Supplementary Material

Charge Transfer Within Excited States Boron/Nitrogen Doped Polycyclic Aromatic Hydrocarbons

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Table of Contents

Table S1: Comparison of excitation energies calculated at the MR-CISD level with three different active spaces explained in the text and different basis sets for three selected structures. All excitation energies are given in eV. CI vector sizes in terms of numbers of configuration state functions (CSFs) are also provided.[a]

Total CSF counts	*2.1 billion*	*511 million*	*2.8 billion*
Schemes	CAS(8,8)/6-31G	R(2)CAS(4,4)A(2)/6-31G	R(2)CAS(4,4)A(2)/6-31G*
		BN-center	
States			
S_1	2.774	2.715	2.733
S_2	2.904	2.904	2.812
S_3	3.145	3.145	3.214
S_4	3.187	3.251	3.329
		BN-vertical	
S_1	0.707	0.709	0.779
S_2	1.380	1.344	1.237
S_3	1.613	1.586	1.536
S_4	2.009	1.969	1.853
		BN-edges-line	
S_1	0.455	0.493	0.501
S_2	1.081	1.107	1.107
S_3	1.257	1.259	1.325
S_4	2.334	2.319	2.283

[a] R stands for RAS and A for auxiliary space.

Table S2: Excitation energies (eV), oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the pristine periacene. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	Pristine Periacene			
	MR-CISD+P			
ΔE	1.987	2.001	2.227	2.809
f	0.002	0.000	0.000	0.152
PR_{NTO}	3.859	3.618	2.003	2.014
	NEVPT2			
ΔE	1.269	1.414	1.608	1.614
f^a	0.005	0.000	0.000	0.177
	ADC(2)[b]			
ΔE	-	-	-	-
f	-	-	-	-
PR_{NTO}	-	-	-	-
	TD-DFT			
ΔE	0.354	0.990	1.122	2.036
f	0.268	0.000	0.000	0.000
PR_{NTO}	1.524	1.390	1.781	1.899

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.
[b]Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value.

Table S3: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-B-top. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	BN-zz-B-top			
	MR-CISD+P			
ΔE	2.665	2.850	2.970	3.257
f	0.261	0.433	0.000	0.000
PR_{NTO}	1.145	1.418	2.533	1.520
	NEVPT2			
ΔE	2.006	2.415	2.453	2.774
f^a	0.234	0.677	0.000	0.000
	ADC(2)			
ΔE	1.630	2.239	2.404	2.666
f	0.201	0.374	0.000	0.000
PR_{NTO}	1.000	1.062	1.000	1.000
	TD-DFT			
ΔE	1.779	2.451	2.598	3.230
f	0.374	0.366	0.000	0.000
PR_{NTO}	1.168	1.301	1.558	1.522

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S4: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-N-top. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	BN-zz-N-top			
	MR-CISD+P			
ΔE	2.879	3.029	3.246	3.426
f	0.288	0.000	0.277	0.000
PR_{NTO}	1.147	2.594	1.653	1.343
	NEVPT2			
ΔE	2.007	2.598	2.754	2.814
f^a	0.274	0.000	0.385	0.000
	ADC(2)			
ΔE	1.995	2.655	2.868	3.068
f	0.233	0.000	0.358	0.000
PR_{NTO}	1.000	1.000	1.202	1.000
	TD-DFT			
ΔE	2.003	2.802	3.017	3.427
f	0.289	0.000	0.306	0.000
PR_{NTO}	1.177	1.489	1.494	1.458

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S5: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-mixed. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	BN-mixed			
	MR-CISD+P			
ΔE	1.981	3.252	3.340	3.543
f	0.206	0.038	0.080	0.027
PR_{NTO}	1.072	1.923	1.910	2.078
	NEVPT2			
ΔE	1.589	3.016	3.104	3.366
f^a	0.221	0.106	0.000	0.056
	ADC(2)			
ΔE	1.413	2.432	2.636	2.981
f	0.182	0.002	0.116	0.130
PR_{NTO}	1.000	1.077	1.000	1.142
	TD-DFT			
ΔE	2.070	2.847	3.360	3.430
f	0.276	0.000	0.002	0.572
PR_{NTO}	1.144	2.235	1.997	2.094

[a]For the NEVPT2 case, the oscillator strength (f) was computed at CASSCF (8,8) level.

Table S6: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-center. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	BN-center			
	MR-CISD+P			
ΔE	2.406	2.625	2.741	2.911
f	0.015	0.380	- [b]	0.136
PR_{NTO}	1.002	1.090	- [b]	1.152
	NEVPT2			
ΔE	1.104	1.645	1.994	2.233
f[a]	0.002	0.541	0.097	- [b]
	ADC(2)			
ΔE	1.255	1.728	2.110	2.423
f	0.001	0.250	0.159	0.000
PR_{NTO}	1.000	1.000	1.000	1.999
	TD-DFT			
ΔE	2.092	2.175	2.227	2.960
f	0.370	0.024	0.120	0.022
PR_{NTO}	1.297	1.053	1.246	1.833

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.
[b]The properties were not computed due to the vanishing of the one-particle transition density matrix in the doubly excited states.

Table S7: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-cross. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	BN-cross			
	MR-CISD+P			
ΔE	3.321	3.461	3.508	3.744
f	0.001	0.859	0.017	0.490
PR_{NTO}	2.016	1.668	1.042	1.230
	NEVPT2			
ΔE	1.963	2.438	2.464	2.638
f^a	0.000	0.959	0.004	0.582
	ADC(2)			
ΔE	2.120	2.493	2.602	2.676
f	0.007	0.001	0.440	0.001
PR_{NTO}	1.000	1.982	1.347	2.065
	TD-DFT			
ΔE	2.842	2.871	2.941	2.986
f	0.001	0.665	0.003	0.142
PR_{NTO}	3.148	1.687	3.281	1.187

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S8: Excitation energies, oscillator strength (f) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-ac. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
		BN-ac		
		MR-CISD+P		
ΔE	1.821	1.982	2.081	3.530
f	0.051	0.028	0.000	0.003
PR_{NTO}	1.358	1.676	1.001	1.904
		NEVPT2		
ΔE	1.726	1.857	2.489	2.541
f^a	0.017	0.015	0.057	0.000
		ADC(2)[b]		
ΔE	-	-	-	-
f	-	-	-	-
PR_{NTO}	-	-	-	-
		TD-DFT		
ΔE	0.181	0.959	1.139	2.213
f	0.043	0.002	0.000	0.027
PR_{NTO}	1.359	1.610	1.856	1.579

[a]For the NEVPT2 case, the oscillator strength (f) was computed at CASSCF (8,8) level.
[b]Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value.

Table S9: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-edges. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
		BN-edges		
		MR-CISD+P		
ΔE	1.771	3.028	3.598	4.556
f	0.040	0.030	0.762	0.478
PR_{NTO}	1.018	1.796	1.784	1.062
		NEVPT2		
ΔE	1.524	2.840	3.240	4.386
f^a	0.034	0.011	0.451	0.352
		ADC(2)		
ΔE	1.013	2.284	2.554	3.364
f	0.007	0.000	0.514	0.283
PR_{NTO}	1.000	1.998	1.998	1.151
		TD-DFT		
ΔE	1.978	2.954	3.453	4.055
f	0.070	0.000	0.762	0.128
PR_{NTO}	1.035	2.150	2.210	2.415

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S10: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-edges-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
	BN-edges-line			
	MR-CISD+P			
ΔE	0.429	1.056	1.179	2.032
f	0.026	0.036	0.174	0.988
PR_{NTO}	1.027	1.245	1.222	1.074
	NEVPT2			
ΔE	0.459	0.980	1.110	1.689
f^a	0.004	0.002	0.254	0.940
	ADC(2)[b]			
ΔE	-	-	-	-
f	-	-	-	-
PR_{NTO}	-	-	-	-
	TD-DFT			
ΔE	1.356	1.357	1.499	1.865
f	0.022	0.005	0.145	0.484
PR_{NTO}	1.452	1.061	1.339	1.302

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.
[b]Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value.

Table S11: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-B-top-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity.

Properties/States	S_1	S_2	S_3	S_4
		BN-zz-B-top-line		
		MR-CISD+P		
ΔE	1.740	2.090	2.507	2.548
f	0.141	0.170	0.000	0.140
PR_{NTO}	1.880	2.176	2.849	2.178
		NEVPT2		
ΔE	1.095	1.144	1.245	1.258
f^a	0.004	0.031	0.211	0.110
		ADC(2)		
ΔE	0.646	0.951	1.160	1.660
f	0.110	0.196	0.095	0.086
PR_{NTO}	1.022	1.016	1.087	1.591
		TD-DFT		
ΔE	0.564	0.829	1.553	1.845
f	0.271	0.080	0.078	0.076
PR_{NTO}	1.234	1.168	1.109	1.219

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S12: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-zz-N-top-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the NEVPT2 case, the oscillator strengths are at CASSCF (8,8) level.

Properties/States	S_1	S_2	S_3	S_4
		BN-zz-N-top-line		
		MR-CISD+P		
ΔE	1.818	1.964	2.119	2.574
f	0.007	0.000	0.080	0.147
PR_{NTO}	2.389	2.486	2.111	2.037
		NEVPT2		
ΔE	1.299	1.471	1.552	1.662
f^a	0.019	0.000	0.076	0.107
		ADC(2)		
ΔE	0.953	1.109	1.433	1.764
f	0.065	0.330	0.103	0.022
PR_{NTO}	1.069	1.057	1.290	1.149
		TD-DFT		
ΔE	0.636	0.873	1.840	1.898
f	0.269	0.007	0.000	0.153
PR_{NTO}	1.373	1.091	1.127	1.164

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S13: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-ac-line. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the NEVPT2 case, the oscillator strengths are at CASSCF (8,8) level.

Properties/States	S_1	S_2	S_3	S_4
		BN-ac-line		
		MR-CISD+P		
ΔE	1.633	2.716	2.941	3.246
f	0.826	0.540	0.018	0.059
PR_{NTO}	1.082	1.252	1.062	1.532
		NEVPT2		
ΔE	1.205	1.989	2.228	2.239
f^a	0.859	0.034	0.431	0.759
		ADC(2)		
ΔE	0.733	1.858	1.958	2.021
f	0.162	0.007	0.138	0.039
PR_{NTO}	1.000	1.903	1.918	1.142
		TD-DFT		
ΔE	1.610	2.509	2.807	2.833
f	0.599	0.004	0.005	0.147
PR_{NTO}	1.168	2.217	1.916	2.166

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.

Table S14: Excitation energies, oscillator strength (*f*) and PR_{NTO} values calculated at the ground-state optimized geometry for the four lowest singlet excited states in four different levels of theory for the BN-vertical. The energies at the MR-CISD level include Pople's correction (+P) for size extensivity. In the NEVPT2 case, the oscillator strengths are at CASSCF (8,8) level.

