Energetics and Optimal Molecular Packingfor Singlet Fission in BN-doped Perylenes: Electronic Adiabatic State Basis Screening - Supporting Information

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1 Ab initio comparison

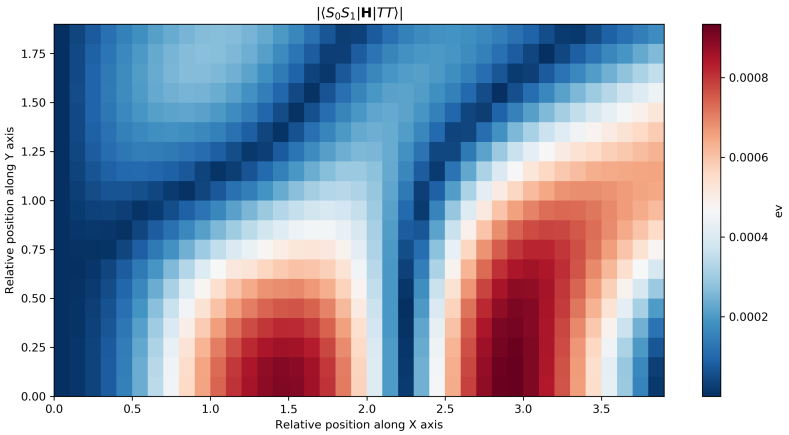

Fig. 1 $|\langle S_0 S_1|\mathbf{H}|TT\rangle|$

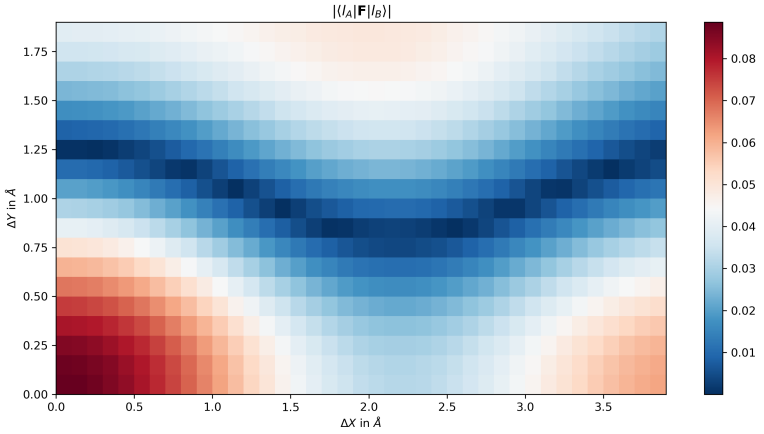

Fig. 2 $|(l_A|\mathbf{F}|l_B)|$

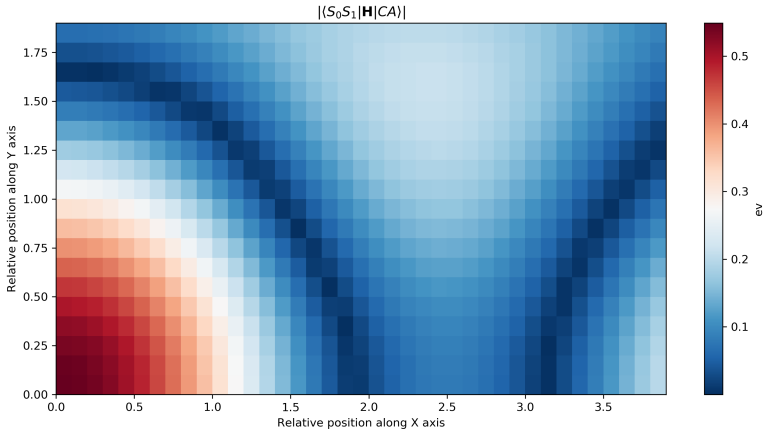

Fig. 3 $|\langle S_0S_1|\mathbf{H}|CA\rangle|$

2 Properties of the BN-doped perylene isomers and undoped perylene and Molecular Structures

Table S1: PG: point group, LS: type of Lewis structure, y_0: biradical character, f: $S_0 \rightarrow S_1$ oscillator strength, diabatic: position and value of maximum of the diabatic coupling $|T_{RP}|^2$ in a scan of the relative displacement of two cofacially stacked dimers (vertical separation $\Delta Z = 3.5$ Å).
† : $E(S_1)_{CASPT2} \geq 1.8eV$
‡ : $E(T_1)_{TD-DFT} \geq 0.8eV$
ε : $\Delta E_{ST\,(TD-DFT)} \geq -0.3eV$
γ : $\Delta E_{TT\,(CASPT2)} \geq -0.3eV$
η : $\Delta E_{TT\,(CASPT2)} \leq -0.2eV$
$*$: $\Delta E_{TT\,(TD-DFT)} \leq -0.2eV$

			CASPT2					TD-DFT					diabatic		
Molecule	PG	LS	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	y_0	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	f	ΔX (Å)	ΔY (Å)	$\lvert T_{RP}\rvert^2$ (eV^2)
BN1-0	C_s	*BN*	3.20	2.15	1.10	1.14	0.07	2.76	1.82	0.88	0.91	0.24	0.70	-0.10	7.58×10^{-05}
BN1-1 † ‡	C_s	*BN*	2.83	1.48	0.13	0.10	0.07	2.43	1.50	0.57	0.50	0.21	0.70	0.30	8.34×10^{-05}
BN1-2 † ‡	C_s	*BN*	2.64	1.58	0.53	0.44	0.06	2.33	1.29	0.25	-0.10	0.27	-0.70	0.10	5.32×10^{-05}
BN1-3	C_s	*BN*	3.13	2.05	0.96	1.02	0.07	2.71	1.78	0.86	0.84	0.25	-0.60	0.30	5.10×10^{-05}
BN1-4 † ‡	C_s	*BN*	2.66	1.57	0.49	0.44	0.06	2.33	1.30	0.26	-0.07	0.27	0.70	0.30	6.58×10^{-05}
BN1-5	C_s	*BN*	3.31	2.73	2.16	1.80	0.02	2.74	1.98	1.23	0.98	0.20	-0.70	-0.20	6.54×10^{-05}
BN1-6	C_s	*BN*	3.11	3.70	4.29	2.50	0.07	2.64	1.90	1.17	0.92	0.19	0.70	-0.20	4.91×10^{-05}
BN1-7	C_s	*B−N+*	1.62	0.80	-0.03	-1.46	0.04	1.67	0.72	-0.23	-0.73	0.17	0.60	0.30	2.77×10^{-05}
BN1-8 † ‡	C_s	*BN*	2.85	1.83	0.82	1.22	0.06	2.36	1.54	0.73	0.80	0.15	-0.70	0.10	5.22×10^{-05}
BN1-9 † ‡	C_s	*BN*	2.66	1.39	0.11	0.43	0.07	2.30	1.46	0.61	0.49	0.17	-0.60	-0.30	4.56×10^{-05}
BN1-10	C_{2v}	*BN*	3.23	1.83	0.43	1.62	0.02	2.68	1.77	0.87	1.02	0.20	0.70	-0.00	7.13×10^{-05}
BN1-11 † ‡	C_s	*BN*	2.73	1.71	0.68	1.10	0.06	2.31	1.52	0.74	0.68	0.16	-0.70	0.10	4.64×10^{-05}
BN1-12	C_{2v}	*BN*	3.19	1.81	0.43	1.59	0.02	2.65	1.74	0.84	0.99	0.21	-0.70	-0.00	5.91×10^{-05}
BN2-0	C_s	*BN*	3.47	2.73	2.00	1.72	0.06	2.87	2.12	1.37	1.24	0.19	0.70	0.20	8.14×10^{-05}
BN2-1	C_s	*BN*	3.33	2.63	1.94	1.80	0.05	2.69	1.95	1.21	1.17	0.17	0.70	-0.20	5.25×10^{-05}
BN2-2	C_s	*B−N+*	1.75	0.66	-0.42	-1.84	0.08	1.80	0.71	-0.37	-0.83	0.19	-0.70	-0.10	3.96×10^{-05}
BN2-3 † ‡	C_s	*B−N+*	2.63	1.45	0.28	0.47	0.15	2.04	1.25	0.46	0.88	0.07	-0.40	2.80	4.45×10^{-05}
BN2-4	C_s	*BN*	3.46	2.95	2.45	1.70	0.08	2.78	2.12	1.45	1.41	0.16	-0.80	-0.20	6.55×10^{-05}
BN2-5 † ‡	C_s	*BN*	2.69	1.69	0.68	0.39	0.08	2.36	1.37	0.39	0.10	0.23	-0.80	-0.30	6.82×10^{-05}
BN2-6	C_s	*BN*	3.28	2.38	1.49	1.56	0.03	2.78	1.97	1.15	1.09	0.19	2.60	0.20	1.26×10^{-05}
BN2-7 † ‡	C_s	*BN*	2.65	1.73	0.80	0.45	0.07	2.35	1.38	0.42	0.27	0.23	0.70	-0.20	5.64×10^{-05}
BN2-8 † ‡	C_s	*BN*	2.97	1.78	0.58	0.28	0.07	2.56	1.62	0.69	0.74	0.18	-0.80	-0.40	8.98×10^{-05}
BN2-9	C_{2h}	*BN*	3.42	2.54	1.66	1.79	0.03	2.92	2.02	1.13	1.43	0.21	0.60	-0.40	1.28×10^{-04}
BN2-10	C_s	*BN*	3.01	1.96	0.91	1.42	0.06	2.55	1.71	0.86	1.11	0.14	2.70	0.70	1.30×10^{-05}
BN2-11	C_s	*B−N+*	1.67	1.02	0.38	-0.04	0.04	1.57	0.79	0.01	-0.10	0.13	-0.70	-0.00	1.92×10^{-05}
BN2-12	C_s	*BN*	3.35	2.87	2.38	2.19	0.01	2.79	2.13	1.46	1.47	0.17	-0.70	0.40	7.72×10^{-05}
BN2-13	C_s	*BN*	3.36	2.30	1.24	2.05	0.08	2.72	1.88	1.04	1.18	0.15	0.70	-0.20	8.18×10^{-05}
BN2-14 † ‡	C_s	*BN*	2.81	1.68	0.55	0.19	0.08	2.37	1.54	0.71	0.44	0.14	-0.60	0.30	5.68×10^{-05}
BN2-15 † ‡	C_s	*B−N+*	2.72	2.19	1.66	1.16	0.04	2.16	1.52	0.88	0.55	0.10	0.80	-0.40	6.01×10^{-05}
BN2-16	C_s	*BN*	3.46	2.51	1.56	2.00	0.07	2.69	1.83	0.96	1.26	0.19	-0.70	-0.20	6.28×10^{-05}
BN2-17 † ‡	C_s	*BN*	2.94	3.07	3.20	2.07	0.06	2.29	1.70	1.11	0.67	0.10	-0.70	-0.00	5.14×10^{-05}
BN2-18	C_s	*BN*	3.52	2.71	1.90	1.49	0.07	2.86	2.05	1.24	1.19	0.16	0.70	-0.40	8.67×10^{-05}
BN2-19 † ‡	C_s	*BN*	2.91	1.78	0.66	0.69	0.08	2.47	1.57	0.67	0.42	0.21	0.70	-0.30	8.07×10^{-05}
BN2-20	C_s	*BN*	3.38	2.15	0.92	2.01	0.08	2.61	1.86	1.11	1.61	0.04	-0.30	3.00	2.65×10^{-05}
BN2-21	C_s	*B−N+*	1.71	0.93	0.15	-0.63	0.05	1.67	0.79	-0.10	-0.55	0.16	0.60	-0.40	2.68×10^{-05}
BN2-22	C_s	*BN*	3.09	2.66	2.23	2.47	0.07	2.65	1.91	1.17	1.46	0.19	0.80	0.30	6.64×10^{-05}
BN2-23	C_s	*BN*	3.12	1.73	0.35	0.20	0.08	2.72	1.67	0.62	0.94	0.21	-0.40	3.10	1.42×10^{-05}
BN2-24	C_{2v}	*BN*	3.34	2.86	2.37	2.80	0.02	2.89	1.97	1.05	1.58	0.04	0.70	-0.00	8.36×10^{-05}

			CASPT2					TD-DFT					diabatic		
Molecule	PG	LS	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	y_0	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	f	ΔX (Å)	ΔY (Å)	$\lvert T_{RP}\rvert^2$ (eV^2)
BN2-25	C_s	*BN*	3.24	3.11	2.98	2.40	0.06	2.65	1.89	1.12	1.16	0.17	-0.70	-0.20	5.69×10^{-05}
BN2-26 † ‡	C_s	*BN*	2.78	1.99	1.20	0.99	0.06	2.40	1.46	0.53	0.40	0.22	-0.70	-0.00	7.38×10^{-05}
BN2-27 † ‡	C_s	*BN*	2.85	1.74	0.63	0.54	0.07	2.46	1.63	0.80	0.69	0.16	0.50	-3.60	1.07×10^{-05}
BN2-28	C_s	*BN*	3.43	2.45	1.47	2.22	0.02	2.71	1.93	1.14	1.33	0.13	0.70	-0.10	8.67×10^{-05}
BN2-29 † ‡	C_s	*BN*	2.63	1.70	0.77	0.70	0.07	2.26	1.52	0.79	0.50	0.12	0.70	0.20	4.10×10^{-05}
BN2-30 † ‡	C_s	*BN*	2.86	1.85	0.83	1.24	0.06	2.40	1.64	0.88	0.79	0.14	0.80	0.10	4.30×10^{-05}
BN2-31	C_s	*BN*	3.48	2.34	1.20	2.22	0.02	2.75	1.92	1.09	1.39	0.17	0.70	-0.20	7.94×10^{-05}
BN2-32 † ‡	C_s	*BN*	2.79	1.70	0.61	1.04	0.06	2.31	1.58	0.86	0.72	0.13	0.70	-0.20	5.37×10^{-05}
BN2-33 † ‡	C_s	*BN*	2.83	1.63	0.42	0.37	0.06	2.42	1.40	0.37	0.17	0.25	-0.70	0.30	8.67×10^{-05}
BN2-34	C_s	*BN*	3.37	3.15	2.94	2.54	0.08	2.78	2.10	1.41	1.40	0.18	0.70	-0.30	8.33×10^{-05}
BN2-35	C_s	*BN*	3.31	3.68	4.06	2.91	0.07	2.82	2.14	1.46	1.47	0.17	0.70	0.10	5.71×10^{-05}
BN2-36 † ‡ ε	C_s	*B−N+*	2.02	1.50	0.98	0.44	0.05	1.80	0.96	0.12	0.27	0.14	-3.10	-0.10	8.90×10^{-06}
BN2-37 † ‡	C_s	*BN*	2.80	1.92	1.04	1.31	0.06	2.32	1.62	0.93	0.90	0.11	0.70	0.30	5.72×10^{-05}
BN2-38	C_{2v}	*BN*	3.38	2.50	1.63	1.70	0.05	2.79	1.97	1.15	1.35	0.18	-0.70	-0.00	8.81×10^{-05}
BN2-39 † ‡	C_s	*BN*	2.97	1.70	0.43	0.41	0.07	2.46	1.62	0.78	0.77	0.16	-0.70	0.40	1.20×10^{-04}
BN2-40 † ‡	C_s	*BN*	2.83	1.79	0.75	0.00	0.05	2.46	1.43	0.40	0.32	0.24	0.80	-0.00	5.66×10^{-05}
BN2-41	C_s	*BN*	3.28	2.34	1.40	1.62	0.07	2.82	1.94	1.06	1.07	0.23	0.70	0.20	5.56×10^{-05}
BN2-42 † ‡	C_s	?	2.70	1.18	-0.35	-0.32	0.08	2.29	1.29	0.29	0.00	0.23	0.70	0.20	9.82×10^{-05}
BN2-43 † ‡	C_s	*BN*	2.65	1.31	-0.04	-0.08	0.07	2.34	1.39	0.44	0.13	0.21	0.70	0.30	8.60×10^{-05}
BN2-44 † ‡	C_s	*B−N+*	2.96	1.92	0.88	0.72	0.06	2.58	1.73	0.88	0.96	0.18	0.70	0.50	1.27×10^{-04}
BN2-45	C_s	*B−N+*	3.14	1.51	-0.12	0.56	0.16	2.03	1.41	0.80	1.33	0.11	0.50	-2.70	7.58×10^{-05}
BN2-46	C_s	*B−N+*	1.55	0.49	-0.57	-1.60	0.07	1.58	0.58	-0.43	-0.75	0.17	-0.70	-0.10	4.88×10^{-05}
BN2-47 † ‡	C_s	*BN*	2.89	1.67	0.45	1.27	0.09	2.38	1.45	0.53	0.94	0.17	0.70	0.20	7.40×10^{-05}
BN2-48	C_s	*BN*	3.22	2.05	0.88	0.74	0.07	2.53	1.78	1.04	1.13	0.17	0.70	0.50	1.24×10^{-04}
BN2-49 † ‡	C_s	*BN*	2.52	1.25	-0.02	-0.06	0.06	2.20	1.21	0.23	0.12	0.23	-0.70	-0.40	1.18×10^{-04}
BN2-50 † ‡	C_s	*BN*	2.75	1.65	0.55	0.28	0.07	2.35	1.55	0.75	0.49	0.16	0.70	0.20	4.27×10^{-05}
BN2-51 † ‡ ε γ η	C_s	*BN*	2.44	1.14	-0.16	-0.23	0.06	2.16	1.17	0.18	-0.06	0.21	0.70	0.20	6.05×10^{-05}
BN2-52 † ‡	C_{2h}	*BN*	2.98	1.58	0.17	0.27	0.06	2.61	1.48	0.36	0.71	0.33	-0.70	-0.50	2.09×10^{-04}
BN2-53 † ‡	C_s	*BN*	2.56	1.55	0.53	1.11	0.07	2.35	1.54	0.73	1.00	0.06	0.70	0.40	8.18×10^{-05}
BN2-54	C_s	*B−N+*	1.40	0.58	-0.24	-1.68	0.06	1.54	0.48	-0.58	-0.89	0.14	2.80	-0.70	5.12×10^{-05}
BN2-55 † ‡	C_s	*BN*	2.72	1.86	1.00	0.47	0.05	2.38	1.72	1.05	0.71	0.13	2.70	-0.30	1.61×10^{-05}
BN2-56	C_s	*BN*	3.41	2.81	2.21	2.04	0.06	2.74	1.82	0.90	0.72	0.26	-0.70	-0.20	8.54×10^{-05}
BN2-57	C_s	*B−N+*	1.37	0.87	0.36	-1.40	0.04	1.42	0.79	0.17	-0.57	0.06	-0.80	-0.60	3.76×10^{-05}
BN2-58	C_s	*BN*	3.41	2.75	2.08	2.35	0.06	2.49	1.98	1.48	1.47	0.09	0.70	-0.30	6.84×10^{-05}
BN2-59 † ‡	C_s	*B−N+*	1.90	1.16	0.41	-0.78	0.05	1.76	0.99	0.22	-0.34	0.11	2.80	0.50	9.87×10^{-06}
BN2-60 † ‡	C_s	*B−N+*	2.58	1.24	-0.11	-0.21	0.17	2.03	1.16	0.29	0.48	0.07	0.70	0.60	1.03×10^{-04}
BN2-61	C_s	*B−N+*	1.60	0.55	-0.50	-1.53	0.07	1.57	0.69	-0.19	-0.85	0.14	-0.70	-0.00	3.53×10^{-05}
BN2-62 † ‡	C_s	*BN*	2.86	1.94	1.03	1.35	0.06	2.48	1.73	0.99	0.77	0.18	0.80	0.30	7.40×10^{-05}
BN2-63 † ‡	C_s	*BN*	2.76	1.60	0.43	0.52	0.07	2.39	1.51	0.62	0.34	0.19	2.50	-1.00	7.09×10^{-06}
BN2-64 † ‡ ε	C_s	*B−N+*	2.44	0.84	-0.76	-0.99	0.20	1.85	0.81	-0.23	-0.73	0.17	2.50	-1.10	4.80×10^{-05}
BN2-65 † ‡	C_s	*BN*	2.55	1.42	0.28	-0.02	0.07	2.36	1.41	0.46	0.31	0.20	0.70	0.20	5.08×10^{-05}
BN2-66	C_s	*BN*	3.01	1.63	0.26	0.44	0.07	2.42	1.57	0.73	0.82	0.12	2.70	-1.00	1.21×10^{-05}
BN2-67 † ‡	C_s	*BN*	2.23	1.29	0.34	-0.21	0.07	2.00	1.28	0.56	0.16	0.13	0.40	3.60	1.26×10^{-05}
BN2-68 † ‡	C_s	*BN*	2.73	1.41	0.09	0.62	0.07	2.35	1.46	0.56	0.57	0.20	0.70	0.30	7.08×10^{-05}
BN2-69 † ‡	C_s	*BN*	2.77	2.46	2.14	1.58	0.07	2.31	1.57	0.83	0.74	0.11	0.70	0.30	6.85×10^{-05}
BN2-70 † ‡	C_s	*BN*	2.44	1.51	0.57	0.41	0.07	2.03	1.33	0.64	0.34	0.12	0.80	0.10	5.43×10^{-05}
BN2-71 † ‡ ε γ	C_s	*BN*	2.46	1.13	-0.20	-0.06	0.07	2.13	1.13	0.14	-0.04	0.23	0.70	-0.10	6.23×10^{-05}
BN2-72	C_s	*BN*	3.12	1.97	0.81	0.87	0.07	2.48	1.72	0.95	0.91	0.17	0.70	0.30	7.08×10^{-05}

