Supporting Information

Charge-driven stability and aromaticity of $C_2N_2B_2H_4$ isomers:

Insights from a combined DFT and machine learning study

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1. List of all possible isomers of molecular formula $(HCNBH)_2$

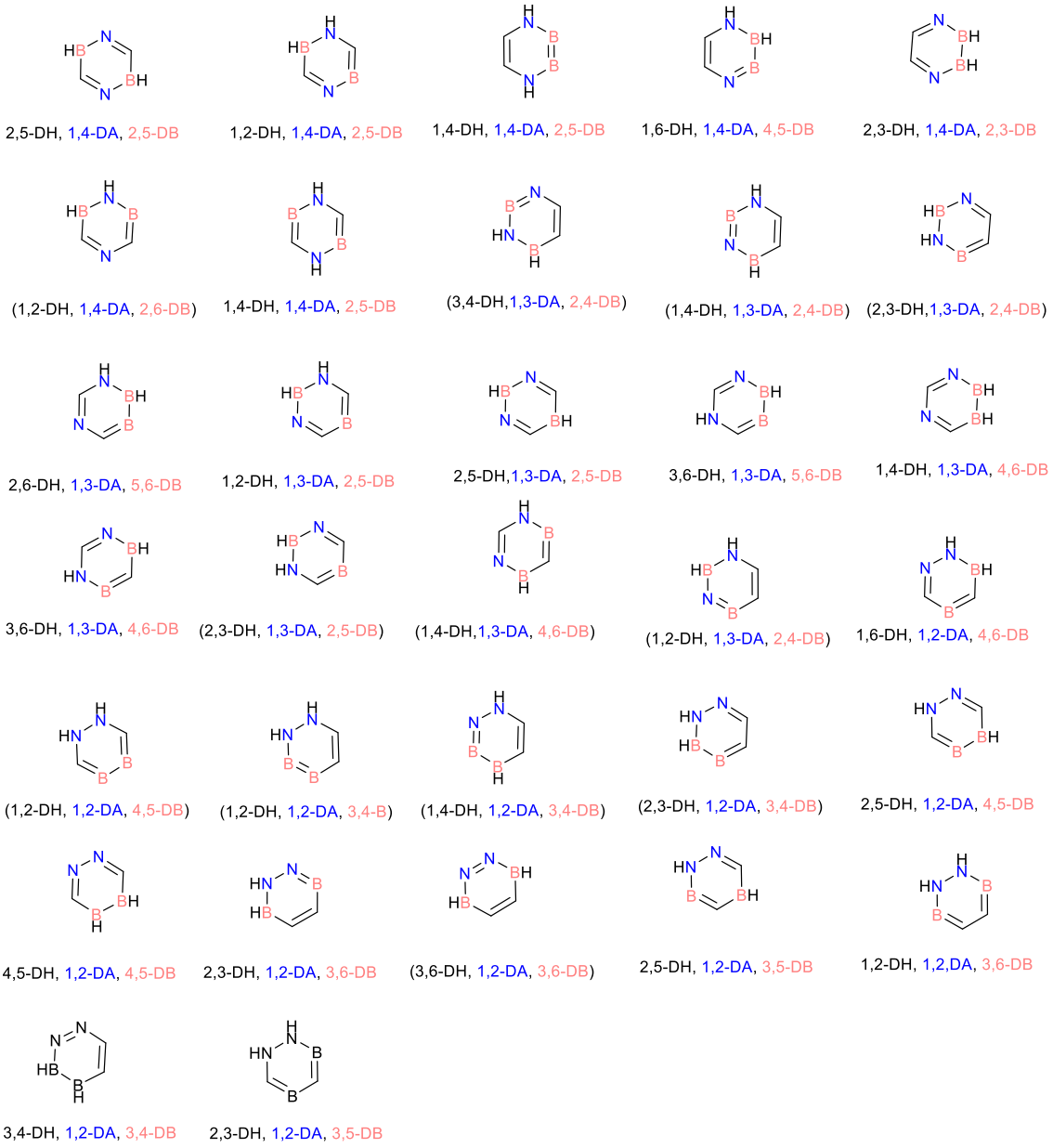

Figure S1. The list of all possible isomers refers to the molecular formula $(HCNBH)_2$.

2. Bond lengths and molecular geometries of 1−13

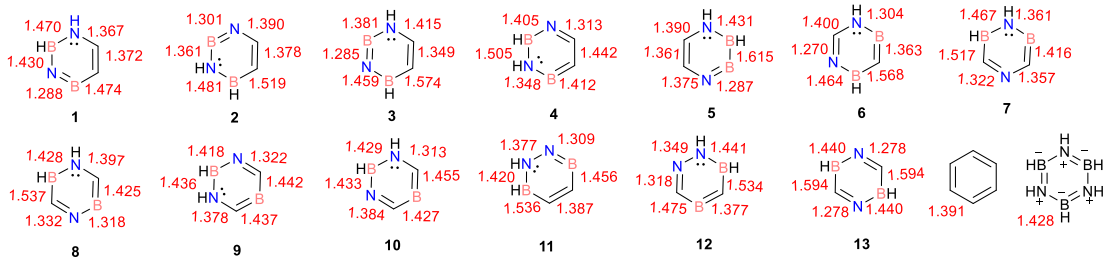

Figure S2. Bond length of **1−13** in the S_0 state.