Properties/States	S_1	S_2	S_3	S_4
	BN-vertical			
	MR-CISD+P			
ΔE	0.770	1.493	1.642	2.021
f	-[c]	0.010	1.608	0.089
PR_{NTO}	-[c]	1.948	1.847	1.432
	NEVPT2			
ΔE	0.535	0.928	1.120	1.174
f[a]	-[c]	0.000	1.105	0.001
	ADC(2)[b]			
ΔE	-	-	-	-
f	-	-	-	-
PR_{NTO}	-	-	-	-
	TD-DFT			
ΔE	1.095	1.105	1.631	1.905
f	0.692	0.003	0.025	0.578
PR_{NTO}	1.168	2.249	1.967	1.442

[a]For the NEVPT2 case, the oscillator strength (*f*) was computed at CASSCF (8,8) level.
[b]Properties at ADC(2) level were not computed for this structure, due to the elevated D1 diagnostic value.
[c]The properties were not computed due to the vanishing of the one-particle transition density matrix in the doubly excited states.

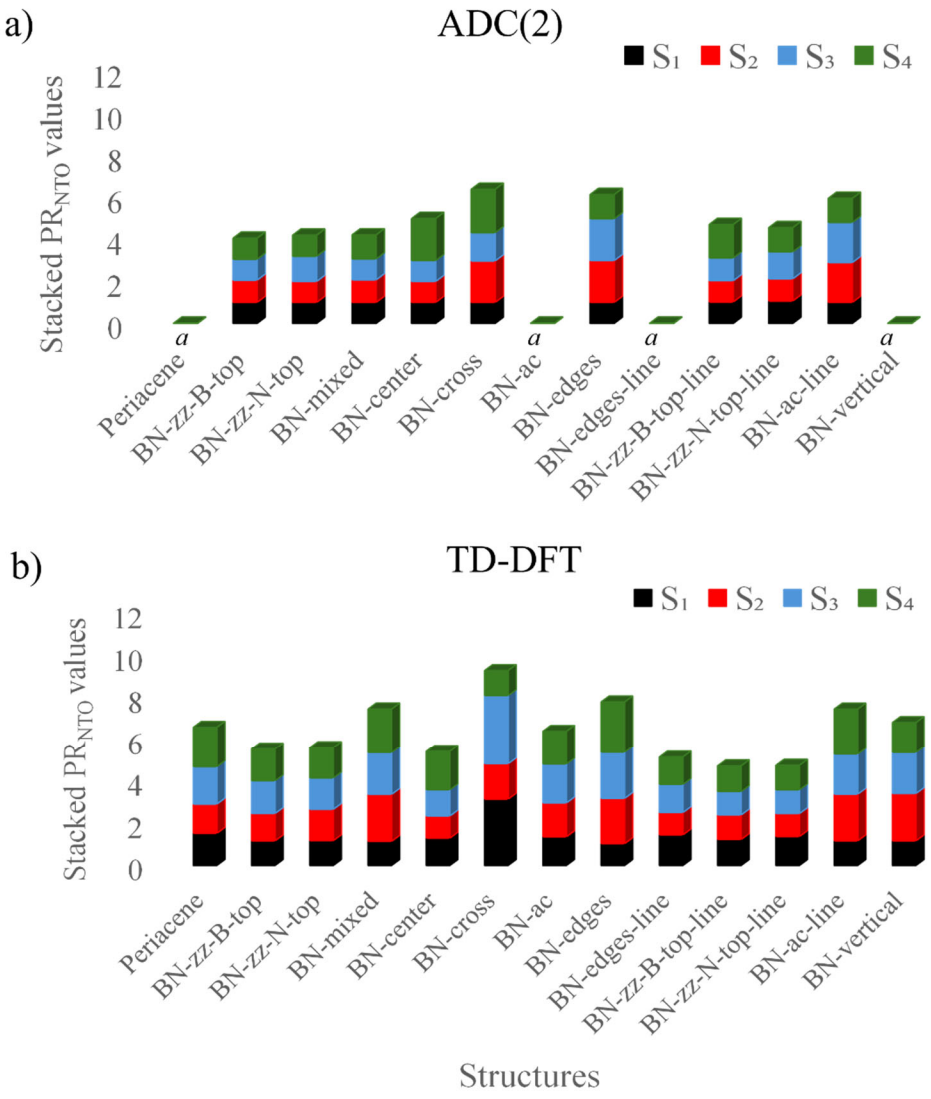

Figure S1: PR_{NTO} values are shown for all computed excited states and all analyzed structures, obtained at ADC(2) (a) and TD-DFT (b) levels of theory.

[a]The PR_{NTO} values at ADC(2) level of theory were not computed for the periacene, BN-ac, BN-edges-line and BN-vertical, due to large D1 diagnostic values exhibited by these structures.

Table S15: Double excitation character values for all computed excited states and all structures, obtained at MR-CISD level of theory.

Structures/States	S_1	S_2	S_3	S_4
Periacene	0.575	0.592	0.600	0.381
BN-zz-B-top	0.195	0.778	0.184	0.486
BN-zz-N-top	0.213	0.773	0.181	0.401
BN-mixed	0.357	0.305	0.241	0.320
BN-center	0.316	0.229	0.986	0.354
BN-cross	0.239	0.196	0.186	0.203
BN-ac	0.575	0.457	0.633	0.691
BN-edges	0.237	0.232	0.235	0.429
BN-edges-line	0.316	0.284	0.273	0.253
BN-zz-B-top-line	0.420	0.517	0.602	0.493
BN-zz-N-top-line	0.684	0.600	0.590	0.528
BN-ac-line	0.363	0.312	0.337	0.286
BN-vertical	0.965	0.320	0.347	0.504

Table S16: Dominant electron configurations and related orbital occupation scheme of the periacene, for the ground state reference wavefunction, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
$1\ ^1A_g$	$(9B_3u)^2(10B_3u)^0(8B_1g)^2(9B_1g)^0$ $(9B_2g)^2(10B_2g)^0(7A_u)^2(8A_u)^0$	31.7	0.098
	$(9B_2g)^2 \rightarrow (10B_3u)^0$	27.4	

Table S17: Dominant electron configurations and related orbital occupation scheme of the BN-ac, for the ground state reference wavefunction, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
$1\ ^1A_1$	$(17B_1)^2(18B_1)^1(19B_1)^1(20B_1)^0$ $(14A_2)^2(15A_2)^2(16A_2)^0(17A_2)^0$	59.5	0.091

Table S18: Dominant electron configurations and related orbital occupation scheme of the BN-vertical, for the ground state reference wavefunction, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
$1\ ^1A_1$	$(17B_1)^2(18B_1)^1(19B_1)^1(20B_1)^0$ $(14A_2)^2(15A_2)^2(16A_2)^0(17A_2)^0$	27.9	0.161
	$(19B_1)^1 \rightarrow (18B_1)^1$	11.1	

Table S19: Dominant electron configurations and related orbital excitation with its respective contribution, of the BN-edges-line, with respect to the ground state reference, using MR-CISD(8,8) method.

State	Electron Configuration	Contribution %	D1 Diagnostic
$1\ ^1A_1$	$(17B_1)^2(18B_1)^2(19B_1)^0(20B_1)^0$ $(14A_2)^2(15A_2)^2(16A_2)^0(17A_2)^0$	57.2	0.093

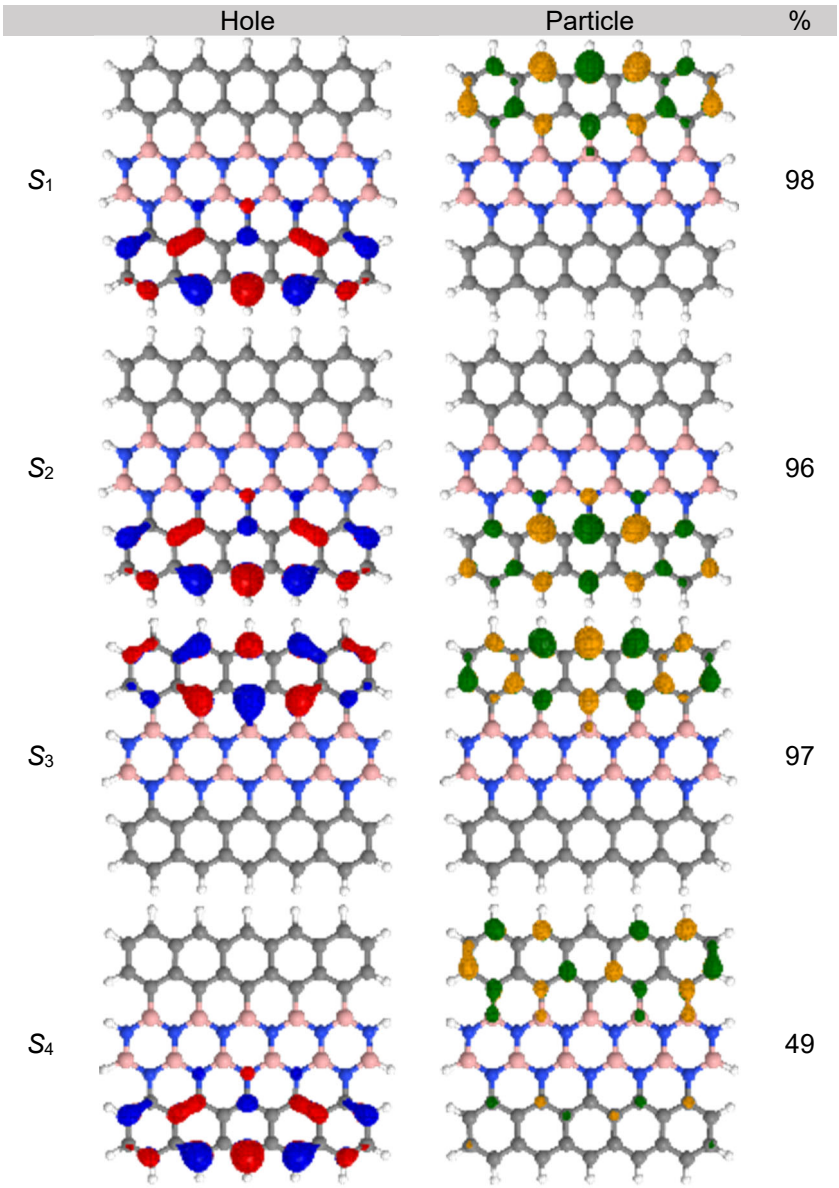

Figure S2: BN-center NTOs obtained using ADC(2)/def2-SV(P) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr^3. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

