	0.02435
H	-0.00004	-0.00060	-0.00002
H	-0.00004	0.00060	0.00002
H	-0.00017	0.00773	0.00005
H	-0.00017	-0.00773	-0.00005
H	0.00000	0.00581	0.00002
H	0.00000	-0.00581	-0.00002
H	-0.00042	0.01037	-0.00050
H	-0.00042	-0.01037	0.00050
H	0.00026	0.01146	0.00041
H	0.00026	-0.01146	-0.00041

Decapentaene			
	$2A_g^-$	$1B_u^+$	$2B_u^-$
C	-0.01088	-0.12008	-0.01974
C	-0.01088	0.12008	0.01974
C	0.00762	0.01559	0.01342
C	0.00762	-0.01559	-0.01342
C	-0.00820	-0.11789	0.00445
C	-0.00820	0.11789	-0.00445
C	0.00936	0.05925	0.00059
C	0.00936	-0.05925	-0.00059
C	0.00250	-0.09716	0.02085
C	0.00250	0.09716	-0.02085
H	0.00007	-0.00937	0.00014
H	0.00007	0.00937	-0.00014
H	-0.00027	-0.00823	-0.00039
H	-0.00027	0.00823	0.00039
H	-0.00002	-0.00480	0.00006
H	-0.00002	0.00480	-0.00006
H	-0.00014	-0.00727	0.00009
H	-0.00014	0.00727	-0.00009
H	-0.00002	-0.00121	0.00006
H	-0.00002	0.00121	-0.00006
H	-0.00001	-0.00344	0.00002
H	-0.00001	0.00344	-0.00002

Dodecahexaene			
	$2A_g^-$	$1B_u^+$	$2B_u^-$
C	0.00831	-0.09883	-0.01461
C	0.00831	0.09883	0.01461
C	-0.00523	0.01204	0.00955
C	-0.00523	-0.01204	-0.00955
C	0.00783	-0.10063	-0.00262
C	0.00783	0.10063	0.00262
C	-0.00778	0.04196	0.00643
C	-0.00778	-0.04196	-0.00643
C	0.00115	-0.09678	0.01761
C	0.00115	0.09678	-0.01761
C	-0.00482	0.07479	-0.01301
C	-0.00482	-0.07479	0.01301
H	0.00023	-0.00654	-0.00029
H	0.00023	0.00654	0.00029
H	0.00000	-0.00766	0.00013
H	0.00000	0.00766	-0.00013
H	0.00004	-0.00404	0.00005
H	0.00004	0.00404	-0.00005
H	0.00015	-0.00630	0.00007
H	0.00015	0.00630	-0.00007
H	0.00005	-0.00205	0.00010
H	0.00005	0.00205	-0.00010
H	0.00009	-0.00435	0.00018
H	0.00009	0.00435	-0.00018
H	-0.00002	0.00123	0.00000
H	-0.00002	-0.00123	0.00000

6 Equilibrium geometries

Equilibrium geometries (Å) obtained at the ωB97X-D/cc-pVTZ level of theory for hexatriene, octatetraene, decapentaene, and dodecahexaene.

Hexatriene			
C	1.199785	2.813176	0.000000
C	1.199785	1.483143	0.000000
C	-0.001156	0.668414	0.000000
C	0.001156	-0.668414	0.000000
C	-1.199785	-1.483143	0.000000
C	-1.199785	-2.813176	0.000000
H	2.120872	3.378561	0.000000
H	0.273669	3.375164	0.000000
H	2.145268	0.949588	0.000000
H	-0.950722	1.196588	0.000000
H	0.950722	-1.196588	0.000000
H	-2.145268	-0.949588	0.000000
H	-2.120872	-3.378561	0.000000
H	-0.273669	-3.375164	0.000000

Octatetraene			
C	0.002067	0.722228	0.000000
C	-0.002067	-0.722228	0.000000
C	1.112008	1.471079	0.000000
C	-1.112008	-1.471079	0.000000
C	1.112008	2.920760	0.000000
C	-1.112008	-2.920760	0.000000
C	2.212462	3.668584	0.000000
C	-2.212462	-3.668584	0.000000
H	-0.965580	1.216443	0.000000
H	0.965580	-1.216443	0.000000
H	2.081206	0.980083	0.000000
H	-2.081206	-0.980083	0.000000
H	0.140113	3.404728	0.000000
H	-0.140113	-3.404728	0.000000
H	3.197764	3.218273	0.000000
H	-3.197764	-3.218273	0.000000
H	2.162014	4.748277	0.000000
H	-2.162014	-4.748277	0.000000

