Supplementary material for the article:

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Supporting Information

A DFT Study of the Modulation of the Antiaromatic and Open-Shell Character of Dibenzo[*a*,*f*]pentalene by Employing Three Strategies: Additional Benzoannulation, BN/CC Isosterism, and Substitution

Marija Baranac-Stojanović*[a]

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Supporting Information

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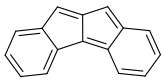
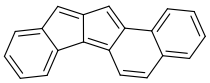
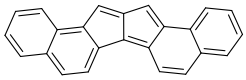
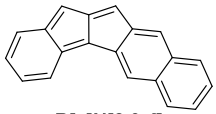
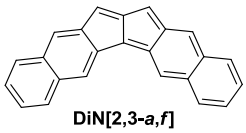
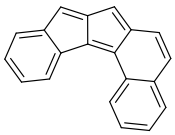
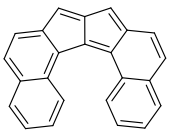
Compound	E_{CS} ZP_{CS}	E_{OS} ZP_{OS}	E_T ZP_T	$\langle S^2 \rangle$ OS/Triplet	*J*	$E_{OS\text{-}AP}$
 **DBP**	-615.8161769 0.203234	-615.8165968 0.201631	-615.8164253 0.202140	0.46/2.02	-0.00011	-615.8166468
 **B[*a*]N[1,2-*f*]**	-769.5060696 0.250271	/ /	-769.4941578 0.248756	0.00/2.02	/	/
 **DiN[2,1-*a*:1,2-*f*]**	-923.1809047 0.296400	/ /	-923.1730585 0.295253	0.00/2.01	/	/
 **B[*a*]N[2,3-*f*]**	-769.5004314 0.249899	-769.5004756 0.248617	-769.497559 0.248497	0.13/2.03	-0.00154	-769.500678
 **DiN[2,3-*a*,*f*]**	-923.1666507 0.295567	-923.1714505 0.298709	-923.1794053 0.294858	0.94/2.03	0.00727	-923.1646372
 **B[*a*]N[2,1-*f*]**	-769.5033093 0.250184	/ /	-769.4910808 0.248651	0.00/2.02	/	/
 **DiN[1,2-*a*:2,1-*f*]**	-923.1700222 0.296836	/ /	-923.1626411 0.295668	0.00/2.01	/	/

Table S2. Absolute energies of closed-shell, open-shell singlet and triplet states of BN-substituted dibenzo[*a*,*f*]pentalenes (E_{CS}, E_{OS} and E_T), zero-point correction to energy (ZP), spin-squared expectation values ($\langle S^2 \rangle$), spin-coupling constant (*J*) and AP-corrected energies for OS singlets ($E_{OS\text{-}AP}$). Energies are in a.u.

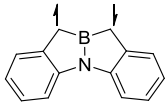
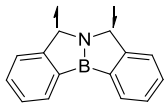
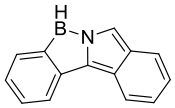
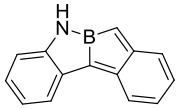
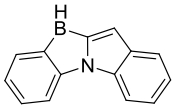
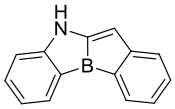
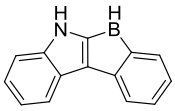
Compound	E_{CS} ZP_{CS}	E_{OS} ZP_{OS}	E_T ZP_T	$\langle S^2 \rangle$ OS/Triplet	*J*	$E_{OS\text{-}AP}$
 **4b,9a-NB**	-619.260011 0.201058	-619.2616593 0.200701	-619.2470344 0.199725	0.44/2.04	-0.00909	-619.2656313
 **9a,4b-NB**	-619.2245922 0.198620	-619.2575435 0.200279	-619.2575164 0.200719	0.87/2.02	-0.00002	-619.2575641
 **9a,9-NB**	-619.293415 0.201302	/ /	-619.2551161 0.199332	0.00/2.02	/	/
 **9,9a-NB**	-619.253421 0.201855	-619.2591592 0.199853	-619.2568933 0.201094	1.07/2.02	-0.00238	-619.2616963
 **4b,9-NB**	-619.2785092 0.201319	/ /	-619.2030623 0.197676	0.00/2.02	/	/
 **9,4b-NB**	-619.2594519 0.201999	/ /	-619.2220105 0.201115	0.00/2.01	/	/
 **9,10-NB**	-619.2726847 0.201439	/ /	-619.2264841 0.199957	0.00/2.01	/	/

Table S3. Absolute energies of closed-shell, open-shell singlet and triplet states of disubstituted dibenzo[*a*,*f*]pentalenes (E_{CS}, E_{OS} and E_T), zero-point correction to energy (ZP), spin-squared expectation values ($\langle S^2 \rangle$), spin-coupling constant (J) and AP-corrected energies for OS singlets ($E_{OS\text{-}AP}$). Energies are in a.u.

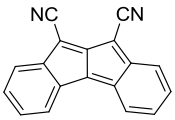
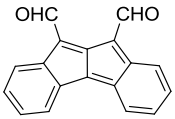
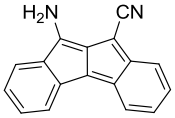
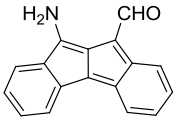
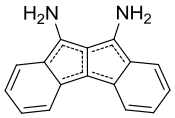
Compound	E_{CS} ZP_{CS}	E_{OS} ZP_{OS}	E_T ZP_T	$\langle S^2 \rangle$ OS/Triplet	J	$E_{OS\text{-}AP}$
	-800.351206 0.200532	-800.3516847 0.206150	-800.3581988 0.199850	0.90/2.03	0.00581	-800.3464280
	-842.5350985 0.222311	-842.537764 0.220285	-842.5393708 0.221529	0.94/2.02	0.00149	-842.5363609
	-763.4932387 0.219615	/ /	-763.4763033 0.218084	0.00/2.02	/	/
	-784.5978313 0.230884	/ /	-784.5738253 0.229058	0.00/2.02	/	/
	-726.5917918 0.236499	/ /	-726.5782955 0.236249	0.00/2.02	/	/

Table S4. Calculated HOMA and FLU_π values for (di)benzo-fused dibenzo[*a*,*f*]pentalene.[a]

Entry	Compound			benz	benz	cpd	cpd	benz	benz	pent	tricycle	DBP	peri
1	DBP	OS	HOMA	/	0.869	0.101	0.127	0.405	/	0.183	0.546	0.685	0.685
2	B[*a*]N[1,2-*f*]	CS	HOMA	/	0.879	-0.020	-0.127	-0.081	0.927	-0.519	0.284	0.480	0.592
			FLU_π	/	0.0223	0.3029	0.3148	0.3009	0.0119	0.3024	0.2594	0.1787	0.1363
3	DiN[2,1-*a*:1,2-*f*]	CS	HOMA	0.720	0.782	0.142	-0.073	-0.062	0.925	0.006	0.337	0.445	0.628
			FLU_π	0.0859	0.0312	0.2362	0.2968	0.2868	0.0125	0.2696	0.2336	0.1847	0.1276
4	B[*a*]N[2,3-*f*]	OS	HOMA	/	0.267	0.026	-0.046	0.493	0.857	0.100	0.349	0.562	0.656
5	DiN[2,3-*a*,*f*]	CS	HOMA	0.856	0.483	0.065	0.049	0.196	0.344	0.117	0.483	0.580	0.700
			FLU_π	0.0321	0.1328	0.2229	0.1830	0.1466	0.2220	0.2001	0.1356	0.1194	0.1073
6	B[*a*]N[2,1-*f*]	CS	HOMA	/	0.869	-0.172	-0.171	-0.155	0.913	-0.093	0.253	0.461	0.582
			FLU_π	/	0.0239	0.3143	0.3089	0.3152	0.0126	0.2978	0.2604	0.3495	0.1364
7	DiN[1,2-*a*:2,1-*f*][b]	CS	HOMA	0.691	0.759	-0.109	-0.203	-0.173	0.913	-0.075	0.264	0.380	0.590
				benz	benz	cpd	cpd	benz	benz	pent			peri
8	DBP	triplet	HOMA	/	0.848	0.263	0.263	0.848	/	0.392			0.782
9	B[*a*]N[1,2-*f*]	triplet	HOMA	/	0.813	0.262	0.325	0.695	0.771	0.464			0.773
10	DiN[2,1-*a*:1,2-*f*]	triplet	HOMA	0.797	0.640	0.319	0.319	0.640	0.797	0.554			0.773
11	B[*a*]N[2,3-*f*]	triplet	HOMA	/	0.859	0.272	0.222	0.506	0.803	0.321			0.771
12	DiN[2,3-*a*,*f*]	triplet	HOMA	0.817	0.508	0.227	0.227	0.508	0.817	0.275			0.770
13	B[*a*]N[2,1-*f*]	triplet	HOMA	/	0.815	0.144	0.212	0.654	0.781	0.421			0.769
14	DiN[1,2-*a*:2,1-*f*]	triplet	HOMA	0.811	0.595	0.181	0.181	0.595	0.811	0.527			0.776

[a] Abbreviations: benz (benzene), cpd (cyclopentadiene), pent (pentalene), tricycle (pent+benz B of DBP, Fig. 4), naphth (naphthalene), DBP (dibenzopentalene substructure), peri (molecular perimeter). [b] FLU_π was not calculated, because this molecule is not planar and lacks clear σ/π separation.

Table S5. Calculated HOMA and FLU_π values for BN substituted dibenzo[*a*,*f*]pentalene.[a]

Entry	Compound			benz	cpd	cpd	benz	ind	ind	pent	peri
1	DBP	OS	HOMA	0.869	0.101	0.127	0.405	0.547	0.635	0.183	0.685
2	4b,9a-NB	OS	HOMA	0.822	0.473	0.473	0.822	0.788	0.788	0.436	0.808
3	9a,4b-NB	OS	HOMA	0.851	0.325	0.325	0.851	0.697	0.697	0.326	0.744
4	9a,9-NB	CS	HOMA	0.908	0.262	0.608	0.531	0.630	0.790	0.377	0.715
			FLU_π	0.0118	0.1743	0.0632	0.1648	0.2341	0.0969	0.2354	0.1959
5	9,9a-NB	OS	HOMA	0.836	0.383	-0.028	0.657	0.727	0.599	0.317	0.793
6	4b,9-NB	CS	HOMA	0.929	0.163	0.649	0.890	0.562	0.837	0.392	0.729
			FLU_π	0.0115	0.2382	0.0888	0.0320	0.3425	0.0569	0.3384	0.2317
7	9,4b-NB	CS	HOMA	0.886	0.168	-0.588	0.851	0.588	0.141	-0.050	0.517
			FLU_π	0.0166	0.3423	1.0238	0.0300	0.2943	0.5147	0.4548	0.2347
8	9,10-NB	CS	HOMA	0.850	0.747	-0.224	0.873	0.885	0.336	0.078	0.562
			FLU_π	0.0486	0.0253	0.6160	0.0270	0.0383	0.5236	0.3818	0.3183
9	DBP	triplet	HOMA	0.848	0.263	0.263	0.848	0.667	0.667	0.392	0.782
10	4b,9a-NB	triplet	HOMA	0.740	0.343	0.343	0.740	0.724	0.724	0.280	0.739
11	9a,4b-NB	triplet	HOMA	0.823	0.224	0.224	0.823	0.647	0.647	0.151	0.664
12	9a,9-NB	triplet	HOMA	0.810	0.336	0.487	0.874	0.700	0.765	0.446	0.790
13	9,9a-NB	triplet	HOMA	0.829	0.400	-0.001	0.725	0.738	0.587	0.329	0.785
14	4b,9-NB	triplet	HOMA	0.896	0.225	0.521	0.854	0.613	0.729	0.299	0.672
15	9,4b-NB	triplet	HOMA	0.896	0.251	0.024	0.623	0.489	0.614	0.183	0.705
16	9,10-NB	triplet	HOMA	0.911	0.373	-0.156	0.654	0.678	0.480	0.292	0.729

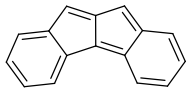
[a] Abbreviations: benz (benzene), cpd (cyclopentadiene), ind (indene), pent (pentalene), peri (molecular perimeter).