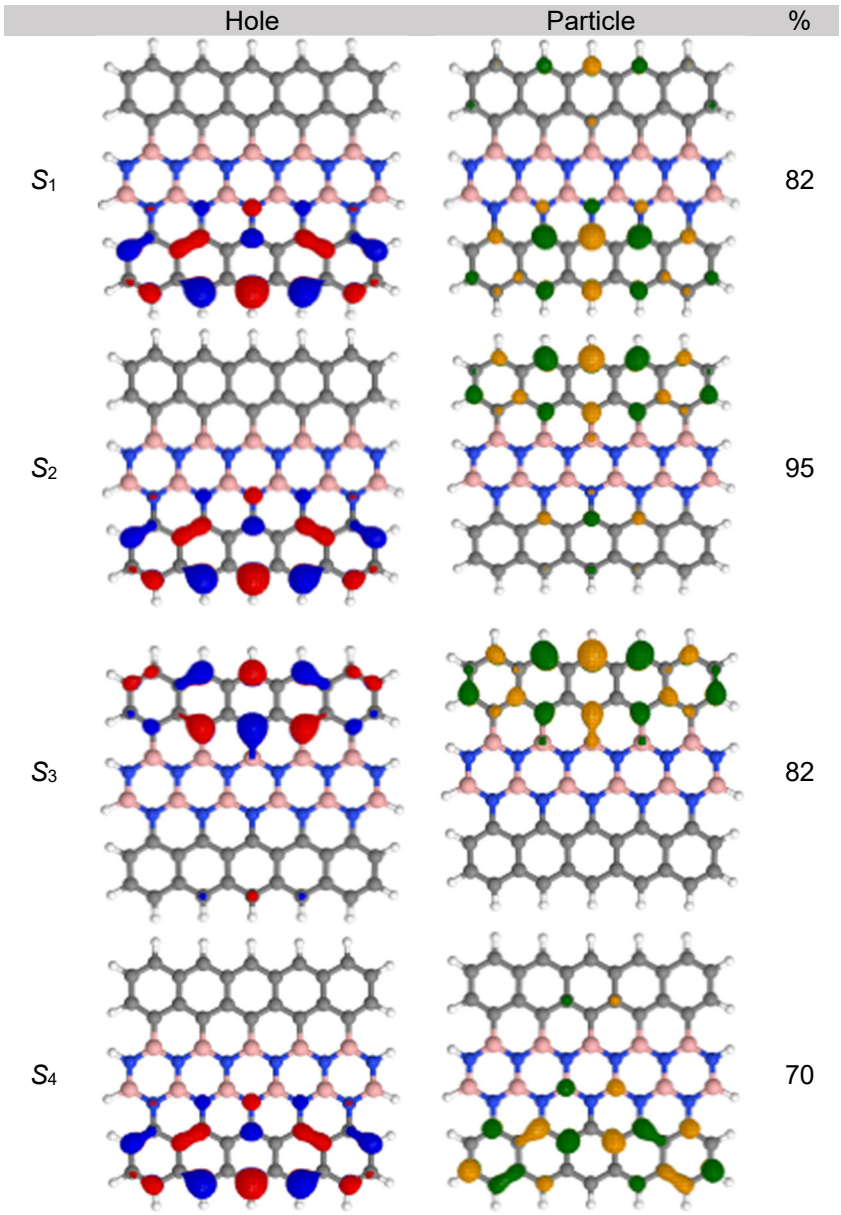

Figure S3: BN-center NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr^3. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

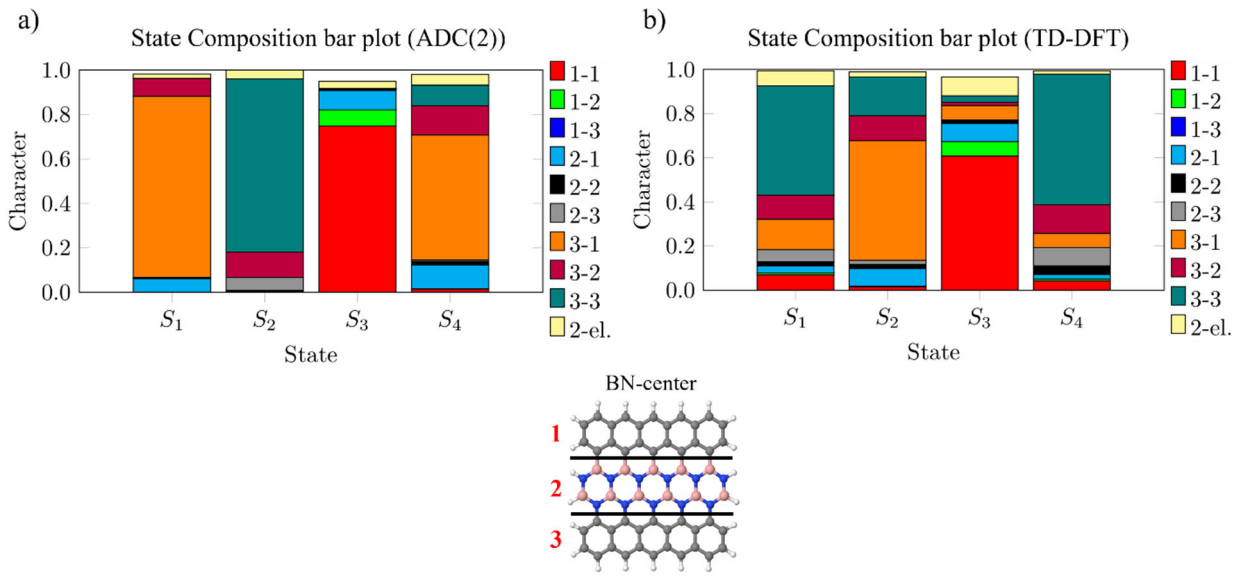

Figure S4: The first four singlet excited states, obtained at ADC(2) and TD-DFT levels, for the BN-center structure decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segments division is indicated by numbers in red.

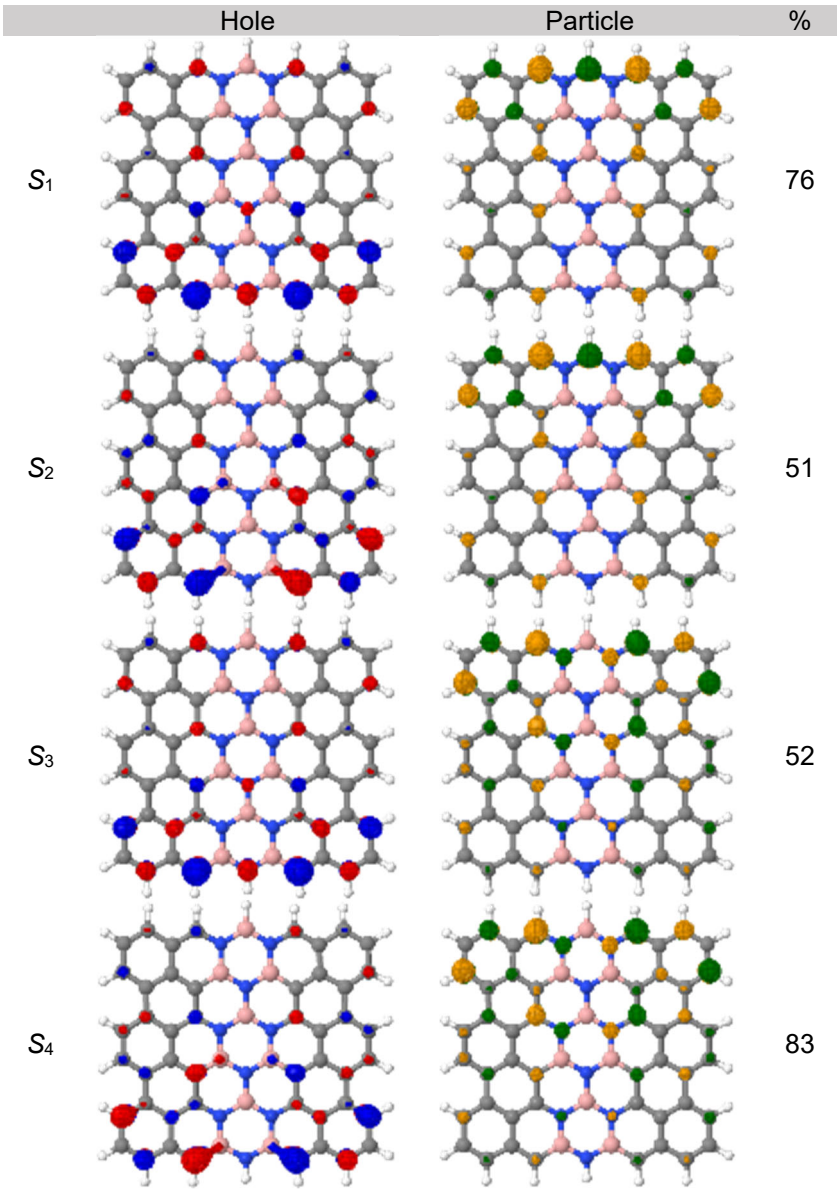

Figure S5: BN-vertical NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr^3. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

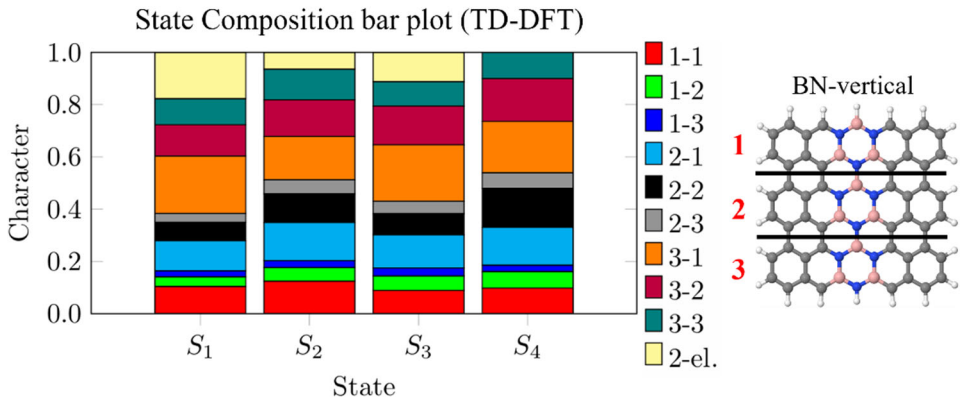

Figure S6: The first four singlet excited states, obtained at TD-DFT level, for the BN-vertical structure decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segments division is indicated by numbers in red.