			CASPT2					TD-DFT					diabatic		
Molecule	PG	LS	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	y_0	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	f	ΔX (Å)	ΔY (Å)	$\lvert T_{RP}\rvert^2$ (eV^2)
BN2-73 † ‡	C_s	BN	2.95	2.12	1.29	0.68	0.07	2.44	1.76	1.09	0.80	0.13	0.70	0.50	8.13×10^{-05}
BN2-74	C_s	$B-N+$	1.65	1.11	0.57	-0.24	0.06	1.53	0.85	0.17	0.19	0.08	0.80	0.40	4.14×10^{-05}
BN2-75 † ‡	C_s	BN	2.53	1.31	0.09	0.57	0.07	2.07	1.30	0.54	0.51	0.11	2.70	-0.50	2.04×10^{-05}
BN2-76 † ‡	C_{2v}	BN	2.39	1.25	0.10	0.14	0.07	2.10	1.25	0.40	0.24	0.14	-0.70	-0.00	6.61×10^{-05}
BN2-77 † ‡	C_s	BN	2.34	1.11	-0.11	-0.09	0.05	2.14	1.20	0.24	0.13	0.20	0.80	0.30	7.06×10^{-05}
BN2-78 † ‡	C_s	BN	3.00	1.68	0.36	0.23	0.07	2.57	1.66	0.74	0.64	0.22	0.20	3.40	8.40×10^{-06}
BN2-79	C_s	$B-N+$	1.14	0.24	-0.65	-1.80	0.04	1.42	0.36	-0.71	-1.30	0.15	-0.50	-1.50	2.84×10^{-05}
BN2-80 † ‡	C_s	BN	2.87	1.88	0.90	0.79	0.07	2.40	1.50	0.61	0.43	0.22	-0.70	0.10	5.91×10^{-05}
BN2-81 † ‡	C_s	BN	2.76	1.90	1.05	0.28	0.05	2.34	1.51	0.67	0.41	0.21	-0.70	-0.00	5.09×10^{-05}
BN2-82 † ‡ ε γ	C_s	BN	2.37	1.09	-0.18	0.10	0.05	2.12	1.02	-0.08	-0.33	0.28	-0.70	-0.20	5.31×10^{-05}
BN2-83 † ‡	C_s	BN	2.66	1.69	0.71	0.36	0.07	2.34	1.34	0.34	0.12	0.24	-0.70	0.20	4.47×10^{-05}
BN2-84 † ‡ ε	C_{2h}	BN	2.50	0.89	-0.73	0.01	0.05	2.16	1.06	-0.03	-0.01	0.28	-0.70	0.10	5.45×10^{-05}
BN2-85 † ‡	C_s	BN	2.40	1.49	0.57	0.63	0.06	2.04	1.19	0.34	0.23	0.16	-0.70	0.10	4.75×10^{-05}
BN2-86	C_s	$B-N+$	1.67	0.69	-0.30	-0.82	0.04	1.67	0.66	-0.34	-0.58	0.18	-0.60	-0.20	3.59×10^{-05}
BN2-87 † ‡	C_s	BN	2.72	1.80	0.87	-0.13	0.06	2.37	1.47	0.57	0.51	0.21	-0.70	0.20	4.00×10^{-05}
BN2-88 † ‡	C_s	BN	2.46	1.21	-0.04	-0.25	0.07	2.20	1.34	0.48	0.21	0.17	-0.70	-0.10	3.86×10^{-05}
BN2-89 † ‡	C_s	$B-N+$	2.76	2.04	1.31	1.11	0.03	2.29	1.34	0.40	0.31	0.21	0.70	0.10	5.23×10^{-05}
BN2-90 † ‡	C_s	$B-N+$	1.99	1.19	0.40	0.17	0.04	1.80	1.05	0.31	0.04	0.11	-0.60	0.10	1.59×10^{-05}
BN2-91 † ‡	C_s	BN	2.56	1.38	0.20	0.47	0.07	2.17	1.30	0.43	0.39	0.19	0.70	-0.10	3.68×10^{-05}
BN2-92 † ‡	C_s	$B-N+$	2.71	1.54	0.38	0.25	0.18	2.15	1.22	0.30	0.45	0.16	0.70	-0.40	7.58×10^{-05}
BN2-93 † ‡ ε	C_s	$B-N+$	2.19	0.94	-0.31	-1.04	0.18	1.76	0.81	-0.13	-0.41	0.12	2.70	-0.00	3.10×10^{-05}
BN2-94 † ‡	C_s	BN	2.90	2.11	1.32	0.85	0.06	2.45	1.61	0.77	0.43	0.23	-0.80	0.20	6.48×10^{-05}
BN2-95 †	C_s	$B-N+$	2.48	0.67	-1.14	-1.11	0.17	1.92	0.74	-0.43	-0.91	0.25	0.70	-0.40	5.45×10^{-05}
BN2-96	C_s	$B-N+$	1.78	1.01	0.24	-0.64	0.04	1.67	0.94	0.22	-0.60	0.11	-0.60	0.40	2.90×10^{-05}
BN2-97	C_s	$B-N+$	1.43	0.28	-0.87	-1.94	0.06	1.58	0.47	-0.63	-1.05	0.18	-2.90	0.60	1.32×10^{-05}
BN2-98 † ‡	C_s	BN	2.89	2.35	1.80	1.87	0.06	2.33	1.70	1.07	0.83	0.14	-0.70	-0.00	3.86×10^{-05}
BN2-99 † ‡	C_s	BN	2.85	1.66	0.47	0.73	0.07	2.46	1.54	0.62	0.36	0.23	-0.60	-0.20	4.52×10^{-05}
BN2-100 † ‡ ε	C_{2v}	$B-N+$	1.83	0.67	-0.49	-0.93	0.03	1.84	0.82	-0.20	-0.67	0.20	0.60	-0.00	2.33×10^{-05}
BN2-101 † ‡ ε	C_s	BN	2.28	0.95	-0.38	-0.26	0.06	1.99	1.07	0.15	-0.09	0.18	-0.70	0.30	4.34×10^{-05}
BN2-102 † ‡	C_s	BN	2.66	1.76	0.86	0.67	0.06	2.31	1.38	0.45	0.41	0.19	-0.70	0.10	5.93×10^{-05}
BN2-103 † ‡	C_s	BN	2.44	1.18	-0.09	-0.19	0.06	2.15	1.19	0.22	0.15	0.21	-0.70	-0.10	4.25×10^{-05}
BN2-104 † ‡	C_s	BN	2.34	1.77	1.20	0.99	0.05	2.02	1.17	0.32	0.28	0.18	-0.70	-0.00	4.25×10^{-05}
BN2-105 † ‡	C_s	BN	2.80	1.58	0.35	0.57	0.06	2.33	1.34	0.34	0.38	0.23	-0.70	-0.00	4.65×10^{-05}
BN2-106 † ‡	C_s	BN	2.38	1.41	0.43	0.49	0.05	2.09	1.20	0.32	0.13	0.19	0.70	-0.10	4.30×10^{-05}
BN2-107 † ‡ ε	C_s	BN	2.11	1.17	0.23	-0.20	0.04	1.97	0.99	0.00	-0.43	0.22	-0.70	0.30	5.06×10^{-05}
BN2-108 † ‡	C_s	BN	2.80	2.14	1.48	0.49	0.05	2.30	1.55	0.81	0.44	0.16	-0.80	0.30	5.78×10^{-05}
BN2-109 † ‡	C_s	BN	2.71	1.90	1.09	0.54	0.06	2.38	1.50	0.64	0.46	0.21	-0.70	-0.00	3.69×10^{-05}
BN2-110	C_s	$B-N+$	1.48	0.55	-0.38	-1.28	0.07	1.53	0.53	-0.47	-0.94	0.17	-0.60	0.10	3.42×10^{-05}
BN2-111 † ‡	C_s	BN	2.55	1.96	1.36	1.18	0.06	2.23	1.30	0.38	0.51	0.18	-0.70	0.10	4.43×10^{-05}
BN2-112 † ‡ ε γ η *	C_{2v}	BN	2.33	1.02	-0.28	-0.44	0.06	2.05	0.96	-0.12	-0.48	0.27	-0.70	-0.00	5.32×10^{-05}
BN2-113 † ‡	C_s	BN	2.76	1.63	0.49	-0.09	0.06	2.36	1.37	0.38	0.20	0.24	-0.70	-0.10	3.92×10^{-05}
BN2-114	C_s	BN	3.60	2.96	2.32	2.32	0.06	2.91	2.11	1.30	1.28	0.21	-0.70	-0.00	6.35×10^{-05}
BN2-115	C_s	BN	3.25	2.59	1.92	1.57	0.06	2.73	2.03	1.32	1.16	0.18	-0.70	0.20	4.30×10^{-05}
BN2-116 † ‡	C_s	$B-N+$	2.04	1.49	0.94	0.64	0.05	1.63	0.94	0.24	0.28	0.10	0.60	-0.00	1.28×10^{-05}
BN2-117 † ‡	C_s	$B-N+$	2.63	2.12	1.60	1.22	0.04	2.16	1.51	0.87	0.61	0.09	-0.60	0.60	4.32×10^{-05}
BN2-118	C_s	BN	3.42	2.87	2.33	2.18	0.07	2.83	2.15	1.47	1.48	0.18	-0.60	0.20	4.70×10^{-05}
BN2-119 † ‡	C_s	BN	2.66	1.78	0.90	0.58	0.03	2.34	1.38	0.42	0.28	0.25	-0.70	-0.20	4.14×10^{-05}
BN2-120	C_{2h}	BN	3.38	2.41	1.44	1.67	0.03	2.80	1.94	1.08	1.33	0.24	-0.50	0.50	6.05×10^{-05}

			CASPT2					TD-DFT					diabatic		
Molecule	PG	LS	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	y_0	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	f	ΔX (Å)	ΔY (Å)	$\lvert T_{RP}\rvert^2$ (eV^2)
BN2-121 † ‡	C_s	BN	2.93	1.78	0.63	1.10	0.06	2.37	1.60	0.83	0.81	0.14	2.70	0.90	1.17×10^{-05}
BN2-122	C_s	$B-N+$	1.71	0.86	0.01	-0.66	0.05	1.67	0.79	-0.10	-0.52	0.16	-0.60	0.30	2.53×10^{-05}
BN2-123	C_s	BN	3.23	2.64	2.06	1.84	0.01	2.66	2.00	1.34	1.24	0.16	-0.70	0.40	4.35×10^{-05}
BN2-124	C_s	BN	3.45	2.58	1.72	2.03	0.07	2.69	1.81	0.93	1.14	0.21	-0.70	0.10	5.90×10^{-05}
BN2-125 † ‡	C_s	BN	2.98	1.61	0.24	0.08	0.06	2.59	1.65	0.70	0.92	0.20	-2.60	0.20	6.85×10^{-06}
BN2-126 † ‡	C_s	$B-N+$	2.59	1.48	0.37	0.84	0.13	1.98	1.26	0.54	0.94	0.11	-2.70	-0.00	1.57×10^{-05}
BN2-127	C_s	BN	3.28	2.21	1.13	2.05	0.07	2.71	1.87	1.03	1.31	0.16	-0.70	0.20	4.39×10^{-05}
BN2-128	C_s	BN	3.19	2.10	1.01	1.99	0.08	2.66	1.83	1.00	1.41	0.19	-0.70	0.10	3.91×10^{-05}
BN2-129	C_s	BN	3.25	2.34	1.43	2.14	0.01	2.70	1.94	1.19	1.44	0.23	-0.70	0.30	5.51×10^{-05}
BN2-130 † ‡	C_s	BN	2.76	1.99	1.23	0.97	0.06	2.41	1.46	0.50	0.37	0.26	0.70	-0.30	5.75×10^{-05}
BN2-131 † ‡	C_s	BN	2.96	2.05	1.14	1.78	0.07	2.35	1.67	1.00	0.61	0.14	0.60	-0.30	4.62×10^{-05}
BN2-132	C_s	$B-N+$	1.68	1.04	0.41	0.04	0.04	1.58	0.77	-0.05	-0.09	0.15	0.60	-0.40	1.66×10^{-05}
BN2-133	C_s	BN	3.38	2.50	1.63	1.30	0.06	2.79	2.00	1.22	1.28	0.15	-0.60	0.20	3.20×10^{-05}
BN2-134	C_{2v}	BN	3.28	2.87	2.46	2.79	0.01	2.84	1.94	1.04	1.44	0.25	-0.70	-0.00	3.71×10^{-05}
BN2-135 † ‡	C_s	BN	2.73	1.60	0.46	0.82	0.07	2.28	1.54	0.80	0.78	0.14	0.50	-3.50	8.16×10^{-06}
BN2-136	C_s	BN	3.35	2.37	1.39	2.19	0.02	2.74	1.92	1.10	1.33	0.18	-0.60	0.30	6.28×10^{-05}
BN2-137 † ‡	C_s	BN	2.81	1.67	0.52	0.70	0.07	2.40	1.54	0.68	0.75	0.15	0.60	0.20	2.69×10^{-05}
BN2-138 † ‡	C_s	BN	2.70	1.78	0.85	1.23	0.06	2.25	1.59	0.94	0.83	0.12	0.70	-0.10	3.14×10^{-05}
BN2-139	C_s	BN	3.32	2.69	2.06	2.42	0.07	2.65	1.86	1.07	1.18	0.16	-0.60	0.30	5.01×10^{-05}
BN2-140 † ‡	C_s	BN	2.90	1.89	0.88	1.43	0.06	2.44	1.65	0.86	0.97	0.16	0.70	-0.30	4.15×10^{-05}
BN2-141 † ‡	C_s	BN	2.81	1.66	0.51	0.47	0.06	2.41	1.43	0.44	0.32	0.24	0.50	-3.20	7.05×10^{-06}
BN2-142	C_s	BN	3.47	3.15	2.83	2.54	0.04	2.88	2.18	1.48	1.50	0.20	0.70	-0.40	8.62×10^{-05}
BN2-143	C_s	BN	3.12	2.75	2.38	2.11	0.07	2.63	1.97	1.30	1.20	0.18	-0.60	0.20	2.95×10^{-05}
BN2-144	C_s	$B-N+$	1.72	0.70	-0.32	-1.60	0.09	1.77	0.66	-0.45	-0.77	0.20	-2.60	-0.40	3.03×10^{-05}
BN2-145 † ‡	C_s	BN	2.98	1.98	0.98	1.38	0.06	2.44	1.66	0.87	0.92	0.15	-0.70	0.10	3.84×10^{-05}
BN2-146	C_{2v}	BN	3.24	2.36	1.49	1.53	0.05	2.69	1.88	1.08	1.23	0.20	0.60	-0.00	2.93×10^{-05}
BN2-147	C_s	$B-N+$	1.57	0.48	-0.60	-2.10	0.07	1.64	0.59	-0.46	-0.96	0.20	0.70	0.20	2.94×10^{-05}
BN2-148 † ‡	C_s	?	2.75	1.55	0.34	0.31	0.08	2.31	1.34	0.38	0.39	0.24	-0.70	-0.10	6.41×10^{-05}
BN2-149 † ‡	C_s	BN	2.93	1.88	0.83	0.10	0.06	2.52	1.55	0.58	0.56	0.25	0.80	0.40	9.95×10^{-05}
BN2-150 † ‡ ε	C_{2h}	BN	2.54	0.92	-0.69	0.12	0.05	2.19	1.11	0.02	0.12	0.28	-0.70	-0.40	9.41×10^{-05}
BN2-151 † ‡	C_s	BN	2.41	1.30	0.19	0.38	0.06	2.07	1.20	0.33	0.19	0.17	0.70	0.40	5.70×10^{-05}
BN2-152	C_s	$B-N+$	1.41	0.39	-0.64	-1.79	0.05	1.56	0.44	-0.68	-1.10	0.19	1.20	1.50	2.67×10^{-05}
BN2-153 † ‡	C_s	BN	2.61	1.81	1.02	-0.02	0.06	2.22	1.44	0.66	0.30	0.19	0.70	0.10	3.50×10^{-05}
BN2-154 † ‡	C_s	BN	2.42	1.07	-0.29	-0.12	0.07	2.13	1.21	0.30	0.16	0.19	-0.60	-0.30	4.76×10^{-05}
BN2-155 † ‡	C_s	$B-N+$	2.68	1.58	0.48	0.21	0.17	2.09	1.26	0.42	0.52	0.11	0.70	0.60	1.01×10^{-04}
BN2-156 † ‡ ε	C_s	$B-N+$	2.09	0.88	-0.34	-1.53	0.18	1.78	0.82	-0.14	-0.60	0.14	0.80	0.10	2.14×10^{-05}
BN2-157 † ‡	C_s	BN	2.73	1.79	0.85	0.72	0.06	2.30	1.50	0.70	0.41	0.19	-0.70	-0.20	3.69×10^{-05}
BN2-158 † ‡	C_s	$B-N+$	2.83	1.80	0.76	0.91	0.02	2.31	1.32	0.34	0.39	0.26	0.80	-0.00	5.12×10^{-05}
BN2-159	C_s	$B-N+$	1.77	0.92	0.06	-0.53	0.04	1.70	0.97	0.23	-0.47	0.12	0.70	0.30	3.54×10^{-05}
BN2-160	C_s	BN	3.11	2.36	1.61	1.82	0.06	2.40	1.76	1.11	0.86	0.15	0.70	0.20	4.42×10^{-05}
BN2-161	C_{2v}	$B-N+$	1.79	0.66	-0.48	-1.54	0.04	1.82	0.80	-0.23	-0.77	0.20	-0.40	3.70	1.45×10^{-05}
BN2-162 †	C_s	$B-N+$	2.25	0.90	-0.45	-1.19	0.20	1.62	0.74	-0.14	-0.69	0.09	-0.70	-0.60	8.90×10^{-05}
BN2-163	C_s	$B-N+$	1.68	0.72	-0.24	-0.62	0.07	1.65	0.70	-0.23	-0.53	0.16	0.70	-0.10	2.19×10^{-05}
BN2-164 † ‡	C_s	BN	2.74	2.06	1.39	0.85	0.07	2.39	1.57	0.75	0.36	0.22	0.70	0.30	6.00×10^{-05}
BN2-165 † ‡	C_s	BN	2.25	1.19	0.14	0.07	0.05	2.03	1.17	0.31	0.17	0.16	0.70	0.20	3.54×10^{-05}
BN2-166 † ‡	C_s	BN	2.85	1.54	0.23	0.41	0.07	2.35	1.36	0.37	0.40	0.22	0.70	0.30	7.31×10^{-05}
BN2-167 † ‡	C_s	BN	2.41	1.22	0.03	-0.09	0.06	2.11	1.16	0.21	-0.05	0.19	0.60	3.40	6.83×10^{-06}
BN2-168 † ‡	C_s	BN	2.54	1.95	1.36	1.21	0.06	2.17	1.30	0.42	0.39	0.18	0.70	0.30	7.01×10^{-05}