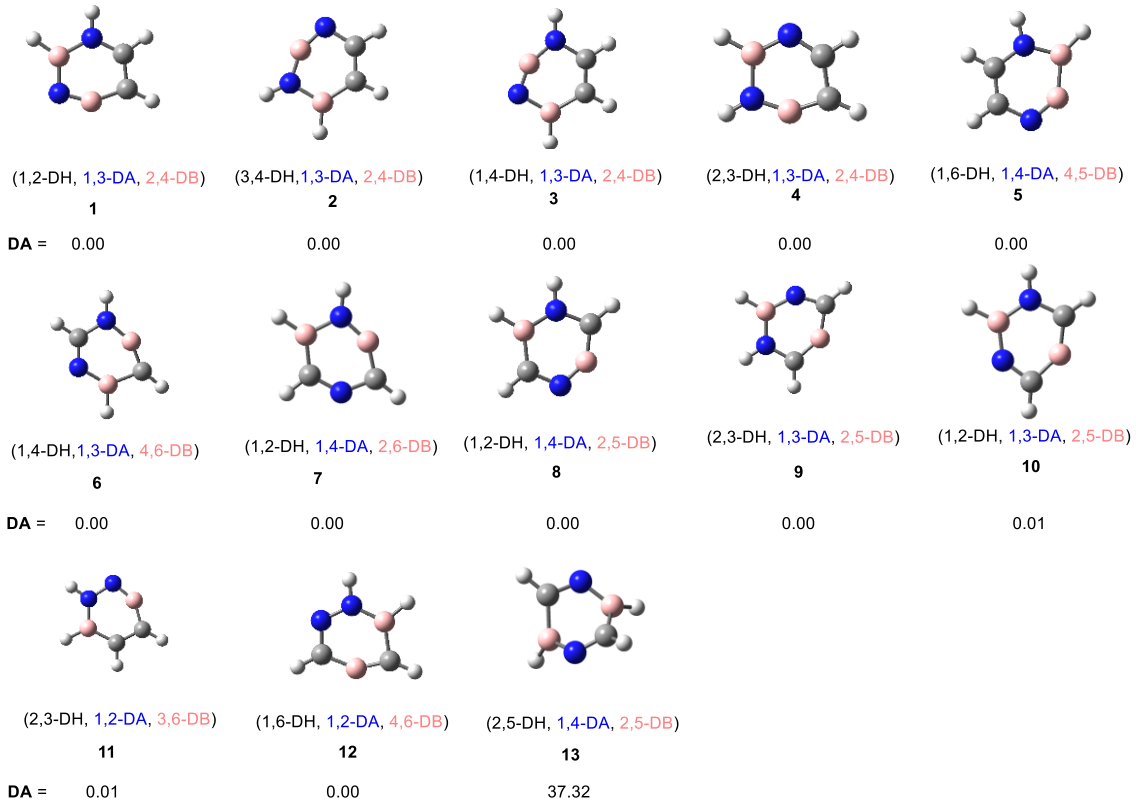

Figure S3. Optimized geometries of the thirteen most stable isomers (**1−13**) in the S_0 state (DA = dihedral angle).

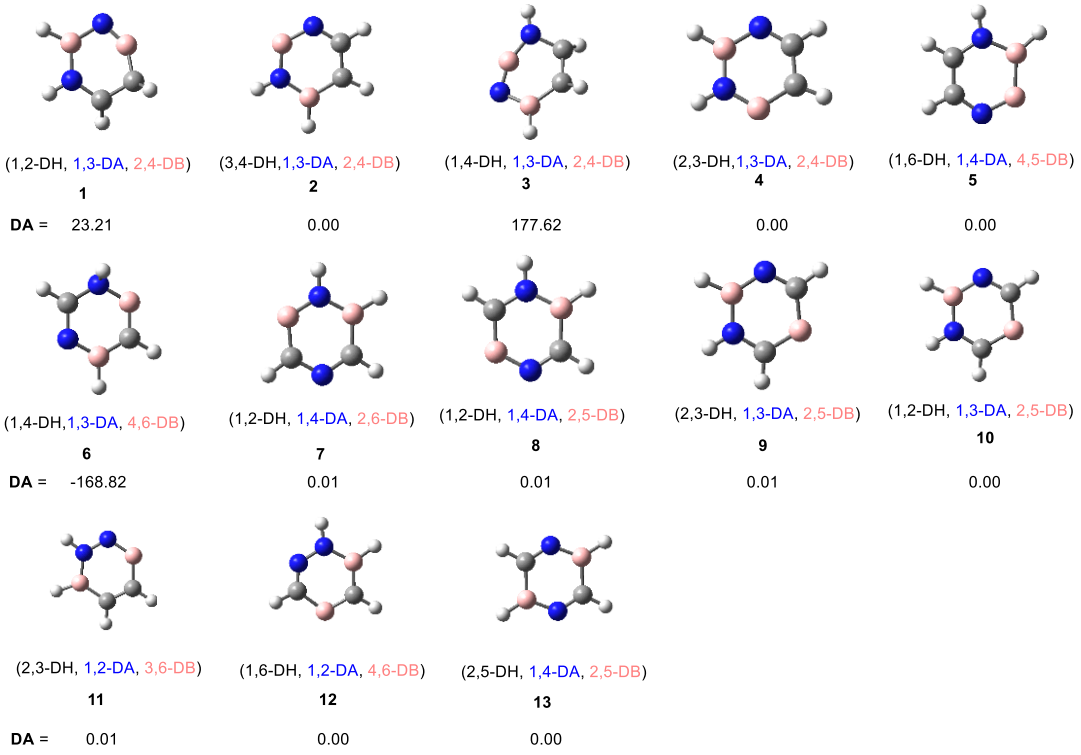

Figure S4. Optimized geometries of the thirteen most stable isomers (**1**−**13**) in the T_1 state (DA = dihedral angle).

3. Correlation analysis between aromaticity indexes

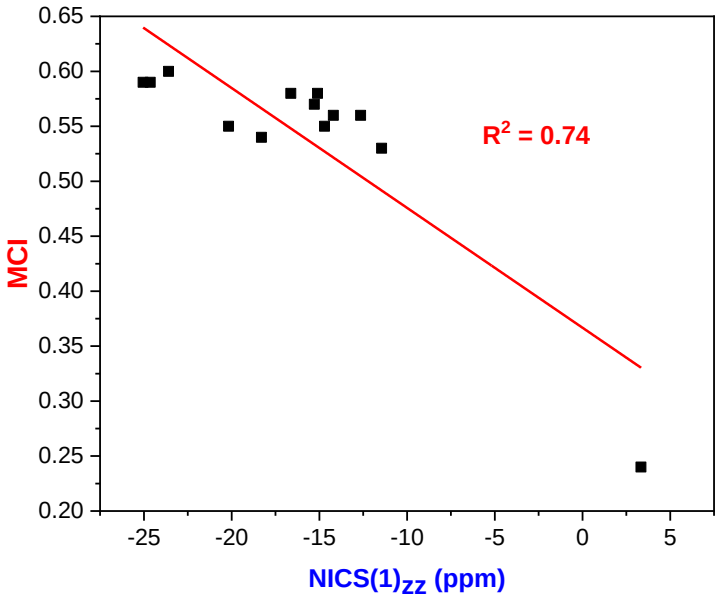

Figure S5. Correlation between MCI and $NICS(1)_{zz}$ values of **1**−**13** in S_0 state.