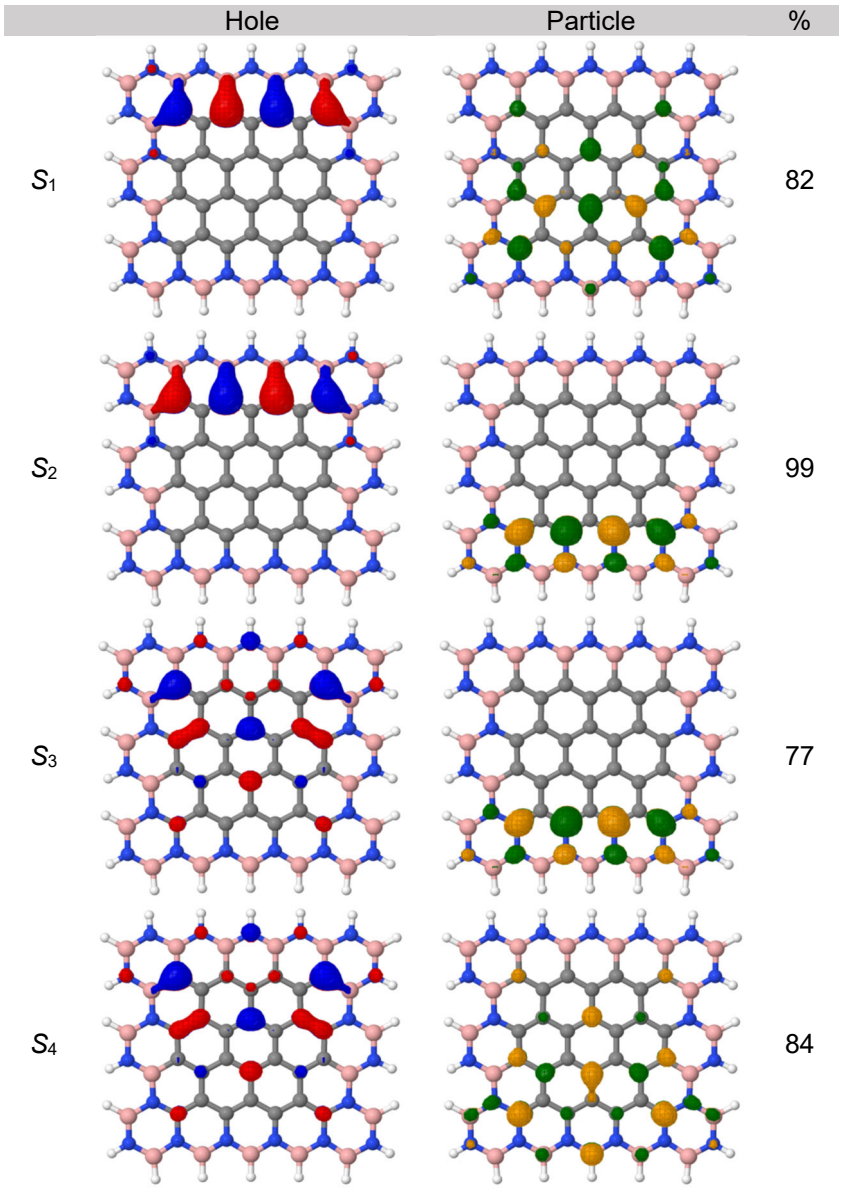

Figure S7: BN-edges-line NTOs obtained using TD-DFT, at wB97XD/def2-SV(P)) level of theory, for the first four excited singlet states, relative to the ground state. Molecular orbitals cutoff value for the isosurface of 0.04 e/bohr^3. Hole orbitals are printed in red and blue, while electron orbitals are in green and yellow.

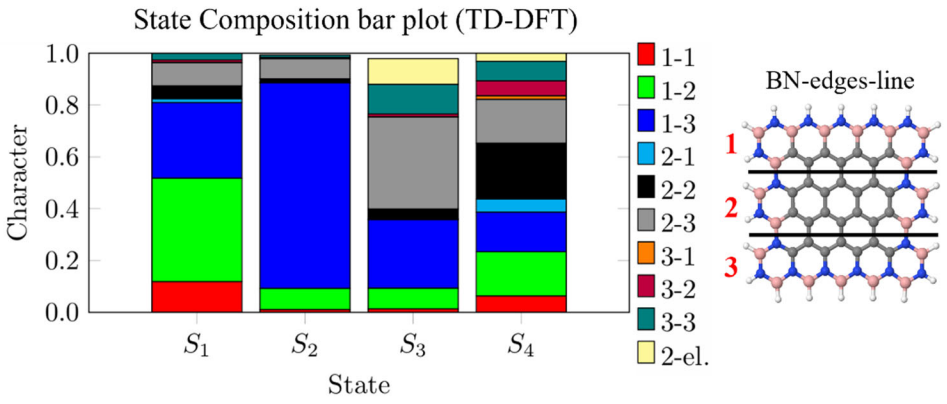

Figure S8: The first four singlet excited states, obtained at TD-DFT level, for the BN-edges-line structure decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segments division is indicated by numbers in red.

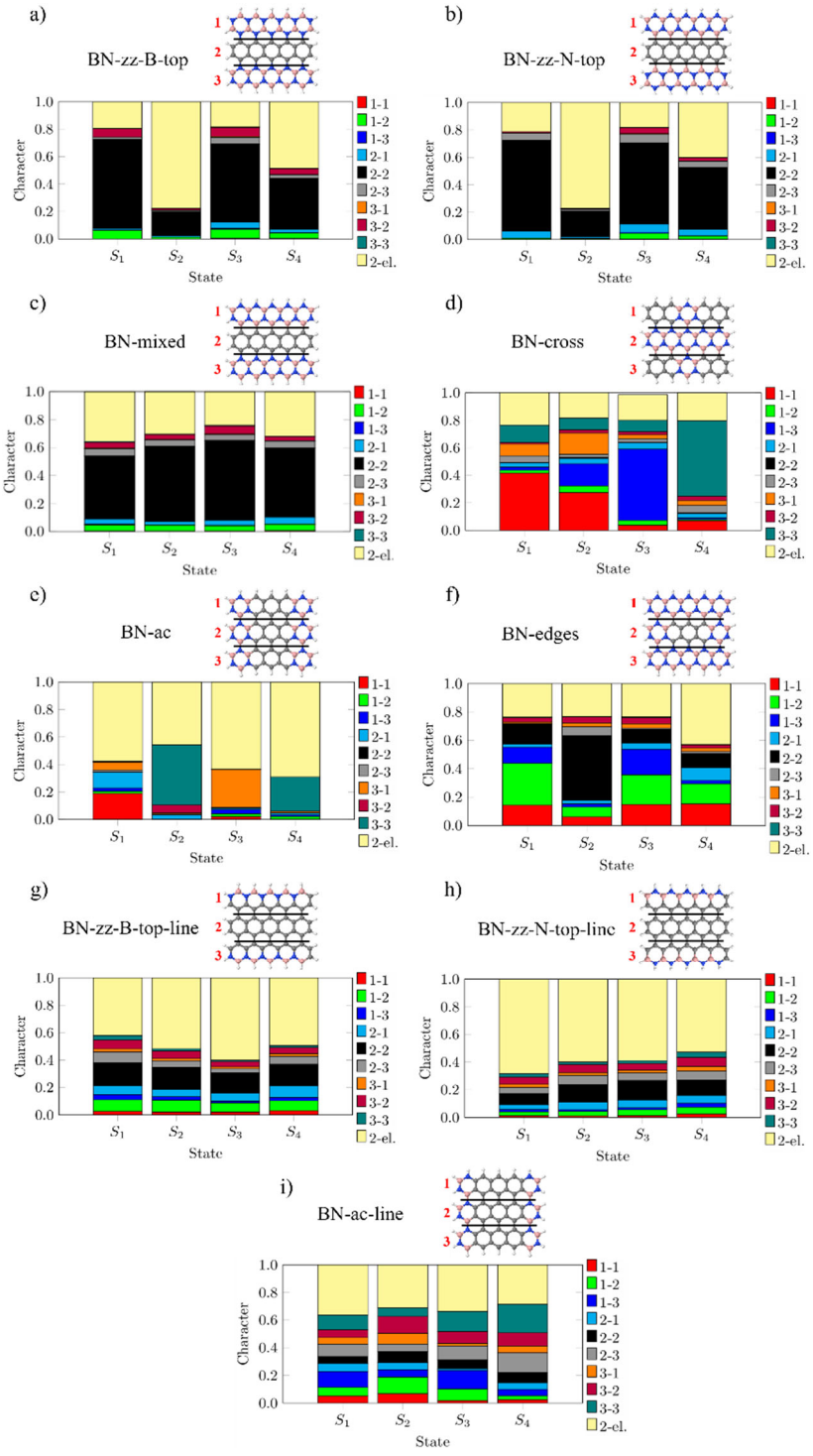

Figure S9: Character of the first four singlet excited states, obtained at the MR-CISD level, for all the structures not analyzed in detail in the main text, decomposed into contributions of local excitations (LE), charge transfer (between segments) and double excitations (2-el.). The segment division is indicated by numbers in red.

Optimized Geometries:

Cartesian coordinates are in Å and geometries are in the x-y plane:

```
Pristine,          wB97XD/def2-SV(P)
     H     4.8846600    6.8225330   -0.0000000
     H     2.4410610    6.7890653   -0.0000000
     H    -0.0000000    6.7819973   -0.0000000
     H    -2.4410610    6.7890653   -0.0000000
     H    -4.8846600    6.8225330   -0.0000000
     C    -6.1004934    5.0477451   -0.0000000
     C    -6.1168148    3.6388849   -0.0000000
     C    -6.1253238    0.6938557   -0.0000000
     C    -6.1253235   -0.6938551    0.0000000
     C    -4.9382981   -1.4266169    0.0000000
     C    -4.9399855   -2.8948803    0.0000000
     C    -6.1168155   -3.6388854    0.0000000
     C    -6.1004941   -5.0477449    0.0000000
     C    -4.9080782   -5.7289205    0.0000000
     C    -2.4487148   -5.6949226   -0.0000000
     C    -3.6737445   -5.0189323    0.0000000
     C    -3.6906963   -3.5832209   -0.0000000
     C    -2.4612866   -2.8629374   -0.0000000
     C    -1.2328603   -3.5611080   -0.0000000
     C    -1.2259415   -5.0062223   -0.0000000
     C     0.0000000   -5.6879600   -0.0000000
     C     4.9080782   -5.7289205    0.0000000
     C     3.6737445   -5.0189323   -0.0000000
     C     2.4487149   -5.6949226   -0.0000000
     C     1.2259415   -5.0062223   -0.0000000
     C     1.2328603   -3.5611080   -0.0000000
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     C     3.6906963   -3.5832209    0.0000000
     C     4.9399855   -2.8948803    0.0000000
     C     6.1168155   -3.6388854    0.0000000
     C     6.1253235   -0.6938551    0.0000000
     C     4.9382981   -1.4266169    0.0000000
     C     3.7048222   -0.7147112    0.0000000
     C     2.4618107   -1.4245279    0.0000000
     C     1.2383407   -0.7200879   -0.0000000
     C     0.0000000   -1.4256325   -0.0000000
     C    -1.2383407   -0.7200879   -0.0000000
     C    -2.4618107   -1.4245279   -0.0000000
     C    -3.7048222   -0.7147112    0.0000000
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     C     6.1004941   -5.0477449    0.0000000
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C	-1.2383410	0.7200874	-0.0000000
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H	-2.4410618	-6.7890650	0.0000000
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H	-7.0879388	1.2072692	-0.0000000
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      B     5.0167669   -1.5001437   -0.0000000
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      N     3.7677347   -0.7663817   -0.0000000
      N     6.2335592   -0.7426943   -0.0000000
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      H     4.9830987   -7.0832610   -0.0000000
      B     2.4883973   -5.8338711    0.0000000
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      B     1.2527011   -3.6517104    0.0000000
      N     1.2473075   -5.1064894    0.0000000
      H     2.4786915   -7.0462364   -0.0000000
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BN-zz-B-top, wB97XD/def2-SV(P)

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H	-0.0000000	-6.9354485	-0.0000000
H	-2.4616248	-6.9445923	-0.0000000
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     B     1.2438208    3.5531032    0.0000000
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     B    -3.7340977    3.5703137    0.0000000
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     B     4.9520159   -5.7721398    0.0000000
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     B    -1.2438208   -3.5531032   -0.0000000
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     B    -6.2168561   -3.6160488    0.0000000
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BN-zz-N-top,         wB97XD/def2-SV(P)
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H	7.3297750	-5.7681962	0.0000000
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H	-7.0881323	-1.2187898	-0.0000000
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B	-2.4939608	3.0100127	0.0000000
B	-3.7609799	5.1924066	-0.0000000
B	-4.9886005	3.0086827	0.0000000
B	-6.2680063	5.1750120	0.0000000
B	6.2680063	-5.1750120	0.0000000
B	3.7609799	-5.1924066	0.0000000
B	4.9886005	-3.0086827	-0.0000000
B	1.2533323	-5.1922662	0.0000000
B	-1.2533323	-5.1922662	0.0000000
B	-3.7609799	-5.1924066	0.0000000
B	-6.2680063	-5.1750120	0.0000000
B	-4.9886005	-3.0086827	-0.0000000
B	-2.4939608	-3.0100127	-0.0000000
B	-0.0000000	-3.0082917	-0.0000000
B	2.4939608	-3.0100127	-0.0000000
N	6.2186822	-3.7475182	0.0000000

BN-mixed, wB97XD/def2-SV(P)

H	4.9515196	-7.0516982	-0.0000000
H	2.4643756	-7.0115267	-0.0000000
H	-0.0000000	-7.0039586	0.0000000

H	-2.4643756	-7.0115267	-0.0000000
H	-4.9515196	-7.0516982	-0.0000000
C	-6.1464144	-0.7810334	0.0000000
C	-6.1142912	0.6269687	0.0000000
C	-4.9498704	1.3568245	0.0000000
C	6.1142912	0.6269687	0.0000000
C	4.9498704	1.3568245	0.0000000
C	3.6941860	0.6384055	0.0000000
C	2.4777234	1.3514128	-0.0000000
C	1.2338831	0.6492883	-0.0000000
C	-0.0000000	1.3542363	-0.0000000
C	-1.2338831	0.6492883	-0.0000000
C	-2.4777234	1.3514128	-0.0000000
C	-3.6941860	0.6384055	-0.0000000
C	3.7109046	-0.8086855	-0.0000000
C	4.9766904	-1.5078087	0.0000000
C	6.1464144	-0.7810334	-0.0000000
C	0.0000000	-1.4987432	0.0000000
C	1.2389265	-0.8011158	-0.0000000
C	2.4834471	-1.5029803	0.0000000
C	-1.2389265	-0.8011158	-0.0000000
C	-2.4834471	-1.5029803	0.0000000
C	-3.7109046	-0.8086855	-0.0000000
C	-4.9766904	-1.5078087	-0.0000000
H	7.0492161	-5.6147188	-0.0000000
H	7.3286615	5.6885426	0.0000000
H	5.0463123	6.8050103	0.0000000
H	2.5034288	6.8091442	0.0000000
H	-0.0000000	6.8046737	-0.0000000
H	-2.5034288	6.8091442	-0.0000000
H	-5.0463123	6.8050103	0.0000000
H	-7.0492161	-5.6147188	-0.0000000
H	-7.3103094	-3.1622424	-0.0000000
H	-7.1123654	-1.2788749	-0.0000000
H	-7.0828015	1.1405661	-0.0000000
H	-7.1034421	3.1671587	0.0000000
H	-7.3286615	5.6885426	0.0000000
H	7.1034421	3.1671587	0.0000000
H	7.0828015	1.1405661	-0.0000000
H	7.1123654	-1.2788749	0.0000000
H	7.3103094	-3.1622424	-0.0000000
B	4.9549384	-5.8406588	-0.0000000
B	2.4775264	-5.8016488	-0.0000000
B	0.0000000	-5.7946780	0.0000000
B	-2.4775264	-5.8016488	0.0000000
B	-4.9549384	-5.8406588	-0.0000000

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      B     6.2264812   -3.6869980   -0.0000000
      B     3.7425122   -3.6399327    0.0000000
      B     1.2460601   -3.6258108    0.0000000
      B    -1.2460601   -3.6258108    0.0000000
      B    -3.7425122   -3.6399327    0.0000000
      B    -6.2264812   -3.6869980   -0.0000000
      N     6.1715060   -5.1082576   -0.0000000
      N     4.9905604   -2.9277521   -0.0000000
      N     3.7221421   -5.0895790   -0.0000000
      N     2.4879235   -2.9041688   -0.0000000
      N     1.2396341   -5.0702773    0.0000000
      N    -0.0000000   -2.8950398    0.0000000
      N    -1.2396341   -5.0702773    0.0000000
      N    -2.4879235   -2.9041688    0.0000000
      N    -3.7221421   -5.0895790    0.0000000
      N    -4.9905604   -2.9277521    0.0000000
      N    -6.1715060   -5.1082576   -0.0000000
      N     5.0271804    5.7921084    0.0000000
      N     6.2220995    3.6653360   -0.0000000
      N     3.7485943    3.6506458   -0.0000000
      N     2.5070827    5.7956078   -0.0000000
      N     1.2503035    3.6430613    0.0000000
      N     0.0000000    5.7912326   -0.0000000
      N    -1.2503035    3.6430613    0.0000000
      N    -2.5070827    5.7956078   -0.0000000
      N    -3.7485943    3.6506458   -0.0000000
      N    -6.2220995    3.6653360   -0.0000000
      N    -5.0271804    5.7921084    0.0000000
      B     6.2676256    5.0915473    0.0000000
      B     3.7602914    5.1027224   -0.0000000
      B     4.9883222    2.9222384   -0.0000000
      B     1.2533016    5.0960318   -0.0000000
      B     2.4944168    2.9141347   -0.0000000
      B    -0.0000000    2.9108930    0.0000000
      B    -1.2533016    5.0960318   -0.0000000
      B    -2.4944168    2.9141347   -0.0000000
      B    -3.7602914    5.1027224   -0.0000000
      B    -4.9883222    2.9222384   -0.0000000
      B    -6.2676256    5.0915473   -0.0000000

BN-center,          wB97XD/def2-SV(P)
      H     4.8767766   -6.9390689   -0.0000000
      H     2.4343880   -6.8970865   -0.0000000
      H    -0.0000000   -6.8841106   -0.0000000
      H    -2.4343880   -6.8970865   -0.0000000
      H    -4.8767766   -6.9390689   -0.0000000
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C	-6.0913392	-5.1724328	-0.0000000
C	-6.0975643	-3.7427977	0.0000000
C	-4.9762619	2.9213672	-0.0000000
C	-6.1266864	3.6730182	0.0000000
C	-6.0807008	5.0969544	0.0000000
C	-4.8962235	5.7655123	0.0000000
C	-2.4483507	5.7081476	-0.0000000
C	-3.6596270	5.0394962	0.0000000
C	-3.6936842	3.5929441	-0.0000000
C	-2.4826767	2.8873895	-0.0000000
C	-1.2317022	3.5749072	0.0000000
C	-1.2196278	5.0184699	0.0000000
C	-0.0000000	5.6986840	-0.0000000
C	4.8962235	5.7655123	-0.0000000
C	3.6596270	5.0394962	-0.0000000
C	2.4483507	5.7081476	-0.0000000
C	1.2196278	5.0184699	-0.0000000
C	1.2317022	3.5749072	-0.0000000
C	2.4826767	2.8873895	-0.0000000
C	3.6936842	3.5929441	-0.0000000
C	4.9762619	2.9213672	-0.0000000
C	6.1266864	3.6730182	0.0000000