			CASPT2					TD-DFT					diabatic		
Molecule	PG	LS	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	y_0	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	f	ΔX (Å)	ΔY (Å)	$\lvert T_{RP}\rvert^2$ (eV^2)
BN2-169 † ‡	C_s	*BN*	2.71	1.74	0.76	0.77	0.06	2.32	1.37	0.42	0.37	0.22	0.70	0.30	6.13×10^{-05}
BN2-170 † ‡	C_s	*BN*	2.42	1.62	0.82	0.55	0.07	2.10	1.24	0.37	0.24	0.18	0.80	0.20	5.86×10^{-05}
BN2-171 † ‡ ε γ η *	C_{2v}	*BN*	2.42	1.14	-0.14	-0.21	0.06	2.11	1.00	-0.12	-0.34	0.30	-0.70	-0.00	5.71×10^{-05}
BN2-172 † ‡	C_s	*BN*	2.99	1.97	0.95	0.88	0.07	2.50	1.57	0.64	0.54	0.25	0.80	0.20	8.06×10^{-05}
BN2-173 † ‡	C_s	*BN*	2.61	1.98	1.35	1.01	0.05	2.17	1.45	0.73	0.27	0.16	0.70	0.40	4.96×10^{-05}
BN2-174	C_s	*B−N+*	1.08	0.29	-0.51	-2.04	0.04	1.36	0.32	-0.72	-1.29	0.14	2.60	-0.90	3.71×10^{-05}
BN2-175 † ‡	C_s	*BN*	2.48	1.54	0.60	0.74	0.06	2.13	1.20	0.27	0.43	0.21	0.70	0.20	4.46×10^{-05}
BN2-176	C_{2h}	*BN*	3.67	3.41	3.14	3.05	0.05	2.96	2.29	1.62	1.68	0.21	0.80	0.50	1.32×10^{-04}
BN2-177 † ‡	C_s	*BN*	2.88	2.33	1.79	1.72	0.07	2.39	1.81	1.23	1.35	0.09	0.70	-0.20	3.59×10^{-05}
BN2-178	C_s	*B−N+*	1.68	1.17	0.67	-0.17	0.04	1.41	0.75	0.09	-0.30	0.11	-0.70	-0.20	8.88×10^{-06}
BN2-179	C_s	*BN*	3.43	3.69	3.94	2.99	0.07	2.69	2.26	1.82	1.58	0.12	-0.70	0.10	3.67×10^{-05}
BN2-180	C_s	*B−N+*	3.14	1.58	0.02	0.97	0.12	1.87	1.35	0.83	1.13	0.08	2.70	-0.50	2.07×10^{-05}
BN2-181	C_s	*BN*	3.58	2.98	2.38	1.95	0.06	2.84	2.17	1.51	1.80	0.01	0.70	-0.10	7.79×10^{-05}
BN2-182 † ‡	C_s	*BN*	2.94	2.44	1.94	1.64	0.06	2.51	1.82	1.12	0.99	0.15	-0.60	0.30	4.45×10^{-05}
BN2-183	C_s	*BN*	3.42	2.52	1.61	1.76	0.07	2.70	1.82	0.94	0.71	0.25	-0.70	-0.20	6.78×10^{-05}
BN2-184	C_s	*BN*	3.28	2.99	2.69	2.73	0.06	2.49	2.01	1.52	1.55	0.12	2.80	-0.50	2.96×10^{-05}
BN2-185	C_{2v}	*BN*	3.94	3.67	3.40	2.62	0.05	3.07	2.45	1.83	1.92	0.10	0.70	-0.00	5.72×10^{-05}
BN2-186	C_s	*BN*	3.03	2.27	1.51	1.74	0.06	2.28	1.75	1.21	1.17	0.05	2.60	-1.10	2.00×10^{-05}
BN2-187 † ‡ ε	C_s	*B−N+*	1.94	1.08	0.22	-0.18	0.05	1.88	0.94	0.01	-0.09	0.20	-0.70	-0.20	3.48×10^{-05}
BN2-188	C_s	*BN*	3.04	2.68	2.32	1.95	0.01	2.68	1.87	1.07	0.78	0.26	-0.80	-0.30	6.96×10^{-05}
BN2-189	C_s	*BN*	3.02	2.16	1.30	1.37	0.07	2.45	1.79	1.14	0.95	0.12	0.70	-0.00	3.67×10^{-05}
BN2-190	C_s	*BN*	3.50	2.86	2.23	2.59	0.02	2.71	2.02	1.33	1.51	0.15	-0.70	-0.30	6.87×10^{-05}
BN2-191 † ‡	C_s	*BN*	2.75	1.93	1.11	1.01	0.07	2.37	1.74	1.10	0.88	0.12	0.60	0.40	5.35×10^{-05}
BN2-192	C_s	*BN*	3.09	2.05	1.01	1.50	0.05	2.50	1.77	1.03	0.94	0.16	0.70	0.30	5.63×10^{-05}
BN2-193	C_s	*BN*	3.41	2.89	2.38	2.64	0.02	2.81	2.12	1.43	1.63	0.16	0.70	-0.00	6.48×10^{-05}
BN2-194	C_s	*BN*	3.02	2.02	1.03	1.50	0.06	2.48	1.81	1.15	1.08	0.14	0.80	-0.10	5.71×10^{-05}
BN2-195	C_{2v}	*BN*	3.42	2.54	1.66	1.41	0.02	2.89	2.19	1.49	1.46	0.22	0.70	-0.00	6.67×10^{-05}
BN2-196	C_s	*BN*	3.55	3.68	3.81	2.88	0.07	2.71	2.25	1.78	1.51	0.11	-0.70	-0.40	5.75×10^{-05}
BN2-197 † ‡	C_s	*BN*	2.89	2.02	1.16	1.35	0.06	2.43	1.73	1.03	1.14	0.13	0.70	0.40	6.11×10^{-05}
BN2-198	C_s	*BN*	3.08	2.08	1.09	1.43	0.07	2.47	1.80	1.14	1.11	0.14	0.70	-0.30	3.50×10^{-05}
BN2-199 † ‡ ε γ η	C_s	*B−N+*	1.95	0.96	-0.02	-0.38	0.05	1.90	0.96	0.01	-0.12	0.20	2.70	0.90	1.64×10^{-05}
BN2-200	C_{2h}	*BN*	3.17	3.75	4.33	3.06	0.07	2.77	2.14	1.51	1.45	0.17	-0.70	0.20	3.90×10^{-05}
BN2-201	C_s	*B−N+*	3.41	2.81	2.21	1.78	0.02	2.48	1.72	0.97	1.16	0.07	-0.40	-3.60	6.76×10^{-06}
BN2-202	C_s	*BN*	3.28	2.43	1.57	1.66	0.07	2.63	1.76	0.89	0.69	0.23	-0.70	0.10	5.48×10^{-05}
BN2-203 † ‡	C_s	*BN*	2.95	2.63	2.31	2.38	0.05	2.30	1.82	1.34	1.17	0.09	-0.60	-0.00	3.55×10^{-05}
BN2-204	C_1	*BN*	3.86	2.96	2.06	2.08	0.06	2.86	2.16	1.46	1.69	0.08	0.70	-0.00	1.21×10^{-03}
BN2-205 † ‡	C_1	*BN*	2.90	2.49	2.09	2.33	0.05	2.39	1.83	1.26	1.25	0.07	2.80	-0.70	3.18×10^{-05}
BN2-206	C_s	*BN*	3.11	2.52	1.93	2.25	0.07	2.50	1.92	1.34	1.51	0.14	0.70	-0.40	4.04×10^{-05}
BN2-207	C_s	*B−N+*	1.67	1.19	0.71	0.00	0.04	1.37	0.73	0.09	-0.28	0.10	-0.60	0.40	1.14×10^{-05}
BN2-208	C_{2v}	*BN*	3.64	3.49	3.34	2.49	0.04	2.91	2.34	1.76	1.92	0.08	-0.70	-0.00	2.84×10^{-05}
BN2-209 † ‡	C_s	*BN*	2.73	1.73	0.72	1.01	0.07	2.30	1.60	0.89	0.79	0.14	0.50	-3.40	7.02×10^{-06}
BN2-210	C_s	*BN*	3.28	2.88	2.49	2.64	0.02	2.74	2.10	1.45	1.56	0.14	0.70	-0.20	6.19×10^{-05}
BN2-211 † ‡	C_s	*BN*	2.86	1.89	0.92	1.07	0.07	2.31	1.65	0.99	0.96	0.13	-2.50	-0.60	9.32×10^{-06}
BN2-212 † ‡	C_s	*BN*	2.64	1.83	1.01	1.30	0.05	2.22	1.64	1.05	0.98	0.10	0.70	-0.00	2.43×10^{-05}
BN2-213	C_1	*BN*	3.46	2.80	2.14	2.52	0.07	2.68	2.04	1.40	1.50	0.14	-0.70	0.20	1.33×10^{-03}
BN2-214 † ‡	C_1	*BN*	2.91	2.29	1.67	1.88	0.06	2.33	1.80	1.27	1.22	0.10	-0.80	0.40	6.23×10^{-04}
BN2-215	C_{2v}	*BN*	3.13	2.94	2.76	2.25	0.05	2.79	2.14	1.50	1.44	0.18	0.70	-0.00	4.60×10^{-05}
BN2-216	C_1	*BN*	3.15	2.21	1.26	1.64	0.07	2.49	1.80	1.11	1.06	0.13	0.80	0.10	6.05×10^{-04}

			CASPT2					TD-DFT					diabatic		
Molecule	PG	LS	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	y_0	$E(S_1)$ (eV)	$E(T_1)$ (eV)	ΔE_{ST} (eV)	ΔE_{TT} (eV)	f	ΔX (Å)	ΔY (Å)	$\lvert T_{RP}\rvert^2$ (eV^2)
BN2-217	C_s	$B-N+$	1.41	0.59	-0.22	-1.85	0.07	1.28	0.48	-0.32	-0.82	0.08	0.50	0.80	3.17×10^{-05}
BN2-218 † ‡	C_{2h}	$B-N+$	2.09	1.14	0.18	0.56	0.01	1.93	1.18	0.44	0.50	0.14	0.60	0.40	2.82×10^{-05}
BN2-219	C_s	$B-N+$	1.57	1.04	0.51	-0.00	0.06	1.40	0.78	0.16	0.23	0.07	0.50	0.70	1.34×10^{-05}
BN2-220	C_s	$B-N+$	1.70	0.71	-0.29	-0.64	0.05	1.79	0.75	-0.29	-0.32	0.17	-3.00	0.10	2.98×10^{-05}
BN2-221	C_s	$B-N+$	1.42	0.47	-0.49	-2.09	0.06	1.57	0.50	-0.57	-0.77	0.14	0.60	0.10	2.67×10^{-05}
BN2-222	C_s	$B-N+$	1.71	0.96	0.21	-0.11	0.07	1.49	0.75	0.02	-0.21	0.10	0.60	0.30	2.00×10^{-05}
BN2-223	C_s	$B-N+$	1.48	0.47	-0.53	-1.18	0.07	1.44	0.54	-0.36	-0.76	0.11	-2.90	0.10	2.42×10^{-05}
BN2-224	C_s	$B-N+$	1.32	0.54	-0.24	-1.31	0.03	1.45	0.59	-0.26	-1.03	0.13	-0.60	-0.20	1.80×10^{-05}
BN2-227	C_s	$B-N+$	1.63	1.11	0.60	-0.06	0.06	1.37	0.74	0.12	-0.21	0.06	0.70	0.20	1.58×10^{-05}
BN2-228	C_s	$B-N+$	1.66	0.68	-0.30	-1.58	0.07	1.60	0.70	-0.20	-0.66	0.15	-0.70	-0.20	3.07×10^{-05}
BN2-229	C_s	$B-N+$	1.50	0.66	-0.17	-0.75	0.04	1.75	0.67	-0.42	-0.39	0.20	-2.70	1.00	3.02×10^{-05}
BN2-230	C_s	$B-N+$	1.24	0.47	-0.30	-1.80	0.04	1.43	0.55	-0.32	-0.92	0.14	-0.70	-0.00	2.05×10^{-05}
BN2-231 † ‡	C_{2h}	BN	2.44	1.79	1.15	1.68	0.01	2.13	1.70	1.27	1.56	0.00	3.40	0.30	9.72×10^{-06}
BN2-232	C_s	BN	3.31	2.42	1.53	1.63	0.07	2.66	1.77	0.87	0.72	0.25	-0.70	-0.00	5.40×10^{-05}
BN2-233	C_s	$B-N+$	1.35	0.79	0.23	-1.67	0.04	1.30	0.74	0.19	-0.68	0.04	-0.50	0.40	1.37×10^{-05}
BN2-234 † ‡	C_s	BN	2.74	1.44	0.15	0.65	0.07	2.35	1.47	0.60	0.70	0.17	0.60	-0.20	3.73×10^{-05}
BN2-235 † ‡	C_s	BN	2.71	1.88	1.05	1.26	0.06	2.17	1.58	1.00	0.99	0.04	-0.70	0.30	3.71×10^{-05}
BN2-236 † ‡	C_s	BN	2.40	1.40	0.41	0.61	0.06	1.93	1.29	0.65	0.29	0.09	0.60	0.30	3.38×10^{-05}
BN2-237 † ‡	C_s	BN	2.74	1.86	0.98	1.30	0.07	2.33	1.48	0.63	0.63	0.19	0.70	0.10	3.81×10^{-05}
BN2-238 † ‡	C_s	BN	2.96	1.80	0.64	1.15	0.06	2.38	1.58	0.77	0.83	0.16	-0.70	0.30	5.96×10^{-05}
BN2-239 † ‡	C_s	BN	2.54	1.89	1.24	1.54	0.07	2.03	1.37	0.70	0.49	0.13	0.70	-0.10	3.40×10^{-05}
BN2-240 † ‡	C_{2v}	BN	2.35	1.35	0.36	0.58	0.07	1.84	1.26	0.68	0.32	0.06	0.70	-0.00	4.16×10^{-05}
BN2-241 † ‡	C_s	BN	2.56	1.49	0.42	1.05	0.08	2.24	1.38	0.51	0.77	0.17	0.60	0.20	3.43×10^{-05}
BN2-242 † ‡	C_s	$B-N+$	2.77	1.41	0.04	0.28	0.16	2.25	1.30	0.36	0.82	0.07	0.40	0.60	2.59×10^{-05}
BN2-243 † ‡	C_{2v}	BN	2.12	1.08	0.03	-0.11	0.07	1.84	1.11	0.38	0.17	0.10	-0.60	-0.00	2.35×10^{-05}
BN2-244 † ‡	C_s	BN	2.61	2.49	2.37	1.48	0.07	2.20	1.55	0.91	0.69	0.08	-0.70	-0.20	4.34×10^{-05}
BN2-245 † ‡	C_{2h}	BN	2.87	1.54	0.21	0.40	0.05	2.50	1.47	0.43	0.80	0.28	-0.50	-3.50	3.99×10^{-06}
BN2-246 † ‡	C_s	BN	2.28	1.18	0.08	0.37	0.07	1.91	1.23	0.54	0.34	0.10	-0.60	-0.30	3.24×10^{-05}
BN2-247 † ‡	C_s	BN	2.77	1.51	0.25	0.40	0.07	2.27	1.50	0.73	0.65	0.11	-0.60	-0.40	4.31×10^{-05}
BN2-248 † ‡	C_s	BN	2.57	1.50	0.43	1.05	0.07	2.43	1.52	0.61	0.90	0.12	0.70	0.10	3.96×10^{-05}
BN2-249	D_{2h}	BN	3.44	1.81	0.19	1.61	0.01	2.50	1.86	1.22	1.59	0.00	-0.70	-0.00	7.99×10^{-05}
BN2-250 † ‡	C_s	BN	2.81	1.70	0.59	1.07	0.06	2.30	1.56	0.82	0.69	0.13	0.70	0.10	4.60×10^{-05}
BN2-251	C_{2v}	BN	3.39	1.86	0.34	1.74	0.01	2.66	1.88	1.10	1.50	0.13	0.70	-0.00	6.40×10^{-05}
BN2-252 † ‡	C_2	BN	2.42	1.49	0.57	0.49	0.04	1.93	1.38	0.82	0.45	0.07	0.70	-0.10	7.23×10^{-04}
BN2-253 † ‡	C_s	BN	2.69	1.83	0.96	1.23	0.05	2.18	1.58	0.97	0.89	0.07	-0.70	0.10	3.94×10^{-05}
BN2-254 † ‡	C_{2h}	BN	2.81	1.56	0.31	1.22	0.01	2.24	1.66	1.07	1.33	0.00	-0.70	0.20	7.50×10^{-05}
BN2-255	D_{2h}	BN	3.35	1.79	0.22	1.57	0.01	2.57	1.82	1.06	1.41	0.10	-0.70	-0.00	5.90×10^{-05}
perylene-undoped	D_{2h}	...	3.05	1.61	0.17	0.43	0.02	2.66	1.66	0.67	0.30	0.28	-0.70	-0.00	6.25×10^{-05}