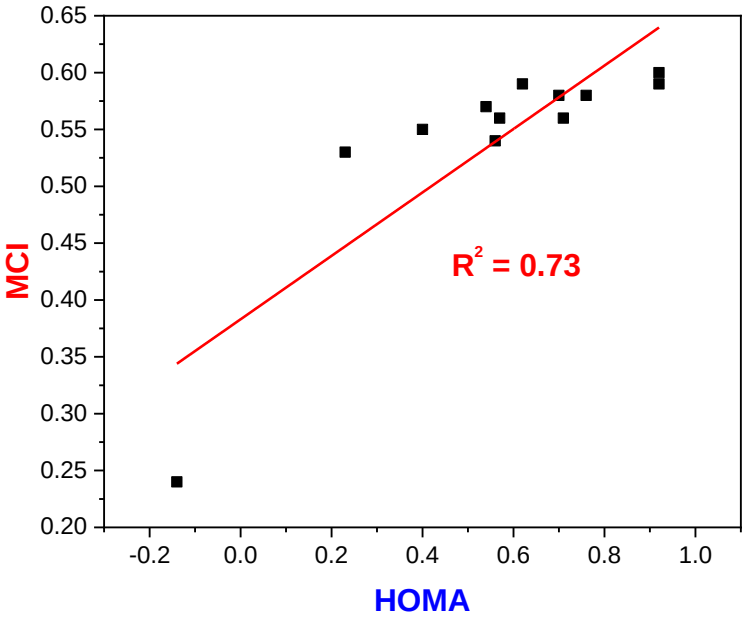

Figure S6. Correlation between MCI and HOMA values of **1**−**13** in S_0 state.

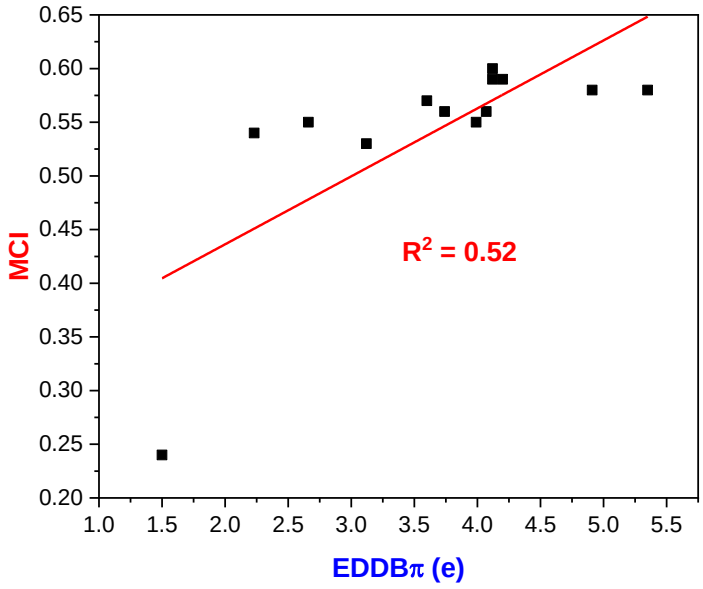

Figure S7. Correlation between MCI and $EDDB_{\pi}$ values of **1**−**13** in S_0 state.

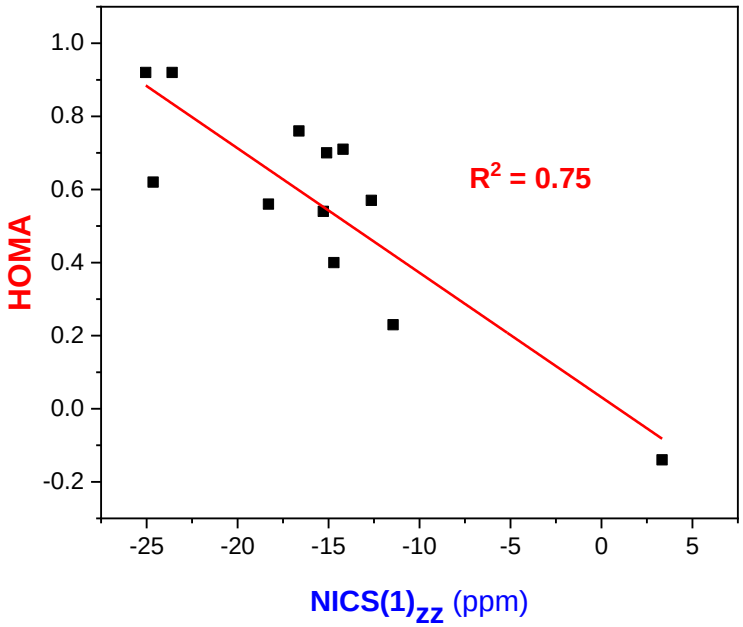

Figure S8. Correlation between HOMA and NICS(1)$_{zz}$ values of **1**−**13** in S_0 state.

4. Linear regression analysis

Code S1: MATLAB Script for Linear Regression Analysis

```
% CSV file

csvFilePath = 'yourcsvPath';


% Read the CSV file data into a matrix

tdata = readmatrix(csvFilePath);


% Separate variables

ty = tdata(:, 1); % Dependent variable

tX = tdata(:, 2:4); % Independent variables

tX_squared = tX.^2;

designMatrix = [tX, tX_squared];
```

```
% Perform a linear regression
tmdl1 = fitlm(designMatrix, ty);
tmdl2 = fitlm(designMatrix(:,1:5), ty);
% Display the model
disp(tmdl1)
disp(tmdl2)
```

Table S1. Data for Linear Regression Analysis

Comp.	ΔE	ΣB.O	Aromaticity	MAV NPA
1	-57.18	8.306	-14.2	0.7345
2	-41.64	8.255	-12.64	0.758833
3	-39.16	8.253	-11.45	0.851833
4	-30.45	8.127	-15.1	0.802333
5	-21.75	8.31	-20.17	0.445667
6	-18.65	8.323	-14.7	0.753
7	-9.7	7.791	-16.62	0.634
8	-8.08	8.083	-24.64	0.550167
9	-3.7	7.887	-25.04	0.429333
10	-3.67	7.857	-23.59	0.5465
11	-2.02	8.086	-18.3	0.5705
12	-1.24	7.798	-15.28	0.619333
13	0	7.946	3.34	0.464
14	2.49	7.878	-1.28	0.492
15	5.3	7.872	-13.89	0.437
16	6.84	8.118	-35.17	0.304667
17	8.7	7.621	-30.33	0.547833
18	15.54	7.885	-23.9	0.385333
19	16.78	7.868	-21.49	0.404167

20	38.88	8.484	-16.5	0.373
21	40.4	7.869	-29.24	0.303667
22	58.42	7.495	-9.63	0.185333
23	80.79	8.041	-19.14	0.375667
24	100.68	7.424	2.08	0.312667

Table S2. Coefficients and Significance Levels for the Iterative Linear Regression Model