C	0.0000000	2.8781780	-0.0000000
C	6.0807008	5.0969544	-0.0000000
C	-4.9452034	-2.9947054	0.0000000
C	-3.6722124	-3.6856418	0.0000000
C	-2.4714643	-2.9649245	0.0000000
C	-1.2252445	-3.6602204	0.0000000
C	-0.0000000	-2.9555984	0.0000000
C	1.2252445	-3.6602204	0.0000000
C	2.4714643	-2.9649245	0.0000000
C	3.6722124	-3.6856418	0.0000000
C	4.9452034	-2.9947054	-0.0000000
C	6.0975643	-3.7427977	-0.0000000
C	6.0913392	-5.1724328	-0.0000000
C	4.9061241	-5.8449656	-0.0000000
C	3.6607532	-5.1314393	0.0000000
C	2.4486298	-5.8021441	0.0000000
C	1.2203387	-5.1048186	0.0000000
C	-0.0000000	-5.7891442	-0.0000000
C	-1.2203387	-5.1048186	0.0000000
C	-2.4486298	-5.8021441	0.0000000
C	-3.6607532	-5.1314393	0.0000000
C	-4.9061241	-5.8449656	-0.0000000
H	7.0394627	-5.7166863	-0.0000000
H	7.0248566	5.6500797	0.0000000

H	4.8551765	6.8583114	0.0000000
H	2.4365225	6.8015594	0.0000000
H	-0.0000000	6.7919161	0.0000000
H	-2.4365225	6.8015594	0.0000000
H	-4.8551765	6.8583114	0.0000000
H	-7.0394627	-5.7166863	-0.0000000
H	-7.0730190	-3.2430497	-0.0000000
H	-7.0725701	-1.1553675	-0.0000000
H	-7.3103790	1.2806527	-0.0000000
H	-7.1000152	3.1885500	0.0000000
H	-7.0248566	5.6500797	0.0000000
H	7.1000152	3.1885500	0.0000000
H	7.3103790	1.2806527	0.0000000
H	7.0725701	-1.1553675	-0.0000000
H	7.0730190	-3.2430497	-0.0000000
B	4.9699104	-1.4252189	0.0000000
B	2.4882706	-1.4059768	0.0000000
B	0.0000000	-1.4042268	0.0000000
B	-2.4882706	-1.4059768	0.0000000
B	-4.9699104	-1.4252189	0.0000000
B	-3.7493744	0.7694603	0.0000000
B	-6.2289752	0.7477611	-0.0000000
B	-1.2489701	0.7612726	0.0000000
B	1.2489701	0.7612726	0.0000000
B	3.7493744	0.7694603	0.0000000
B	6.2289752	0.7477611	0.0000000
N	6.1831380	-0.6714061	0.0000000
N	4.9938235	1.4986622	0.0000000
N	2.4901356	1.4867462	-0.0000000
N	0.0000000	1.4828294	-0.0000000
N	-2.4901356	1.4867462	-0.0000000
N	-4.9938235	1.4986622	-0.0000000
N	-3.7355992	-0.6769658	0.0000000
N	-6.1831380	-0.6714061	-0.0000000
N	-1.2455294	-0.6759734	0.0000000
N	1.2455294	-0.6759734	0.0000000
N	3.7355992	-0.6769658	0.0000000

BN-cross, wB97XD/def2-SV(P)

H	4.8629704	-6.9614034	-0.0000000
H	2.4007367	-6.8646993	0.0000000
H	-0.0000000	-7.0708785	0.0000000
H	-2.4007367	-6.8646993	0.0000000
H	-4.8629704	-6.9614034	-0.0000000
C	-6.0967528	-5.2141099	-0.0000000
C	-6.1407238	-3.7774132	-0.0000000

C	-5.0102022	2.9211069	0.0000000
C	-6.1777441	3.6422789	0.0000000
C	-6.1757770	5.0675629	0.0000000
C	-5.0108411	5.7586223	0.0000000
C	-2.5710212	5.7884225	-0.0000000
C	-3.7422576	5.0712144	0.0000000
C	-3.7249478	3.6072404	-0.0000000
C	-2.5056717	2.9089379	-0.0000000
C	5.0108411	5.7586223	-0.0000000
C	3.7422576	5.0712144	-0.0000000
C	2.5710212	5.7884225	-0.0000000
C	2.5056717	2.9089379	-0.0000000
C	3.7249478	3.6072404	-0.0000000
C	5.0102022	2.9211069	-0.0000000
C	6.1777441	3.6422789	-0.0000000
C	6.1757771	5.0675629	-0.0000000
C	-5.0097208	-3.0004318	-0.0000000
C	-3.7227858	-3.6715389	0.0000000
C	-2.5528512	-2.9348967	0.0000000
C	2.5528512	-2.9348967	0.0000000
C	3.7227858	-3.6715389	0.0000000
C	5.0097208	-3.0004318	-0.0000000
C	6.1407238	-3.7774132	-0.0000000
C	6.0967528	-5.2141099	0.0000000
C	4.9007527	-5.8668326	0.0000000
C	3.6657904	-5.1251067	0.0000000
C	2.4437770	-5.7700010	0.0000000
C	-2.4437770	-5.7700010	0.0000000
C	-3.6657904	-5.1251067	0.0000000
C	-4.9007527	-5.8668326	-0.0000000
H	7.0339463	-5.7779970	-0.0000000
H	7.1356565	5.5948090	0.0000000
H	4.9951023	6.8522626	0.0000000
H	2.6436072	6.8828081	0.0000000
H	-0.0000000	6.7051594	0.0000000
H	-2.6436072	6.8828081	0.0000000
H	-4.9951023	6.8522626	0.0000000
H	-7.0339463	-5.7779970	-0.0000000
H	-7.1327198	-3.3089374	-0.0000000
H	-7.1169624	-1.1444428	-0.0000000
H	-7.3418039	1.2808356	-0.0000000
H	-7.1376429	3.1344091	0.0000000
H	-7.1356565	5.5948090	0.0000000
H	7.1376429	3.1344091	-0.0000000
H	7.3418039	1.2808356	-0.0000000
H	7.1169624	-1.1444428	-0.0000000

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      H     7.1327198   -3.3089374   -0.0000000
      B     5.0126457   -1.4209001   -0.0000000
      B     2.5352140   -1.4009353    0.0000000
      B     0.0000000   -1.4464151    0.0000000
      B    -2.5352140   -1.4009353    0.0000000
      B    -5.0126457   -1.4209001   -0.0000000
      B    -3.7734003    0.7840419   -0.0000000
      B    -6.2592961    0.7517002   -0.0000000
      B    -1.2544595    0.7397257   -0.0000000
      B     1.2544595    0.7397257   -0.0000000
      B     3.7734003    0.7840419   -0.0000000
      B     6.2592961    0.7517002   -0.0000000
      N     6.2240428   -0.6661524   -0.0000000
      N     5.0202181    1.5017712   -0.0000000
      N     2.4984356    1.5027791   -0.0000000
      N    -0.0000000    1.4464524   -0.0000000
      N    -2.4984356    1.5027791   -0.0000000
      N    -5.0202181    1.5017712   -0.0000000
      N    -3.7764064   -0.6606254   -0.0000000
      N    -6.2240428   -0.6661524   -0.0000000
      N    -1.2613512   -0.7025060    0.0000000
      N     1.2613512   -0.7025060    0.0000000
      N     3.7764064   -0.6606254   -0.0000000
      N     1.2882979    3.5745640   -0.0000000
      N    -1.2882979    3.5745640   -0.0000000
      N    -0.0000000    5.6923853    0.0000000
      N    -0.0000000   -2.9107791    0.0000000
      N     1.2385916   -5.1192359    0.0000000
      N    -1.2385916   -5.1192359    0.0000000
      B     1.2678319    5.0550201    0.0000000
      B    -1.2678319    5.0550201    0.0000000
      B    -0.0000000    2.8707464   -0.0000000
      B     1.2363815   -3.6426494    0.0000000
      B    -1.2363815   -3.6426494    0.0000000
      B     0.0000000   -5.8585958    0.0000000

BN-ac,          wB97XD/def2-SV(P)
      H     5.0273516    6.7437537    0.0000000
      H     2.3872304    6.9019186    0.0000000
      H     0.0000000    6.8632268    0.0000000
      H    -2.3872304    6.9019186    0.0000000
      H    -5.0273516    6.7437537    0.0000000
      C    -2.4178268   -5.6773807    0.0000000
      C    -2.4349626   -2.8120697   -0.0000000
      C    -1.2264196   -3.5006305   -0.0000000
      C    -1.2213052   -4.9601077    0.0000000
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C	-0.0000001	-5.6523718	0.0000000
C	2.4178267	-5.6773807	0.0000000
C	1.2213054	-4.9601077	0.0000000
C	1.2264192	-3.5006305	-0.0000000
C	2.4349629	-2.8120696	-0.0000000
C	2.4580101	-1.3855118	-0.0000000
C	1.2488127	-0.6552343	-0.0000000
C	-0.0000002	-1.3671050	-0.0000000
C	-1.2488124	-0.6552343	-0.0000000
C	-2.4580102	-1.3855119	0.0000000
C	0.0000003	-2.7928172	-0.0000000
C	0.0000002	1.5048635	0.0000000
C	1.2399311	0.8033191	-0.0000000
C	2.4517458	1.5008665	-0.0000000
C	-1.2399314	0.8033191	-0.0000000
C	-2.4517457	1.5008665	-0.0000000
C	-2.4726770	2.9330798	-0.0000000
C	-1.2522540	3.6460251	-0.0000000
C	-0.0000001	2.9323561	-0.0000000
C	1.2522541	3.6460251	-0.0000000
C	2.4726770	2.9330799	-0.0000000
C	2.4494615	5.8055393	0.0000000
C	1.2390156	5.1131026	-0.0000000
C	0.0000000	5.7685102	0.0000000
C	-1.2390157	5.1131026	-0.0000000
C	-2.4494615	5.8055393	0.0000000
H	6.9394406	-5.7344570	0.0000000
H	2.4005395	-6.7726745	0.0000000
H	0.0000000	-6.7476941	0.0000000
H	-2.4005395	-6.7726744	0.0000000
H	-7.0672467	3.0971606	0.0000000
H	-7.0533053	-1.2634942	0.0000000
H	-6.9394406	-5.7344570	0.0000000
H	7.0533053	-1.2634941	0.0000000
H	7.0672467	3.0971606	0.0000000
B	-4.8556880	-5.8906259	0.0000000
H	-4.7790625	-7.0992149	-0.0000000
B	-6.1935789	-3.7579876	0.0000000
H	-7.3017967	-3.2679692	0.0000000
B	-3.7211545	-3.6165405	-0.0000000
B	-4.9644737	-1.4994827	-0.0000000
B	-6.2388988	0.6678346	-0.0000000
H	-7.3355942	1.1878971	0.0000000
B	-3.7583732	0.7096708	-0.0000000
B	-4.9777245	2.8737306	-0.0000000
B	-6.2695382	5.0470164	0.0000000

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      H    -7.3450208    5.6194136    0.0000000
      B    -3.7461897    5.0697502    0.0000000
      B     4.8556880   -5.8906259    0.0000000
      H     4.7790625   -7.0992149   -0.0000000
      B     6.1935789   -3.7579876    0.0000000
      H     7.3017967   -3.2679692    0.0000000
      B     3.7211545   -3.6165405   -0.0000000
      B     4.9644737   -1.4994827   -0.0000000
      B     3.7583732    0.7096708   -0.0000000
      B     6.2388988    0.6678346    0.0000000
      H     7.3355942    1.1878971    0.0000000
      B     4.9777245    2.8737306   -0.0000000
      B     3.7461897    5.0697502    0.0000000
      B     6.2695382    5.0470164    0.0000000
      H     7.3450208    5.6194136    0.0000000
      N    -3.6311420   -5.0884476    0.0000000
      N    -4.9963330   -2.9699771    0.0000000
      N    -6.0811987   -5.1940462    0.0000000
      N    -6.1769239   -0.7564086   -0.0000000
      N    -3.7058877   -0.7542846   -0.0000000
      N    -5.0175453    1.4058013   -0.0000000
      N    -3.7101296    3.5887479   -0.0000000
      N    -5.0409338    5.7311024    0.0000000
      N    -6.1990981    3.6157888    0.0000000
      N     5.0409338    5.7311024    0.0000000
      N     6.1990981    3.6157888   -0.0000000
      N     3.7101297    3.5887479    0.0000000
      N     5.0175453    1.4058013   -0.0000000
      N     3.7058877   -0.7542847   -0.0000000
      N     6.1769239   -0.7564086   -0.0000000