Column 1	Column 2	Column 3	Column 4	Column 5
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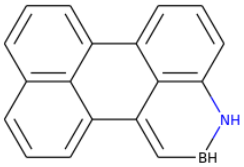	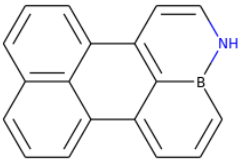	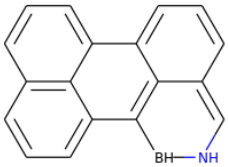	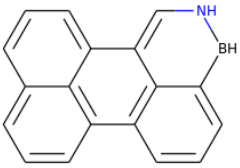	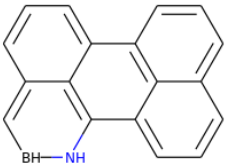
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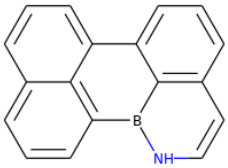	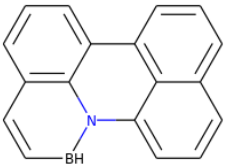	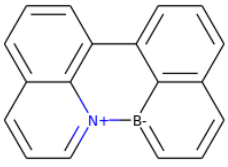	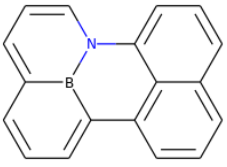	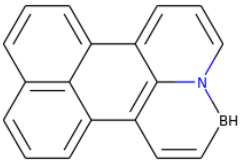
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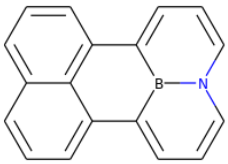	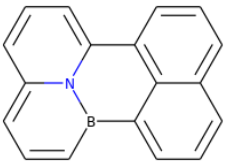	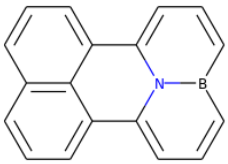	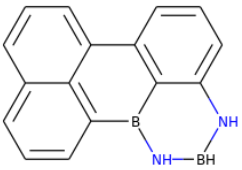	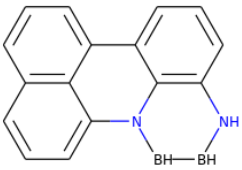
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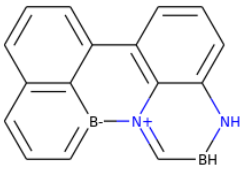	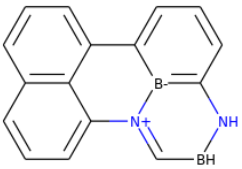	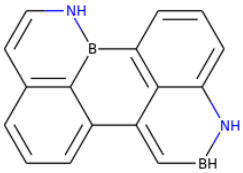	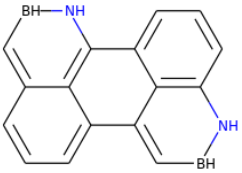	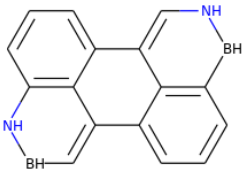
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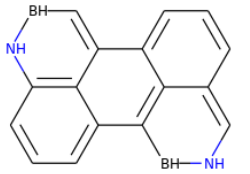	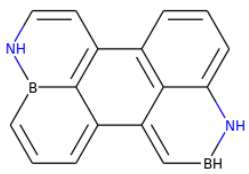	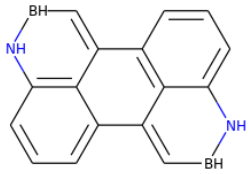	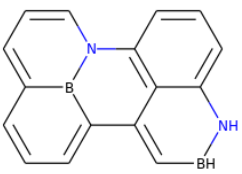	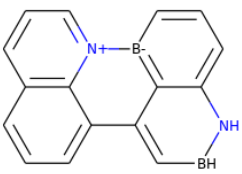
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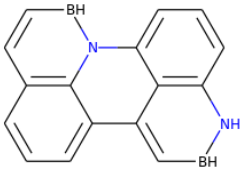	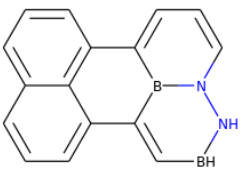	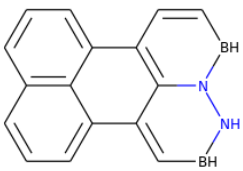	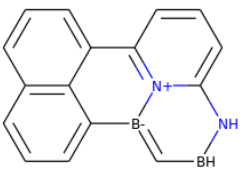	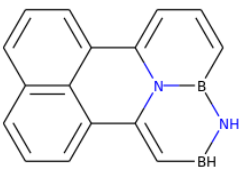
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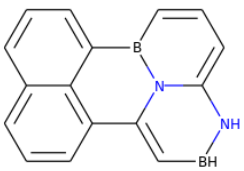	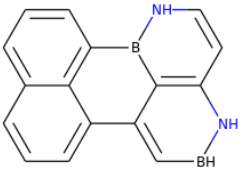	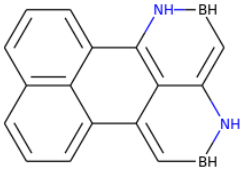	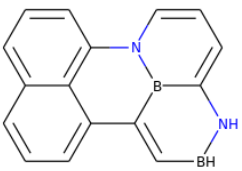	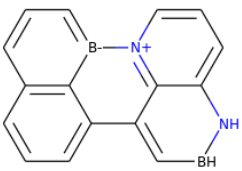
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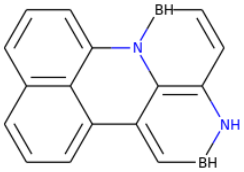	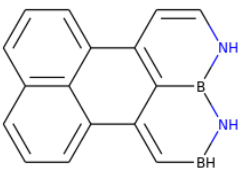	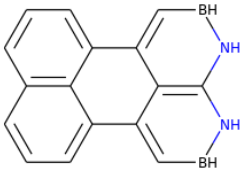	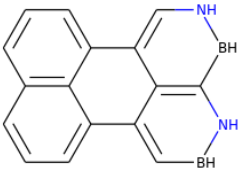	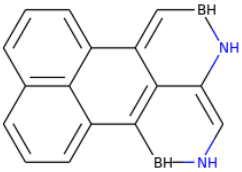

Column 1	Column 2	Column 3	Column 4	Column 5
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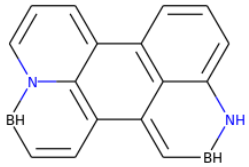	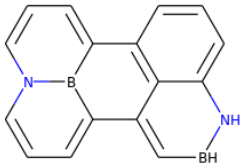	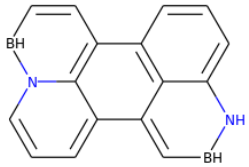	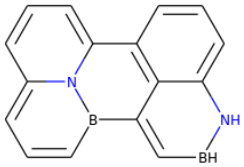	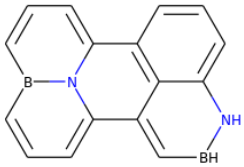
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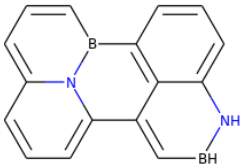	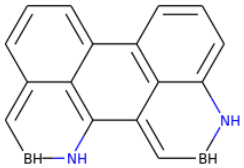	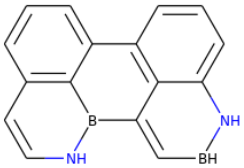	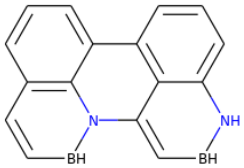	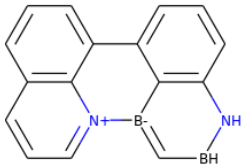
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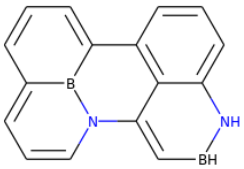	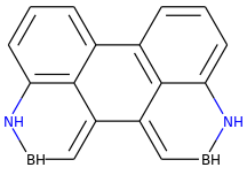	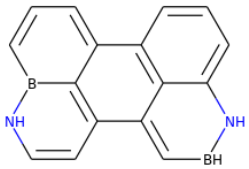	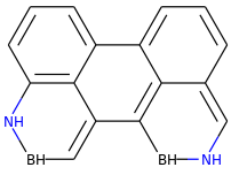	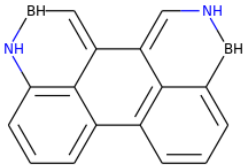
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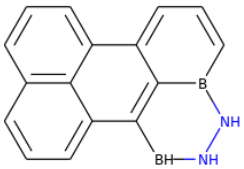	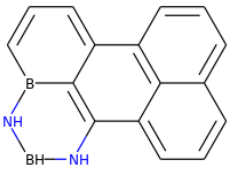	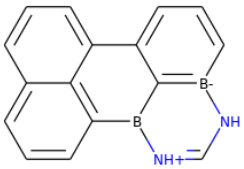	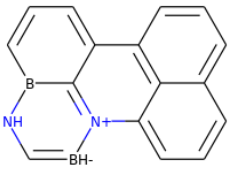	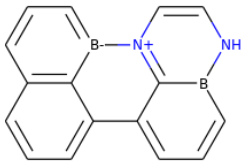
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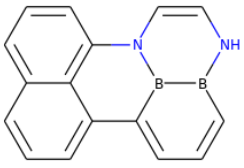	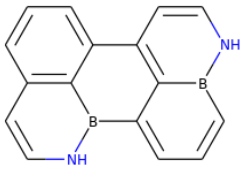	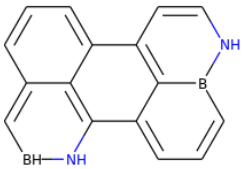	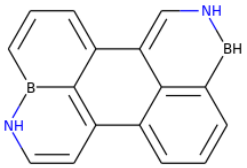	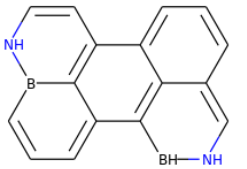
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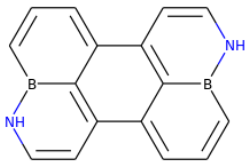	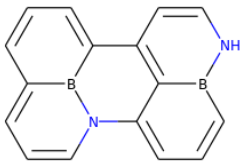	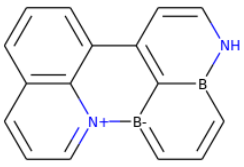	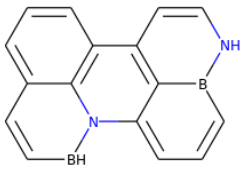	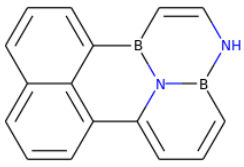
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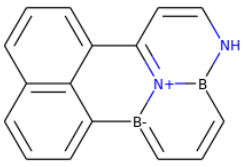	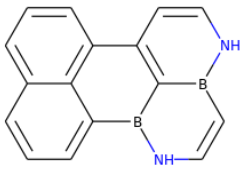	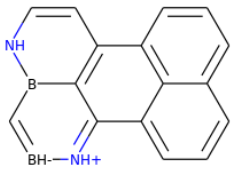	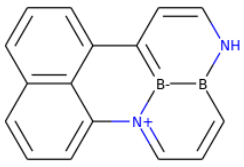	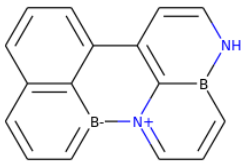
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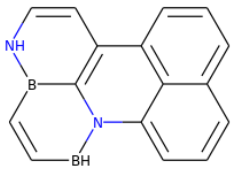	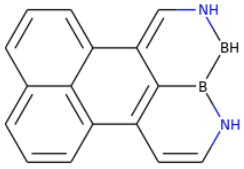	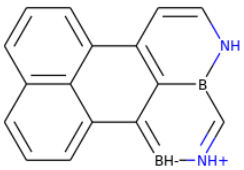	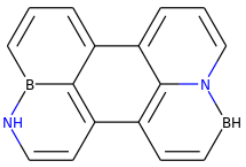	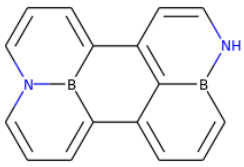

Column 1	Column 2	Column 3	Column 4	Column 5
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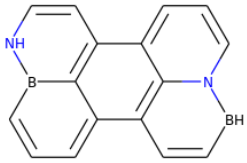	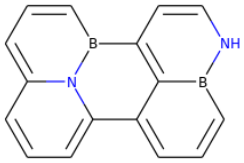	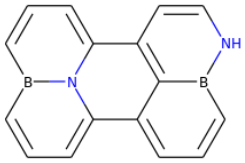	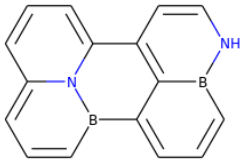	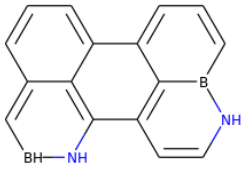
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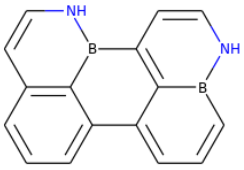	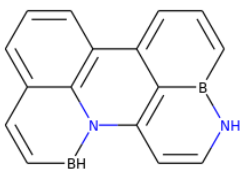	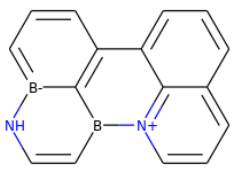	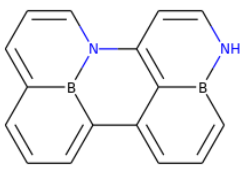	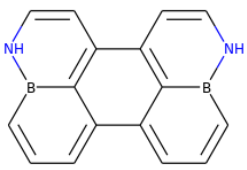
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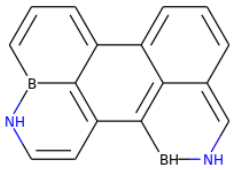	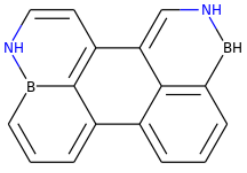	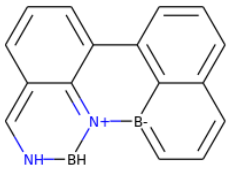	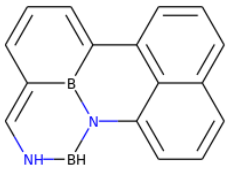	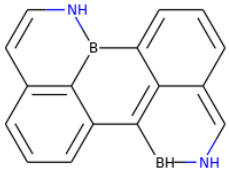
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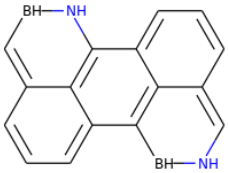	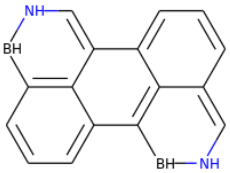	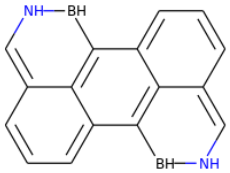	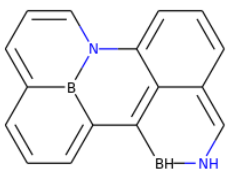	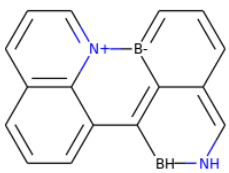
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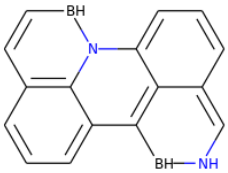	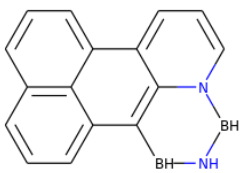	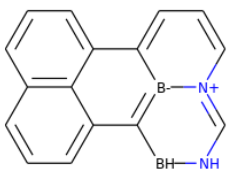	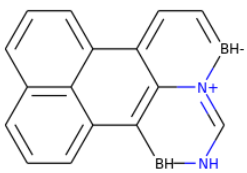	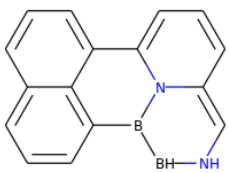
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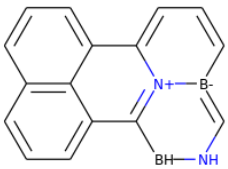	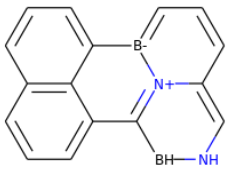	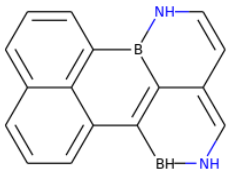	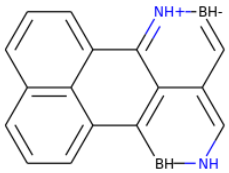	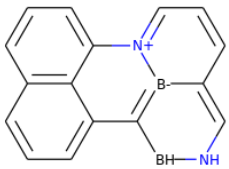
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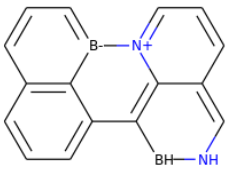
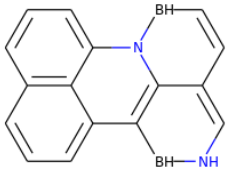
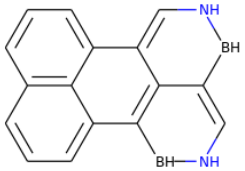
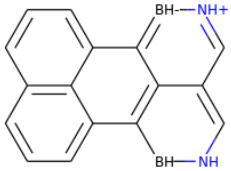
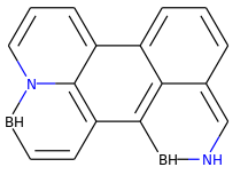
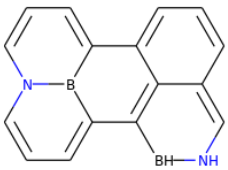
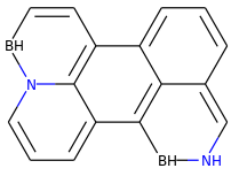
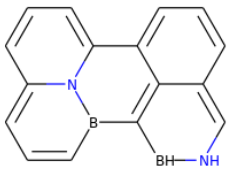
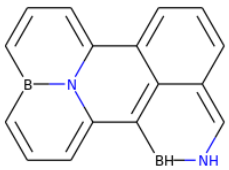
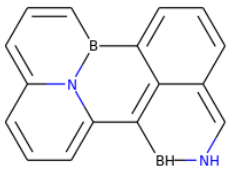
				
perylene-BN2-0102	perylene-BN2-0103	perylene-BN2-0104	perylene-BN2-0105	perylene-BN2-0106
				