Variable	Estimate	SE	tStat	pValue
Intercept	5598.2	4108.9	1.3625	0.19083
X1	-1351.7	1035.7	-1.3051	0.20924
X2	-0.2682	1.4031	-0.19115	0.85067
X3	-153.98	174.36	-0.88308	0.38951
X4	82.722	64.837	1.2758	0.21917
X5	-0.021096	0.043993	-0.47953	0.63767
X6	10.2	157.02	0.064962	0.94896

Table S3. Performance Statistics for the Iterative Linear Regression Model

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
22.2	0.734	0.64	7.81	0.000376

Table S4. Coefficients and Significance Levels for the Refined Linear Regression Model

Variable	Estimate	SE	tStat	p-Value
Intercept	5704.4	3664.4	1.5567	0.13695
X1	-1379	919.97	-1.499	0.15121
X2	-0.2719	1.3626	-0.19954	0.84408
X3	-142.87	32.847	-4.3494	0.00038637
X4	84.433	57.582	1.4663	0.15982
X5	-0.021209	0.042726	-0.4964	0.62562

Table S5. Performance Statistics for the Refined Linear Regression Model

RMSE	R^2	Adjusted R^2	F-statistic	p-Value
21.6	0.734	0.66	9.92	0.00011

Table S6. Variable Contribution of Principal Component Analysis

Variable	ΔE	Bond Order	Aromaticity	MAV NPA
Contribution	0.317292	0.00015	0.088742	0.285949

Table S7. Eigen Vectors for Principal Component Analysis

Eigenvectors					
Principle Component	Eigenvalues	ΔE	Bond Order	Aromaticity	MAV NPA
PC_1	2.23385	-0.61829	0.013436	0.326983	0.714578
PC_2	1.06496	0.516684	-0.193	0.831168	0.070355
PC_3	0.52560	-0.05002	0.945154	0.26603	-0.18278
PC_4	0.17557	0.590133	0.263164	-0.36259	0.671579

Table S8. Variable contributions to the principal components.

Variable	NICS(1)$_{zz}$	HOMA	EDDB$_{\pi}$	MCI
PC1	27.00%	19.89%	23.65%	29.46%
PC2	15.84%	77.55%	2.17%	4.44%

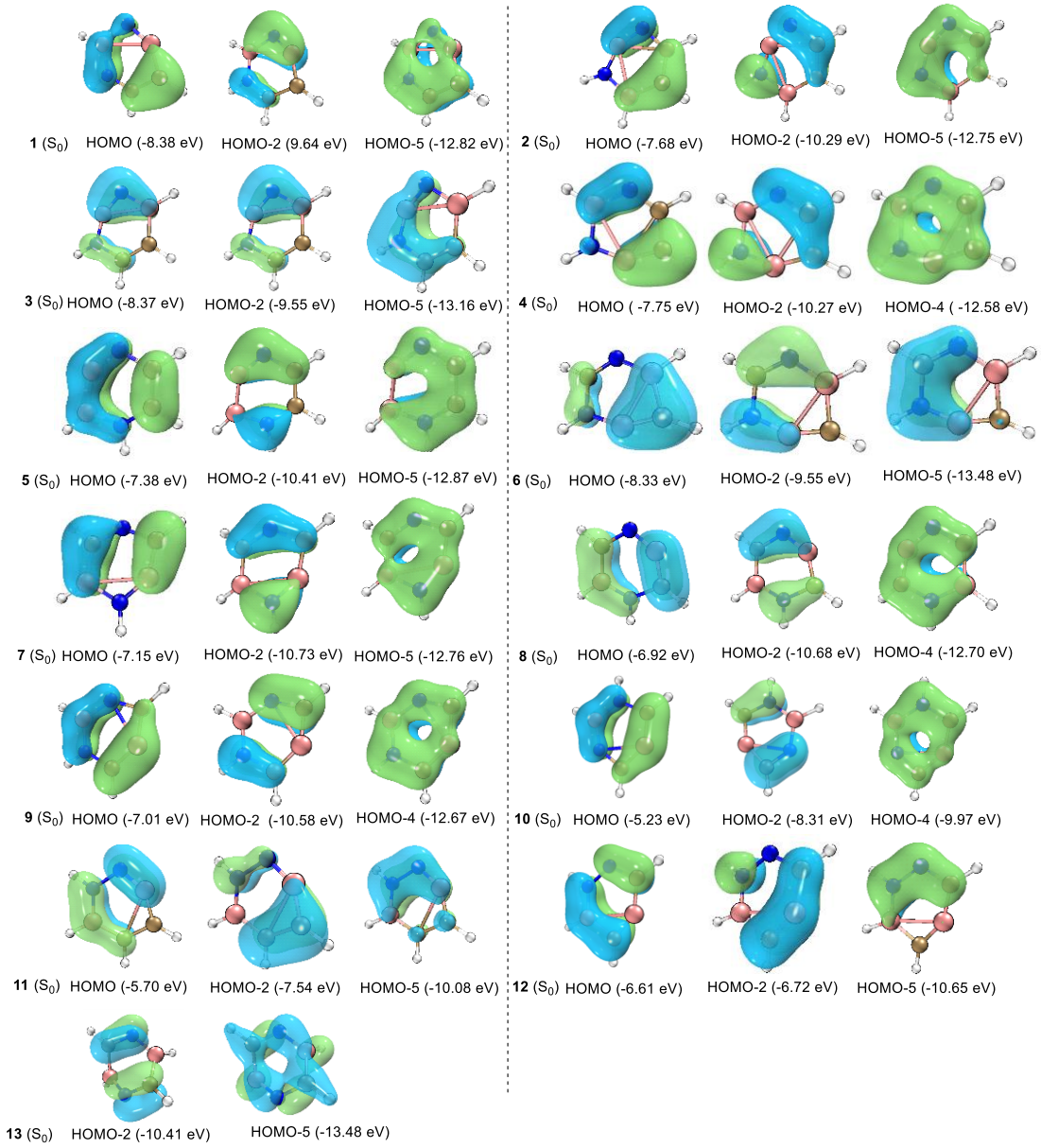

Figure S9. All delocalized π-orbital of compounds **1**−**12** and localized π-orbital of **13**. Energies of molecular orbitals are given in the parenthesis.

5. DFT vs. Hückel Theory:

We have provided a comparison between HOMO and LUMO energies from the Hückel model and DFT calculations for selected isomers **1**, **5**, and **13** (Table S10). The DFT-calculated HOMO-LUMO gaps are 8.74 eV, 7.37 eV, and 6.25 eV for isomers **1**,

5, and **13**, respectively, while the Hückel model predicts gaps of 1.38 β, 1.33 β, and 1.18 β. The observed trend (**1** > **5** > **13**) in DFT results aligns with the Hückel model's qualitative prediction, confirming that isomer **1** exhibits the greatest electronic stability, while isomer **13** is the least stable. However, the absolute energy values differ due to the Hückel model's neglect of electronic interactions and heteroatom effects.