      N     4.9963330   -2.9699771    0.0000000
      N     3.6311420   -5.0884476    0.0000000
      N     6.0811987   -5.1940462    0.0000000

BN-edges,          wB97XD/def2-SV(P)
      H     4.9178923   -7.0744632   -0.0000000
      H     2.4285619   -7.0036774   -0.0000000
      H    -0.0000000   -6.9683996   -0.0000000
      H    -2.4285619   -7.0036774   -0.0000000
      H    -4.9178923   -7.0744632   -0.0000000
      C     2.4463464    1.4000856   -0.0000000
      C     1.2334992    0.6939813    0.0000000
      C    -0.0000000    1.3873165   -0.0000000
      C    -1.2334992    0.6939813   -0.0000000
      C    -2.4463464    1.4000856    0.0000000
      C     0.0000000   -1.4755684    0.0000000
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C	1.2492167	-0.7769188	0.0000000
C	2.4922570	-1.4744389	0.0000000
C	-1.2492167	-0.7769188	0.0000000
C	-2.4922570	-1.4744389	0.0000000
H	7.0411722	-5.6834159	-0.0000000
H	7.3505634	5.6409551	0.0000000
H	5.0775625	6.7759221	0.0000000
H	2.5583394	6.8084177	0.0000000
H	-0.0000000	6.8441519	0.0000000
H	-2.5583394	6.8084177	0.0000000
H	-5.0775625	6.7759221	0.0000000
H	-7.0411722	-5.6834159	-0.0000000
H	-7.3235644	-3.1944149	-0.0000000
H	-7.0544309	-1.2630337	-0.0000000
H	-7.3288185	1.1832839	-0.0000000
H	-7.1115411	3.1223173	0.0000000
H	-7.3505633	5.6409551	0.0000000
H	7.1115411	3.1223173	0.0000000
H	7.3288185	1.1832839	-0.0000000
H	7.0544309	-1.2630337	-0.0000000
H	7.3235644	-3.1944149	-0.0000000
B	4.9419469	-5.8636232	-0.0000000
B	2.4619599	-5.7949748	0.0000000
B	0.0000000	-5.7599759	0.0000000
B	-2.4619599	-5.7949748	0.0000000
B	-4.9419469	-5.8636232	-0.0000000
B	6.2392266	-3.7354644	-0.0000000
B	3.7528180	-3.6529988	-0.0000000
B	1.2510989	-3.5944636	0.0000000
B	-1.2510989	-3.5944636	0.0000000
B	-3.7528180	-3.6529988	0.0000000
B	-6.2392266	-3.7354644	-0.0000000
N	6.1757094	-5.1563247	-0.0000000
N	5.0105120	-2.9775741	0.0000000
N	3.7117078	-5.0995393	0.0000000
N	2.5026831	-2.8735442	0.0000000
N	1.2393078	-5.0381257	0.0000000
N	-0.0000000	-2.8660202	0.0000000
N	-1.2393078	-5.0381257	0.0000000
N	-2.5026831	-2.8735442	0.0000000
N	-3.7117078	-5.0995393	0.0000000
N	-5.0105120	-2.9775741	0.0000000
N	-6.1757094	-5.1563247	-0.0000000
N	5.0513356	5.7634390	-0.0000000
N	6.2346329	3.6266085	-0.0000000
N	3.7645779	3.6263679	-0.0000000

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     N     2.5324285    5.7950686   -0.0000000
     N     1.2466293    3.6817031   -0.0000000
     N    -0.0000000    5.8305494   -0.0000000
     N    -1.2466293    3.6817031   -0.0000000
     N    -2.5324285    5.7950686   -0.0000000
     N    -3.7645779    3.6263679   -0.0000000
     N    -6.2346329    3.6266085   -0.0000000
     N    -5.0513356    5.7634390   -0.0000000
     B     6.2840965    5.0514913   -0.0000000
     B     3.7796560    5.0782273   -0.0000000
     B     5.0001492    2.8793377   -0.0000000
     B     1.2565379    5.1281023   -0.0000000
     B     2.4775391    2.9311773   -0.0000000
     B    -0.0000000    2.9430279    0.0000000
     B    -1.2565379    5.1281023   -0.0000000
     B    -2.4775391    2.9311773   -0.0000000
     B    -3.7796560    5.0782273    0.0000000
     B    -5.0001492    2.8793377    0.0000000
     B    -6.2840965    5.0514913   -0.0000000
     B     6.2279185    0.6676311   -0.0000000
     B     4.9829121   -1.5278874   -0.0000000
     B     3.7364516    0.6784463   -0.0000000
     B    -6.2279185    0.6676311   -0.0000000
     B    -4.9829121   -1.5278874   -0.0000000
     B    -3.7364516    0.6784463   -0.0000000
     N    -5.0136891    1.3992752   -0.0000000
     N    -3.6955668   -0.8256783    0.0000000
     N    -6.1741439   -0.7635225   -0.0000000
     N     5.0136891    1.3992752   -0.0000000
     N     6.1741439   -0.7635225   -0.0000000
     N     3.6955668   -0.8256783    0.0000000

BN-edges-line,          wB97XD/def2-SV(P)
     H     4.7871573   -7.0181844    0.0000000
     H     2.4128258   -6.9140816    0.0000000
     H     0.0000000   -6.9007249   -0.0000000
     H    -2.4128258   -6.9140816    0.0000000
     H    -4.7871573   -7.0181844   -0.0000000
     C    -3.6899081    3.5923083    0.0000000
     C    -2.4723684    2.9011235    0.0000000
     C    -1.2304418    3.5956748    0.0000000
     C     1.2304418    3.5956748   -0.0000000
     C     2.4723684    2.9011235   -0.0000000
     C     3.6899081    3.5923083    0.0000000
     C     3.6972621    0.7184576   -0.0000000
     C     2.4853661    1.4359563   -0.0000000
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C	1.2356260	0.7213912	-0.0000000
C	-0.0000000	1.4319666	-0.0000000
C	-1.2356260	0.7213912	-0.0000000
C	-2.4853661	1.4359563	0.0000000
C	-3.6972621	0.7184576	0.0000000
C	0.0000000	2.8966328	-0.0000000
C	3.6707930	-0.7172505	0.0000000
C	-0.0000000	-1.4182626	-0.0000000
C	1.2241669	-0.7148495	-0.0000000
C	2.4670173	-1.4194180	-0.0000000
C	-1.2241669	-0.7148495	-0.0000000
C	-2.4670173	-1.4194180	-0.0000000
C	-3.6707930	-0.7172505	0.0000000
C	-3.6869422	-3.6110676	-0.0000000
C	-2.4774078	-2.8844990	-0.0000000
C	-1.2298202	-3.5739595	-0.0000000
C	0.0000000	-2.8722154	-0.0000000
C	1.2298202	-3.5739595	0.0000000
C	2.4774078	-2.8844990	0.0000000
C	3.6869422	-3.6110676	-0.0000000
H	6.9910661	-5.6669450	0.0000000
H	7.3341021	5.6002168	0.0000000
H	5.1098215	6.7769711	0.0000000
H	2.4991117	6.8706145	0.0000000
H	-0.0000000	6.8681089	0.0000000
H	-2.4991117	6.8706145	0.0000000
H	-5.1098215	6.7769711	0.0000000
H	-6.9910661	-5.6669450	-0.0000000
H	-7.2122500	-3.1519096	-0.0000000
H	-7.0955586	-1.2490941	-0.0000000
H	-7.2367938	1.2045551	0.0000000
H	-7.1226298	3.1145382	0.0000000
H	-7.3341021	5.6002168	0.0000000
H	7.1226298	3.1145382	0.0000000
H	7.2367938	1.2045551	0.0000000
H	7.0955586	-1.2490941	-0.0000000
H	7.2122500	-3.1519096	-0.0000000
B	4.8875144	-5.8174221	0.0000000
B	6.1557083	-3.7275635	-0.0000000
B	4.9691499	-1.5053523	-0.0000000
B	6.1721108	0.6313884	-0.0000000
B	4.9904958	2.8464054	0.0000000
B	6.2580088	5.0216548	-0.0000000
B	3.7379880	5.1283807	-0.0000000
B	1.2485140	5.1496072	0.0000000
B	-1.2485140	5.1496072	0.0000000

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      B    -3.7379880    5.1283807    0.0000000
      B    -6.2580088    5.0216548    0.0000000
      B    -4.9904958    2.8464054    0.0000000
      B    -6.1721108    0.6313884   -0.0000000
      B    -4.9691499   -1.5053523   -0.0000000
      B    -6.1557083   -3.7275635   -0.0000000
      B    -4.8875144   -5.8174221    0.0000000
      B    -2.4416065   -5.7134812    0.0000000
      B    -0.0000000   -5.6996819    0.0000000
      B     2.4416065   -5.7134812    0.0000000
      N     6.1236094   -5.1436004    0.0000000
      N     4.9085638   -2.9862560   -0.0000000
      N     6.1922337   -0.7954127   -0.0000000
      N     4.9428727    1.3605041    0.0000000
      N     6.2299153    3.5890957    0.0000000
      N     5.0441005    5.7653308   -0.0000000
      N     2.5048978    5.8547072   -0.0000000
      N    -0.0000000    5.8522060    0.0000000
      N    -2.5048978    5.8547072    0.0000000
      N    -5.0441005    5.7653308    0.0000000
      N    -6.2299153    3.5890957    0.0000000
      N    -4.9428727    1.3605041    0.0000000
      N    -6.1922337   -0.7954127   -0.0000000
      N    -4.9085638   -2.9862560   -0.0000000
      N    -3.6784228   -5.0043627    0.0000000
      N    -6.1236094   -5.1436004   -0.0000000
      N    -1.2232534   -4.9640655    0.0000000
      N     1.2232534   -4.9640655    0.0000000
      N     3.6784228   -5.0043627    0.0000000

BN-zz-B-top-line,         wB97XD/def2-SV(P)
      H    -4.9103946    6.9507733   -0.0000000
      H    -2.4155474    6.9160417   -0.0000000
      H     0.0368956    6.9018724   -0.0000000
      H     2.4720479    6.9021166   -0.0000000
      H     4.8501061    6.9771591   -0.0000000
      C     6.1283095    0.6987579   -0.0000000
      C     6.1283081   -0.6987606   -0.0000000
      C     4.9520219   -1.4334846   -0.0000000
      C    -6.1043008   -0.6977744   -0.0000000
      C    -4.9249612   -1.4263384   -0.0000000
      C    -3.6809771   -0.7174261    0.0000000
      C    -2.4494900   -1.4269422   -0.0000000
      C    -1.2231887   -0.7212107    0.0000000
      C     0.0171136   -1.4249063   -0.0000000
      C     1.2460540   -0.7220201    0.0000000
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C	2.4824699	-1.4282814	-0.0000000
C	3.7073973	-0.7196553	0.0000000
C	-3.6809761	0.7174102	-0.0000000
C	-4.9249647	1.4263256	0.0000000
C	-6.1043029	0.6977639	-0.0000000
C	0.0171187	1.4248957	0.0000000
C	-1.2231859	0.7211957	-0.0000000
C	-2.4494883	1.4269284	-0.0000000
C	1.2460577	0.7220092	0.0000000
C	2.4824743	1.4282755	0.0000000
C	3.7074000	0.7196492	0.0000000
C	4.9520240	1.4334816	0.0000000
H	-7.0118767	5.4492381	-0.0000000
H	-7.0118540	-5.4492287	0.0000000
H	-4.9103913	-6.9507513	0.0000000
H	-2.4155478	-6.9160201	0.0000000
H	0.0368940	-6.9018569	0.0000000
H	2.4720465	-6.9021084	0.0000000
H	4.8501049	-6.9771557	-0.0000000
H	7.2532214	5.4653209	0.0000000
H	7.1143309	3.0549819	0.0000000
H	7.0974113	1.1985437	-0.0000000
H	7.0974105	-1.1985448	0.0000000
H	7.1143280	-3.0549834	-0.0000000
H	7.2532186	-5.4653206	-0.0000000