Column 1	Column 2	Column 3	Column 4	Column 5
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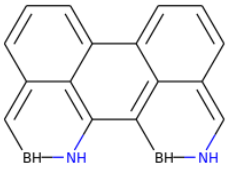	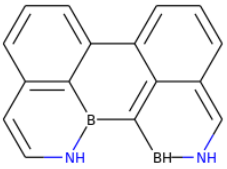	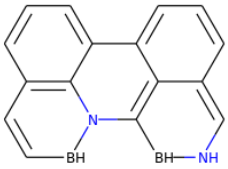	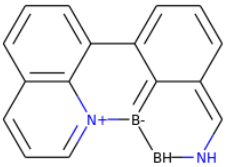	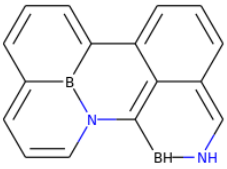
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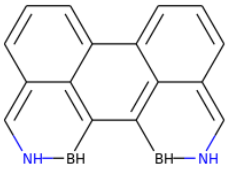	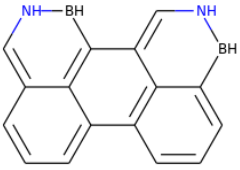	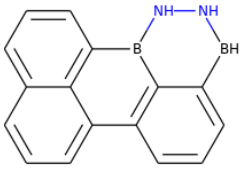	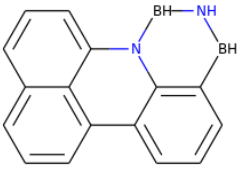	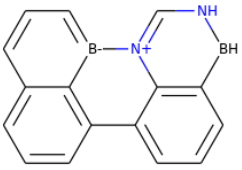
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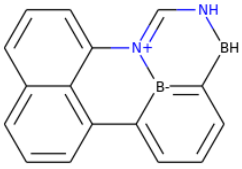	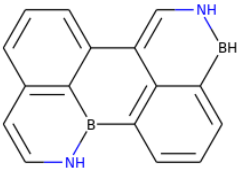	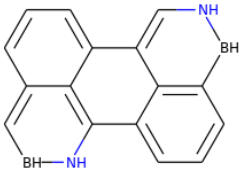	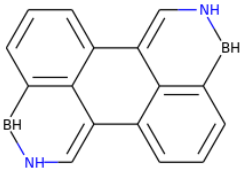	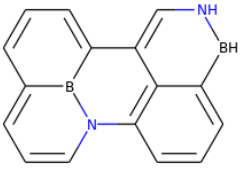
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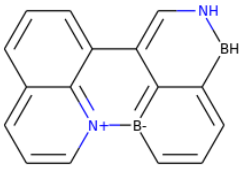	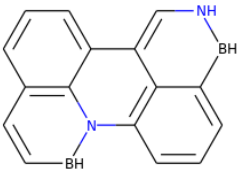	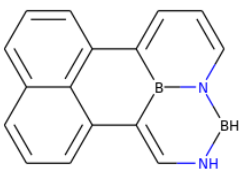	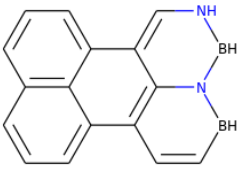	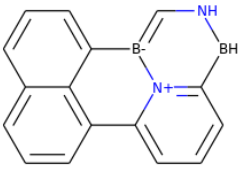
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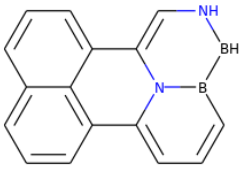	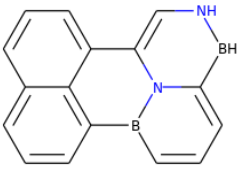	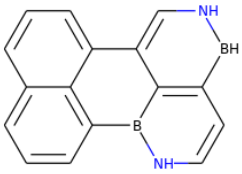	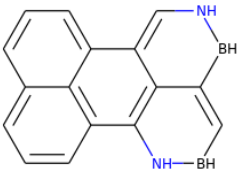	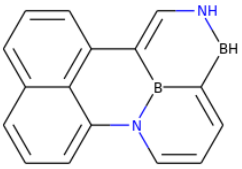
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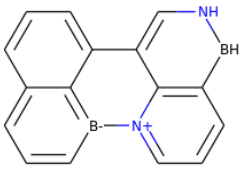	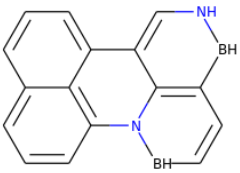	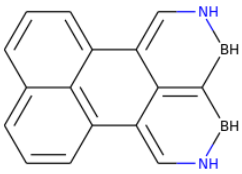	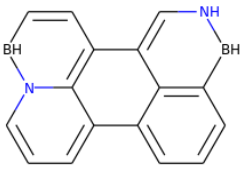	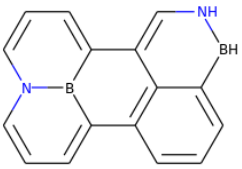
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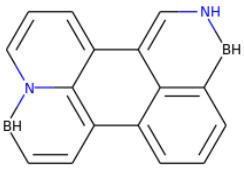	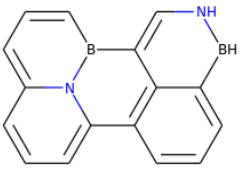	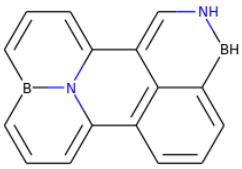	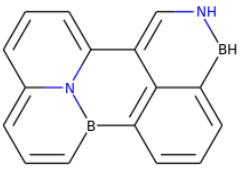	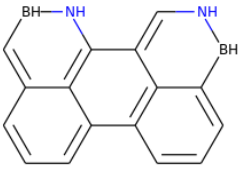
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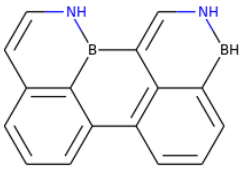	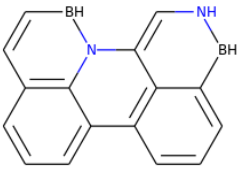	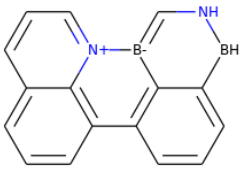	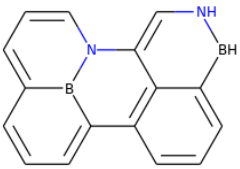	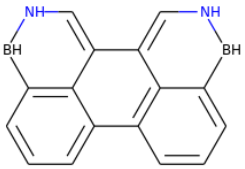

Column 1	Column 2	Column 3	Column 4	Column 5
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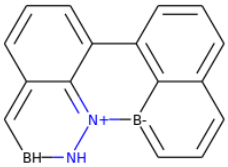	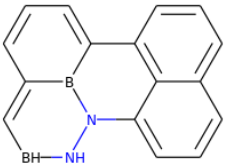	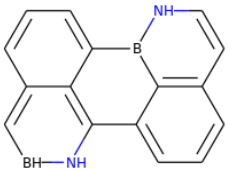	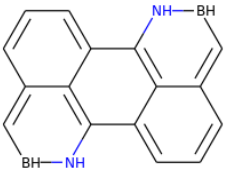	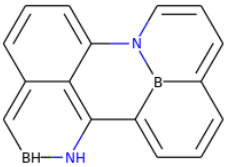
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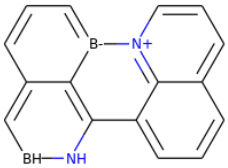
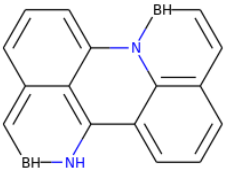
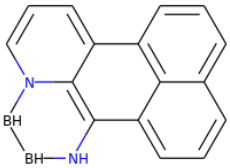
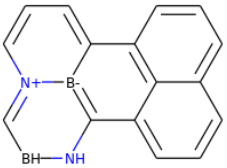
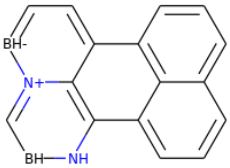
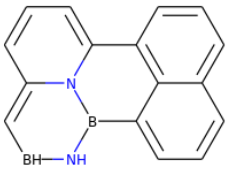
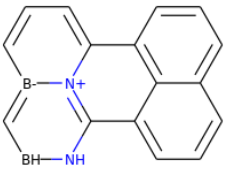
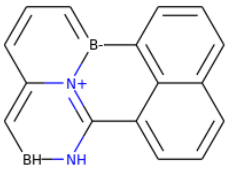
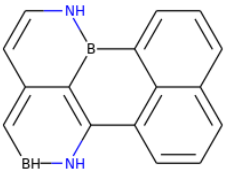
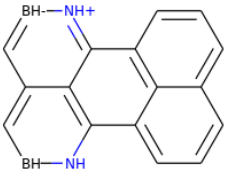
				
perylene-BN2-0157	perylene-BN2-0158	perylene-BN2-0159	perylene-BN2-0160	perylene-BN2-0161
				
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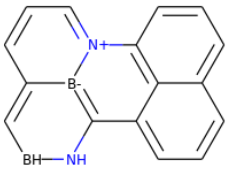	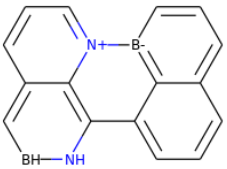	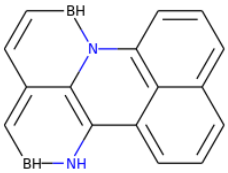	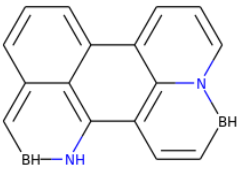	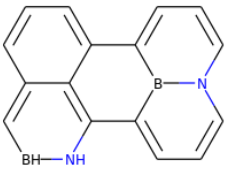
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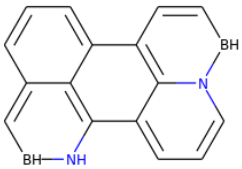	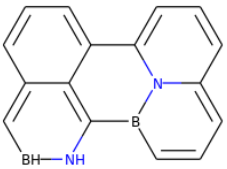	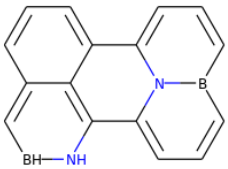	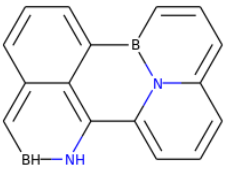	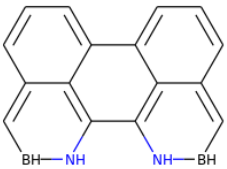
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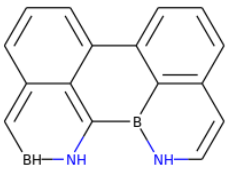	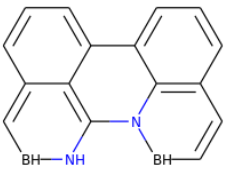	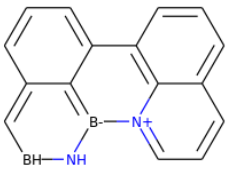	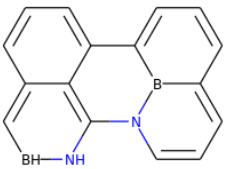	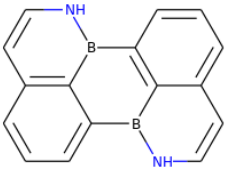
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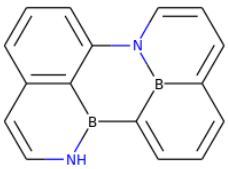	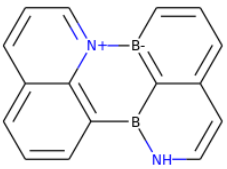	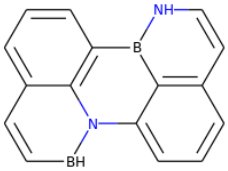	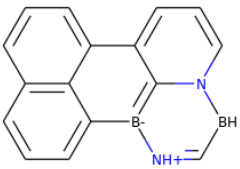	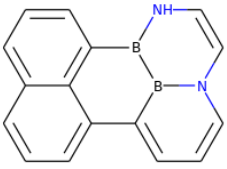
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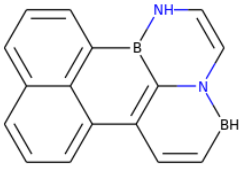	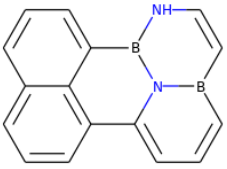	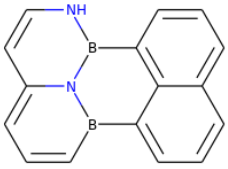	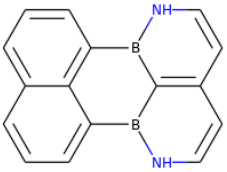	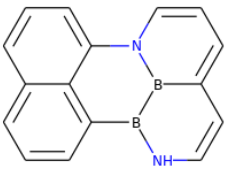

Column 1	Column 2	Column 3	Column 4	Column 5
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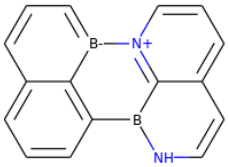	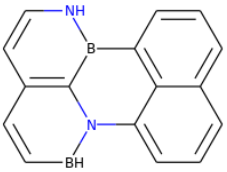	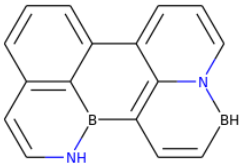	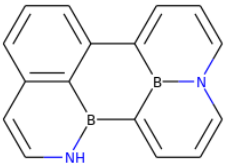	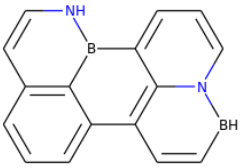
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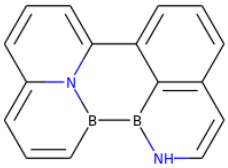	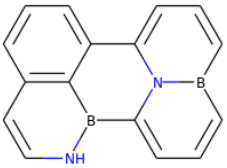	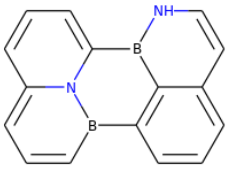	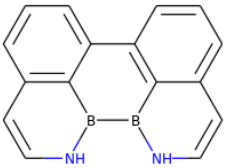	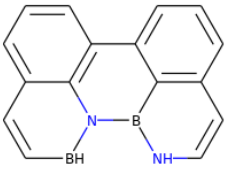
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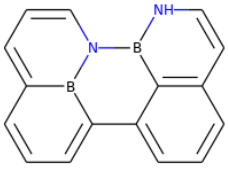	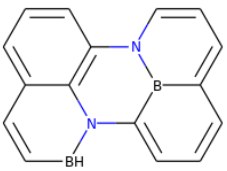	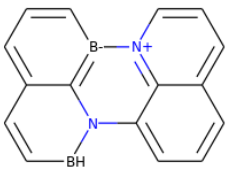	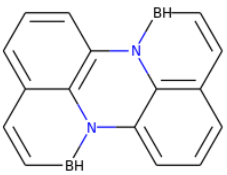	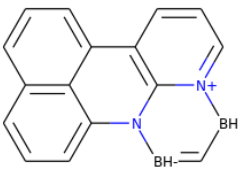
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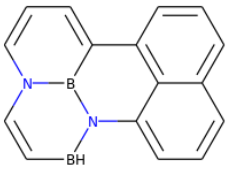
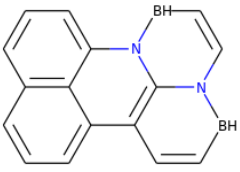
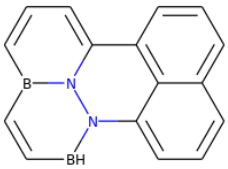
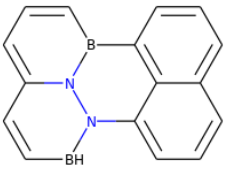
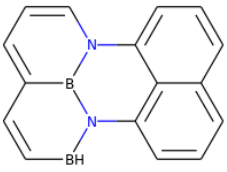
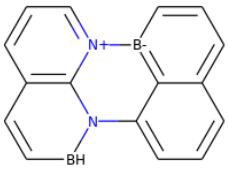
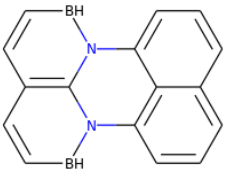
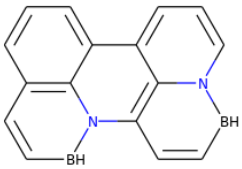
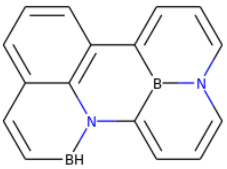
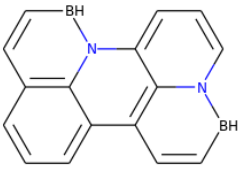
				
perylene-BN2-0207	perylene-BN2-0208	perylene-BN2-0209	perylene-BN2-0210	perylene-BN2-0211
				
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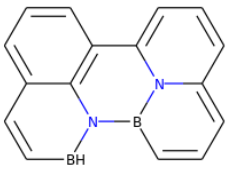	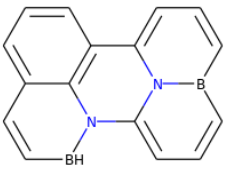	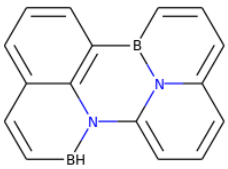	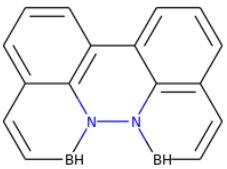	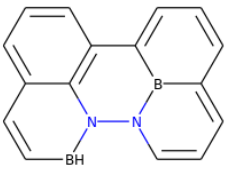
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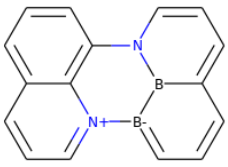	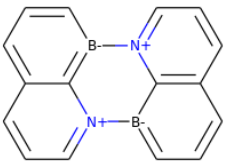	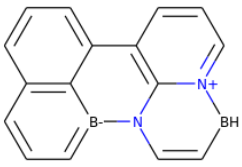	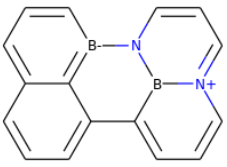	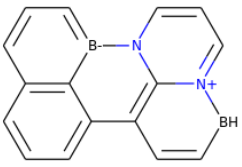
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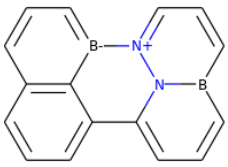	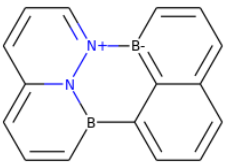	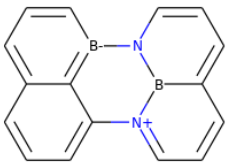	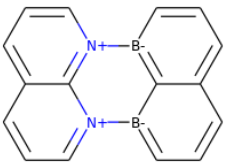	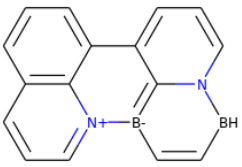