Table S6. Calculated HOMA and FLU values for disubstituted dibenzo[*a*,*f*]pentalene.[a]

Entry	Substituents			benz	cpd	cpd	benz	ind	ind	pent	peri
1	DBP	OS	HOMA	0.869	0.101	0.127	0.405	0.547	0.635	0.183	0.685
2	CN,CN	CS	HOMA	0.895	-0.338	-0.005	0.222	0.437	0.506	-0.032	0.526
			FLU	0.0054	0.0434	0.0395	0.0293	0.0218	0.0247	0.0369	0.0187
3	CHO,CHO	OS	HOMA	0.878	0.069	0.168	0.748	0.537	0.621	0.303	0.728
4	CN,NH_2	CS	HOMA	0.897	0.099	0.485	0.573	0.524	0.781	0.185	0.644
			FLU	0.0051	0.0416	0.0281	0.0177	0.0205	0.0158	0.0351	0.0162
5	CHO,NH_2	CS	HOMA	0.894	0.068	0.491	0.680	0.431	0.793	0.121	0.616
			FLU	0.0051	0.0420	0.0275	0.0132	0.0209	0.0143	0.0379	0.0170
6	NH_2,NH_2	CS	HOMA	0.767	0.472	0.472	0.767	0.787	0.787	0.467	0.824
			FLU	0.0104	0.0314	0.0314	0.0104	0.0150	0.0150	0.0291	0.0118
7	DBP	triplet	HOMA	0.848	0.263	0.263	0.848	0.667	0.667	0.392	0.782
8	CN,CN	triplet	HOMA	0.883	0.275	0.275	0.883	0.652	0.652	0.303	0.713
9	CHO,CHO	triplet	HOMA	0.877	0.235	0.208	0.887	0.633	0.613	0.255	0.690
10	CN,NH_2	triplet	HOMA	0.846	0.345	0.207	0.884	0.713	0.606	0.291	0.714
11	CHO,NH_2	triplet	HOMA	0.830	0.331	0.109	0.880	0.709	0.552	0.232	0.688
12	NH_2,NH_2	triplet	HOMA	0.861	0.352	0.352	0.861	0.706	0.706	0.329	0.739

[a] Abbreviations: benz (benzene), cpd (cyclopentadiene), ind (indene), pent (pentalene), peri (molecular perimeter).

X, Y, Z Coordinates of the Optimized Structures



DBP

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-2.297194	0.354070	0.000000
3	6	0	-1.272246	-0.648955	0.000000
4	6	0	0.000000	0.069797	0.000000
5	6	0	-0.297697	1.489964	0.000000
6	6	0	1.370554	-0.070761	0.000000
7	6	0	1.960190	1.304709	0.000000
8	6	0	0.949336	2.238590	0.000000
9	1	0	1.060566	3.313405	0.000000
10	6	0	3.385232	1.454372	0.000000
11	1	0	3.821274	2.447713	0.000000
12	6	0	4.173607	0.344300	0.000000
13	1	0	5.253172	0.441760	0.000000
14	6	0	3.601504	-0.983043	0.000000
15	1	0	4.277155	-1.831674	0.000000
16	6	0	2.253863	-1.195093	0.000000
17	1	0	1.854030	-2.202521	0.000000
18	6	0	-3.637311	0.008463	0.000000
19	1	0	-4.407950	0.772326	0.000000
20	6	0	-1.630566	-1.985502	0.000000
21	6	0	-3.988291	-1.354242	0.000000
22	1	0	-5.032716	-1.642627	0.000000
23	6	0	-2.998180	-2.328127	0.000000
24	1	0	-3.279519	-3.375541	0.000000
25	1	0	-2.188492	2.614782	0.000000
26	1	0	-0.880080	-2.767601	0.000000

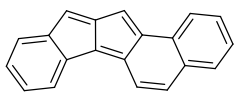
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.536128	1.797768	0.000000
2	6	0	-2.266197	0.527113	0.000000
3	6	0	-1.312289	-0.546807	0.000000
4	6	0	0.000000	0.077785	0.000000
5	6	0	-0.194336	1.519925	0.000000
6	6	0	1.368779	-0.166970	0.000000
7	6	0	2.050114	1.150228	0.000000
8	6	0	1.098679	2.167565	0.000000
9	1	0	1.294066	3.230277	0.000000
10	6	0	3.471870	1.197875	0.000000
11	1	0	3.981242	2.155577	0.000000
12	6	0	4.183989	0.025708	0.000000
13	1	0	5.267759	0.049869	0.000000

14	6	0	3.523652	-1.246283	0.000000
15	1	0	4.130240	-2.145261	0.000000
16	6	0	2.154796	-1.350714	0.000000
17	1	0	1.677689	-2.323929	0.000000
18	6	0	-3.627090	0.267307	0.000000
19	1	0	-4.347277	1.078814	0.000000
20	6	0	-1.759088	-1.859361	0.000000
21	6	0	-4.065415	-1.068677	0.000000
22	1	0	-5.126991	-1.286518	0.000000
23	6	0	-3.143701	-2.110500	0.000000
24	1	0	-3.496236	-3.135942	0.000000
25	1	0	-2.005730	2.773647	0.000000
26	1	0	-1.060589	-2.688313	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.328627	2.014669
2	6	0	0.000000	2.183502	0.842246
3	6	0	0.000000	1.361568	-0.344691
4	6	0	0.000000	0.000000	0.106256
5	6	0	0.000000	0.000000	1.563961
6	6	0	0.000000	-1.361568	-0.344691
7	6	0	0.000000	-2.183502	0.842246
8	6	0	0.000000	-1.328627	2.014669
9	1	0	0.000000	-1.676130	3.038345
10	6	0	0.000000	-3.569828	0.721956
11	1	0	0.000000	-4.201576	1.603628
12	6	0	0.000000	-4.143738	-0.555854
13	1	0	0.000000	-5.223448	-0.655307
14	6	0	0.000000	-3.348198	-1.705559
15	1	0	0.000000	-3.818102	-2.682213
16	6	0	0.000000	-1.953028	-1.607708
17	1	0	0.000000	-1.345453	-2.505463
18	6	0	0.000000	3.569828	0.721956
19	1	0	0.000000	4.201576	1.603628
20	6	0	0.000000	1.953028	-1.607708
21	6	0	0.000000	4.143738	-0.555854
22	1	0	0.000000	5.223448	-0.655307
23	6	0	0.000000	3.348198	-1.705559
24	1	0	0.000000	3.818102	-2.682213
25	1	0	0.000000	1.676130	3.038345
26	1	0	0.000000	1.345453	-2.505463



B[*a*]N[1,2-*f*]

Closed-shell

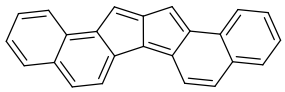
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579178	-2.570934	0.000000

2	6	0	2.840520	-1.810960	0.000000
3	6	0	2.528634	-0.413257	0.000000
4	6	0	1.068545	-0.324617	0.000000
5	6	0	0.545058	-1.682225	0.000000
6	6	0	0.000000	0.535601	0.000000
7	6	0	-1.248544	-0.293310	0.000000
8	6	0	-0.908986	-1.620629	0.000000
9	1	0	-1.579643	-2.467281	0.000000
10	6	0	-2.545861	0.364617	0.000000
11	6	0	-2.572657	1.786479	0.000000
12	6	0	-1.331355	2.545513	0.000000
13	1	0	-1.413526	3.627830	0.000000
14	6	0	-0.105857	1.962852	0.000000
15	1	0	0.791284	2.571098	0.000000
16	6	0	4.154099	-2.245842	0.000000
17	1	0	4.388996	-3.305105	0.000000
18	6	0	3.552789	0.516752	0.000000
19	6	0	5.187696	-1.290427	0.000000
20	1	0	6.221355	-1.616043	0.000000
21	6	0	4.887853	0.065336	0.000000
22	1	0	5.692642	0.792076	0.000000
23	1	0	1.518988	-3.652468	0.000000
24	1	0	3.344529	1.580599	0.000000
25	6	0	-3.761619	-0.333774	0.000000
26	1	0	-3.753110	-1.417778	0.000000
27	6	0	-3.810242	2.448381	0.000000
28	1	0	-3.825913	3.533492	0.000000
29	6	0	-4.976873	0.340694	0.000000
30	1	0	-5.904518	-0.220473	0.000000
31	6	0	-5.004059	1.737883	0.000000
32	1	0	-5.951006	2.265251	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.417702	-2.727482	0.000000
2	6	0	2.689851	-2.034506	0.000000
3	6	0	2.456465	-0.606416	0.000000
4	6	0	1.039285	-0.430354	0.000000
5	6	0	0.413356	-1.750848	0.000000
6	6	0	0.000000	0.557249	0.000000
7	6	0	-1.239787	-0.153221	0.000000
8	6	0	-0.977753	-1.578717	0.000000
9	1	0	-1.726167	-2.357830	0.000000
10	6	0	-2.470723	0.554092	0.000000
11	6	0	-2.421827	1.991608	0.000000
12	6	0	-1.164862	2.662168	0.000000
13	1	0	-1.159276	3.746739	0.000000
14	6	0	0.023284	1.965693	0.000000
15	1	0	0.966900	2.498960	0.000000
16	6	0	3.996667	-2.517908	0.000000
17	1	0	4.191166	-3.584996	0.000000
18	6	0	3.535340	0.282553	0.000000
19	6	0	5.059577	-1.609353	0.000000
20	1	0	6.078237	-1.981015	0.000000

21	6	0	4.834092	-0.225807	0.000000
22	1	0	5.678565	0.453494	0.000000
23	1	0	1.294086	-3.801353	0.000000
24	1	0	3.369782	1.353905	0.000000
25	6	0	-3.737817	-0.085921	0.000000
26	1	0	-3.783016	-1.168702	0.000000
27	6	0	-3.641955	2.712171	0.000000
28	1	0	-3.605953	3.796673	0.000000
29	6	0	-4.901372	0.647161	0.000000
30	1	0	-5.860651	0.142121	0.000000
31	6	0	-4.853969	2.060053	0.000000
32	1	0	-5.776991	2.628726	0.000000



DiN[2,1-*a*:1,2-*f*]