H	-7.0656490	-3.1371151	-0.0000000
H	-7.0717745	-1.2034299	-0.0000000
H	-7.0717779	1.2034289	-0.0000000
H	-7.0656693	3.1371044	-0.0000000
B	-4.9026804	5.7448723	-0.0000000
B	-2.4279864	5.7111941	-0.0000000
B	0.0349219	5.6977329	0.0000000
B	2.4948948	5.6988257	0.0000000
B	4.9630303	5.7716405	-0.0000000
B	-4.9026658	-5.7448584	0.0000000
B	-2.4279851	-5.7111803	0.0000000
B	0.0349162	-5.6977233	0.0000000
B	2.4948883	-5.6988207	-0.0000000
B	4.9630256	-5.7716384	-0.0000000
N	-6.1045667	5.0018271	-0.0000000
N	-3.6691267	4.9991155	-0.0000000
N	-1.2010736	4.9769207	-0.0000000
N	1.2646888	4.9689472	0.0000000
N	3.7404410	4.9864687	0.0000000
N	-3.6691200	-4.9991058	0.0000000
N	-6.1045499	-5.0018211	0.0000000

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      N    -1.2010759   -4.9769146    0.0000000
      N     1.2646829   -4.9689443   -0.0000000
      N     3.7404356   -4.9864678   -0.0000000
      C    -6.0891681    3.6211762   -0.0000000
      C    -4.9269118    2.8995912   -0.0000000
      C    -3.6562470    3.5862619   -0.0000000
      C    -2.4551384    2.8832116   -0.0000000
      C    -1.1941760    3.5667957   -0.0000000
      C     0.0112518    2.8701702   -0.0000000
      C     1.2746255    3.5628752    0.0000000
      C     2.4781941    2.8784807    0.0000000
      C     3.7476681    3.5904737    0.0000000
      C     4.9524457    2.9004849    0.0000000
      C     6.2617188    4.9993172   -0.0000000
      C     6.1871394    3.6347198    0.0000000
      C    -6.0891524   -3.6211793    0.0000000
      C    -4.9269048   -2.8995966    0.0000000
      C    -3.6562444   -3.5862625    0.0000000
      C    -2.4551405   -2.8832167    0.0000000
      C    -1.1941833   -3.5667972    0.0000000
      C     0.0112436   -2.8701753    0.0000000
      C     1.2746160   -3.5628761   -0.0000000
      C     2.4781858   -2.8784837   -0.0000000
      C     3.7476616   -3.5904739   -0.0000000
      C     4.9524411   -2.9004872   -0.0000000
      C     6.1871360   -3.6347208   -0.0000000
      C     6.2617155   -4.9993181   -0.0000000

BN-zz-N-top-line,         wB97XD/def2-SV(P)
      H     5.0053940    6.8814756   -0.0000000
      H     2.4899685    6.8780695   -0.0000000
      H     0.0076530    6.8686492   -0.0000000
      H    -2.4867593    6.8675884   -0.0000000
      H    -5.1231563    6.7503923   -0.0000000
      C    -6.0721874    0.6973981    0.0000000
      C    -6.0721928   -0.6973921   -0.0000000
      C    -4.8907186   -1.4281646    0.0000000
      C     6.1605916   -0.6967710    0.0000000
      C     4.9834782   -1.4285283    0.0000000
      C     3.7427428   -0.7171760    0.0000000
      C     2.5120374   -1.4296517   -0.0000000
      C     1.2858585   -0.7221888   -0.0000000
      C     0.0491970   -1.4322984   -0.0000000
      C    -1.1792708   -0.7213262    0.0000000
      C    -2.4130728   -1.4253270   -0.0000000
      C    -3.6455247   -0.7175726   -0.0000000
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C	3.7427449	0.7171710	0.0000000
C	4.9834721	1.4285301	-0.0000000
C	6.1605975	0.6967764	0.0000000
C	0.0491937	1.4322988	0.0000000
C	1.2858569	0.7221858	0.0000000
C	2.5120329	1.4296502	0.0000000
C	-1.1792706	0.7213262	-0.0000000
C	-2.4130764	1.4253283	0.0000000
C	-3.6455202	0.7175756	0.0000000
C	-4.8907209	1.4281657	-0.0000000
H	7.2783374	5.7874093	-0.0000000
H	7.2783499	-5.7874101	0.0000000
H	5.0054090	-6.8814766	0.0000000
H	2.4899723	-6.8780707	0.0000000
H	0.0076486	-6.8686502	0.0000000
H	-2.4867664	-6.8675882	0.0000000
H	-5.1231636	-6.7503871	0.0000000
H	-7.0944489	5.5511943	-0.0000000
H	-7.0912368	3.1257078	-0.0000000
H	-7.0356912	1.2083837	0.0000000
H	-7.0356930	-1.2083765	-0.0000000
H	-7.0912468	-3.1257037	0.0000000
H	-7.0944587	-5.5511934	0.0000000
H	7.1207622	-3.0699937	0.0000000
H	7.1243911	-1.2069171	-0.0000000
H	7.1243897	1.2069314	0.0000000
H	7.1207556	3.0699868	-0.0000000
N	4.9954152	5.8665896	-0.0000000
N	-5.0062633	5.7431508	-0.0000000
N	-2.4876097	5.8525344	0.0000000
N	0.0053646	5.8531596	0.0000000
N	2.4938750	5.8625247	0.0000000
N	4.9954269	-5.8665906	-0.0000000
N	2.4938816	-5.8625260	-0.0000000
N	0.0053658	-5.8531606	-0.0000000
N	-2.4876132	-5.8525356	-0.0000000
N	-5.0062673	-5.7431582	0.0000000
B	6.2301010	5.1673531	-0.0000000
B	3.7391487	5.1671092	-0.0000000
B	1.2522105	5.1572353	-0.0000000
B	-1.2375225	5.1526955	-0.0000000
B	-3.7100326	5.1184747	-0.0000000
B	6.2301101	-5.1673547	-0.0000000
B	3.7391578	-5.1671140	-0.0000000
B	1.2522152	-5.1572386	-0.0000000
B	-1.2375219	-5.1526964	0.0000000

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      B    -3.7100369   -5.1184718    0.0000000
      C    -6.1496684    4.9992909    0.0000000
      C    -6.1296330    3.6373608    0.0000000
      C    -4.8926308    2.8959738   -0.0000000
      C    -3.6860004    3.5804627   -0.0000000
      C    -2.4151961    2.8728360    0.0000000
      C    -1.2175804    3.5843253    0.0000000
      C     0.0473482    2.8802408    0.0000000
      C     1.2594978    3.5883843    0.0000000
      C     2.5172212    2.8874429    0.0000000
      C     3.7281131    3.5991591    0.0000000
      C     4.9979570    2.9053347   -0.0000000
      C     6.1772185    3.6232245    0.0000000
      C     6.1772232   -3.6232247   -0.0000000
      C     4.9979678   -2.9053437   -0.0000000
      C     3.7281200   -3.5991612   -0.0000000
      C     2.5172295   -2.8874497   -0.0000000
      C     1.2595013   -3.5883851   -0.0000000
      C     0.0473538   -2.8802435   -0.0000000
      C    -1.2175801   -3.5843250   -0.0000000
      C    -2.4151969   -2.8728361   -0.0000000
      C    -3.6860009   -3.5804644    0.0000000
      C    -4.8926350   -2.8959658    0.0000000
      C    -6.1296360   -3.6373710   -0.0000000
      C    -6.1496750   -4.9992762   -0.0000000

BN-ac-line,          wB97XD/def2-SV(P)
      H     4.9501247   -7.0944891    0.0000000
      H     2.4183951   -6.7926508    0.0000000
      H    -0.0000000   -6.7768626   -0.0000000
      H    -2.4183951   -6.7926508    0.0000000
      H    -4.9501247   -7.0944891    0.0000000
      C    -2.4619528    5.7167553   -0.0000000
      C    -3.6547308    5.0302693   -0.0000000
      C    -3.6686493    3.5982390   -0.0000000
      C    -2.4670956    2.8870290    0.0000000
      C    -1.2217060    3.5813767    0.0000000
      C    -1.2217970    5.0184219    0.0000000
      C     0.0000000    5.6998658    0.0000000
      C     3.6547308    5.0302693   -0.0000000
      C     2.4619528    5.7167553    0.0000000
      C     1.2217970    5.0184219    0.0000000
      C     1.2217060    3.5813767    0.0000000
      C     2.4670956    2.8870290    0.0000000
      C     3.6686493    3.5982390   -0.0000000
      C     3.6974321    0.7186730    0.0000000
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C	2.4820691	1.4348464	0.0000000
C	1.2363977	0.7207616	0.0000000
C	0.0000000	1.4251321	0.0000000
C	-1.2363977	0.7207616	0.0000000
C	-2.4820691	1.4348464	0.0000000
C	-3.6974321	0.7186730	0.0000000
C	-0.0000000	2.8711053	0.0000000
C	3.6803924	-0.7109107	-0.0000000
C	-0.0000000	-1.4139835	0.0000000
C	1.2279080	-0.7097289	-0.0000000
C	2.4715164	-1.4136489	-0.0000000
C	-1.2279080	-0.7097289	0.0000000
C	-2.4715164	-1.4136489	0.0000000
C	-3.6803924	-0.7109107	-0.0000000
C	-3.6828034	-3.6087154	-0.0000000
C	-2.4817292	-2.8686357	-0.0000000
C	-1.2301133	-3.5649131	-0.0000000
C	0.0000000	-2.8574230	-0.0000000
C	1.2301133	-3.5649131	-0.0000000
C	2.4817292	-2.8686357	-0.0000000
C	3.6828034	-3.6087154	0.0000000
C	3.6560475	-5.0492563	0.0000000
C	2.4442551	-5.6980118	0.0000000
C	1.2137803	-4.9963827	-0.0000000
C	-0.0000000	-5.6822501	-0.0000000
C	-1.2137803	-4.9963827	-0.0000000
C	-2.4442551	-5.6980119	0.0000000
C	-3.6560475	-5.0492563	0.0000000
H	7.0643637	-5.6240824	0.0000000
H	7.1594783	5.7137346	-0.0000000
H	4.8279437	6.6968012	-0.0000000
H	2.4470987	6.8113935	-0.0000000
H	-0.0000000	6.7943280	0.0000000
H	-2.4470987	6.8113935	-0.0000000
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H	-7.2206578	-3.1385223	0.0000000
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H	-7.2332392	1.2384668	-0.0000000
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      B     4.9807962   -1.5105787   -0.0000000
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      B     6.1501255    5.0393332   -0.0000000
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      N     6.2022699   -0.7690341   -0.0000000
      N     4.9354603    1.3785564   -0.0000000
      N     6.1977298    3.6136816   -0.0000000
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      B    -6.1631845   -3.7241671   -0.0000000
      B    -4.9807962   -1.5105787   -0.0000000
      B    -6.1799185    0.6426534   -0.0000000
      B    -4.9872562    2.8419200   -0.0000000
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      N    -6.1705464   -5.1454746    0.0000000


BN-vertical,          wB97XD/def2-SV(P)
      H    -4.8735713    6.8499324    0.0000000
      H    -2.4416012    6.7954756   -0.0000000
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      C     6.1336227    3.6651862    0.0000000
      C     6.1530840    0.7002440   -0.0000000
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