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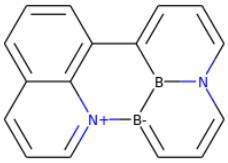	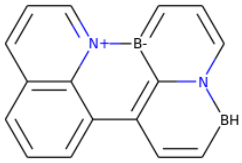	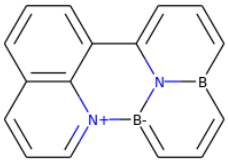	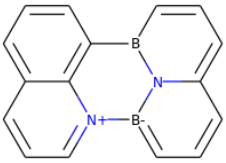	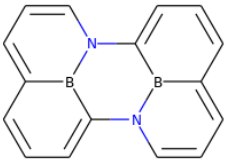
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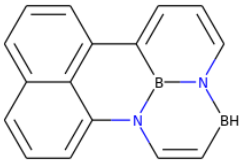	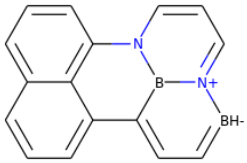	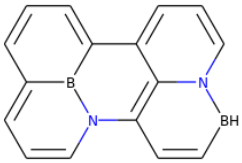	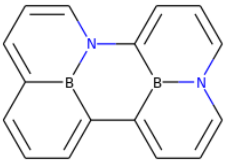	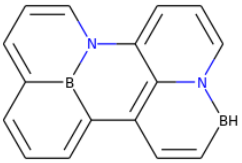
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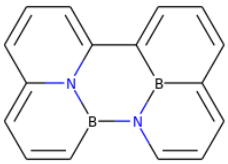	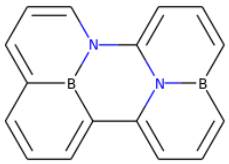	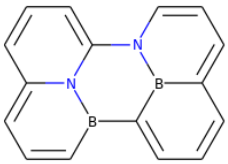	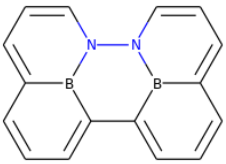	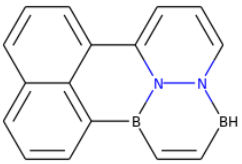
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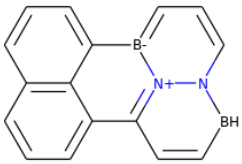	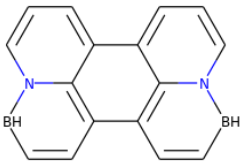	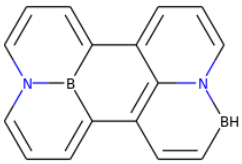	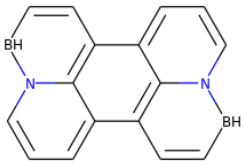	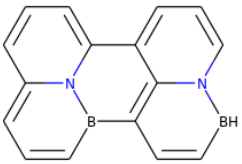
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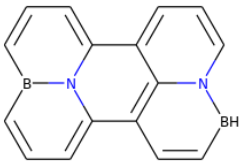	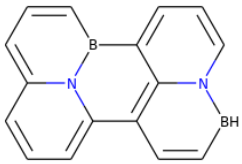	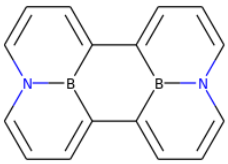	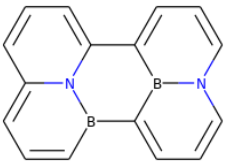	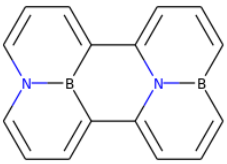
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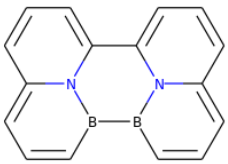
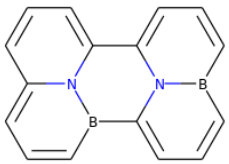
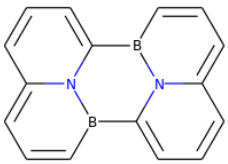
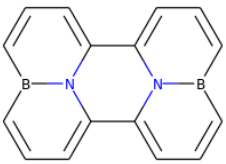
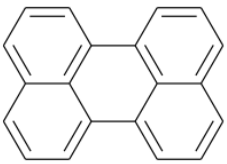
				

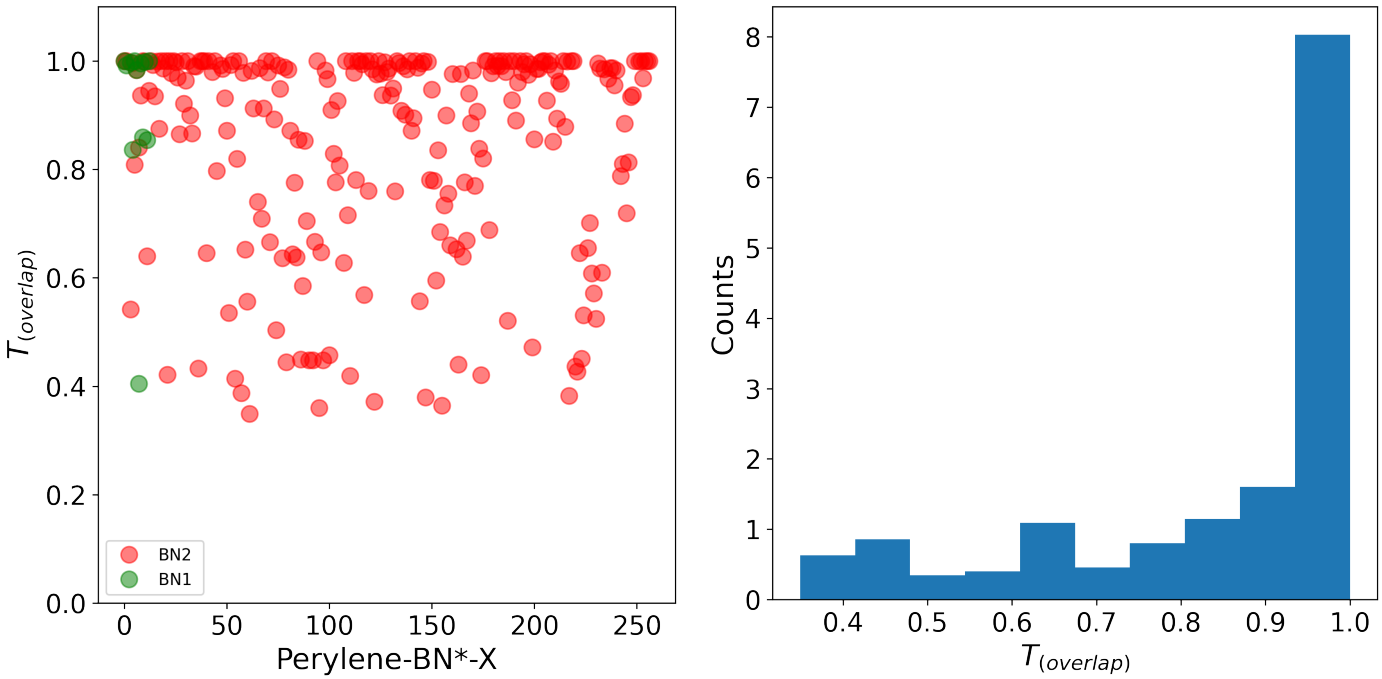


Fig. 4 (a)Maximum ($T_{(\text{overlap})}$) of BN doped and undoped perylene molecule, (b) Histogram of distribution of Max($T_{(\text{overlap})}$)

3 Appendix: Effect of Derivative on density matrix

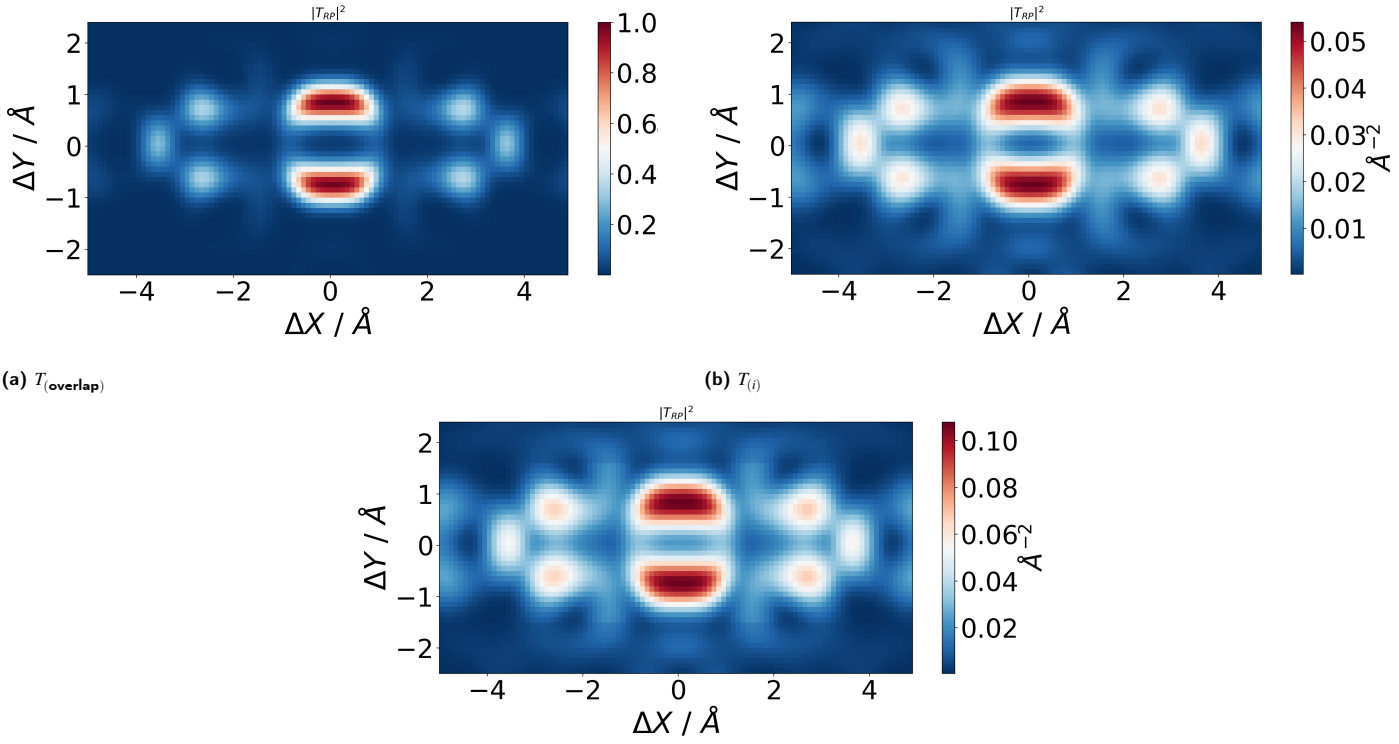
The $|T_{RP}|^2_{NAC}$ is calculated by using jacobian vector product of singlet exciton wave function $|S^*\rangle$ and biexciton wave function $|TT^*\rangle$. It is drastically influenced by various geometrical factors primarily bond distance, bond strength, stacking distance. For an optimal geometry the density matrix does not change for slight change in geometry therefore it's derivative is zero. While performing rigid scan the geometry of dimer is not optimal through out the scan. This effects value of $|T_{RP}|^2_{NAC}$. We addressed the effect of derivative on density matrix (DDM) on $|T_{RP}|^2_{NAC}$ and stacking position in this section. Scan of $|T_{RP}|^2_{NAC}$ is done with (i) ignoring the DDM ($T_{(i)}$) and (ii) considering DDM ($T_{(ii)}$) Where the DDM is calculated using automatic differentiation [1 2 3].

To study the correlation between $T(i)$ and $T(ii)$ the two $|T_{RP}|^2_{NAC}$ scan plots are merged. In both the cases all the scan points are factorised with their respective maximum and multiplied as shown by equation 1, where subscript x,y corresponds to the stacking position. The products are plotted showing the overlap of high $|T_{RP}|^2_{NAC}$ by both the method.

$$T_{(\text{overlap})x,y} = \frac{T_{(i)x,y}}{\text{Max}(T_{(i)})} \times \frac{T_{(ii)x,y}}{\text{Max}(T_{(ii)})} \tag{1}$$

When both methods show same stacking position of maximum $|T_{RP}|^2_{NAC}$, maximum $T_{(\text{overlap})}$ is 1 and it is lower than 1 when $T(i)$ and $T(ii)$ differ. Maximum of $T_{(\text{overlap})}$ of all the molecules and their distribution are shown in figure 4. It is closed to 1 for most of the molecules. Therefore both the methods predict similar stacking position for high $|T_{RP}|^2_{NAC}$. In perylene Max($T_{(\text{overlap})}$) is 1 so both the methods show exactly same stacking position for maximum $|T_{RP}|^2_{NAC}$. In BN2-150 Max($T_{(\text{overlap})}$) is slightly lower ie. 0.95 . It is because $T_{(ii)}$ is overestimated at fully stacked orientation. In BN2-100 has Max($T_{(\text{overlap})}$) of 0.46 because the two methods show very different maxima of $|T_{RP}|^2_{NAC}$. Though the second local maxima of $T(i)$ is the maxima of $T(ii)$ and vice versa.

Involving derivative on density matrix gives complete picture of $|T_{RP}|^2_{NAC}$ yet increases computation cost and causes computational failure due to lack of memory. Since, when SCF operation converges, it returns the density matrix with error ε. Due to this error in density matrix, error in calculation of $|T_{RP}|^2_{NAC}$ is induced.Thus highly converged density matrix is needed which adds in computational cost.

