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Cyclic π Electron Delocalization in Fluoroborazines

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Supporting Information

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Table S1. Calculated B–N bond lengths (d/Å) used for calculations of HOMA, and HOMA values for **1**-**20**.

Molecule		$d_{N(1)B(2)}$	$d_{B(2)N(3)}$	$d_{N(3)B(4)}$	$d_{B(4)N(5)}$	$d_{N(5)B(6)}$	$d_{B(6)B(1)}$	HOMA
borazine	**1**	1.43095	1.43095	1.43095	1.43095	1.43095	1.43095	0.940
2-fluoroborazine	**2**	1.42549	1.42549	1.43107	1.43159	1.43159	1.43107	0.945
2,4-difluoroborazine	**3**	1.42650	1.42612	1.42612	1.42650	1.43155	1.43155	0.951
2,4,6-trifluoroborazine	**4**	1.42687	1.42687	1.42687	1.42687	1.42687	1.42687	0.955
1-fluoroborazine	**5**	1.42762	1.42911	1.43186	1.43186	1.42911	1.42762	0.945
1,3-difluoroborazine	**6**	1.42664	1.42664	1.42877	1.42991	1.42991	1.42877	0.950
1,3,5-trifluoroborazine	**7**	1.42727	1.42727	1.42727	1.42727	1.42727	1.42727	0.954
1,2,6-trifluoroborazine	**8**	1.43376	1.42492	1.43213	1.43213	1.42492	1.43376	0.941
1,2,4-trifluoroborazine	**9**	1.43502	1.42451	1.42782	1.42788	1.42888	1.42775	0.948
1,2,4,6-tetrafluoroborazine	**10**	1.43479	1.42493	1.42806	1.42806	1.42493	1.43479	0.945
1,2,3,4,6-pentafluoroborazine	**11**	1.43392	1.43392	1.43533	1.42622	1.42622	1.43533	0.935
1,2-difluoroborazine	**12**	1.43360	1.42451	1.43180	1.43233	1.42942	1.42676	0.944
1,4-difluoroborazine	**13**	1.42875	1.42857	1.42731	1.42731	1.42857	1.42875	0.950
1,2,3,4-tetrafluoroborazine	**14**	1.43438	1.43326	1.43503	1.42589	1.42989	1.42781	0.938
1,2,4,5-tetrafluoroborazine	**15**	1.43582	1.42614	1.42614	1.43582	1.42606	1.42606	0.945
1,2,3,4,5,6-hexafluoroborazine	**16**	1.43481	1.43481	1.43481	1.43481	1.43481	1.43481	0.922
1,2,3-trifluoroborazine	**17**	1.43358	1.43358	1.42760	1.43011	1.43011	1.42760	0.941
1,2,5-trifluoroborazine	**18**	1.43502	1.42581	1.42966	1.42915	1.42736	1.42545	0.948
1,2,3,5-tetrafluoroborazine	**19**	1.43487	1.43487	1.42645	1.42767	1.42767	1.42645	0.944
1,2,3,4,5-pentafluoroborazine	**20**	1.43511	1.43469	1.43469	1.43511	1.42653	1.42653	0.934
benzene		1.39435	1.39435	1.39435	1.39435	1.39435	1.39435	0.990