Table S9. Comparison of Hückel and DFT Molecular Orbital Energies for selected BN-heterocycles **1**, **5**, and **13**.

Isomer	Hückel HOMO (β)	Hückel LUMO (β)	Hückel HOMO–LUMO Gap (β)	DFT HOMO (eV)	DFT LUMO (eV)	DFT HOMO–LUMO Gap (eV)
1	0.0000	1.3845	1.38	-8.38	0.37	8.74
5	-0.1273	1.2049	1.33	-7.38	-0.01	7.37
13	0.0877	1.2657	1.18	-8.15	-1.90	6.25

The Hückel calculations in this work utilize a single electronegativity parameter, Z, for the Coulomb integrals, where the atomic Coulomb parameters are defined as $\alpha_B = \alpha - Z\beta$ for boron and $\alpha_N = \alpha + Z\beta$ for nitrogen. The resonance integrals between adjacent atoms are taken as β. This approach allows for a simplified yet insightful description of the π-electronic structure of BN-doped heterocycles.

6. Cartesian coordinates

1,2-DH, 1,3-DA, 2,4-DB (1, S_0)

C	0.87536	2.3139	-0.0012
C	-1.21707	1.10561	-0.00068
H	1.42556	3.26604	-0.00126
H	-2.31667	1.1058	-0.00086
N	1.57301	1.10539	0.0000
N	0.87547	-0.10236	0.0000
H	1.30524	-0.52087	0.8001
B	-0.51969	-0.10236	0.0000
B	-0.51947	2.31382	-0.00168
H	-1.10928	3.33584	-0.00293

1,2-DH, 1,3-DA, 2,4-DB (1, T_1)

C	0.33336	-0.65943	-0.1802
C	1.65793	-0.64789	0.14691
H	-0.24761	-1.51683	-0.44898
H	2.22648	-1.55328	0.10312
H	3.26877	0.64772	0.20128
H	2.21992	2.90702	-0.44891
B	1.59667	2.02438	0.02535
B	-0.17792	0.82603	-0.09245
N	0.0193	2.10127	0.11771
N	2.34106	0.67247	0.57376

3,4-DH, 1,3-DA, 2,4-DB (2, S_0)

C	0.0187	-0.58153	-0.27964
C	1.29826	-0.6322	0.30785
H	-0.32627	-1.41459	-0.85576

H	1.79768	-1.56314	0.47763
H	-0.56479	2.95213	-0.14462
H	-2.07618	0.76653	0.26714
B	1.0488	1.57145	0.20668
B	-0.96358	0.78917	-0.12529
N	-0.20495	2.08999	-0.50132
N	1.94625	0.66655	0.64204

3,4-DH, 1,3-DA, 2,4-DB (2, T_1)

C	0.0187	-0.58153	-0.27964
C	1.29826	-0.6322	0.30785
H	-0.32627	-1.41459	-0.85576
H	1.79768	-1.56314	0.47763
H	-0.56479	2.95213	-0.14462
H	-2.07618	0.76653	0.26714
B	1.0488	1.57145	0.20668
B	-0.96358	0.78917	-0.12529
N	-0.20495	2.08999	-0.50132
N	1.94625	0.66655	0.64204

1,4-DH, 1,3-DA, 2,4-DB (3, S_0)

C	-0.65298	-0.11318	-0.07456
C	0.6889	-0.2274	0.32617
H	-1.21705	-0.96635	-0.38893
H	1.14582	-1.17697	0.51178
H	2.40965	0.97901	0.1619
H	-2.19573	1.76115	0.63612
B	-1.31465	1.42321	-0.07233
B	0.60042	1.93483	-0.50899
N	-0.55422	2.38369	-1.03238
N	1.4517	1.05268	0.4392

1,4-DH, 1,3-DA, 2,4-DB (3, T_1)

C	-0.65298	-0.11318	-0.07456
C	0.6889	-0.2274	0.32617
H	-1.21705	-0.96635	-0.38893
H	1.14582	-1.17697	0.51178
H	2.40965	0.97901	0.1619
H	-2.19573	1.76115	0.63612
B	-1.31465	1.42321	-0.07233
B	0.60042	1.93483	-0.50899
N	-0.55422	2.38369	-1.03238
N	1.4517	1.05268	0.4392

2,3-DH, 1,3-DA, 2,4-DB (4, S_0)

C	-0.51248	0.09281	0.17521
C	-1.35321	1.38788	0.24968
H	-0.86733	-0.91633	0.15045
H	2.68017	1.43446	-0.33479
H	1.20982	3.59571	-0.97276
H	-2.42208	1.36251	0.2918
N	-0.666	2.55655	0.28199
N	1.87218	1.60028	0.2306
B	0.87683	2.72026	-0.25505
B	0.80464	0.52985	0.13809

2,3-DH, 1,3-DA, 2,4-DB (4, T_1)

C	-0.51248	0.09281	0.17521

C	-1.35321	1.38788	0.24968
H	-0.86733	-0.91633	0.15045
H	2.68017	1.43446	-0.33479
H	1.20982	3.59571	-0.97276
H	-2.42208	1.36251	0.2918
N	-0.666	2.55655	0.28199
N	1.87218	1.60028	0.2306
B	0.87683	2.72026	-0.25505
B	0.80464	0.52985	0.13809

1,6-DH, 1,4-DA, 4,5-DB (5, S_0)

C	-0.56165	-0.58771	-0.12083
C	0.89393	-0.56937	-0.00334
H	-1.03909	-1.50666	-0.39005
H	1.38682	-1.48459	-0.25697
H	2.69774	0.54917	-0.06234
H	1.55375	2.99263	-0.16942
B	1.10959	1.94299	0.13618
B	-0.4631	1.45971	0.31096
N	-1.41844	0.61852	0.11376
N	1.83431	0.59937	0.43963

1,6-DH, 1,4-DA, 4,5-DB (5, T_1)

C	-0.56165	-0.58771	-0.12083
C	0.89393	-0.56937	-0.00334
H	-1.03909	-1.50666	-0.39005
H	1.38682	-1.48459	-0.25697
H	2.69774	0.54917	-0.06234
H	1.55375	2.99263	-0.16942
B	1.10959	1.94299	0.13618
B	-0.4631	1.45971	0.31096
N	-1.41844	0.61852	0.11376
N	1.83431	0.59937	0.43963

1,4-DH,1,3-DA, 4,6-DB (6, S_0)