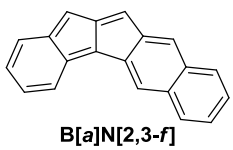
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.230446	-1.739870	0.000000
2	6	0	-2.163239	-0.604851	0.000000
3	6	0	-1.408965	0.592450	0.000000
4	6	0	0.000000	0.198475	0.000000
5	6	0	0.045426	-1.246324	0.000000
6	6	0	1.294968	0.660604	0.000000
7	6	0	2.201862	-0.533160	0.000000
8	6	0	1.438375	-1.671190	0.000000
9	1	0	1.790484	-2.692657	0.000000
10	6	0	3.642664	-0.343043	0.000000
11	6	0	4.138698	0.989994	0.000000
12	6	0	3.217370	2.114192	0.000000
13	1	0	3.651858	3.109016	0.000000
14	6	0	1.866721	1.971058	0.000000
15	1	0	1.223197	2.843171	0.000000
16	6	0	-3.575832	-0.584877	0.000000
17	6	0	-2.054580	1.834611	0.000000
18	6	0	-4.225053	0.702251	0.000000
19	6	0	-3.439579	1.878932	0.000000
20	1	0	-3.946527	2.838315	0.000000
21	1	0	-1.522213	-2.782192	0.000000
22	1	0	-1.483894	2.756146	0.000000
23	6	0	4.561128	-1.402949	0.000000
24	1	0	4.197014	-2.424061	0.000000
25	6	0	5.525378	1.207989	0.000000
26	1	0	5.896923	2.227683	0.000000
27	6	0	5.930488	-1.165717	0.000000
28	1	0	6.621425	-2.001338	0.000000
29	6	0	6.418416	0.144298	0.000000
30	1	0	7.486415	0.328869	0.000000
31	6	0	-4.388239	-1.752673	0.000000
32	1	0	-3.915701	-2.728265	0.000000
33	6	0	-5.645423	0.753937	0.000000
34	1	0	-6.129233	1.725453	0.000000

35	6	0	-6.397118	-0.394283	0.000000
36	1	0	-7.479680	-0.339412	0.000000
37	6	0	-5.757989	-1.659718	0.000000
38	1	0	-6.360257	-2.561545	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.327035	1.735947
2	6	0	0.000000	2.171562	0.564588
3	6	0	0.000000	1.353777	-0.616504
4	6	0	0.000000	0.000000	-0.175049
5	6	0	0.000000	0.000000	1.292311
6	6	0	0.000000	-1.353777	-0.616504
7	6	0	0.000000	-2.171562	0.564588
8	6	0	0.000000	-1.327035	1.735947
9	1	0	0.000000	-1.668240	2.760825
10	6	0	0.000000	-3.589515	0.452359
11	6	0	0.000000	-4.161461	-0.865566
12	6	0	0.000000	-3.312560	-2.015291
13	1	0	0.000000	-3.775935	-2.995850
14	6	0	0.000000	-1.943783	-1.899404
15	1	0	0.000000	-1.321943	-2.787195
16	6	0	0.000000	3.589515	0.452359
17	6	0	0.000000	1.943783	-1.899404
18	6	0	0.000000	4.161461	-0.865566
19	6	0	0.000000	3.312560	-2.015291
20	1	0	0.000000	3.775935	-2.995850
21	1	0	0.000000	1.668240	2.760825
22	1	0	0.000000	1.321943	-2.787195
23	6	0	0.000000	-4.457187	1.573756
24	1	0	0.000000	-4.032515	2.570775
25	6	0	0.000000	-5.570296	-0.992720
26	1	0	0.000000	-6.003937	-1.987379
27	6	0	0.000000	-5.824577	1.412649
28	1	0	0.000000	-6.473436	2.281081
29	6	0	0.000000	-6.386780	0.117968
30	1	0	0.000000	-7.464425	-0.000728
31	6	0	0.000000	4.457187	1.573756
32	1	0	0.000000	4.032515	2.570775
33	6	0	0.000000	5.570296	-0.992720
34	1	0	0.000000	6.003937	-1.987379
35	6	0	0.000000	6.386780	0.117968
36	1	0	0.000000	7.464425	-0.000728
37	6	0	0.000000	5.824577	1.412649
38	1	0	0.000000	6.473436	2.281081



B[*a*]N[2,3-*f*]

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.769573	-2.064219	0.000000
2	6	0	-1.776220	-3.023236	0.000000
3	6	0	-0.436287	-2.366523	0.000000
4	6	0	-0.649582	-1.005138	0.000000
5	6	0	-2.095228	-0.785237	0.000000
6	6	0	0.000000	0.294900	0.000000
7	6	0	-1.076726	1.275396	0.000000
8	6	0	-2.351584	0.557121	0.000000
9	1	0	-3.321644	1.039511	0.000000
10	6	0	-0.817155	2.616348	0.000000
11	1	0	-1.622974	3.344054	0.000000
12	6	0	0.538824	3.080733	0.000000
13	6	0	1.602342	2.121758	0.000000
14	6	0	1.299058	0.718005	0.000000
15	1	0	2.122624	0.012019	0.000000
16	6	0	-1.845896	-4.453818	0.000000
17	1	0	-2.812702	-4.945689	0.000000
18	6	0	0.736006	-3.183852	0.000000
19	6	0	-0.692789	-5.179738	0.000000
20	1	0	-0.734074	-6.263218	0.000000
21	6	0	0.602523	-4.541518	0.000000
22	1	0	1.486280	-5.170083	0.000000
23	1	0	-3.835932	-2.236190	0.000000
24	1	0	1.718683	-2.726251	0.000000
25	6	0	0.852804	4.455692	0.000000
26	1	0	0.042361	5.177727	0.000000
27	6	0	2.931940	2.592386	0.000000
28	1	0	3.742669	1.871021	0.000000
29	6	0	2.166420	4.887417	0.000000
30	1	0	2.391818	5.947571	0.000000
31	6	0	3.211423	3.947297	0.000000
32	1	0	4.241100	4.286892	0.000000

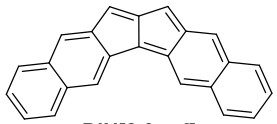
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.793707	-2.029420	0.000000
2	6	0	-1.808206	-3.002594	0.000000
3	6	0	-0.464496	-2.362510	0.000000
4	6	0	-0.663736	-0.995148	0.000000
5	6	0	-2.107563	-0.758745	0.000000
6	6	0	0.000000	0.295356	0.000000
7	6	0	-1.065065	1.289099	0.000000
8	6	0	-2.348216	0.587507	0.000000
9	1	0	-3.312062	1.081795	0.000000
10	6	0	-0.786853	2.626772	0.000000
11	1	0	-1.582988	3.365037	0.000000
12	6	0	0.574869	3.072913	0.000000
13	6	0	1.626292	2.100870	0.000000
14	6	0	1.305416	0.701986	0.000000
15	1	0	2.119222	-0.015200	0.000000
16	6	0	-1.894896	-4.429495	0.000000

17	1	0	-2.867467	-4.909925	0.000000
18	6	0	0.697811	-3.189722	0.000000
19	6	0	-0.748470	-5.170618	0.000000
20	1	0	-0.802682	-6.253508	0.000000
21	6	0	0.551097	-4.548400	0.000000
22	1	0	1.428286	-5.185998	0.000000
23	1	0	-3.861807	-2.190728	0.000000
24	1	0	1.684910	-2.741675	0.000000
25	6	0	0.906612	4.444122	0.000000
26	1	0	0.105567	5.176367	0.000000
27	6	0	2.962431	2.554408	0.000000
28	1	0	3.763513	1.822511	0.000000
29	6	0	2.225872	4.858615	0.000000
30	1	0	2.463665	5.916101	0.000000
31	6	0	3.258931	3.905647	0.000000
32	1	0	4.293097	4.231355	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.085077	-1.484864	0.000000
2	6	0	-2.247199	-2.671272	0.000000
3	6	0	-0.862870	-2.271441	0.000000
4	6	0	-0.858134	-0.830079	0.000000
5	6	0	-2.234552	-0.368390	0.000000
6	6	0	0.000000	0.310984	0.000000
7	6	0	-0.877772	1.485256	0.000000
8	6	0	-2.249568	1.039341	0.000000
9	1	0	-3.115170	1.686781	0.000000
10	6	0	-0.332765	2.748192	0.000000
11	1	0	-0.968035	3.628420	0.000000
12	6	0	1.082898	2.921196	0.000000
13	6	0	1.942596	1.769365	0.000000
14	6	0	1.370087	0.465979	0.000000
15	1	0	2.029851	-0.395226	0.000000
16	6	0	-2.578470	-4.022003	0.000000
17	1	0	-3.616332	-4.337342	0.000000
18	6	0	0.142618	-3.232710	0.000000
19	6	0	-1.551409	-4.976980	0.000000
20	1	0	-1.802822	-6.031593	0.000000
21	6	0	-0.211102	-4.589395	0.000000
22	1	0	0.565795	-5.345245	0.000000
23	1	0	-4.166343	-1.486490	0.000000
24	1	0	1.187871	-2.945308	0.000000
25	6	0	1.674758	4.206323	0.000000
26	1	0	1.028299	5.077920	0.000000
27	6	0	3.344966	1.964298	0.000000
28	1	0	3.991832	1.092874	0.000000
29	6	0	3.045540	4.361512	0.000000
30	1	0	3.478127	5.355612	0.000000
31	6	0	3.889078	3.231095	0.000000
32	1	0	4.965198	3.361162	0.000000



DiN[2,3-*a*,*f*]

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.342219	2.663140	0.000000
2	6	0	-2.207282	1.491344	0.000000
3	6	0	-1.364984	0.300364	0.000000
4	6	0	0.000000	0.783884	0.000000
5	6	0	-0.037009	2.239088	0.000000
6	6	0	1.335312	0.402137	0.000000
7	6	0	2.147896	1.654673	0.000000
8	6	0	1.306828	2.759993	0.000000
9	1	0	1.603313	3.798557	0.000000
10	6	0	3.560699	1.563564	0.000000
11	1	0	4.161192	2.467895	0.000000
12	6	0	4.182532	0.328079	0.000000
13	6	0	3.382288	-0.902514	0.000000
14	6	0	1.996454	-0.843605	0.000000
15	1	0	1.425834	-1.766123	0.000000
16	6	0	-3.571871	1.403470	0.000000
17	1	0	-4.190264	2.296059	0.000000
18	6	0	-1.953279	-0.935213	0.000000
19	6	0	-4.203558	0.118530	0.000000
20	6	0	-3.384052	-1.056841	0.000000
21	1	0	-1.699421	3.686135	0.000000
22	1	0	-1.359198	-1.842621	0.000000
23	6	0	5.616541	0.205994	0.000000
24	1	0	6.205837	1.117196	0.000000
25	6	0	4.082027	-2.158194	0.000000
26	1	0	3.494632	-3.070571	0.000000
27	6	0	6.225179	-1.010271	0.000000
28	1	0	7.306886	-1.081167	0.000000
29	6	0	5.442051	-2.214128	0.000000
30	1	0	5.947200	-3.173534	0.000000
31	6	0	-5.607146	-0.017329	0.000000
32	1	0	-6.219381	0.878915	0.000000
33	6	0	-4.021209	-2.315256	0.000000
34	1	0	-3.409840	-3.211730	0.000000
35	6	0	-6.203088	-1.265546	0.000000
36	1	0	-7.283140	-1.354659	0.000000
37	6	0	-5.401465	-2.419640	0.000000
38	1	0	-5.867517	-3.398693	0.000000