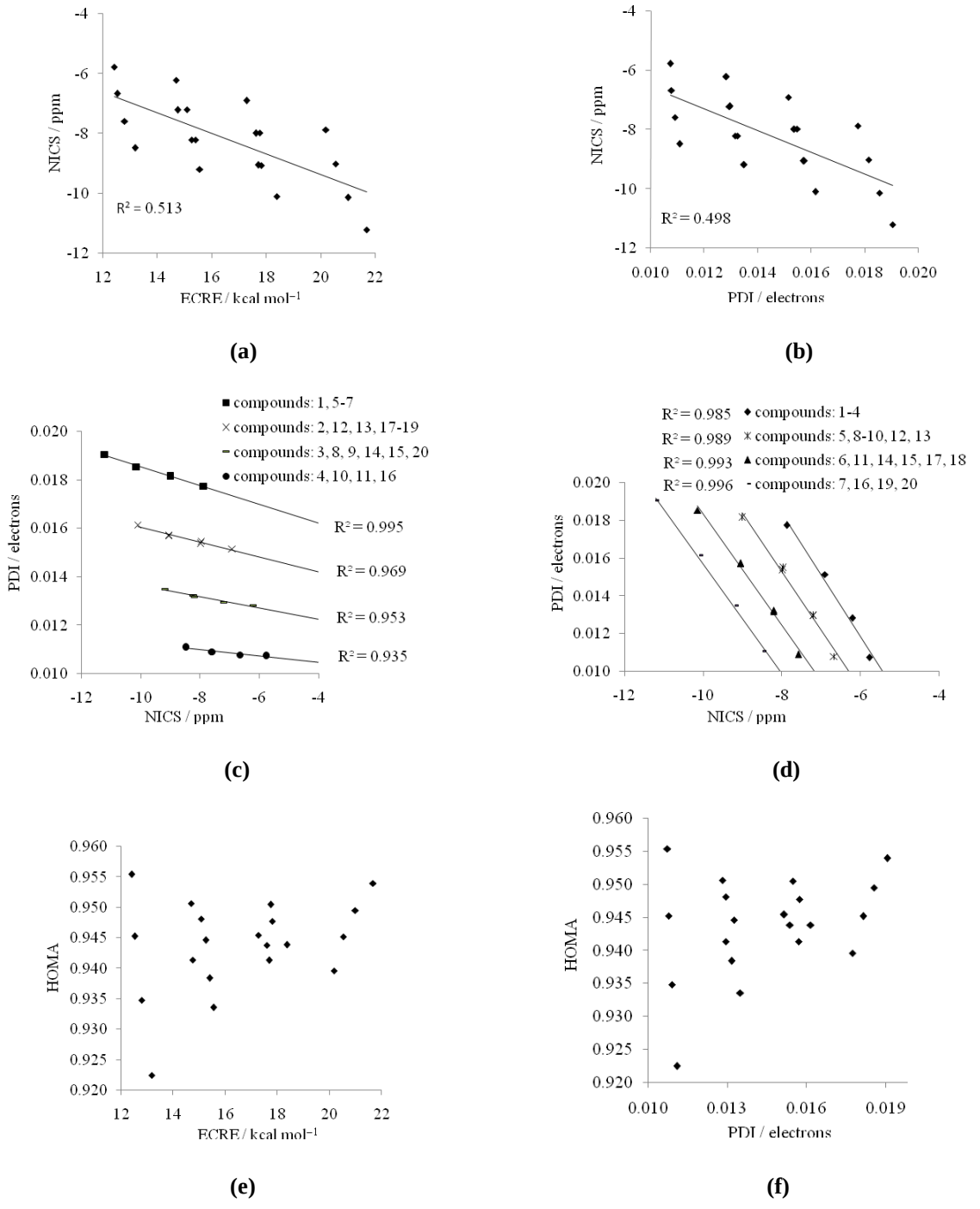


Figure S1. NICS(0)$_{\pi zz}$ vs ECRE and PDI for **1-20**, (a) and (b), respectively; PDI vs NICS(0)$_{\pi zz}$ for structurally similar compounds, (c) and (d); HOMA vs ECRE and PDI for **1-20**, (e) and (f), respectively.

Absolute energies (atomic units) and x, y, z coordinates (Å) of the optimized structures

Borazine (**1**)

E = -242.7485061 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.409784	0.000000
2	1	0	0.000000	2.418791	0.000000
3	7	0	1.220909	-0.704892	0.000000
4	1	0	2.094734	-1.209395	0.000000
5	7	0	-1.220909	-0.704892	0.000000
6	1	0	-2.094734	-1.209395	0.000000
7	5	0	1.256794	0.725610	0.000000
8	1	0	2.288954	1.321528	0.000000
9	5	0	0.000000	-1.451221	0.000000
10	1	0	0.000000	-2.643056	0.000000
11	5	0	-1.256794	0.725610	0.000000
12	1	0	-2.288954	1.321528	0.000000

2-Fluoroborazine (**2**)