C	0.48819	0.08661	0.0000
C	1.88323	2.50287	-0.0012
H	-0.06157	-0.8657	0.00045
H	2.43343	3.45502	-0.00126
B	1.88335	0.08661	0.0000
H	2.47356	-0.93518	0.0000
B	-0.20919	1.29459	-0.00068
N	2.58089	1.29437	0.0000
N	0.48841	2.5028	-0.00168
H	0.18791	2.99498	-0.81866

1,4-DH,1,3-DA, 4,6-DB (6, T_1)

C	0.48819	0.08661	0.0000
C	1.88323	2.50287	-0.0012
H	-0.06157	-0.8657	0.00045
H	2.43343	3.45502	-0.00126
B	1.88335	0.08661	0.0000
H	2.47356	-0.93518	0.0000
B	-0.20919	1.29459	-0.00068
N	2.58089	1.29437	0.0000
N	0.48841	2.5028	-0.00168
H	0.18791	2.99498	-0.81866

1,2-DH, 1,4-DA, 2,6-DB (7, S_0)

C	-0.4983	-0.08127	0.27627
C	1.66763	1.0001	0.01899
H	-1.18203	-0.84228	0.58977
H	2.66979	0.9575	-0.35351
N	1.0088	-0.11361	0.43865
N	-0.42814	2.36545	-0.81943
H	-0.78693	2.98292	-1.51944
B	-0.83935	1.12869	-0.37858
B	0.8131	2.43097	0.09471
H	1.06104	3.32036	0.8295

1,2-DH, 1,4-DA, 2,6-DB (7, T_1)

C	-0.4983	-0.08127	0.27627
C	1.66763	1.0001	0.01899
H	-1.18203	-0.84228	0.58977
H	2.66979	0.9575	-0.35351
N	1.0088	-0.11361	0.43865
N	-0.42814	2.36545	-0.81943
H	-0.78693	2.98292	-1.51944
B	-0.83935	1.12869	-0.37858
B	0.8131	2.43097	0.09471
H	1.06104	3.32036	0.8295

1,2-DH, 1,4-DA, 2,5-DB (8, S_0)

C	-0.32629	-0.64662	0.03099
C	1.10455	-0.80552	0.01338
H	-0.92053	-1.52529	-0.1094
H	1.66197	-1.71725	-0.04077
H	-0.93919	2.84305	0.08654
H	-2.02682	0.66093	-0.10968
B	1.655	0.63845	0.08245
B	0.89955	1.80966	0.01662
N	-1.10955	0.75115	0.27823
N	-0.54636	2.00726	-0.29703

1,2-DH, 1,4-DA, 2,5-DB (8, T_1)

C	0.56514	1.71956	0.0000
C	-2.22494	1.71979	-0.00068
H	1.66482	1.71964	0.00063
H	-3.32455	1.71997	-0.00086
B	-0.13252	2.92807	-0.0012
H	0.4571	3.9502	-0.00181
B	-1.52756	0.51181	0.0000
N	-1.52734	2.92799	-0.00168
H	-1.80381	3.43404	-0.81867
N	-0.1324	0.51181	0.0000

2,3-DH, 1,3-DA, 2,5-DB (9, S_0)

C	2.31877	0.95134	0.19516
C	-0.242	2.42088	-0.21515
H	-0.58625	-1.13456	0.02714
H	3.28396	1.02256	0.65148
H	-0.66999	3.28236	-0.68374
B	1.25439	2.06115	-0.01493
B	0.00265	-0.11211	0.01368
N	1.54765	-0.22133	-0.30968
N	-0.86349	1.17574	0.32153
H	-0.96306	1.29838	1.30897

2,3-DH, 1,3-DA, 2,5-DB (9, T_1)

C	2.31877	0.95134	0.19516
C	-0.242	2.42088	-0.21515
H	-0.58625	-1.13456	0.02714
H	3.28396	1.02256	0.65148
H	-0.66999	3.28236	-0.68374
B	1.25439	2.06115	-0.01493
B	0.00265	-0.11211	0.01368
N	1.54765	-0.22133	-0.30968
N	-0.86349	1.17574	0.32153
H	-0.96306	1.29838	1.30897

1,2-DH, 1,3-DA, 2,5-DB (S_0, 10)

C	-0.83465	0.40157	0.0000
C	-0.83443	2.81776	-0.00168
H	-1.3844	-0.55074	0.00045
H	2.35773	1.60941	0.00063
H	-1.38455	3.77004	-0.00263
N	0.5604	2.81783	-0.0012
N	0.56051	0.40157	0.0000
H	0.84912	-0.09846	-0.8165
B	1.25805	1.60933	0.0000
B	-1.53203	1.60955	-0.00068

1,2-DH, 1,3-DA, 2,5-DB (T_1, 10)

C	-0.83465	0.40157	0.0000
C	-0.83443	2.81776	-0.00168
H	-1.3844	-0.55074	0.00045
H	2.35773	1.60941	0.00063
H	-1.38455	3.77004	-0.00263
N	0.5604	2.81783	-0.0012
N	0.56051	0.40157	0.0000
H	0.84912	-0.09846	-0.8165
B	1.25805	1.60933	0.0000
B	-1.53203	1.60955	-0.00068

2,3-DH, 1,2-DA, 3,6-DB (11, S_0)

C	1.28492	-0.03937	0.0000
C	1.98246	1.16838	0.0000
H	1.83443	-0.99188	0.00132
H	3.08214	1.16846	0.00063
H	1.83501	3.32903	-0.00126
H	-0.66014	3.32909	-0.00263
B	1.28481	2.37689	-0.0012
B	-0.11024	-0.03937	0.0000
N	-0.11002	2.37681	-0.00168
N	-0.80762	1.16861	-0.00068

2,3-DH, 1,2-DA, 3,6-DB (11, T_1)

C	1.28492	-0.03937	0.0000
C	1.98246	1.16838	0.0000
H	1.83443	-0.99188	0.00132
H	3.08214	1.16846	0.00063
H	1.83501	3.32903	-0.00126
H	-0.66014	3.32909	-0.00263
B	1.28481	2.37689	-0.0012
B	-0.11024	-0.03937	0.0000
N	-0.11002	2.37681	-0.00168

N	-0.80762	1.16861	-0.00068

1,6-DH, 1,2-DA, 4,6-DB (12, S_0)

C	-0.17323	-0.30709	0.0000
C	-0.17301	2.1091	-0.00168
H	-0.72299	-1.2594	0.00045
H	3.01915	0.90074	0.00063
H	1.77202	3.06132	-0.00126
H	-0.72313	3.06138	-0.00263
B	-0.87061	0.90089	-0.00068
B	1.22182	2.10917	-0.0012
N	1.22193	-0.30709	0.0000
N	1.91947	0.90066	0.0000