Open-shell singlet

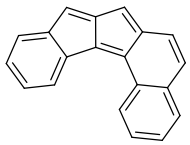
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.336037	2.727569
2	6	0	0.000000	2.192373	1.584939
3	6	0	0.000000	1.360705	0.375499

4	6	0	0.000000	0.000000	0.826242
5	6	0	0.000000	0.000000	2.249855
6	6	0	0.000000	-1.360705	0.375499
7	6	0	0.000000	-2.192373	1.584939
8	6	0	0.000000	-1.336037	2.727569
9	1	0	0.000000	-1.663304	3.758273
10	6	0	0.000000	-3.572749	1.484740
11	1	0	0.000000	-4.192872	2.375844
12	6	0	0.000000	-4.194779	0.210505
13	6	0	0.000000	-3.378716	-0.976920
14	6	0	0.000000	-1.960201	-0.864537
15	1	0	0.000000	-1.367401	-1.773096
16	6	0	0.000000	3.572749	1.484740
17	1	0	0.000000	4.192872	2.375844
18	6	0	0.000000	1.960201	-0.864537
19	6	0	0.000000	4.194779	0.210505
20	6	0	0.000000	3.378716	-0.976920
21	1	0	0.000000	1.663304	3.758273
22	1	0	0.000000	1.367401	-1.773096
23	6	0	0.000000	-5.605744	0.069094
24	1	0	0.000000	-6.217988	0.965157
25	6	0	0.000000	-4.023253	-2.238285
26	1	0	0.000000	-3.412291	-3.135168
27	6	0	0.000000	-6.197930	-1.174323
28	1	0	0.000000	-7.278267	-1.262802
29	6	0	0.000000	-5.397969	-2.338574
30	1	0	0.000000	-5.869691	-3.314734
31	6	0	0.000000	5.605744	0.069094
32	1	0	0.000000	6.217988	0.965157
33	6	0	0.000000	4.023253	-2.238285
34	1	0	0.000000	3.412291	-3.135168
35	6	0	0.000000	6.197930	-1.174323
36	1	0	0.000000	7.278267	-1.262802
37	6	0	0.000000	5.397969	-2.338574
38	1	0	0.000000	5.869691	-3.314734

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.329197	2.751287
2	6	0	0.000000	2.190837	1.593729
3	6	0	0.000000	1.360025	0.387944
4	6	0	0.000000	0.000000	0.839907
5	6	0	0.000000	0.000000	2.289070
6	6	0	0.000000	-1.360025	0.387944
7	6	0	0.000000	-2.190837	1.593729
8	6	0	0.000000	-1.329197	2.751287
9	1	0	0.000000	-1.665948	3.778306
10	6	0	0.000000	-3.561697	1.485732
11	1	0	0.000000	-4.189182	2.371548
12	6	0	0.000000	-4.181993	0.200480
13	6	0	0.000000	-3.366765	-0.981593
14	6	0	0.000000	-1.945607	-0.857176
15	1	0	0.000000	-1.343870	-1.759886
16	6	0	0.000000	3.561697	1.485732

17	1	0	0.000000	4.189182	2.371548
18	6	0	0.000000	1.945607	-0.857176
19	6	0	0.000000	4.181993	0.200480
20	6	0	0.000000	3.366765	-0.981593
21	1	0	0.000000	1.665948	3.778306
22	1	0	0.000000	1.343870	-1.759886
23	6	0	0.000000	-5.588541	0.053985
24	1	0	0.000000	-6.205710	0.946592
25	6	0	0.000000	-4.000715	-2.245988
26	1	0	0.000000	-3.383708	-3.138816
27	6	0	0.000000	-6.176523	-1.194703
28	1	0	0.000000	-7.256819	-1.285491
29	6	0	0.000000	-5.376325	-2.354779
30	1	0	0.000000	-5.844050	-3.332690
31	6	0	0.000000	5.588541	0.053985
32	1	0	0.000000	6.205710	0.946592
33	6	0	0.000000	4.000715	-2.245988
34	1	0	0.000000	3.383708	-3.138816
35	6	0	0.000000	6.176523	-1.194703
36	1	0	0.000000	7.256819	-1.285491
37	6	0	0.000000	5.376325	-2.354779
38	1	0	0.000000	5.844050	-3.332690



B[*a*]N[2,1-*f*]

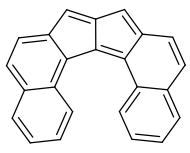
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.595993	1.913187	0.000905
2	6	0	3.067133	0.524321	0.000518
3	6	0	1.929723	-0.350028	-0.000284
4	6	0	0.739875	0.524131	-0.000171
5	6	0	1.236339	1.901306	0.000300
6	6	0	-0.638725	0.585432	-0.000072
7	6	0	-1.014138	2.039837	-0.000049
8	6	0	0.113883	2.814620	0.000289
9	1	0	0.156483	3.894215	0.000314
10	6	0	-2.392990	2.431171	-0.000534
11	1	0	-2.643283	3.486644	-0.000682
12	6	0	-3.361813	1.487804	-0.000894
13	1	0	-4.407861	1.775393	-0.001340
14	6	0	-3.059262	0.064852	-0.000467
15	6	0	-1.710076	-0.399852	0.000158
16	6	0	4.360383	0.034446	0.000624
17	1	0	5.206847	0.713156	0.001268
18	6	0	2.153947	-1.717115	-0.001339
19	6	0	4.564999	-1.356906	-0.000199
20	1	0	5.572098	-1.756888	-0.000094
21	6	0	3.474536	-2.212210	-0.001236
22	1	0	3.632202	-3.285005	-0.002008

23	1	0	3.245771	2.779646	0.001519
24	1	0	1.342078	-2.430555	-0.002420
25	6	0	-1.485218	-1.784738	0.001176
26	1	0	-0.471090	-2.151891	0.002103
27	6	0	-4.104404	-0.870416	-0.000425
28	1	0	-5.127816	-0.509765	-0.000966
29	6	0	-2.534554	-2.695376	0.001281
30	1	0	-2.325994	-3.759079	0.002094
31	6	0	-3.852719	-2.236916	0.000385
32	1	0	-4.676893	-2.941180	0.000415

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.678530	1.900486	0.077841
2	6	0	-3.088734	0.520798	0.039982
3	6	0	-1.919269	-0.335369	-0.009723
4	6	0	-0.770595	0.536597	0.021295
5	6	0	-1.280057	1.916692	0.053928
6	6	0	0.666857	0.602716	0.008890
7	6	0	1.001632	1.997996	-0.006856
8	6	0	-0.203004	2.798855	0.031005
9	1	0	-0.232009	3.879427	0.034210
10	6	0	2.335641	2.428168	-0.061180
11	1	0	2.564298	3.488123	-0.082590
12	6	0	3.348280	1.493038	-0.092243
13	1	0	4.383583	1.813488	-0.142203
14	6	0	3.074516	0.098844	-0.046836
15	6	0	1.714612	-0.369756	0.021163
16	6	0	-4.369885	-0.031459	0.029100
17	1	0	-5.242490	0.611397	0.070851
18	6	0	-2.104896	-1.720024	-0.098754
19	6	0	-4.516971	-1.416429	-0.043972
20	1	0	-5.509741	-1.852210	-0.054302
21	6	0	-3.394707	-2.251059	-0.113475
22	1	0	-3.528064	-3.324402	-0.182657
23	1	0	-3.344937	2.750876	0.107851
24	1	0	-1.266315	-2.397557	-0.172657
25	6	0	1.507671	-1.767150	0.117808
26	1	0	0.501470	-2.142939	0.214182
27	6	0	4.134235	-0.842231	-0.052248
28	1	0	5.152949	-0.472949	-0.111020
29	6	0	2.560617	-2.655670	0.117980
30	1	0	2.365465	-3.719357	0.197211
31	6	0	3.889983	-2.193870	0.023169
32	1	0	4.711413	-2.900931	0.019892



DiN[1,2-*a*:2,1-*f*]

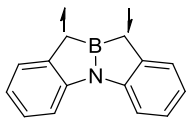
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.163880	-3.112239	-0.253621
2	6	0	2.081189	-1.969354	-0.339858
3	6	0	1.368142	-0.782962	-0.050666
4	6	0	-0.046433	-1.179739	0.102374
5	6	0	-0.070400	-2.643038	0.074042
6	6	0	-1.362508	-0.763209	0.096075
7	6	0	-2.217882	-1.983623	0.290638
8	6	0	-1.435185	-3.103668	0.243661
9	1	0	-1.762500	-4.127542	0.355173
10	6	0	-3.625460	-1.842629	0.522120
11	1	0	-4.218637	-2.725480	0.735107
12	6	0	-4.194791	-0.615750	0.484222
13	1	0	-5.255529	-0.495785	0.676854
14	6	0	-3.444324	0.570964	0.099213
15	6	0	-2.042333	0.500059	-0.155939
16	6	0	3.458012	-1.961803	-0.598862
17	1	0	3.971555	-2.883366	-0.851464
18	6	0	2.088668	0.413911	0.177379
19	6	0	4.151228	-0.768745	-0.526339
20	1	0	5.213522	-0.737427	-0.742196
21	6	0	3.503770	0.419835	-0.115121
22	1	0	1.447711	-4.140740	-0.439975
23	6	0	-1.405902	1.619494	-0.714888
24	1	0	-0.365936	1.549134	-1.001410
25	6	0	-4.112435	1.786484	-0.107198
26	1	0	-5.174640	1.842996	0.106900
27	6	0	-2.093732	2.806505	-0.938245
28	1	0	-1.577762	3.654016	-1.374480
29	6	0	-3.447226	2.898995	-0.609041
30	1	0	-3.986011	3.826147	-0.769049
31	6	0	4.236178	1.624978	0.072741
32	1	0	5.292624	1.630535	-0.175045
33	6	0	3.638943	2.748465	0.584410
34	1	0	4.215864	3.654369	0.732537
35	6	0	2.270437	2.717155	0.953898
36	1	0	1.817759	3.591238	1.408588
37	6	0	1.520724	1.585858	0.753852
38	1	0	0.486620	1.566235	1.069385

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.327728	-1.276846	3.138759
2	6	0	-0.463058	-2.113983	1.977534
3	6	0	-0.168488	-1.357803	0.784968
4	6	0	0.000000	0.000000	1.204046
5	6	0	0.000000	0.000000	2.684455
6	6	0	0.168488	1.357803	0.784968
7	6	0	0.463058	2.113983	1.977534
8	6	0	0.327728	1.276846	3.138759
9	1	0	0.456205	1.601671	4.161564