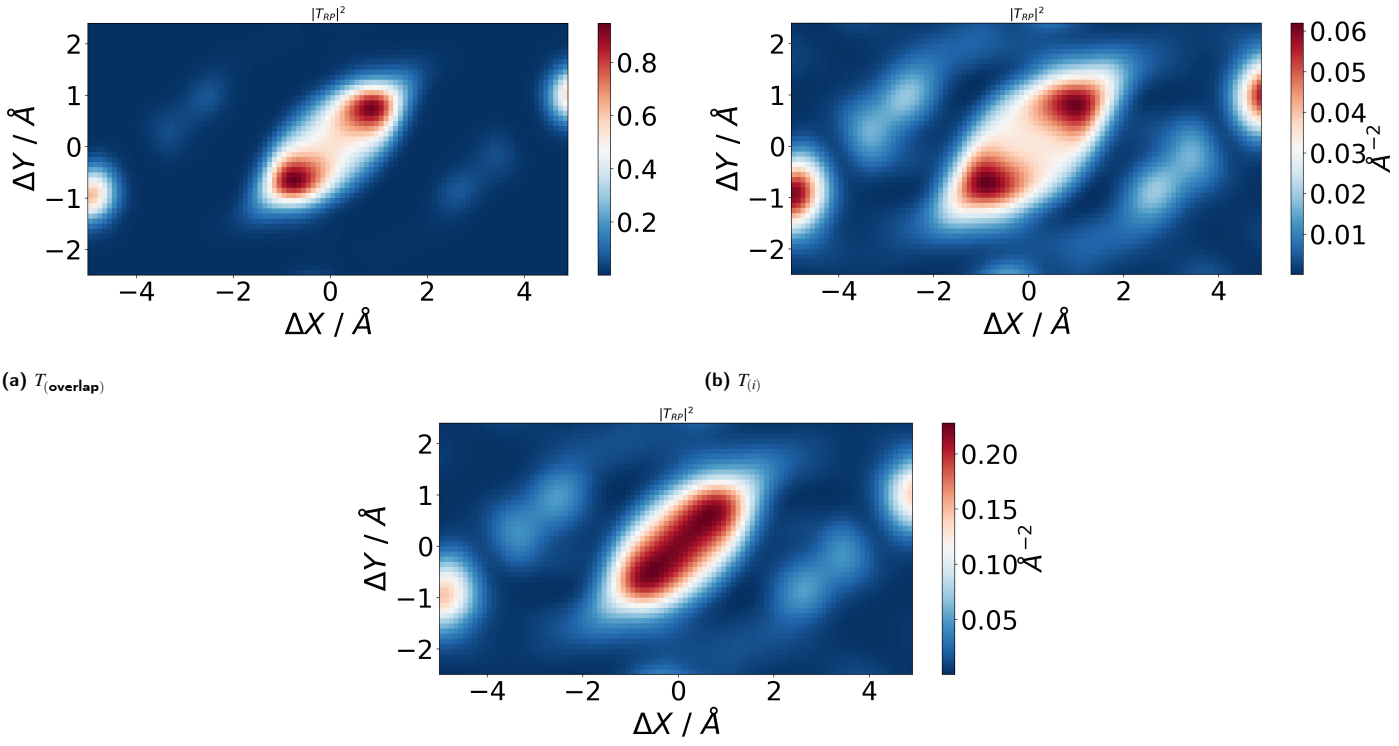


(a) $T_{(\mathbf{overlap})}$

(b) $T_{(i)}$

(c) $T_{(ii)}$

Fig. 5 Perylene Undoped

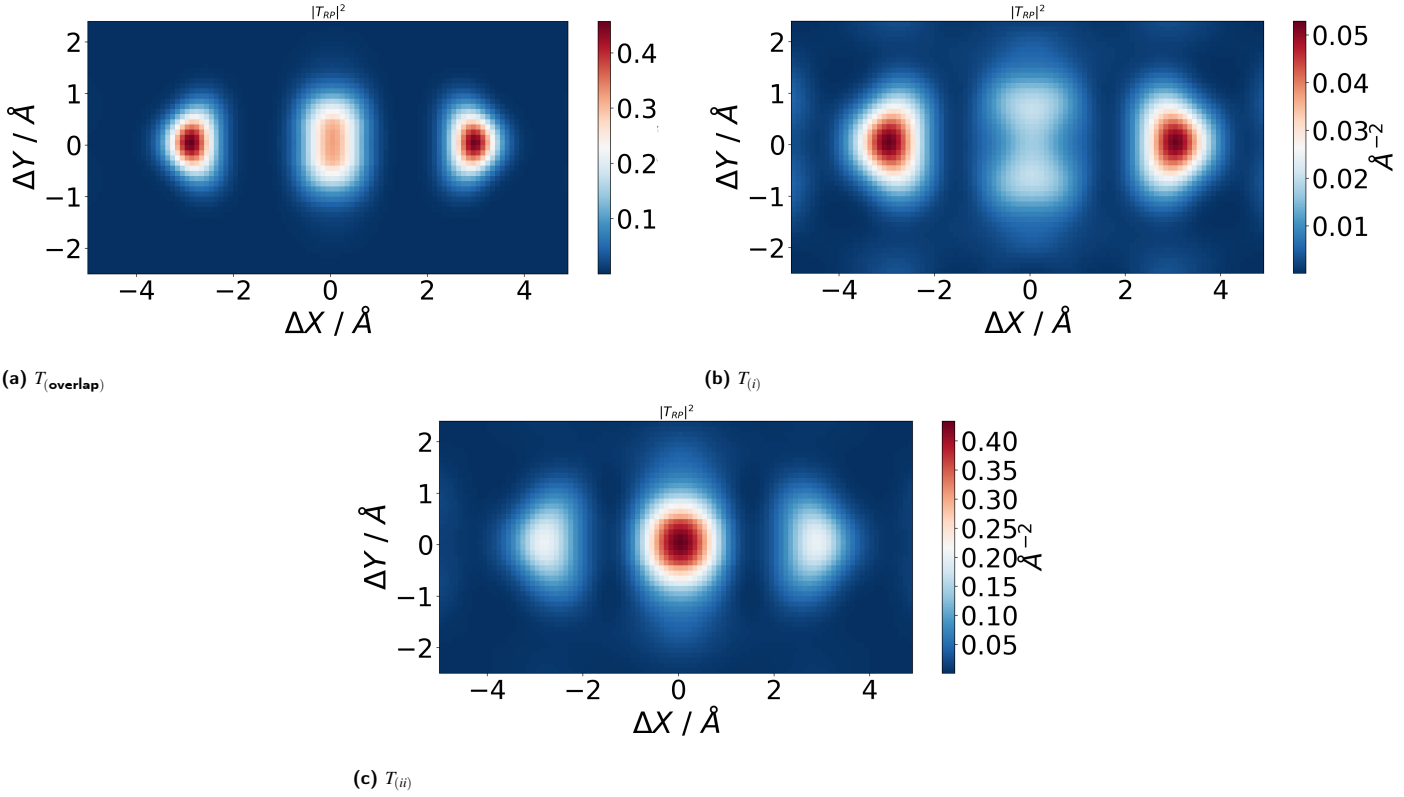


(a) $T_{(\mathbf{overlap})}$

(b) $T_{(i)}$

(c) $T_{(ii)}$

Fig. 6 BN2-150



(a) $T_{(\mathbf{overlap})}$

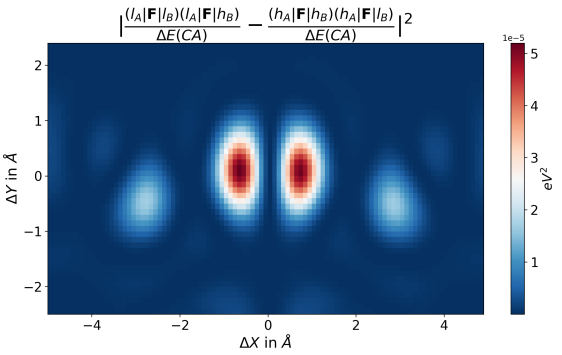
(b) $T_{(i)}$

(c) $T_{(ii)}$

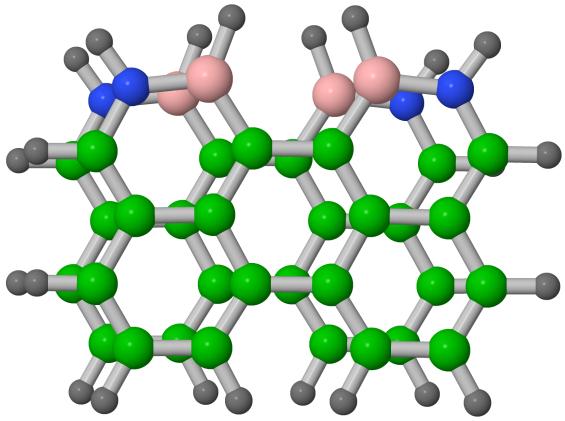
Fig. 7 BN2-100

4 Appendix: Rotation of Best molecule

The Rotation along the principle axis of molecule highly affect singlet fission .[4–6] In the case of BN2-112 rotation did not increase the singlet fission rate. BN2-112 upon rotation ,from rotation 0° (Fig. 8b) to 180° (Fig. 9b) the stacking position of the maximum of $|T_{RP}|^2$ changes from $\Delta X = \pm 0.7$ Å and $\Delta Y = 0.1$ Å (see Fig. 8a) to $\Delta X = \pm 2.7$ Å and $\Delta Y = -0.9$ Å(see Fig. 9a). Though the $|T_{RP}|^2$ reduces upon rotation.Then value $|T_{RP}|^2$ at $\Delta X = \pm 0.7$ Å and $\Delta Y = 0.1$ Å reduces drastically upon rotation from 0° to 180° where as $|T_{RP}|^2$ at $\Delta X = \pm 2.7$ Å and $\Delta Y = -0.9$ Å varies less.

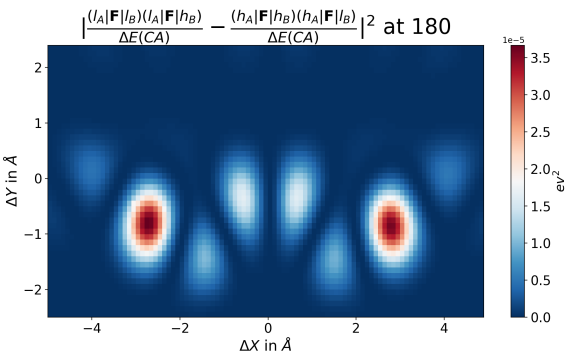


(a) $|T_{RP}|^2$

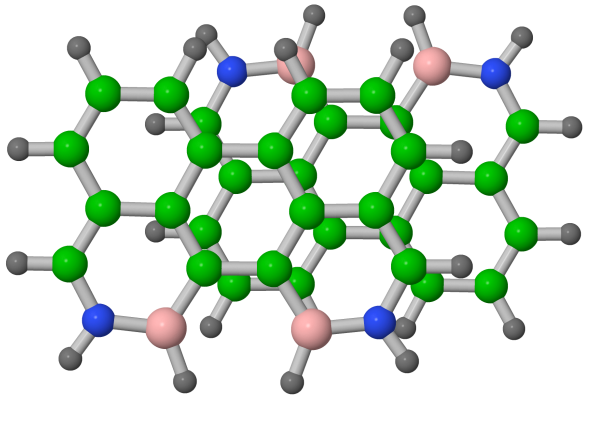


(b) Slipped stacked molecular structure

Fig. 8 BN2-112. at 0°



(a) $|T_{RP}|^2$



(b) Slipped stacked molecular structure

Fig. 9 BN2-112. at 180°

Table S2 :Maxima $|T_{RP}|^2_{NAC}$ Ignoring derivative on density matrix(DDM), with (DDM) and their ovelap

Molecule	Without DDM			With DDM			Overlap		
	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})
BN1-0	∓0.50	±0.80	0.19	∓0.50	±0.80	0.38	∓0.50	±0.80	1.00
BN1-1	∓1.30	∓0.90	0.20	∓1.20	∓0.90	0.39	∓1.20	∓0.90	0.99
BN1-2	±2.70	±0.80	0.07	0.00	0.00	0.32	±0.20	∓0.50	0.80
BN1-3	∓0.30	±0.90	0.13	∓0.20	±0.80	0.27	∓0.20	±0.80	1.00
BN1-4	±0.70	±0.80	0.09	0.00	0.00	0.34	∓0.60	∓0.60	0.84
BN1-5	∓3.60	±0.30	0.24	∓3.60	±0.30	0.48	∓3.60	±0.30	1.00
BN1-6	±0.40	∓0.80	0.13	±0.40	∓0.70	0.28	±0.40	∓0.80	0.98
BN1-7	±3.00	±0.10	0.12	0.00	0.00	1.04	±2.90	∓0.10	0.41
BN1-8	±0.40	±0.70	0.30	±0.30	±0.70	0.68	±0.40	±0.70	1.00
BN1-9	0.00	∓0.80	0.09	0.00	∓0.40	0.27	0.00	∓0.70	0.86
BN1-10	−0.50	±0.80	0.13	−0.40	±0.80	0.27	∓0.40	±0.80	1.00
BN1-11	±3.60	±0.10	0.10	0.00	0.50	0.29	0.00	±0.50	0.85
BN1-12	−0.50	±0.80	0.18	−0.50	±0.80	0.36	−0.50	±0.80	1.00
BN2-0	±1.70	±1.10	0.33	±1.70	±1.10	0.65	±1.70	±1.10	1.00
BN2-1	±0.20	∓0.80	0.18	±0.20	∓0.80	0.36	±0.20	∓0.80	1.00
BN2-2	±3.20	∓0.20	0.54	±3.20	∓0.10	1.67	±3.20	∓0.20	0.99
BN2-3	±2.10	±0.80	0.41	0.00	0.00	3.98	±0.80	±0.10	0.54
BN2-4	∓2.80	∓0.80	0.27	∓2.80	±0.70	0.55	±2.80	±0.70	1.00
BN2-5	∓0.80	∓0.70	0.12	0.00	0.00	0.46	∓0.60	∓0.60	0.81
BN2-6	±0.70	∓1.00	0.17	±0.60	∓0.90	0.31	±0.60	∓1.00	0.98
BN2-7	±0.50	∓0.70	0.10	0.00	0.00	0.43	±0.40	∓0.60	0.84
BN2-8	±1.20	±0.80	0.29	±0.50	∓0.40	0.61	±1.20	±0.80	0.94
BN2-9	∓1.00	±0.90	0.68	∓1.00	±0.90	1.17	∓1.00	±0.90	1.00
BN2-10	∓1.50	±0.90	1.29	±1.50	∓0.90	2.82	∓1.50	±0.90	1.00
BN2-11	∓2.80	±0.50	0.16	0.00	0.00	0.74	∓2.80	±0.50	0.64
BN2-12	∓1.20	±0.70	0.22	∓0.80	±0.70	0.43	∓1.10	±0.70	0.94
BN2-13	0.00	∓0.80	0.20	0.00	∓0.80	0.38	0.00	∓0.80	1.00
BN2-14	∓0.30	±0.90	0.12	∓0.30	±0.80	0.26	∓0.30	±0.90	0.99
BN2-15	±0.70	±0.90	0.12	±0.70	∓0.10	0.45	±0.90	∓0.10	0.93
BN2-16	∓0.50	±0.70	0.19	∓0.40	±0.70	0.37	∓0.50	±0.70	1.00
BN2-17	±3.80	∓0.20	0.11	0.40	0.40	0.26	3.80	∓0.20	0.87
BN2-18	∓0.20	±0.80	0.22	∓0.30	±0.80	0.42	∓0.20	±0.80	1.00
BN2-19	∓0.70	±0.80	0.12	∓0.50	±0.70	0.29	∓0.60	±0.80	0.99
BN2-20	∓2.20	∓1.00	1.68	∓2.20	∓1.00	4.15	∓2.20	∓1.00	1.00
BN2-21	∓3.00	±0.30	0.18	0.00	0.00	1.27	∓3.00	±0.30	0.42
BN2-22	∓1.50	∓0.60	0.44	∓1.50	∓0.60	0.84	∓1.50	∓0.60	1.00
BN2-23	∓0.70	∓0.60	0.20	∓0.60	∓0.50	0.47	∓0.70	∓0.50	0.98
BN2-24	±0.70	−0.80	1.80	±0.70	−0.80	3.69	±0.70	−0.80	1.00
BN2-25	∓0.10	∓0.80	0.18	∓0.20	∓0.80	0.33	∓0.20	∓0.80	1.00
BN2-26	±0.40	±0.60	0.13	0.30	±0.40	0.34	±0.40	±0.50	0.97
BN2-27	∓0.20	±0.90	0.12	0.00	0.10	0.39	−0.10	±0.70	0.86
BN2-28	∓0.80	±0.80	0.50	∓0.80	±0.80	1.08	∓0.80	±0.80	1.00
BN2-29	∓0.10	±0.70	0.13	0.00	±0.10	0.41	∓0.10	±0.60	0.92
BN2-30	∓0.10	±0.70	0.15	∓0.10	±0.50	0.42	∓0.10	±0.60	0.96
BN2-31	±0.80	∓1.00	0.62	±0.80	∓1.00	1.29	±0.80	∓1.00	1.00
BN2-32	0.00	∓0.70	0.14	0.00	∓0.10	0.46	0.00	∓0.60	0.90
BN2-33	∓0.90	±0.80	0.13	0.00	0.00	0.45	∓0.70	±0.70	0.87

Molecule	Without DDM			With DDM			Overlap		
	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})
BN2-34	∓1.50	±1.00	0.23	∓0.50	±0.90	0.47	∓0.50	±0.90	0.99
BN2-35	∓0.90	∓0.70	0.21	∓0.80	∓0.60	0.43	∓0.80	∓0.60	0.99
BN2-36	∓2.90	∓0.30	0.24	0.00	−0.10	1.52	0.00	−0.10	0.43
BN2-37	∓0.40	±0.70	0.65	∓0.40	±0.70	1.53	∓0.40	±0.70	1.00
BN2-38	±0.60	0.80	0.49	±0.60	0.80	0.82	±0.60	0.80	1.00
BN2-39	±1.40	∓0.90	0.41	±1.40	∓0.90	0.74	±1.40	∓0.90	1.00
BN2-40	∓2.80	±0.80	0.13	0.00	0.00	0.49	∓0.20	∓0.60	0.65
BN2-41	∓0.30	∓0.80	0.20	∓0.40	∓0.80	0.39	∓0.30	∓0.80	1.00
BN2-42	∓1.00	∓0.80	0.14	±0.70	±0.90	0.31	∓0.90	∓0.80	0.97
BN2-43	±1.40	±0.80	0.20	±1.30	±0.90	0.40	±1.30	±0.90	0.98
BN2-44	±1.20	±0.60	0.58	±1.20	±0.60	1.14	±1.20	±0.60	1.00
BN2-45	∓0.80	∓0.30	0.30	0.00	0.00	3.26	∓0.70	∓0.10	0.80
BN2-46	∓3.20	∓0.40	0.29	0.00	0.00	3.15	∓3.20	∓0.30	0.37
BN2-47	±0.70	∓0.40	0.31	±0.60	∓0.40	0.70	±0.70	∓0.40	0.99
BN2-48	±1.70	±1.00	0.77	±1.70	±1.10	1.62	±1.70	±1.10	0.99
BN2-49	±1.10	±0.90	0.16	±0.80	±0.70	0.53	±1.00	±0.80	0.93
BN2-50	∓1.10	∓0.70	0.18	±0.20	∓0.60	0.36	±0.20	∓0.70	0.87
BN2-51	±0.90	±0.80	0.11	0.00	0.00	0.49	±0.70	±0.80	0.54
BN2-52	±1.50	±1.00	0.41	±1.30	±1.00	0.87	±1.40	±1.00	0.99
BN2-53	∓1.00	∓0.90	0.61	∓1.00	∓0.90	1.47	∓1.00	∓0.90	1.00
BN2-54	±2.90	∓0.10	0.21	0.00	0.00	2.59	∓0.20	−0.30	0.41
BN2-55	∓0.80	∓0.90	0.13	0.20	−0.10	0.35	∓0.70	∓0.90	0.82
BN2-56	∓0.50	∓0.80	0.14	∓0.60	∓0.80	0.30	∓0.50	∓0.80	1.00
BN2-57	±3.10	∓0.50	0.12	0.00	0.00	1.17	±3.00	∓0.50	0.39
BN2-58	±0.70	∓0.60	1.67	±0.70	∓0.50	3.66	±0.70	∓0.60	0.98
BN2-59	∓0.60	∓1.00	0.16	0.00	0.00	1.59	−0.30	−0.80	0.65
BN2-60	±1.80	±1.20	0.32	0.00	0.00	8.04	0.00	0.00	0.56
BN2-61	∓3.00	∓0.30	0.11	0.00	0.00	1.13	∓2.90	∓0.30	0.35
BN2-62	∓1.20	∓0.70	0.33	∓1.10	∓0.60	0.72	∓1.10	∓0.70	0.98
BN2-63	∓0.60	∓0.90	0.13	−0.10	∓0.20	0.38	∓0.50	∓0.80	0.91
BN2-64	±1.50	±1.10	0.28	0.00	0.00	3.87	0.00	0.00	0.41
BN2-65	±1.00	±0.50	0.11	0.00	0.00	0.50	±0.50	±0.60	0.74
BN2-66	∓1.50	∓0.90	0.29	∓1.50	∓1.00	0.51	∓1.50	∓0.90	0.99
BN2-67	±1.00	±0.80	0.12	0.00	0.00	0.38	±0.70	±0.90	0.71
BN2-68	−3.80	±0.30	0.16	∓0.80	∓0.50	0.43	∓0.90	∓0.80	0.91
BN2-69	±1.10	±0.80	0.50	±1.10	±0.80	1.04	±1.10	±0.80	1.00
BN2-70	∓0.90	∓0.70	0.17	∓0.70	∓0.60	0.43	∓0.90	∓0.60	0.98
BN2-71	∓2.90	∓0.60	0.11	0.00	0.00	0.50	−0.50	±0.40	0.67
BN2-72	±1.00	±0.90	0.48	±1.00	±0.90	1.05	±1.00	±0.90	1.00
BN2-73	±1.40	±0.80	0.22	±0.80	±0.40	0.49	±1.20	±0.70	0.89
BN2-74	∓2.80	±0.50	0.18	0.00	0.00	0.92	∓2.80	±0.60	0.50
BN2-75	±3.50	∓0.50	0.26	∓3.50	±0.40	0.56	∓3.50	±0.40	0.99
BN2-76	±0.70	−0.70	0.21	0.50	∓0.60	0.51	±0.70	−0.60	0.95
BN2-77	±3.20	∓0.60	0.17	0.00	0.00	0.56	±3.10	∓0.60	0.64
BN2-78	±1.30	±0.80	0.24	±1.20	±0.90	0.44	±1.20	±0.90	0.99
BN2-79	±4.90	±1.10	0.25	0.00	0.10	2.90	±4.90	±1.10	0.44
BN2-80	∓0.50	±0.70	0.15	∓0.50	±0.60	0.40	∓0.50	±0.70	0.98
BN2-81	0.00	∓0.60	0.12	0.00	0.00	0.51	0.00	−0.40	0.87