1,6-DH, 1,2-DA, 4,6-DB (12, T_1)

C	-0.17323	-0.30709	0.0000
C	-0.17301	2.1091	-0.00168
H	-0.72299	-1.2594	0.00045
H	3.01915	0.90074	0.00063
H	1.77202	3.06132	-0.00126
H	-0.72313	3.06138	-0.00263
B	-0.87061	0.90089	-0.00068
B	1.22182	2.10917	-0.0012
N	1.22193	-0.30709	0.0000
N	1.91947	0.90066	0.0000

2,5-DH, 1,4-DA, 2,5-DB (13, S_0)

C	-2.86625	2.5481	-0.01105
C	-4.45568	5.04931	-0.27757
H	-4.69596	5.95607	-0.79232
B	-3.11875	4.77319	0.64762
H	-2.92548	5.29033	1.6905
B	-4.38006	2.85564	0.57047
H	-4.79923	2.40461	1.57709
N	-2.18728	3.65066	0.03834
N	-5.15768	3.91359	-0.30765
H	-2.5085	1.60433	-0.36632

2,5-DH, 1,4-DA, 2,5-DB (13, S_0)

C	-2.86625	2.5481	-0.01105
C	-4.45568	5.04931	-0.27757
H	-4.69596	5.95607	-0.79232
B	-3.11875	4.77319	0.64762
H	-2.92548	5.29033	1.6905
B	-4.38006	2.85564	0.57047
H	-4.79923	2.40461	1.57709
N	-2.18728	3.65066	0.03834
N	-5.15768	3.91359	-0.30765
H	-2.5085	1.60433	-0.36632

2,5-DH, 1,3-DA, 2,5-DB (S_0, 14)

N	-0.80359	1.14454	0.42405
N	1.3194	-0.00781	-0.22593
B	0.01882	-0.05629	0.06499
H	-0.40243	-1.1569	0.00497
B	1.4089	2.7593	0.12563
H	2.12636	3.64768	0.42299
C	1.80201	1.48648	-0.10678

H	2.54821	1.4673	0.65985
C	-0.18591	2.54411	-0.14001
H	-0.6181	3.41326	0.31021

2,5-DH, 1,3-DA, 2,5-DB (T_1, 14)

N	-0.80359	1.14454	0.42405
N	1.3194	-0.00781	-0.22593
B	0.01882	-0.05629	0.06499
H	-0.40243	-1.1569	0.00497
B	1.4089	2.7593	0.12563
H	2.12636	3.64768	0.42299
C	1.80201	1.48648	-0.10678
H	2.54821	1.4673	0.65985
C	-0.18591	2.54411	-0.14001
H	-0.6181	3.41326	0.31021

2,6-DH, 1,3-DA, 5,6-DB (S_0, 15)

C	1.17469	0.03937	0.0000
C	-0.91785	1.24735	-0.00068
H	1.7242	-0.91314	0.00132
H	1.72477	3.40777	-0.00126
H	-2.01746	1.24753	-0.00086
B	1.17457	2.45563	-0.0012
B	1.87223	1.24712	0.0000
N	-0.22025	2.45555	-0.00168
H	-0.5085	2.9548	-0.81878
N	-0.22047	0.03937	0.0000

2,6-DH, 1,3-DA, 5,6-DB (T_1, 15)

C	1.17469	0.03937	0.0000
C	-0.91785	1.24735	-0.00068
H	1.7242	-0.91314	0.00132
H	1.72477	3.40777	-0.00126
H	-2.01746	1.24753	-0.00086
B	1.17457	2.45563	-0.0012
B	1.87223	1.24712	0.0000
N	-0.22025	2.45555	-0.00168
H	-0.5085	2.9548	-0.81878
N	-0.22047	0.03937	0.0000

3,6-DH, 1,2-DA, 3,6-DB (S_0, 16)

C	0.68241	1.13676	0.00019
C	-0.68014	1.13835	0.00014
H	2.7461	-0.2824	-0.0009
H	1.21685	2.08691	-0.00003
H	-1.21261	2.08957	-0.00028
H	-2.74679	-0.27874	-0.00062
N	-0.58862	-1.1366	0.00007
N	0.58655	-1.13737	0.00023
B	-1.57828	-0.13366	-0.0002
B	1.57774	-0.13599	-0.00025

3,6-DH, 1,2-DA, 3,6-DB (T_1, 16)

C	0.68241	1.13676	0.00019
C	-0.68014	1.13835	0.00014
H	2.7461	-0.2824	-0.0009
H	1.21685	2.08691	-0.00003
H	-1.21261	2.08957	-0.00028

H	-2.74679	-0.27874	-0.00062
N	-0.58862	-1.1366	0.00007
N	0.58655	-1.13737	0.00023
B	-1.57828	-0.13366	-0.0002
B	1.57774	-0.13599	-0.00025

2,5-DH, 1,2-DA, 3,5-DB (S_0, 17)

C	0.87536	2.3139	-0.0012
C	-1.21707	1.10561	-0.00068
H	1.42556	3.26604	-0.00126
H	-2.31667	1.1058	-0.00086
N	1.57301	1.10539	0.0000
N	0.87547	-0.10236	0.0000
H	1.30524	-0.52087	0.8001
B	-0.51969	-0.10236	0.0000
B	-0.51947	2.31382	-0.00168
H	-1.10928	3.33584	-0.00293

2,5-DH, 1,2-DA, 3,5-DB (T_1, 17)

C	0.87536	2.3139	-0.0012
C	-1.21707	1.10561	-0.00068
H	1.42556	3.26604	-0.00126
H	-2.31667	1.1058	-0.00086
N	1.57301	1.10539	0.0000
N	0.87547	-0.10236	0.0000
H	1.30524	-0.52087	0.8001
B	-0.51969	-0.10236	0.0000
B	-0.51947	2.31382	-0.00168
H	-1.10928	3.33584	-0.00293

1,4-DH, 1,2-DA, 3,4-DB (S_0, 18)

C	1.28492	0.2126	0.0000
C	-0.11002	2.62878	-0.00168
H	1.83443	-0.73991	0.00132
H	-0.66014	3.58106	-0.00263
B	1.28481	2.62886	-0.0012
H	1.87442	3.65099	-0.00181
B	1.98246	1.42035	0.0000
H	3.16246	1.41971	0.00101
N	-0.11024	0.2126	0.0000
N	-0.80762	1.42057	-0.00068

1,4-DH, 1,2-DA, 3,4-DB (T_1, 18)