E = -342.0912174 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.983077
2	5	0	0.000000	-1.259776	-1.172842
3	1	0	0.000000	-2.290963	-1.768073
4	5	0	0.000000	1.259776	-1.172842
5	1	0	0.000000	2.290963	-1.768073
6	7	0	0.000000	-1.227227	0.257854
7	1	0	0.000000	-2.094064	0.775292
8	7	0	0.000000	0.000000	-1.852860
9	1	0	0.000000	0.000000	-2.861723
10	7	0	0.000000	1.227227	0.257854
11	1	0	0.000000	2.094064	0.775292
12	9	0	0.000000	0.000000	2.335597

2,4-Difluoroborazine (**3**)

E = -441.4335372 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-1.240621	0.331892
2	5	0	0.000000	1.240621	0.331892
3	5	0	0.000000	0.000000	-1.841194
4	1	0	0.000000	0.000000	-3.030687
5	7	0	0.000000	0.000000	1.035232
6	1	0	0.000000	0.000000	2.045372
7	7	0	0.000000	1.221374	-1.094483
8	1	0	0.000000	2.102443	-1.587231
9	7	0	0.000000	-1.221374	-1.094483
10	1	0	0.000000	-2.102443	-1.587231
11	9	0	0.000000	2.409817	1.006832
12	9	0	0.000000	-2.409817	1.006832

2,4,6-Trifluoroborazine (**4**)

E = -540.7753353 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.417696	0.000000
2	1	0	0.000000	2.427951	0.000000
3	7	0	1.227761	-0.708848	0.000000
4	1	0	2.102667	-1.213975	0.000000
5	7	0	-1.227761	-0.708848	0.000000
6	1	0	-2.102667	-1.213975	0.000000
7	5	0	1.243503	0.717937	0.000000
8	5	0	0.000000	-1.435873	0.000000
9	5	0	-1.243503	0.717937	0.000000
10	9	0	-2.410708	1.391823	0.000000
11	9	0	2.410708	1.391823	0.000000
12	9	0	0.000000	-2.783645	0.000000

1-Fuoroborazine (**5**)

E = -341.9351713 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.278623	0.280976
2	1	0	0.000000	2.283683	0.906581
3	5	0	0.000000	0.000000	-1.894520
4	1	0	0.000000	0.000000	-3.083949
5	5	0	0.000000	-1.278623	0.280976
6	1	0	0.000000	-2.283683	0.906581
7	7	0	0.000000	0.000000	0.915975
8	7	0	0.000000	1.221236	-1.146985
9	1	0	0.000000	2.094619	-1.652935
10	7	0	0.000000	-1.221236	-1.146985
11	1	0	0.000000	-2.094619	-1.652935
12	9	0	0.000000	0.000000	2.320608

1,3-Difluoroborazine (**6**)

E = -441.1190614 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.267702	1.127792
2	1	0	0.000000	2.309354	1.687125
3	5	0	0.000000	0.000000	-1.099503
4	1	0	0.000000	0.000000	-2.277556
5	5	0	0.000000	-1.267702	1.127792
6	1	0	0.000000	-2.309354	1.687125
7	7	0	0.000000	1.180421	-0.298305
8	7	0	0.000000	-1.180421	-0.298305
9	7	0	0.000000	0.000000	1.789286
10	1	0	0.000000	0.000000	2.799167
11	9	0	0.000000	2.393001	-1.001388
12	9	0	0.000000	-2.393001	-1.001388

1,3,5-Trifluoroborazine (**7**)

E = -540.3000541 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.363536	0.000000
2	7	0	-1.180857	-0.681768	0.000000
3	7	0	1.180857	-0.681768	0.000000
4	5	0	0.000000	-1.483445	0.000000
5	1	0	0.000000	-2.660815	0.000000
6	5	0	1.284701	0.741722	0.000000
7	1	0	2.304333	1.330407	0.000000
8	5	0	-1.284701	0.741722	0.000000
9	1	0	-2.304333	1.330407	0.000000
10	9	0	0.000000	2.763467	0.000000
11	9	0	-2.393233	-1.381734	0.000000
12	9	0	2.393233	-1.381734	0.000000

1,2,6-Trifluoroborazine (**8**)