10	6	0	0.815396	3.474037	1.900997
11	1	0	1.082854	4.016466	2.801263
12	6	0	0.816442	4.105456	0.678544
13	1	0	1.102001	5.149668	0.605848
14	6	0	0.383066	3.439912	-0.506871
15	6	0	0.000000	2.055738	-0.455253
16	6	0	-0.815396	-3.474037	1.900997
17	1	0	-1.082854	-4.016466	2.801263
18	6	0	0.000000	-2.055738	-0.455253
19	6	0	-0.816442	-4.105456	0.678544
20	1	0	-1.102001	-5.149668	0.605848
21	6	0	-0.383066	-3.439912	-0.506871
22	1	0	-0.456205	-1.601671	4.161564
23	6	0	-0.607931	1.496226	-1.603885
24	1	0	-1.001061	0.490603	-1.556823
25	6	0	0.254826	4.148633	-1.724293
26	1	0	0.569566	5.186692	-1.755996
27	6	0	-0.746755	2.223861	-2.768658
28	1	0	-1.225295	1.770289	-3.629519
29	6	0	-0.288002	3.553366	-2.842861
30	1	0	-0.389717	4.112659	-3.765736
31	6	0	-0.254826	-4.148633	-1.724293
32	1	0	-0.569566	-5.186692	-1.755996
33	6	0	0.288002	-3.553366	-2.842861
34	1	0	0.389717	-4.112659	-3.765736
35	6	0	0.746755	-2.223861	-2.768658
36	1	0	1.225295	-1.770289	-3.629519
37	6	0	0.607931	-1.496226	-1.603885
38	1	0	1.001061	-0.490603	-1.556823



4b,9a-NB

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.456362	2.095673
2	6	0	0.000000	2.195337	0.872536
3	6	0	0.000000	1.291451	-0.257735
4	6	0	0.000000	-1.291451	-0.257735
5	6	0	0.000000	-2.195337	0.872536
6	6	0	0.000000	-1.456362	2.095673
7	1	0	0.000000	-1.957800	3.056214
8	6	0	0.000000	-3.580874	0.642534
9	1	0	0.000000	-4.265251	1.484209
10	6	0	0.000000	-4.063848	-0.661900
11	1	0	0.000000	-5.131143	-0.847916
12	6	0	0.000000	-3.171753	-1.741489
13	1	0	0.000000	-3.563720	-2.752690
14	6	0	0.000000	-1.782916	-1.556231
15	1	0	0.000000	-1.122153	-2.412895
16	6	0	0.000000	3.580874	0.642534

17	1	0	0.000000	4.265251	1.484209
18	6	0	0.000000	1.782916	-1.556231
19	6	0	0.000000	4.063848	-0.661900
20	1	0	0.000000	5.131143	-0.847916
21	6	0	0.000000	3.171753	-1.741489
22	1	0	0.000000	3.563720	-2.752690
23	1	0	0.000000	1.957800	3.056214
24	1	0	0.000000	1.122153	-2.412895
25	5	0	0.000000	0.000000	1.714841
26	7	0	0.000000	0.000000	0.235897

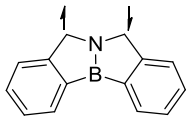
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.466990	2.099146
2	6	0	0.000000	2.199721	0.874105
3	6	0	0.000000	1.293597	-0.254002
4	6	0	0.000000	-1.293597	-0.254002
5	6	0	0.000000	-2.199721	0.874105
6	6	0	0.000000	-1.466990	2.099146
7	1	0	0.000000	-1.968887	3.059116
8	6	0	0.000000	-3.585394	0.638394
9	1	0	0.000000	-4.272620	1.477736
10	6	0	0.000000	-4.064024	-0.667475
11	1	0	0.000000	-5.130842	-0.856462
12	6	0	0.000000	-3.168985	-1.744729
13	1	0	0.000000	-3.557225	-2.757321
14	6	0	0.000000	-1.780211	-1.553434
15	1	0	0.000000	-1.116384	-2.407749
16	6	0	0.000000	3.585394	0.638394
17	1	0	0.000000	4.272620	1.477736
18	6	0	0.000000	1.780211	-1.553434
19	6	0	0.000000	4.064024	-0.667475
20	1	0	0.000000	5.130842	-0.856462
21	6	0	0.000000	3.168985	-1.744729
22	1	0	0.000000	3.557225	-2.757321
23	1	0	0.000000	1.968887	3.059116
24	1	0	0.000000	1.116384	-2.407749
25	5	0	0.000000	0.000000	1.715549
26	7	0	0.000000	0.000000	0.241080

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.496284	2.104072
2	6	0	0.000000	2.203861	0.885848
3	6	0	0.000000	1.293992	-0.250339
4	6	0	0.000000	-1.293992	-0.250339
5	6	0	0.000000	-2.203861	0.885848
6	6	0	0.000000	-1.496284	2.104072
7	1	0	0.000000	-1.995444	3.064145
8	6	0	0.000000	-3.599014	0.631514
9	1	0	0.000000	-4.291696	1.466122

10	6	0	0.000000	-4.063609	-0.670751
11	1	0	0.000000	-5.129282	-0.867669
12	6	0	0.000000	-3.160710	-1.751824
13	1	0	0.000000	-3.545942	-2.765250
14	6	0	0.000000	-1.775848	-1.552281
15	1	0	0.000000	-1.107211	-2.402811
16	6	0	0.000000	3.599014	0.631514
17	1	0	0.000000	4.291696	1.466122
18	6	0	0.000000	1.775848	-1.552281
19	6	0	0.000000	4.063609	-0.670751
20	1	0	0.000000	5.129282	-0.867669
21	6	0	0.000000	3.160710	-1.751824
22	1	0	0.000000	3.545942	-2.765250
23	1	0	0.000000	1.995444	3.064145
24	1	0	0.000000	1.107211	-2.402811
25	5	0	0.000000	0.000000	1.716088
26	7	0	0.000000	0.000000	0.239375



9a,4b-NB

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.276987	1.827272
2	6	0	0.000000	-2.196833	0.792540
3	6	0	0.000000	-1.488357	-0.505847
4	6	0	0.000000	1.488357	-0.505847
5	6	0	0.000000	2.196833	0.792540
6	6	0	0.000000	1.276987	1.827272
7	1	0	0.000000	1.451801	2.894904
8	6	0	0.000000	3.620017	0.860305
9	1	0	0.000000	4.118873	1.824205
10	6	0	0.000000	4.339915	-0.304542
11	1	0	0.000000	5.423218	-0.281105
12	6	0	0.000000	3.668903	-1.565510
13	1	0	0.000000	4.267803	-2.470427
14	6	0	0.000000	2.290691	-1.663907
15	1	0	0.000000	1.826950	-2.644881
16	6	0	0.000000	-3.620017	0.860305
17	1	0	0.000000	-4.118873	1.824205
18	6	0	0.000000	-2.290691	-1.663907
19	6	0	0.000000	-4.339915	-0.304542
20	1	0	0.000000	-5.423218	-0.281105
21	6	0	0.000000	-3.668903	-1.565510
22	1	0	0.000000	-4.267803	-2.470427
23	1	0	0.000000	-1.451801	2.894904
24	1	0	0.000000	-1.826950	-2.644881
25	7	0	0.000000	0.000000	1.276634
26	5	0	0.000000	0.000000	-0.173115

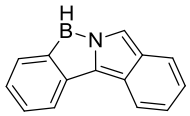
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.271867	1.886411
2	6	0	0.000000	-2.197531	0.787450
3	6	0	0.000000	-1.495636	-0.473082
4	6	0	0.000000	1.495636	-0.473082
5	6	0	0.000000	2.197531	0.787450
6	6	0	0.000000	1.271867	1.886411
7	1	0	0.000000	1.492668	2.944211
8	6	0	0.000000	3.596942	0.819356
9	1	0	0.000000	4.130898	1.763821
10	6	0	0.000000	4.300304	-0.385285
11	1	0	0.000000	5.384794	-0.368556
12	6	0	0.000000	3.631253	-1.614514
13	1	0	0.000000	4.200650	-2.536800
14	6	0	0.000000	2.231873	-1.654345
15	1	0	0.000000	1.725076	-2.614079
16	6	0	0.000000	-3.596942	0.819356
17	1	0	0.000000	-4.130898	1.763821
18	6	0	0.000000	-2.231873	-1.654345
19	6	0	0.000000	-4.300304	-0.385285
20	1	0	0.000000	-5.384794	-0.368556
21	6	0	0.000000	-3.631253	-1.614514
22	1	0	0.000000	-4.200650	-2.536800
23	1	0	0.000000	-1.492668	2.944211
24	1	0	0.000000	-1.725076	-2.614079
25	7	0	0.000000	0.000000	1.393827
26	5	0	0.000000	0.000000	-0.105173

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.271363	1.866127
2	6	0	0.000000	-2.199122	0.782495
3	6	0	0.000000	-1.500594	-0.484290
4	6	0	0.000000	1.500594	-0.484290
5	6	0	0.000000	2.199122	0.782495
6	6	0	0.000000	1.271363	1.866127
7	1	0	0.000000	1.476194	2.927672
8	6	0	0.000000	3.602995	0.833181
9	1	0	0.000000	4.121405	1.786541
10	6	0	0.000000	4.318696	-0.356513
11	1	0	0.000000	5.402674	-0.332294
12	6	0	0.000000	3.653707	-1.594295
13	1	0	0.000000	4.234081	-2.510295
14	6	0	0.000000	2.259566	-1.655946
15	1	0	0.000000	1.768968	-2.623932
16	6	0	0.000000	-3.602995	0.833181
17	1	0	0.000000	-4.121405	1.786541
18	6	0	0.000000	-2.259566	-1.655946
19	6	0	0.000000	-4.318696	-0.356513
20	1	0	0.000000	-5.402674	-0.332294
21	6	0	0.000000	-3.653707	-1.594295

22	1	0	0.000000	-4.234081	-2.510295
23	1	0	0.000000	-1.476194	2.927672
24	1	0	0.000000	-1.768968	-2.623932
25	7	0	0.000000	0.000000	1.352934
26	5	0	0.000000	0.000000	-0.131007



9a,9-NB

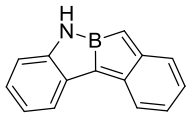
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.246524	0.816161	0.000000
2	6	0	1.382151	-0.323067	0.000000
3	6	0	-1.318634	-0.301032	0.000000
4	6	0	-2.155455	0.898807	0.000000
5	6	0	-1.310339	1.997640	0.000000
6	1	0	-1.527244	3.053767	0.000000
7	6	0	-3.573761	0.773714	0.000000
8	1	0	-4.200304	1.658988	0.000000
9	6	0	-4.125692	-0.477794	0.000000
10	1	0	-5.203458	-0.594127	0.000000
11	6	0	-3.305779	-1.653818	0.000000
12	1	0	-3.790918	-2.623656	0.000000
13	6	0	-1.938172	-1.581878	0.000000
14	1	0	-1.339334	-2.485000	0.000000
15	6	0	3.625418	0.631384	0.000000
16	1	0	4.291832	1.488122	0.000000
17	6	0	1.910343	-1.609991	0.000000
18	6	0	4.157186	-0.664158	0.000000
19	1	0	5.230632	-0.813431	0.000000
20	6	0	3.302236	-1.765726	0.000000
21	1	0	3.721788	-2.766096	0.000000
22	1	0	1.575268	3.233430	0.000000
23	1	0	1.268283	-2.483112	0.000000
24	6	0	0.000000	0.136195	0.000000
25	7	0	-0.013996	1.529899	0.000000
26	5	0	1.339054	2.072642	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.052693	1.239733	0.000000
2	6	0	1.397704	-0.049867	0.000000
3	6	0	-1.255847	-0.540455	0.000000
4	6	0	-2.279616	0.467128	0.000000
5	6	0	-1.635139	1.742200	0.000000
6	1	0	-2.069895	2.729238	0.000000
7	6	0	-3.624679	0.098217	0.000000
8	1	0	-4.407688	0.847865	0.000000