C	0.2548	1.80032	-0.88805
C	-0.55488	0.70483	-0.47498
H	-0.53471	-1.14798	0.52807
H	1.77355	3.48268	0.33208
H	0.24467	2.14144	-1.90217
H	-1.37778	0.44765	-1.10869
B	1.26783	2.42324	0.2128
B	1.29609	1.07382	1.15162
N	1.03009	-0.17806	1.34641
N	-0.32282	-0.20786	0.79506

2,3-DH, 1,2-DA, 3,4-DB (S_0, 19)

C	0.71557	-1.2146	0.25636
C	2.11073	-1.2146	0.25636
H	0.16581	-2.16691	0.25681
H	2.66024	-2.16711	0.25767

H	2.66082	2.15381	0.2551
H	0.16567	2.15387	0.25373
N	0.01819	-0.00662	0.25568
N	0.71579	1.20159	0.25468
B	2.80827	-0.00685	0.25636
B	2.11062	1.20166	0.25516

2,3-DH, 1,2-DA, 3,4-DB (T_1, 19)

C	0.71557	-1.2146	0.25636
C	2.11073	-1.2146	0.25636
H	0.16581	-2.16691	0.25681
H	2.66024	-2.16711	0.25767
H	2.66082	2.15381	0.2551
H	0.16567	2.15387	0.25373
N	0.01819	-0.00662	0.25568
N	0.71579	1.20159	0.25468
B	2.80827	-0.00685	0.25636
B	2.11062	1.20166	0.25516

1,4-DH, 1,4-DA, 2,5-DB (S_0, 20)

C	0.28346	-0.79528	0.0000
C	1.67862	-0.79528	0.0000
H	-0.26629	-1.74759	0.00045
H	2.22813	-1.74779	0.00132
H	3.47584	0.41256	0.00063
H	-1.51352	0.41288	-0.00086
B	1.67851	1.62098	-0.0012
B	0.28368	1.62091	-0.00168
N	-0.41392	0.4127	-0.00068
N	2.37616	0.41248	0.0000

1,4-DH, 1,4-DA, 2,5-DB (T_1, 20)

C	0.28346	-0.79528	0.0000
C	1.67862	-0.79528	0.0000
H	-0.26629	-1.74759	0.00045
H	2.22813	-1.74779	0.00132
H	3.47584	0.41256	0.00063
H	-1.51352	0.41288	-0.00086
B	1.67851	1.62098	-0.0012
B	0.28368	1.62091	-0.00168
N	-0.41392	0.4127	-0.00068
N	2.37616	0.41248	0.0000

2,5-DH, 1,2-DA, 4,5-DB (S_0, 21)

C	2.15367	1.5393	-0.0358
C	-0.91017	1.45193	0.03389
H	3.12224	1.35948	0.38187
H	-1.97466	1.48271	0.1379
B	1.48383	3.03122	-0.02334
H	1.94658	4.1167	-0.02566
B	-0.06799	2.50016	-0.07361
N	-0.03491	0.22635	-0.0844
H	-0.47107	-0.38494	-0.74477
N	1.4007	0.50481	-0.52288

2,5-DH, 1,2-DA, 4,5-DB (T_1, 21)

C	2.15367	1.5393	-0.0358
C	-0.91017	1.45193	0.03389

H	3.12224	1.35948	0.38187
H	-1.97466	1.48271	0.1379
B	1.48383	3.03122	-0.02334
H	1.94658	4.1167	-0.02566
B	-0.06799	2.50016	-0.07361
N	-0.03491	0.22635	-0.0844
H	-0.47107	-0.38494	-0.74477
N	1.4007	0.50481	-0.52288

1,2-DH, 1,2-DA, 4,5-DB (S_0, 22)

C	0.54704	-0.18843	0.28566
C	-0.71243	2.63935	-0.81094
H	0.89722	-1.16661	0.5415
H	-1.05454	3.61879	-1.07278
B	0.46825	2.06298	-1.13062
B	1.04963	0.65211	-0.64671
N	-0.64925	0.59327	0.91664
H	-1.29461	-0.08633	1.26542
N	-1.47183	1.55072	0.01277
H	-2.10849	2.02912	0.61758

1,2-DH, 1,2-DA, 4,5-DB (T_1, 22)

C	-0.32629	-0.64662	0.03099
C	1.10455	-0.80552	0.01338
H	-0.92053	-1.52529	-0.1094
H	1.66197	-1.71725	-0.04077
H	-0.93919	2.84305	0.08654
H	-2.02682	0.66093	-0.10968
B	1.655	0.63845	0.08245
B	0.89955	1.80966	0.01662
N	-1.10955	0.75115	0.27823
N	-0.54636	2.00726	-0.29703

1,2-DH, 1,2-DA, 3,4-B (S_0, 23)

C	-0.32629	-0.64662	0.03099
C	1.10455	-0.80552	0.01338
H	-0.92053	-1.52529	-0.1094
H	1.66197	-1.71725	-0.04077
H	-0.93919	2.84305	0.08654
H	-2.02682	0.66093	-0.10968
B	1.655	0.63845	0.08245
B	0.89955	1.80966	0.01662
N	-1.10955	0.75115	0.27823
N	-0.54636	2.00726	-0.29703

1,2-DH, 1,2-DA, 3,4-DB (T_1, 23)

C	-0.32629	-0.64662	0.03099
C	1.10455	-0.80552	0.01338
H	-0.92053	-1.52529	-0.1094
H	1.66197	-1.71725	-0.04077
H	-0.93919	2.84305	0.08654
H	-2.02682	0.66093	-0.10968
B	1.655	0.63845	0.08245
B	0.89955	1.80966	0.01662
N	-1.10955	0.75115	0.27823
N	-0.54636	2.00726	-0.29703

4,5-DH, 1,2-DA, 4,5-DB (S_0, 24)

C	1.28492	0.2126	0.0000
C	-0.11002	2.62878	-0.00168
H	1.83443	-0.73991	0.00132
H	-0.66014	3.58106	-0.00263
B	1.28481	2.62886	-0.0012
H	1.87442	3.65099	-0.00181
B	1.98246	1.42035	0.0000
H	3.16246	1.41971	0.00101
N	-0.11024	0.2126	0.0000
N	-0.80762	1.42057	-0.00068

4,5-DH, 1,2-DA, 4,5-DB (T_1, 24)

C	1.28492	0.2126	0.0000
C	-0.11002	2.62878	-0.00168
H	1.83443	-0.73991	0.00132
H	-0.66014	3.58106	-0.00263
B	1.28481	2.62886	-0.0012
H	1.87442	3.65099	-0.00181
B	1.98246	1.42035	0.0000
H	3.16246	1.41971	0.00101
N	-0.11024	0.2126	0.0000
N	-0.80762	1.42057	-0.00068