Decapentaene			
C	2.398511	4.962720	0.000000
C	2.392909	3.631995	0.000000
C	1.191228	2.821795	0.000000
C	1.191228	1.482319	0.000000
C	-0.001340	0.670478	0.000000
C	0.001340	-0.670478	0.000000
C	-1.191228	-1.482319	0.000000
C	-1.191228	-2.821795	0.000000
C	-2.392909	-3.631995	0.000000
C	-2.398511	-4.962720	0.000000
H	3.322048	5.523983	0.000000
H	1.474714	5.528448	0.000000
H	3.336944	3.095691	0.000000
H	0.242564	3.351439	0.000000
H	2.142576	0.957164	0.000000
H	-0.953055	1.194701	0.000000
H	0.953055	-1.194701	0.000000
H	-2.142576	-0.957164	0.000000
H	-0.242564	-3.351439	0.000000
H	-3.336944	-3.095691	0.000000
H	-1.474714	-5.528448	0.000000
H	-3.322048	-5.523983	0.000000

Dodecahexaene			
C	0.080392	6.739396	0.000000
C	0.651879	5.537613	0.000000
C	-0.080392	4.286915	0.000000
C	0.500160	3.079561	0.000000
C	-0.223280	1.831635	0.000000
C	0.360806	0.623803	0.000000
C	-0.360806	-0.623803	0.000000
C	0.223280	-1.831635	0.000000
C	-0.500160	-3.079561	0.000000
C	0.080392	-4.286915	0.000000
C	-0.651879	-5.537613	0.000000
C	-0.080392	-6.739396	0.000000
H	-0.997217	6.850054	0.000000
H	0.669422	7.645568	0.000000
H	1.735021	5.463469	0.000000
H	-1.164771	4.353107	0.000000
H	1.584980	3.017966	0.000000
H	-1.307984	1.891932	0.000000
H	1.445625	0.564353	0.000000
H	-1.445625	-0.564353	0.000000
H	1.307984	-1.891932	0.000000
H	-1.584980	-3.017966	0.000000
H	1.164771	-4.353107	0.000000
H	-1.735021	-5.463469	0.000000
H	0.997217	-6.850054	0.000000
H	-0.669422	-7.645568	0.000000

7 Analytical harmonic frequencies

Analytical harmonic frequencies (cm^{-1}) obtained at the ωB97X-D/cc-pVTZ level of theory for hexatriene, octatetraene, decapentaene, and dodecahexaene.

Hexatriene		
95.1336	150.7519	211.5209
255.9578	358.0191	449.7425
552.9187	623.9102	723.5179
922.7781	955.8464	956.0392
961.8523	985.5939	990.8484
1040.3897	1066.1807	1161.3261
1227.9621	1291.7130	1328.4505
1340.8802	1345.6464	1446.5141
1473.9792	1671.2505	1723.0189
1746.7017	3149.7507	3150.2842
3154.8230	3156.4427	3164.5415
3165.1372	3249.6232	3249.6284

Octatetraene		
58.0065	89.0457	146.4513
175.5533	227.9791	240.0637
344.6555	354.0860	398.7137
551.7074	580.3276	652.7047
695.0033	888.7538	938.3310
955.8429	956.6633	958.9506
976.4411	980.2533	1011.2405
1049.5024	1064.4052	1166.2661
1168.0533	1222.3243	1266.3935
1319.7383	1330.9599	1335.5178
1349.4858	1354.2800	1454.1398
1471.3191	1661.5676	1705.9223
1734.7093	1739.2413	3148.1013
3148.7343	3149.8237	3153.2998
3155.0322	3157.3526	3163.2744
3163.2856	3248.6255	3248.6352

Decapentaene		
39.4430	57.8961	102.6391
135.8017	153.3818	188.0334
236.1301	280.1418	280.8487
288.1648	399.2763	422.3690
496.9841	558.7764	611.5585
664.1020	682.5410	866.8573
917.9226	944.6001	954.3713
957.4848	968.9806	969.7571
970.2775	994.8173	1026.4846
1054.9110	1064.4060	1152.0253
1174.2786	1183.1725	1218.5637
1253.4684	1294.2542	1326.8542
1334.1048	1339.2740	1340.2768
1351.3754	1369.1895	1458.2054
1468.7348	1654.9311	1692.9295
1722.7413	1726.9375	1741.5269
3147.5963	3148.5767	3150.0570
3150.2509	3153.3100	3155.4337
3156.7557	3158.7931	3164.1468
3164.2666	3250.2006	3250.2055

Dodecahexaene		
27.6903	41.0313	74.1112
109.8725	111.5806	144.5454
191.3733	205.0345	236.7164
242.8161	250.2331	318.1396
338.1497	422.0856	423.0473
458.9032	527.6242	598.2838
614.5657	669.4709	677.4618
852.4118	899.0680	930.3173
947.2338	955.0495	956.3252
964.1880	967.9921	971.4348
983.6979	1008.9724	1035.8579
1057.4033	1063.7771	1154.2571
1156.0488	1184.5556	1188.2643
1215.0575	1244.8060	1277.1561
1313.3899	1330.6529	1333.0156
1338.0394	1344.1399	1345.3504
1352.6804	1382.8629	1460.6322
1467.4463	1649.8524	1683.0881
1712.0727	1714.6204	1736.3313
1737.6193	3148.3766	3148.5279
3149.7143	3150.0582	3150.6570
3153.3075	3154.9248	3156.1179
3157.9038	3159.9644	3163.9478
3164.0574	3248.9081	3248.9105