9	6	0	-3.947727	-1.266528	0.000000
10	1	0	-4.989715	-1.565725	0.000000
11	6	0	-2.954141	-2.243989	0.000000
12	1	0	-3.231441	-3.291451	0.000000
13	6	0	-1.594436	-1.887612	0.000000
14	1	0	-0.831681	-2.656812	0.000000
15	6	0	3.449964	1.266358	0.000000
16	1	0	3.976353	2.215360	0.000000
17	6	0	2.139870	-1.246353	0.000000
18	6	0	4.175574	0.076499	0.000000
19	1	0	5.259733	0.106984	0.000000
20	6	0	3.522891	-1.173062	0.000000
21	1	0	4.111649	-2.083241	0.000000
22	1	0	0.988702	3.513718	0.000000
23	1	0	1.644479	-2.210671	0.000000
24	6	0	0.000000	0.160467	0.000000
25	7	0	-0.272897	1.556140	0.000000
26	5	0	0.955423	2.329068	0.000000



9,9a-NB

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.281996	-0.330903	0.000000
2	6	0	-1.013419	-0.989450	0.000000
3	6	0	1.329923	0.328423	0.000000
4	6	0	1.513789	1.848414	0.000000
5	6	0	0.338445	2.544115	0.000000
6	1	0	0.301589	3.625910	0.000000
7	6	0	2.870981	2.361188	0.000000
8	1	0	3.027216	3.434801	0.000000
9	6	0	3.919634	1.507020	0.000000
10	1	0	4.933429	1.892849	0.000000
11	6	0	3.738839	0.058607	0.000000
12	1	0	4.625146	-0.566375	0.000000
13	6	0	2.507883	-0.506514	0.000000
14	1	0	2.394529	-1.584863	0.000000
15	6	0	-3.465629	-1.039016	0.000000
16	1	0	-4.424270	-0.531181	0.000000
17	6	0	-0.983693	-2.381729	0.000000
18	6	0	-3.405836	-2.445500	0.000000
19	1	0	-4.328654	-3.014362	0.000000
20	6	0	-2.183988	-3.107428	0.000000
21	1	0	-2.157179	-4.190936	0.000000
22	1	0	-2.951851	1.677907	0.000000
23	1	0	-0.035046	-2.906643	0.000000
24	5	0	-0.759125	1.423868	0.000000
25	6	0	0.000000	0.049058	0.000000
26	7	0	-2.128410	1.095120	0.000000

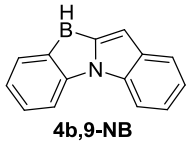
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.231455	0.650818	0.000000
2	6	0	-1.314808	-0.464802	0.000000
3	6	0	1.389314	-0.239527	0.000000
4	6	0	2.144865	1.023107	0.000000
5	6	0	1.296263	2.175231	0.000000
6	1	0	1.713885	3.175418	0.000000
7	6	0	3.551862	0.975346	0.000000
8	1	0	4.123000	1.897814	0.000000
9	6	0	4.205673	-0.253470	0.000000
10	1	0	5.289426	-0.286269	0.000000
11	6	0	3.478876	-1.459518	0.000000
12	1	0	4.013785	-2.402631	0.000000
13	6	0	2.083730	-1.456397	0.000000
14	1	0	1.539976	-2.394373	0.000000
15	6	0	-3.603031	0.451735	0.000000
16	1	0	-4.289931	1.291427	0.000000
17	6	0	-1.842007	-1.768773	0.000000
18	6	0	-4.089790	-0.861976	0.000000
19	1	0	-5.161158	-1.028446	0.000000
20	6	0	-3.220269	-1.959976	0.000000
21	1	0	-3.626783	-2.964663	0.000000
22	1	0	-2.059819	2.743879	0.000000
23	1	0	-1.173999	-2.622685	0.000000
24	5	0	-0.135811	1.618397	0.000000
25	6	0	0.000000	0.077917	0.000000
26	7	0	-1.540665	1.880036	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.215957	0.708932	0.000000
2	6	0	-1.324689	-0.428419	0.000000
3	6	0	1.387030	-0.273027	0.000000
4	6	0	2.170209	0.963333	0.000000
5	6	0	1.347591	2.141445	0.000000
6	1	0	1.792998	3.129712	0.000000
7	6	0	3.572628	0.883075	0.000000
8	1	0	4.165535	1.791721	0.000000
9	6	0	4.196728	-0.361240	0.000000
10	1	0	5.279345	-0.420553	0.000000
11	6	0	3.441472	-1.544733	0.000000
12	1	0	3.951360	-2.501644	0.000000
13	6	0	2.046109	-1.504940	0.000000
14	1	0	1.477788	-2.428209	0.000000
15	6	0	-3.591353	0.539370	0.000000
16	1	0	-4.259632	1.393949	0.000000
17	6	0	-1.881440	-1.721268	0.000000
18	6	0	-4.107116	-0.763320	0.000000
19	1	0	-5.181987	-0.905786	0.000000
20	6	0	-3.262885	-1.881412	0.000000

21	1	0	-3.692484	-2.876418	0.000000
22	1	0	-1.996383	2.796631	0.000000
23	1	0	-1.232461	-2.589705	0.000000
24	5	0	-0.097540	1.623890	0.000000
25	6	0	0.000000	0.082949	0.000000
26	7	0	-1.498049	1.920910	0.000000



4b,9-NB

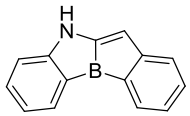
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.225258	0.907698	0.000000
2	6	0	1.327661	-0.197764	0.000000
3	6	0	-1.270448	-0.260209	0.000000
4	6	0	-2.179516	0.844833	0.000000
5	6	0	-1.392263	2.042909	0.000000
6	1	0	-1.769546	3.054880	0.000000
7	6	0	-3.561637	0.605373	0.000000
8	1	0	-4.259815	1.435173	0.000000
9	6	0	-4.017772	-0.703732	0.000000
10	1	0	-5.082302	-0.906229	0.000000
11	6	0	-3.110444	-1.779670	0.000000
12	1	0	-3.493157	-2.794080	0.000000
13	6	0	-1.735260	-1.579079	0.000000
14	1	0	-1.060803	-2.424151	0.000000
15	6	0	3.596078	0.647764	0.000000
16	1	0	4.299380	1.474078	0.000000
17	6	0	1.776661	-1.510633	0.000000
18	6	0	4.066749	-0.668257	0.000000
19	1	0	5.131622	-0.869072	0.000000
20	6	0	3.160535	-1.727855	0.000000
21	1	0	3.529641	-2.747677	0.000000
22	1	0	1.753481	3.339224	0.000000
23	1	0	1.097106	-2.351827	0.000000
24	5	0	1.383875	2.212468	0.000000
25	6	0	-0.063098	1.681358	0.000000
26	7	0	0.000000	0.272989	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.155781	1.104677	0.000000
2	6	0	1.341370	-0.073702	0.000000
3	6	0	-1.253205	-0.350018	0.000000
4	6	0	-2.249552	0.673355	0.000000
5	6	0	-1.580707	1.932172	0.000000
6	1	0	-2.049124	2.904607	0.000000
7	6	0	-3.596123	0.303481	0.000000

8	1	0	-4.373748	1.058437	0.000000
9	6	0	-3.931406	-1.063877	0.000000
10	1	0	-4.975463	-1.354848	0.000000
11	6	0	-2.948728	-2.039619	0.000000
12	1	0	-3.221192	-3.087743	0.000000
13	6	0	-1.572941	-1.685223	0.000000
14	1	0	-0.821306	-2.461602	0.000000
15	6	0	3.536892	0.911302	0.000000
16	1	0	4.201672	1.768606	0.000000
17	6	0	1.862735	-1.366012	0.000000
18	6	0	4.078166	-0.381314	0.000000
19	1	0	5.154890	-0.511957	0.000000
20	6	0	3.250971	-1.510439	0.000000
21	1	0	3.685922	-2.502575	0.000000
22	1	0	1.498061	3.504420	0.000000
23	1	0	1.229854	-2.242790	0.000000
24	5	0	1.218230	2.351192	0.000000
25	6	0	-0.163373	1.702126	0.000000
26	7	0	0.000000	0.318290	0.000000



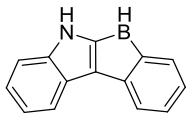
9,4b-NB

Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.110940	-0.934501	0.000000
2	6	0	1.516443	0.371598	0.000000
3	6	0	-1.490218	0.616936	0.000000
4	6	0	-2.269548	-0.587260	0.000000
5	6	0	-1.405433	-1.812796	0.000000
6	1	0	-1.819888	-2.815729	0.000000
7	6	0	-3.649247	-0.530727	0.000000
8	1	0	-4.245462	-1.437609	0.000000
9	6	0	-4.287920	0.729445	0.000000
10	1	0	-5.371751	0.775200	0.000000
11	6	0	-3.549283	1.899065	0.000000
12	1	0	-4.050636	2.860217	0.000000
13	6	0	-2.138014	1.838273	0.000000
14	1	0	-1.568045	2.762181	0.000000
15	6	0	3.495021	-1.104407	0.000000
16	1	0	3.939599	-2.093904	0.000000
17	6	0	2.369925	1.483820	0.000000
18	6	0	4.299971	0.033179	0.000000
19	1	0	5.378199	-0.086617	0.000000
20	6	0	3.752007	1.322574	0.000000
21	1	0	4.406391	2.186164	0.000000
22	1	0	1.408375	-2.940648	0.000000
23	1	0	1.945766	2.482588	0.000000
24	6	0	-0.112298	-1.426533	0.000000
25	7	0	1.160483	-1.964052	0.000000
26	5	0	0.000000	0.132903	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.145733	-0.841974	0.000000
2	6	0	1.526569	0.449908	0.000000
3	6	0	-1.490510	0.579440	0.000000
4	6	0	-2.255593	-0.678538	0.000000
5	6	0	-1.414610	-1.824434	0.000000
6	1	0	-1.770650	-2.848010	0.000000
7	6	0	-3.669204	-0.657301	0.000000
8	1	0	-4.225849	-1.589128	0.000000
9	6	0	-4.331538	0.553921	0.000000
10	1	0	-5.415315	0.580644	0.000000
11	6	0	-3.606011	1.769793	0.000000
12	1	0	-4.150042	2.708264	0.000000
13	6	0	-2.214754	1.777451	0.000000
14	1	0	-1.688858	2.726708	0.000000
15	6	0	3.519679	-1.029594	0.000000
16	1	0	3.953856	-2.024329	0.000000
17	6	0	2.387383	1.554532	0.000000
18	6	0	4.336480	0.105040	0.000000
19	1	0	5.414016	-0.012419	0.000000
20	6	0	3.773749	1.384722	0.000000
21	1	0	4.423362	2.253005	0.000000
22	1	0	1.422220	-2.857593	0.000000
23	1	0	1.974844	2.558078	0.000000
24	6	0	-0.067128	-1.351483	0.000000
25	7	0	1.174420	-1.877375	0.000000
26	5	0	0.000000	0.179503	0.000000