E = -540.6099912 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-1.271912	0.037327
2	5	0	0.000000	1.271912	0.037327
3	5	0	0.000000	0.000000	-2.132235
4	1	0	0.000000	0.000000	-3.320081
5	7	0	0.000000	0.000000	0.699069
6	7	0	0.000000	1.222805	-1.386749
7	1	0	0.000000	2.101489	-1.885372
8	7	0	0.000000	-1.222805	-1.386749
9	1	0	0.000000	-2.101489	-1.885372
10	9	0	0.000000	2.415598	0.725835
11	9	0	0.000000	0.000000	2.092744
12	9	0	0.000000	-2.415598	0.725835

1,2,4-Trifluoroborazine (**9**)

E = -540.6140465 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-1.120283	0.000000
2	5	0	-1.253892	1.038960	0.000000
3	5	0	1.254818	1.104603	0.000000
4	1	0	2.290925	1.675082	0.000000
5	7	0	-1.222186	-0.388504	0.000000
6	1	0	-2.093873	-0.900615	0.000000
7	7	0	-0.017962	1.754018	0.000000
8	1	0	-0.047274	2.763567	0.000000
9	7	0	1.192338	-0.321777	0.000000
10	9	0	2.406944	-1.014899	0.000000
11	9	0	0.042831	-2.453886	0.000000
12	9	0	-2.429746	1.695386	0.000000

1,2,4,6-Tetrafluoroborazine (**10**)

E = -639.9509083 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-1.274111	-0.412890
2	5	0	0.000000	0.000000	1.737944
3	5	0	0.000000	1.274111	-0.412890
4	7	0	0.000000	-1.229392	1.011343
5	1	0	0.000000	-2.101835	1.522136
6	7	0	0.000000	1.229392	1.011343
7	1	0	0.000000	2.101835	1.522136
8	7	0	0.000000	0.000000	-1.072627
9	9	0	0.000000	0.000000	-2.465647
10	9	0	0.000000	-2.416166	-1.100518
11	9	0	0.000000	0.000000	3.082738
12	9	0	0.000000	2.416166	-1.100518

1,2,3,4,6-Pentafluoroborazine (**11**)

E = -739.1243436 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.257942	-1.017408
2	5	0	0.000000	0.000000	1.209220
3	5	0	0.000000	-1.257942	-1.017408
4	7	0	0.000000	1.194895	0.416532
5	7	0	0.000000	-1.194895	0.416532
6	7	0	0.000000	0.000000	-1.689476
7	1	0	0.000000	0.000000	-2.701360
8	9	0	0.000000	2.400990	1.111054
9	9	0	0.000000	0.000000	2.529681
10	9	0	0.000000	-2.400990	1.111054
11	9	0	0.000000	-2.421064	-1.663438
12	9	0	0.000000	2.421064	-1.663438

1,2-Difluoroborazine (**12**)

E = -441.2727486 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.912539	-0.243690	0.000000
2	5	0	1.424180	0.776139	0.000000
3	1	0	2.098217	1.749090	0.000000
4	5	0	1.112109	-1.730795	0.000000
5	1	0	1.582399	-2.822598	0.000000
6	7	0	0.000000	0.861970	0.000000
7	7	0	1.935416	-0.558729	0.000000
8	1	0	2.937668	-0.677518	0.000000
9	7	0	-0.305899	-1.532575	0.000000
10	1	0	-0.915658	-2.338207	0.000000
11	9	0	-0.566244	2.141578	0.000000
12	9	0	-2.236867	-0.065323	0.000000

1,4-Difluoroborazine (**13**)

E = -441.2766962 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	1.427291
2	5	0	0.000000	-1.281112	-0.727092
3	1	0	0.000000	-2.285590	-1.352296
4	5	0	0.000000	1.281112	-0.727092
5	1	0	0.000000	2.285590	-1.352296
6	7	0	0.000000	-1.228411	0.700502
7	1	0	0.000000	-2.094738	1.219719
8	7	0	0.000000	0.000000	-1.359612
9	7	0	0.000000	1.228411	0.700502
10	1	0	0.000000	2.094738	1.219719
11	9	0	0.000000	0.000000	-2.763909
12	9	0	0.000000	0.000000	2.776117

1,2,3,4-Tetrafluoroborazine (**14**)