Molecule	Without DDM			With DDM			Overlap		
	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})
BN2-82	∓0.80	∓0.80	0.07	0.00	−0.10	0.40	−0.10	−0.20	0.64
BN2-83	−2.70	−0.80	0.08	0.00	0.00	0.38	±0.20	−0.50	0.78
BN2-84	±3.20	±0.60	0.09	0.00	0.00	0.42	0.00	∓0.20	0.64
BN2-85	2.80	±0.80	0.10	0.00	0.00	0.46	0.20	∓0.50	0.86
BN2-86	±3.00	±0.40	0.13	0.00	∓0.10	1.26	±2.90	±0.40	0.45
BN2-87	∓2.70	∓0.80	0.13	0.00	0.00	0.45	∓2.80	∓0.70	0.59
BN2-88	0.00	±0.80	0.06	0.00	0.00	0.22	∓0.10	±0.60	0.85
BN2-89	∓3.00	∓0.30	0.12	0.00	0.00	0.44	∓2.90	∓0.30	0.70
BN2-90	±2.80	±0.20	0.09	0.00	0.00	0.70	0.00	0.40	0.45
BN2-91	±3.60	±0.20	0.08	0.00	0.00	0.24	±3.60	±0.20	0.66
BN2-92	∓2.80	∓0.60	0.22	0.00	0.00	1.45	±0.80	∓0.90	0.45
BN2-93	±3.00	±0.20	0.09	0.00	0.00	1.24	0.00	0.10	0.67
BN2-94	±3.50	±0.40	0.19	3.50	0.40	0.37	±3.50	±0.40	1.00
BN2-95	±2.80	±0.70	0.24	∓0.10	0.20	2.39	∓0.10	0.20	0.36
BN2-96	±3.00	±0.10	0.11	0.00	0.00	0.64	±2.90	±0.10	0.65
BN2-97	∓2.90	∓0.30	0.11	0.00	0.00	1.61	0.00	−0.10	0.45
BN2-98	0.00	∓0.80	0.10	0.00	∓0.70	0.21	0.00	∓0.70	0.98
BN2-99	±0.20	±0.90	0.09	0.00	∓0.60	0.21	0.00	±0.80	0.97
BN2-100	∓3.00	0.00	0.11	0.00	0.00	0.87	∓2.90	0.00	0.46
BN2-101	0.00	∓0.60	0.06	0.00	∓0.10	0.48	0.00	∓0.10	0.91
BN2-102	∓0.40	0.70	0.08	0.00	0.00	0.39	∓0.30	±0.60	0.83
BN2-103	0.00	∓0.80	0.06	0.00	0.00	0.37	0.00	−0.30	0.78
BN2-104	±0.20	−0.50	0.06	0.00	0.00	0.33	0.00	0.00	0.93
BN2-105	±2.70	±0.70	0.12	0.00	0.00	0.36	±2.70	±0.60	0.81
BN2-106	∓3.60	∓0.20	0.08	0.00	0.00	0.26	∓3.60	∓0.20	0.62
BN2-107	∓2.90	∓0.60	0.12	−0.10	±0.20	0.47	∓2.90	∓0.50	0.63
BN2-108	∓3.60	∓0.40	0.30	∓3.60	∓0.40	0.64	∓3.60	∓0.40	1.00
BN2-109	∓2.60	∓0.80	0.09	0.00	0.00	0.42	−0.10	±0.40	0.72
BN2-110	∓3.00	0.00	0.19	0.00	0.00	4.93	0.00	0.00	0.42
BN2-111	∓2.50	∓0.80	0.20	∓2.50	∓0.80	0.52	∓2.50	∓0.80	1.00
BN2-112	0.00	0.40	0.07	0.00	0.00	0.55	0.00	0.00	0.98
BN2-113	∓0.10	∓0.80	0.09	0.00	0.00	0.37	0.00	∓0.50	0.78
BN2-114	∓0.10	∓0.80	0.26	∓0.20	∓0.80	0.46	∓0.20	∓0.80	1.00
BN2-115	±0.20	∓0.80	0.17	±0.20	∓0.80	0.34	±0.20	∓0.80	1.00
BN2-116	±2.80	∓0.20	0.19	±2.80	∓0.10	0.62	±2.80	∓0.10	0.99
BN2-117	∓1.50	±1.00	0.13	±0.20	−0.10	0.48	∓1.40	±1.00	0.57
BN2-118	∓0.10	±0.80	0.31	∓0.10	±0.80	0.56	∓0.10	±0.80	1.00
BN2-119	∓0.20	∓0.70	0.10	0.00	0.00	0.41	−0.20	∓0.50	0.76
BN2-120	±0.30	∓1.00	0.16	±0.30	∓1.00	0.27	±0.30	∓1.00	1.00
BN2-121	0.00	±0.70	0.22	0.00	±0.60	0.56	0.00	±0.70	0.98
BN2-122	±2.90	∓0.10	0.10	0.00	0.00	1.39	0.00	0.00	0.37
BN2-123	±0.30	∓0.90	0.16	±0.30	∓0.80	0.31	±0.30	∓0.90	0.98
BN2-124	∓0.10	±0.80	0.15	∓0.20	±0.80	0.30	∓0.20	±0.80	1.00
BN2-125	∓0.20	±0.90	0.10	∓0.20	±0.80	0.22	∓0.20	±0.80	0.98
BN2-126	±0.20	∓1.10	0.36	±0.20	∓0.90	0.91	∓0.20	±1.10	0.94
BN2-127	∓2.80	±0.40	0.47	∓2.70	±0.50	0.83	∓2.70	±0.50	1.00
BN2-128	∓0.10	±0.80	0.10	∓0.10	±0.70	0.21	∓0.10	±0.70	0.98
BN2-129	±0.20	∓0.90	0.16	±0.20	∓0.80	0.29	±0.20	∓0.80	0.99

Molecule	Without DDM			With DDM			Overlap		
	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})
BN2-130	∓0.70	±0.80	0.09	∓0.40	0.40	0.26	∓0.60	±0.70	0.94
BN2-131	±0.30	∓0.80	0.16	0.40	∓0.50	0.41	±0.30	∓0.80	0.95
BN2-132	±2.50	±0.60	0.20	0.00	0.00	0.63	±2.50	±0.60	0.76
BN2-133	0.00	∓0.80	0.23	0.00	∓0.80	0.42	0.00	∓0.80	1.00
BN2-134	0.00	±0.90	0.19	0.00	±0.80	0.35	0.00	±0.80	1.00
BN2-135	0.00	∓0.90	0.13	0.00	∓0.60	0.32	0.00	∓0.70	0.91
BN2-136	∓0.50	±1.10	0.15	∓0.40	±1.00	0.30	∓0.50	±1.00	0.99
BN2-137	0.00	∓0.80	0.14	0.00	−0.50	0.36	0.00	∓0.70	0.90
BN2-138	∓0.20	±0.70	0.16	∓0.20	±0.60	0.42	∓0.20	±0.70	0.98
BN2-139	±0.60	∓0.90	0.23	±0.60	∓0.90	0.48	±0.60	∓0.90	1.00
BN2-140	0.00	±0.70	0.16	0.00	0.00	0.53	0.00	±0.50	0.87
BN2-141	±0.70	∓0.90	0.11	0.30	−0.30	0.41	±0.50	∓0.70	0.89
BN2-142	±3.40	±0.50	0.28	±3.40	±0.50	0.48	±3.40	±0.50	1.00
BN2-143	0.00	±0.80	0.14	0.00	±0.70	0.26	0.00	±0.80	0.99
BN2-144	∓0.60	±1.40	0.24	0.00	0.00	3.22	∓0.10	0.30	0.56
BN2-145	∓0.40	±0.80	0.56	∓0.30	±0.70	1.29	∓0.40	±0.70	1.00
BN2-146	0.00	±0.80	0.20	0.00	±0.80	0.37	0.00	±0.80	1.00
BN2-147	∓5.00	∓0.90	0.16	0.00	0.00	1.74	∓5.00	∓0.90	0.38
BN2-148	∓0.70	−0.60	0.13	∓0.80	∓0.40	0.28	∓0.70	∓0.60	1.00
BN2-149	∓1.40	∓1.00	0.18	0.00	0.00	0.54	∓0.90	∓0.80	0.78
BN2-150	∓0.90	∓0.80	0.12	∓0.60	∓0.50	0.46	∓0.80	∓0.70	0.95
BN2-151	∓0.60	∓0.80	0.10	0.00	0.00	0.38	∓0.50	∓0.70	0.78
BN2-152	∓0.90	∓1.20	0.13	0.00	−0.10	2.82	0.00	−0.10	0.60
BN2-153	∓0.60	∓0.60	0.08	0.00	0.00	0.39	0.00	0.00	0.83
BN2-154	∓0.40	∓0.80	0.05	0.00	0.00	0.34	±0.20	−0.10	0.68
BN2-155	±2.70	∓0.70	0.23	0.00	0.00	1.68	0.00	±0.10	0.36
BN2-156	∓0.40	∓0.80	0.10	0.00	0.00	1.85	∓0.10	−0.20	0.73
BN2-157	±3.60	0.00	0.07	0.40	0.50	0.17	±0.40	±0.60	0.90
BN2-158	±0.30	±1.00	0.15	0.00	0.00	0.81	±0.30	±0.70	0.76
BN2-159	±3.00	∓0.50	0.16	0.00	0.00	0.65	±3.00	∓0.40	0.66
BN2-160	±0.30	±0.80	0.13	±0.50	±0.70	0.30	±0.40	±0.70	0.98
BN2-161	0.00	±0.70	0.11	0.00	0.00	2.06	0.00	0.00	0.91
BN2-162	±2.70	∓0.80	0.18	0.00	0.00	5.48	0.00	0.00	0.65
BN2-163	∓2.90	∓0.10	0.12	0.00	0.00	0.85	∓2.90	∓0.10	0.44
BN2-164	∓1.10	∓0.70	0.19	∓0.90	∓0.50	0.46	∓1.00	∓0.60	0.98
BN2-165	±2.70	∓0.60	0.09	0.00	0.00	0.45	∓0.30	−0.20	0.64
BN2-166	∓0.90	∓0.80	0.10	0.00	0.00	0.41	∓0.70	∓0.70	0.78
BN2-167	∓0.90	∓0.80	0.08	0.00	0.00	0.38	∓0.50	∓0.70	0.67
BN2-168	±3.60	∓0.20	0.17	0.00	0.00	0.44	±3.60	∓0.20	0.94
BN2-169	∓0.80	∓0.80	0.12	±0.30	±0.30	0.40	∓0.60	∓0.70	0.89
BN2-170	±1.00	±0.70	0.17	±0.80	±0.60	0.46	±0.90	±0.70	0.98
BN2-171	±3.50	0.00	0.09	0.00	0.00	0.51	0.00	±0.10	0.77
BN2-172	±3.80	0.00	0.19	0.00	0.00	0.46	±3.80	0.00	0.91
BN2-173	∓0.90	∓0.50	0.12	0.00	0.00	0.43	∓0.70	∓0.40	0.84
BN2-174	±4.90	±1.10	0.36	0.00	0.10	5.46	±4.90	±1.10	0.42
BN2-175	±0.80	±0.50	0.08	0.00	0.00	0.28	±0.70	±0.50	0.82
BN2-176	∓3.70	±0.40	2.57	∓3.70	±0.40	5.68	∓3.70	±0.40	1.00
BN2-177	∓1.40	±0.80	9.05	∓1.40	±0.80	26.42	∓1.40	±0.80	1.00

Molecule	Without DDM			With DDM			Overlap		
	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})
BN2-178	±2.80	∓0.40	0.20	0.00	0.00	0.81	±2.90	∓0.30	0.69
BN2-179	±0.60	∓0.70	0.18	±0.60	∓0.60	0.34	±0.70	∓0.60	0.98
BN2-180	∓0.20	∓1.10	0.37	∓0.20	∓0.90	0.82	∓0.20	∓1.00	0.99
BN2-181	∓0.20	∓0.90	0.36	∓0.20	∓0.90	0.69	∓0.20	∓0.90	1.00
BN2-182	0.00	∓0.90	0.14	0.00	∓0.80	0.28	0.00	∓0.90	0.99
BN2-183	∓0.40	∓0.80	0.14	∓0.40	∓0.80	0.29	∓0.40	∓0.80	1.00
BN2-184	∓3.50	±0.40	0.21	±3.60	∓0.40	0.42	∓3.60	±0.40	0.99
BN2-185	∓3.80	0.00	0.73	∓3.80	0.00	1.67	∓3.80	0.00	1.00
BN2-186	±0.80	0.00	0.25	±0.60	∓0.10	0.66	±0.70	∓0.10	0.98
BN2-187	±3.10	∓0.60	0.19	0.00	0.00	0.91	±3.00	∓0.50	0.52
BN2-188	∓1.50	∓0.80	0.16	∓1.50	∓0.80	0.32	∓1.50	∓0.80	1.00
BN2-189	∓3.60	±0.20	0.17	∓0.30	∓0.50	0.45	∓0.30	∓0.60	0.93
BN2-190	±1.80	±1.20	0.30	±1.80	±1.20	0.61	±1.80	±1.20	1.00
BN2-191	0.00	±0.80	0.17	0.00	0.20	0.51	0.00	±0.70	0.89
BN2-192	∓0.10	±0.70	0.20	∓0.20	±0.30	0.53	∓0.10	±0.60	0.96
BN2-193	∓0.60	±0.90	0.64	∓0.60	±0.90	1.27	∓0.60	±0.90	1.00
BN2-194	±0.40	±0.60	0.41	±0.40	0.50	1.07	±0.40	±0.50	0.98
BN2-195	±3.80	0.00	0.55	±3.80	∓0.10	1.06	±3.80	0.00	0.99
BN2-196	∓1.60	∓1.00	0.21	∓1.60	∓1.00	0.40	∓1.60	∓1.00	1.00
BN2-197	∓0.30	±0.60	0.53	−0.20	±0.50	1.48	∓0.30	±0.50	0.97
BN2-198	∓0.30	∓0.70	0.32	∓0.30	∓0.60	0.75	∓0.30	∓0.60	0.99
BN2-199	∓0.50	∓1.50	0.10	0.00	0.00	1.30	0.00	−0.20	0.47
BN2-200	±1.10	∓0.60	0.18	0.00	0.00	0.41	±0.90	∓0.50	0.86
BN2-201	∓0.90	±0.20	0.32	∓0.80	±0.30	0.86	∓0.80	±0.30	0.99
BN2-202	∓0.30	±0.80	0.12	∓0.30	±0.70	0.25	∓0.30	±0.80	0.99
BN2-203	0.00	∓0.90	0.37	0.00	∓0.80	0.75	0.00	∓0.80	1.00
BN2-204	−2.70	0.20	36.88	−2.70	0.20	88.62	−2.70	0.20	1.00
BN2-205	±3.00	∓0.10	12.86	±3.00	∓0.10	30.96	±3.00	∓0.10	1.00
BN2-206	±0.60	∓0.70	0.21	∓0.70	±0.50	0.67	±0.70	∓0.60	0.93
BN2-207	±2.80	∓0.10	0.14	±2.80	0.00	0.47	±2.80	∓0.10	0.99
BN2-208	2.70	±0.70	3.92	2.70	±0.70	6.65	2.70	±0.70	1.00
BN2-209	0.00	±0.80	0.12	0.00	0.00	0.40	0.00	±0.60	0.85
BN2-210	0.00	±0.90	0.17	±0.30	±0.60	0.38	±0.20	±0.80	0.98
BN2-211	0.00	∓0.80	0.10	0.00	∓0.20	0.27	±0.20	∓0.60	0.89
BN2-212	±0.30	∓0.60	0.12	0.30	−0.40	0.33	0.30	−0.50	0.96
BN2-213	−4.90	0.50	18.79	∓2.40	−0.50	43.90	−4.90	0.50	0.96
BN2-214	∓3.00	0.10	17.53	−3.00	0.10	48.49	−3.00	0.10	1.00
BN2-215	∓0.70	∓0.50	0.13	0.00	0.00	0.32	−0.50	±0.50	0.88
BN2-216	∓0.20	−2.50	2.19	∓0.10	−2.50	4.68	∓0.10	−2.50	1.00
BN2-217	∓3.00	−0.10	0.18	0.00	0.00	3.26	0.00	±0.10	0.38
BN2-218	∓2.90	∓0.10	0.42	∓2.90	∓0.10	1.16	∓2.90	∓0.10	1.00
BN2-219	∓2.70	∓0.50	0.12	∓2.70	∓0.40	0.36	∓2.70	∓0.40	1.00
BN2-220	∓2.90	±0.40	0.12	0.00	0.00	1.66	0.00	∓0.10	0.44
BN2-221	∓2.80	±0.30	0.14	0.00	0.10	1.56	0.00	∓0.10	0.43
BN2-222	∓2.90	0.00	0.16	0.00	0.00	0.81	∓2.90	0.00	0.65
BN2-223	∓2.90	±0.10	0.12	0.00	0.00	1.83	0.00	0.00	0.45
BN2-224	∓2.80	±0.60	0.11	0.00	0.00	0.75	∓2.80	±0.50	0.53
BN2-225									

Molecule	Without DDM			With DDM			Overlap		
	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})	x (Å)	y (Å)	$\lvert T_{RP}\rvert^2_{NAC}$ (Å^{-2})
BN2-226	±0.20	∓1.30	0.22	0.00	0.00	6.82	0.00	−0.30	0.65
BN2-227	∓3.00	0.00	0.25	0.00	0.00	1.34	∓3.00	∓0.10	0.70
BN2-228	±0.50	±1.40	0.07	0.00	0.00	1.05	0.00	0.00	0.61
BN2-229	±2.70	∓0.30	0.14	0.00	±0.10	2.58	0.00	±0.10	0.57
BN2-230	±3.00	±0.40	0.11	0.00	0.00	0.69	±3.00	±0.30	0.52
BN2-231	±0.90	∓0.40	2.70	±0.90	∓0.50	8.52	±0.90	∓0.50	1.00
BN2-232	0.00	±0.80	0.13	∓0.10	±0.70	0.29	0.00	±0.80	0.99
BN2-233	∓2.70	∓0.20	0.05	0.00	0.00	0.76	−0.10	0.30	0.61
BN2-234	±4.80	∓0.60	0.13	∓0.10	±0.50	0.33	±4.80	∓0.60	0.98
BN2-235	±0.60	±0.50	0.57	±0.50	±0.50	1.40	±0.60	±0.50	0.99
BN2-236	0.00	±0.80	0.13	0.00	±0.60	0.35	0.00	±0.70	0.97
BN2-237	±0.20	∓0.70	0.14	±0.30	∓0.60	0.42	±0.20	∓0.70	0.99
BN2-238	∓0.30	∓0.70	0.35	∓0.30	∓0.60	0.90	∓0.40	∓0.60	0.99
BN2-239	±0.20	±0.60	0.09	∓0.10	0.30	0.28	0.00	±0.50	0.96
BN2-240	±0.50	0.80	0.23	0.30	±0.70	0.63	±0.50	0.70	0.98
BN2-241	∓0.10	∓0.60	0.06	0.00	0.00	0.22	0.00	∓0.30	0.88
BN2-242	±0.50	∓0.30	0.09	0.00	0.00	1.00	0.20	−0.20	0.79
BN2-243	0.00	∓0.70	0.08	0.00	−0.20	0.42	0.00	−0.30	0.81
BN2-244	±0.20	±0.90	0.12	0.00	±0.50	0.34	±0.20	±0.80	0.88
BN2-245	∓0.40	∓1.10	0.07	0.00	0.00	0.28	0.00	∓0.30	0.72
BN2-246	0.00	±0.70	0.06	0.00	0.00	0.28	−0.10	0.40	0.81
BN2-247	0.00	±0.80	0.11	0.00	∓0.50	0.33	0.00	±0.70	0.93
BN2-248	∓0.20	±0.70	0.12	∓0.10	0.30	0.36	∓0.20	±0.50	0.94
BN2-249	±1.80	−1.30	8.01	±1.80	−1.30	22.02	±1.80	−1.30	1.00
BN2-250	±3.70	∓0.10	0.10	0.00	−0.40	0.33	0.20	−0.50	0.87
BN2-251	∓0.70	−0.90	1.20	∓0.70	−0.80	2.77	∓0.70	−0.80	1.00
BN2-252	2.90	0.00	6.35	2.90	0.00	17.94	2.90	0.00	1.00
BN2-253	0.00	±0.70	0.16	0.20	0.40	0.45	±0.20	±0.60	0.97
BN2-254	±3.80	±0.10	0.59	±3.80	±0.10	1.42	±3.80	±0.10	1.00
BN2-255	0.70	∓0.90	0.17	0.70	∓0.90	0.33	0.70	∓0.90	1.00
perylene-undoped	0.00	±0.80	0.11	0.00	±0.80	0.22	0.00	±0.80	1.00

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