9,10-NB

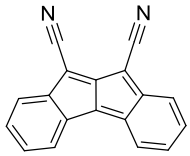
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.211039	1.006729	0.000000
2	6	0	1.434757	-0.194181	0.000000
3	6	0	-1.292733	-0.419051	0.000000
4	6	0	-2.222384	0.673807	0.000000
5	1	0	-1.907001	2.770971	0.000000
6	6	0	-3.606611	0.465899	0.000000
7	1	0	-4.300896	1.298954	0.000000
8	6	0	-4.060680	-0.842475	0.000000
9	1	0	-5.127568	-1.034536	0.000000
10	6	0	-3.163603	-1.934560	0.000000
11	1	0	-3.561191	-2.942870	0.000000
12	6	0	-1.795536	-1.736120	0.000000
13	1	0	-1.118935	-2.582549	0.000000

14	6	0	3.592645	0.917967	0.000000
15	1	0	4.199004	1.818537	0.000000
16	6	0	2.044756	-1.432037	0.000000
17	6	0	4.222279	-0.344702	0.000000
18	1	0	5.304271	-0.412273	0.000000
19	6	0	3.455548	-1.497549	0.000000
20	1	0	3.940960	-2.467599	0.000000
21	1	0	1.504678	3.393718	0.000000
22	1	0	1.464421	-2.347865	0.000000
23	6	0	-0.152972	1.558421	0.000000
24	7	0	-1.505140	1.847812	0.000000
25	5	0	1.227842	2.237624	0.000000
26	6	0	0.000000	0.174970	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.942677	1.441064	0.000000
2	6	0	1.409382	0.075012	0.000000
3	6	0	-1.177134	-0.678764	0.000000
4	6	0	-2.284716	0.220523	0.000000
5	1	0	-2.368790	2.361585	0.000000
6	6	0	-3.594216	-0.219462	0.000000
7	1	0	-4.426608	0.475097	0.000000
8	6	0	-3.815643	-1.606345	0.000000
9	1	0	-4.833374	-1.978817	0.000000
10	6	0	-2.750075	-2.507937	0.000000
11	1	0	-2.951419	-3.572671	0.000000
12	6	0	-1.428181	-2.055283	0.000000
13	1	0	-0.609381	-2.764678	0.000000
14	6	0	3.338548	1.589362	0.000000
15	1	0	3.773499	2.583606	0.000000
16	6	0	2.272396	-1.042771	0.000000
17	6	0	4.169182	0.477152	0.000000
18	1	0	5.246165	0.607695	0.000000
19	6	0	3.636816	-0.838729	0.000000
20	1	0	4.313210	-1.685865	0.000000
21	1	0	0.836497	3.660418	0.000000
22	1	0	1.870350	-2.049934	0.000000
23	6	0	-0.427553	1.544529	0.000000
24	7	0	-1.788044	1.537604	0.000000
25	5	0	0.783453	2.473111	0.000000
26	6	0	0.000000	0.140780	0.000000



Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.269454	1.266125	0.000000
2	6	0	2.187873	0.101698	0.000000
3	6	0	1.397055	-1.084597	0.000000
4	6	0	0.000000	-0.651959	0.000000
5	6	0	-0.018593	0.797196	0.000000
6	6	0	-1.304551	-1.094034	0.000000
7	6	0	-2.185626	0.106182	0.000000
8	6	0	-1.406568	1.255999	0.000000
9	6	0	-3.603490	-0.059713	0.000000
10	1	0	-4.248273	0.811371	0.000000
11	6	0	-4.116134	-1.321899	0.000000
12	1	0	-5.189966	-1.468607	0.000000
13	6	0	-3.264148	-2.489878	0.000000
14	1	0	-3.733577	-3.467031	0.000000
15	6	0	-1.905132	-2.391562	0.000000
16	1	0	-1.284184	-3.279139	0.000000
17	6	0	3.567754	0.054846	0.000000
18	1	0	4.157459	0.964790	0.000000
19	6	0	2.023312	-2.317265	0.000000
20	6	0	4.194151	-1.206715	0.000000
21	1	0	5.275599	-1.267756	0.000000
22	6	0	3.433141	-2.366336	0.000000
23	1	0	3.927385	-3.331056	0.000000
24	1	0	1.452054	-3.237988	0.000000
25	6	0	1.714240	2.610507	0.000000
26	6	0	-1.873018	2.583723	0.000000
27	7	0	2.130553	3.689481	0.000000
28	7	0	-2.275526	3.670734	0.000000

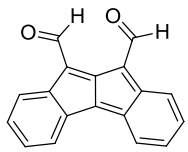
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.345145	1.266965
2	6	0	0.000000	-2.197206	0.098976
3	6	0	0.000000	-1.360730	-1.076715
4	6	0	0.000000	0.000000	-0.618332
5	6	0	0.000000	0.000000	0.797436
6	6	0	0.000000	1.360730	-1.076715
7	6	0	0.000000	2.197206	0.098976
8	6	0	0.000000	1.345145	1.266965
9	6	0	0.000000	3.588241	-0.012184
10	1	0	0.000000	4.212513	0.874166
11	6	0	0.000000	4.155363	-1.285400
12	1	0	0.000000	5.233373	-1.393151
13	6	0	0.000000	3.346397	-2.431938
14	1	0	0.000000	3.814120	-3.409809
15	6	0	0.000000	1.953462	-2.339906
16	1	0	0.000000	1.349367	-3.239306
17	6	0	0.000000	-3.588241	-0.012184
18	1	0	0.000000	-4.212513	0.874166
19	6	0	0.000000	-1.953462	-2.339906
20	6	0	0.000000	-4.155363	-1.285400
21	1	0	0.000000	-5.233373	-1.393151
22	6	0	0.000000	-3.346397	-2.431938

23	1	0	0.000000	-3.814120	-3.409809
24	1	0	0.000000	-1.349367	-3.239306
25	6	0	0.000000	-1.804567	2.594358
26	6	0	0.000000	1.804567	2.594358
27	7	0	0.000000	-2.218764	3.677978
28	7	0	0.000000	2.218764	3.677978

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.334670	1.283113
2	6	0	0.000000	2.191227	0.095223
3	6	0	0.000000	1.359557	-1.075561
4	6	0	0.000000	0.000000	-0.618831
5	6	0	0.000000	0.000000	0.826211
6	6	0	0.000000	-1.359557	-1.075561
7	6	0	0.000000	-2.191227	0.095223
8	6	0	0.000000	-1.334670	1.283113
9	6	0	0.000000	-3.574198	-0.018664
10	1	0	0.000000	-4.203772	0.863806
11	6	0	0.000000	-4.140246	-1.299753
12	1	0	0.000000	-5.218852	-1.404832
13	6	0	0.000000	-3.337037	-2.444451
14	1	0	0.000000	-3.802264	-3.423091
15	6	0	0.000000	-1.943956	-2.343138
16	1	0	0.000000	-1.332765	-3.237795
17	6	0	0.000000	3.574198	-0.018664
18	1	0	0.000000	4.203772	0.863806
19	6	0	0.000000	1.943956	-2.343138
20	6	0	0.000000	4.140246	-1.299753
21	1	0	0.000000	5.218852	-1.404832
22	6	0	0.000000	3.337037	-2.444451
23	1	0	0.000000	3.802264	-3.423091
24	1	0	0.000000	1.332765	-3.237795
25	6	0	0.000000	1.808065	2.604785
26	6	0	0.000000	-1.808065	2.604785
27	7	0	0.000000	2.240323	3.681493
28	7	0	0.000000	-2.240323	3.681493



Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.028975	1.369578	0.000000
2	6	0	-2.079211	0.310152	0.000000
3	6	0	-1.436347	-0.960956	0.000000
4	6	0	0.000000	-0.694703	0.000000
5	6	0	0.197858	0.752342	0.000000

6	6	0	1.230407	-1.307399	0.000000
7	6	0	2.256181	-0.233989	0.000000
8	6	0	1.639934	1.022589	0.000000
9	6	0	3.634210	-0.611555	0.000000
10	1	0	4.411715	0.142101	0.000000
11	6	0	3.961700	-1.936244	0.000000
12	1	0	5.005895	-2.228413	0.000000
13	6	0	2.961847	-2.977127	0.000000
14	1	0	3.290141	-4.009965	0.000000
15	6	0	1.633305	-2.680201	0.000000
16	1	0	0.887166	-3.465552	0.000000
17	6	0	-3.457374	0.403992	0.000000
18	1	0	-3.941780	1.370800	0.000000
19	6	0	-2.184377	-2.122976	0.000000
20	6	0	-4.214698	-0.788243	0.000000
21	1	0	-5.296769	-0.728838	0.000000
22	6	0	-3.591774	-2.024949	0.000000
23	1	0	-4.187860	-2.930261	0.000000
24	1	0	-1.710683	-3.097734	0.000000
25	6	0	2.330949	2.288140	0.000000
26	1	0	3.435601	2.211407	0.000000
27	8	0	1.806185	3.394538	0.000000
28	6	0	-1.289498	2.829297	0.000000
29	1	0	-0.393532	3.466834	0.000000
30	8	0	-2.416774	3.285854	0.000000

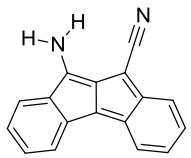
Open-shell singlet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.052712	-1.387040	0.000000
2	6	0	2.068705	-0.320021	0.000000
3	6	0	1.408466	0.955811	0.000000
4	6	0	0.000000	0.687635	0.000000
5	6	0	-0.196209	-0.766459	0.000000
6	6	0	-1.260746	1.313056	0.000000
7	6	0	-2.258907	0.255589	0.000000
8	6	0	-1.605461	-1.030778	0.000000
9	6	0	-3.620985	0.598897	0.000000
10	1	0	-4.389639	-0.164189	0.000000
11	6	0	-3.980528	1.939245	0.000000
12	1	0	-5.030531	2.208567	0.000000
13	6	0	-3.008046	2.966624	0.000000
14	1	0	-3.331226	4.000996	0.000000
15	6	0	-1.658309	2.665585	0.000000
16	1	0	-0.918657	3.457122	0.000000
17	6	0	3.456097	-0.388160	0.000000
18	1	0	3.953335	-1.348286	0.000000
19	6	0	2.152515	2.135427	0.000000
20	6	0	4.188343	0.809360	0.000000
21	1	0	5.271481	0.767747	0.000000
22	6	0	3.548412	2.051090	0.000000
23	1	0	4.139963	2.959278	0.000000
24	1	0	1.665085	3.103273	0.000000
25	6	0	-2.299932	-2.299519	0.000000
26	1	0	-3.404250	-2.226695	0.000000