E = -639.7883034 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.059967	-0.003585	0.000000
2	5	0	1.404857	0.668399	0.000000
3	5	0	0.787156	-1.780193	0.000000
4	1	0	1.073162	-2.926600	0.000000
5	7	0	0.000000	0.961147	0.000000
6	7	0	1.743072	-0.716799	0.000000
7	1	0	2.725149	-0.956112	0.000000
8	7	0	-0.575452	-1.353655	0.000000
9	9	0	-1.558403	-2.346521	0.000000
10	9	0	-2.340959	0.320696	0.000000
11	9	0	-0.377441	2.301186	0.000000
12	9	0	2.317705	1.638501	0.000000

1,2,4,5-Tetrafluoroborazine (**15**)

E = -639.7921707 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-1.256912	0.740020
2	5	0	0.000000	1.256912	0.740020
3	5	0	0.000000	0.000000	-1.488254
4	1	0	0.000000	0.000000	-2.665840
5	7	0	0.000000	0.000000	1.413852
6	1	0	0.000000	0.000000	2.425695
7	7	0	0.000000	1.184380	-0.693962
8	7	0	0.000000	-1.184380	-0.693962
9	9	0	0.000000	-2.399791	-1.381444
10	9	0	0.000000	-2.420627	1.386984
11	9	0	0.000000	2.420627	1.386984
12	9	0	0.000000	2.399791	-1.381444

1,2,3,4,5,6-Hexafluoroborazine (**16**)

E = -838.2952438 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.284766	0.741760	0.000000
2	5	0	-1.284766	0.741760	0.000000
3	5	0	0.000000	-1.483520	0.000000
4	7	0	0.000000	1.380552	0.000000
5	7	0	-1.195594	-0.690276	0.000000
6	7	0	1.195594	-0.690276	0.000000
7	9	0	2.399866	-1.385563	0.000000
8	9	0	2.426322	1.400838	0.000000
9	9	0	0.000000	2.771126	0.000000
10	9	0	-2.426322	1.400838	0.000000
11	9	0	-2.399866	-1.385563	0.000000
12	9	0	0.000000	-2.801676	0.000000

1,2,3-Trifluoroborazine (**17**)

E = -540.4518511 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	0.000000	0.800023
2	5	0	0.000000	-1.268098	-1.424467
3	1	0	0.000000	-2.310370	-1.982483
4	5	0	0.000000	1.268098	-1.424467
5	1	0	0.000000	2.310370	-1.982483
6	7	0	0.000000	-1.190270	0.001012
7	7	0	0.000000	0.000000	-2.085629
8	1	0	0.000000	0.000000	-3.095312
9	7	0	0.000000	1.190270	0.001012
10	9	0	0.000000	2.394541	0.710427
11	9	0	0.000000	0.000000	2.122487
12	9	0	0.000000	-2.394541	0.710427

1,2,5-Trifluoroborazine (**18**)

E = -540.455689 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.284986	-0.415956	0.000000
2	1	0	2.299251	-1.014819	0.000000
3	5	0	-1.269802	-0.364488	0.000000
4	5	0	0.009511	1.810555	0.000000
5	1	0	0.056638	2.991453	0.000000
6	7	0	0.000000	-1.032989	0.000000
7	7	0	-1.207252	1.059951	0.000000
8	1	0	-2.082819	1.565094	0.000000
9	7	0	1.192305	1.008395	0.000000
10	9	0	-0.025990	-2.429484	0.000000
11	9	0	-2.420424	-1.037895	0.000000
12	9	0	2.413979	1.696293	0.000000

1,2,3,5-Tetrafluoroborazine (**19**)

E = -639.6320506 a.u.

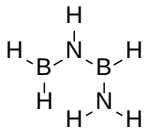
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	1.285909	1.048362
2	1	0	0.000000	2.305983	1.635506
3	5	0	0.000000	0.000000	-1.174616
4	5	0	0.000000	-1.285909	1.048362
5	1	0	0.000000	-2.305983	1.635506
6	7	0	0.000000	1.191377	-0.374952
7	7	0	0.000000	-1.191377	-0.374952
8	7	0	0.000000	0.000000	1.668588
9	9	0	0.000000	2.393851	-1.082143
10	9	0	0.000000	0.000000	-2.494399
11	9	0	0.000000	-2.393851	-1.082143
12	9	0	0.000000	0.000000	3.068424

1,2,3,4,5-Pentafluoroborazine (**20**)

E = -738.9638954 a.u.