27	8	0	-1.770267	-3.402393	0.000000
28	6	0	1.338668	-2.829174	0.000000
29	1	0	0.457073	-3.485678	0.000000
30	8	0	2.475091	-3.274501	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.064789	-1.405664	0.000000
2	6	0	2.069656	-0.337086	0.000000
3	6	0	1.403574	0.936675	0.000000
4	6	0	0.000000	0.665327	0.000000
5	6	0	-0.202087	-0.767976	0.000000
6	6	0	-1.275451	1.319439	0.000000
7	6	0	-2.267789	0.282233	0.000000
8	6	0	-1.597374	-1.024981	0.000000
9	6	0	-3.617866	0.618692	0.000000
10	1	0	-4.388953	-0.142258	0.000000
11	6	0	-3.981280	1.971297	0.000000
12	1	0	-5.031478	2.239271	0.000000
13	6	0	-3.013815	2.979923	0.000000
14	1	0	-3.323197	4.018498	0.000000
15	6	0	-1.653940	2.662525	0.000000
16	1	0	-0.910358	3.450462	0.000000
17	6	0	3.460123	-0.394838	0.000000
18	1	0	3.962778	-1.352107	0.000000
19	6	0	2.141444	2.123337	0.000000
20	6	0	4.181215	0.805199	0.000000
21	1	0	5.264751	0.771942	0.000000
22	6	0	3.533669	2.046434	0.000000
23	1	0	4.121983	2.956714	0.000000
24	1	0	1.647050	3.087575	0.000000
25	6	0	-2.300197	-2.293033	0.000000
26	1	0	-3.403963	-2.217662	0.000000
27	8	0	-1.771317	-3.395253	0.000000
28	6	0	1.354190	-2.836639	0.000000
29	1	0	0.477840	-3.499734	0.000000
30	8	0	2.495114	-3.281984	0.000000



Closed-shell

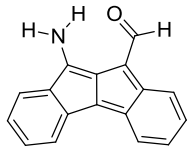
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.493469	1.249692	0.000000
2	6	0	2.270875	-0.013614	0.000000
3	6	0	1.338127	-1.095400	0.000000
4	6	0	0.000000	-0.505623	0.000000

5	6	0	0.135439	0.908736	0.000000
6	6	0	-1.366921	-0.807614	0.000000
7	6	0	-2.093054	0.466345	0.000000
8	6	0	-1.157212	1.525951	0.000000
9	6	0	-3.508859	0.469257	0.000000
10	1	0	-4.050992	1.408407	0.000000
11	6	0	-4.176902	-0.730639	0.000000
12	1	0	-5.260968	-0.743026	0.000000
13	6	0	-3.474144	-1.973648	0.000000
14	1	0	-4.044721	-2.895714	0.000000
15	6	0	-2.102241	-2.021660	0.000000
16	1	0	-1.585152	-2.974427	0.000000
17	6	0	3.634779	-0.230046	0.000000
18	1	0	4.343343	0.592894	0.000000
19	6	0	1.817369	-2.395543	0.000000
20	6	0	4.109047	-1.554297	0.000000
21	1	0	5.174900	-1.746154	0.000000
22	6	0	3.207925	-2.611840	0.000000
23	1	0	3.582737	-3.629418	0.000000
24	1	0	1.138912	-3.240073	0.000000
25	6	0	-1.383536	2.912362	0.000000
26	7	0	-1.487454	4.069906	0.000000
27	7	0	2.026878	2.469465	0.000000
28	1	0	1.436291	3.290030	0.000000
29	1	0	3.024711	2.607356	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.263075	1.548522	-0.003010
2	6	0	2.226355	0.460978	-0.002444
3	6	0	1.514197	-0.795216	0.001111
4	6	0	0.120150	-0.478590	-0.006224
5	6	0	-0.020125	0.957687	-0.010221
6	6	0	-1.196235	-1.065691	-0.003317
7	6	0	-2.135945	0.017961	-0.004462
8	6	0	-1.388736	1.285636	-0.007570
9	6	0	-3.498024	-0.231105	-0.001567
10	1	0	-4.212128	0.584870	-0.002031
11	6	0	-3.941253	-1.564702	0.001872
12	1	0	-5.005399	-1.770859	0.003753
13	6	0	-3.034327	-2.622195	0.002765
14	1	0	-3.399143	-3.642691	0.005247
15	6	0	-1.653696	-2.380870	0.000444
16	1	0	-0.957149	-3.211313	0.001213
17	6	0	3.620403	0.470095	-0.006107
18	1	0	4.178987	1.400300	-0.020684
19	6	0	2.222638	-1.999686	0.007772
20	6	0	4.305150	-0.746651	0.001214
21	1	0	5.389188	-0.747716	-0.001804
22	6	0	3.615661	-1.968647	0.009093
23	1	0	4.174821	-2.896831	0.013960
24	1	0	1.697907	-2.947997	0.010444
25	6	0	-1.940415	2.574236	0.002396
26	7	0	-2.372696	3.653496	0.014995

27	7	0	1.563876	2.878700	-0.044344
28	1	0	0.828785	3.552820	0.106420
29	1	0	2.492634	3.183469	0.198452



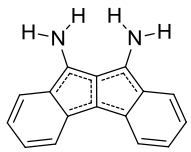
Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.399558	-1.291207	0.000000
2	6	0	2.246082	-0.071399	0.000000
3	6	0	1.371844	1.058233	0.000000
4	6	0	0.000000	0.538848	0.000000
5	6	0	0.054061	-0.866127	0.000000
6	6	0	-1.359671	0.921945	0.000000
7	6	0	-2.148149	-0.305646	0.000000
8	6	0	-1.261388	-1.430995	0.000000
9	6	0	-3.556460	-0.217711	0.000000
10	1	0	-4.165012	-1.115131	0.000000
11	6	0	-4.156406	1.024270	0.000000
12	1	0	-5.238355	1.096517	0.000000
13	6	0	-3.387538	2.218013	0.000000
14	1	0	-3.899178	3.173932	0.000000
15	6	0	-2.010875	2.176718	0.000000
16	1	0	-1.434125	3.094799	0.000000
17	6	0	3.618538	0.073764	0.000000
18	1	0	4.281170	-0.786236	0.000000
19	6	0	1.916607	2.331706	0.000000
20	6	0	4.160632	1.372400	0.000000
21	1	0	5.235130	1.508628	0.000000
22	6	0	3.316962	2.475624	0.000000
23	1	0	3.744460	3.472210	0.000000
24	1	0	1.282779	3.210224	0.000000
25	7	0	1.800709	-2.545999	0.000000
26	1	0	1.050782	-3.261590	0.000000
27	1	0	2.778281	-2.794305	0.000000
28	6	0	-1.552479	-2.821337	0.000000
29	1	0	-2.616474	-3.111800	0.000000
30	8	0	-0.691541	-3.723481	0.000000

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.296021	1.448466	-0.006055
2	6	0	-2.213872	0.321310	-0.002338
3	6	0	-1.449681	-0.906445	0.001041
4	6	0	-0.073766	-0.534544	-0.003106
5	6	0	0.010749	0.907624	-0.006200
6	6	0	1.267296	-1.065584	-0.002017

7	6	0	2.159616	0.058450	-0.003108
8	6	0	1.361460	1.305017	-0.003482
9	6	0	3.529228	-0.149628	-0.002569
10	1	0	4.223772	0.682789	-0.003241
11	6	0	4.023827	-1.466659	-0.001331
12	1	0	5.095319	-1.631249	-0.001214
13	6	0	3.159008	-2.557137	-0.000212
14	1	0	3.560924	-3.563639	0.000753
15	6	0	1.770931	-2.363933	-0.000395
16	1	0	1.103913	-3.218380	0.000487
17	6	0	-3.607948	0.273193	-0.002706
18	1	0	-4.202863	1.180687	-0.009285
19	6	0	-2.111825	-2.140580	0.006567
20	6	0	-4.241914	-0.968629	0.003061
21	1	0	-5.325032	-1.014549	0.002828
22	6	0	-3.502105	-2.164500	0.007995
23	1	0	-4.024808	-3.113776	0.012223
24	1	0	-1.549701	-3.067252	0.009096
25	6	0	1.852967	2.650069	0.007206
26	1	0	2.950078	2.775446	0.006077
27	8	0	1.133804	3.658144	0.019579
28	7	0	-1.615922	2.760580	-0.027902
29	1	0	-2.568300	3.071470	0.057716
30	1	0	-0.849976	3.430303	0.009127



Closed-shell

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.026695	-1.335519	1.537969
2	6	0	-0.000827	-2.191409	0.384812
3	6	0	-0.009435	-1.351645	-0.799893
4	6	0	0.000000	0.000000	-0.368875
5	6	0	0.000000	0.000000	1.063453
6	6	0	0.009435	1.351645	-0.799893
7	6	0	0.000827	2.191409	0.384812
8	6	0	-0.026695	1.335519	1.537969
9	6	0	0.000000	3.589503	0.283076
10	1	0	-0.002877	4.216332	1.170953
11	6	0	0.011972	4.177999	-0.971287
12	1	0	0.014654	5.256782	-1.069567
13	6	0	0.022618	3.367256	-2.129157
14	1	0	0.032123	3.846901	-3.102521
15	6	0	0.020657	1.983467	-2.059685
16	1	0	0.028127	1.394437	-2.969593
17	6	0	0.000000	-3.589503	0.283076
18	1	0	0.002877	-4.216332	1.170953
19	6	0	-0.020657	-1.983467	-2.059685
20	6	0	-0.011972	-4.177999	-0.971287
21	1	0	-0.014654	-5.256782	-1.069567

22	6	0	-0.022618	-3.367256	-2.129157
23	1	0	-0.032123	-3.846901	-3.102521
24	1	0	-0.028127	-1.394437	-2.969593
25	7	0	0.058132	-1.750810	2.839094
26	1	0	0.249898	-2.726346	3.011723
27	1	0	0.457509	-1.130054	3.526625
28	7	0	-0.058132	1.750810	2.839094
29	1	0	-0.249898	2.726346	3.011723
30	1	0	-0.457509	1.130054	3.526625

Triplet

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029680	-1.338728	1.561397
2	6	0	0.003383	-2.194704	0.388155
3	6	0	-0.005716	-1.364726	-0.789330
4	6	0	0.000000	0.000000	-0.326693
5	6	0	0.000000	0.000000	1.107871
6	6	0	0.005716	1.364726	-0.789330
7	6	0	-0.003383	2.194704	0.388155
8	6	0	-0.029680	1.338728	1.561397
9	6	0	0.000000	3.581651	0.260435
10	1	0	0.001824	4.230086	1.131212
11	6	0	0.011170	4.147407	-1.021381
12	1	0	0.017166	5.226560	-1.126764
13	6	0	0.017579	3.343776	-2.163329
14	1	0	0.026579	3.804592	-3.144241
15	6	0	0.013718	1.946710	-2.052377
16	1	0	0.016747	1.331804	-2.945235
17	6	0	0.000000	-3.581651	0.260435
18	1	0	-0.001824	-4.230086	1.131212
19	6	0	-0.013718	-1.946710	-2.052377
20	6	0	-0.011170	-4.147407	-1.021381
21	1	0	-0.017166	-5.226560	-1.126764
22	6	0	-0.017579	-3.343776	-2.163329
23	1	0	-0.026579	-3.804592	-3.144241
24	1	0	-0.016747	-1.331804	-2.945235
25	7	0	0.051363	-1.785082	2.872567
26	1	0	0.296235	-2.757114	2.998866
27	1	0	0.532347	-1.190015	3.533239
28	7	0	-0.051363	1.785082	2.872567
29	1	0	-0.296235	2.757114	2.998866
30	1	0	-0.532347	1.190015	3.533239