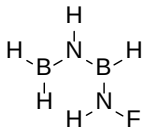
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000000	-1.284024	0.464616
2	5	0	0.000000	1.284024	0.464616
3	5	0	0.000000	0.000000	-1.761011
4	1	0	0.000000	0.000000	-2.937812
5	7	0	0.000000	0.000000	1.104622
6	7	0	0.000000	1.185187	-0.967090
7	7	0	0.000000	-1.185187	-0.967090
8	9	0	0.000000	-2.398804	-1.655295
9	9	0	0.000000	-2.425956	1.124534
10	9	0	0.000000	0.000000	2.495256
11	9	0	0.000000	2.425956	1.124534
12	9	0	0.000000	2.398804	-1.655295

Reference molecules



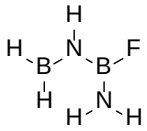
E = -162.985 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.689302	-1.559325	0.000000
2	1	0	0.437879	-1.955849	0.000000
3	1	0	-1.597847	-2.332278	0.000000
4	5	0	0.000000	0.932480	0.000000
5	1	0	-0.427695	2.046543	0.000000
6	7	0	-0.943591	-0.177029	0.000000
7	1	0	-1.916339	0.100946	0.000000
8	7	0	1.385751	0.739227	0.000000
9	1	0	1.822456	-0.169933	0.000000
10	1	0	2.032938	1.509412	0.000000



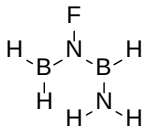
E = -262.1667083 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.151375	0.690005	0.000000
2	1	0	-1.555782	1.725496	0.000000
3	1	0	-3.342272	0.674186	0.000000
4	5	0	0.000000	-0.739599	0.000000
5	1	0	0.458135	-1.832711	0.000000
6	7	0	-1.433948	-0.520938	0.000000
7	1	0	-1.981499	-1.371824	0.000000
8	7	0	0.880781	0.344757	0.000000
9	1	0	0.739970	1.342806	0.000000
10	9	0	2.256721	0.104810	0.000000



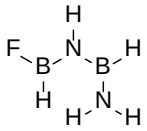
E = -262.3279122 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.071137	-2.108747	0.000000
2	1	0	1.118536	-2.213808	0.000000
3	1	0	-0.766265	-3.076427	0.000000
4	5	0	0.000000	0.463627	0.000000
5	7	0	-0.651446	-0.829271	0.000000
6	1	0	-1.663213	-0.776577	0.000000
7	7	0	1.384428	0.662653	0.000000
8	1	0	1.784397	1.586342	0.000000
9	1	0	2.050608	-0.091422	0.000000
10	9	0	-0.811028	1.551535	0.000000



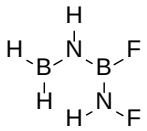
E = -262.1765222 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.271352	1.053455	0.000000
2	1	0	2.173955	0.276722	0.000000
3	1	0	1.418732	2.227818	0.000000
4	5	0	-0.511783	-0.880794	0.000000
5	1	0	-1.685355	-1.039608	0.000000
6	7	0	0.000000	0.487379	0.000000
7	7	0	0.364552	-1.966027	0.000000
8	1	0	0.023973	-2.913249	0.000000
9	1	0	1.369758	-1.887689	0.000000
10	9	0	-1.072308	1.424804	0.000000



E = -262.3304203 a.u.

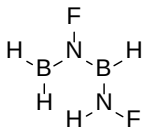
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.067189	-0.249246	0.000000
2	1	0	0.915198	-1.429855	0.000000
3	5	0	-1.429130	0.409034	0.000000
4	1	0	-2.171623	1.341926	0.000000
5	7	0	0.000000	0.664357	0.000000
6	1	0	0.265419	1.642130	0.000000
7	7	0	-1.971949	-0.883068	0.000000
8	1	0	-2.966247	-1.037472	0.000000
9	1	0	-1.426866	-1.731018	0.000000
10	9	0	2.333052	0.216258	0.000000



imaginary frequency: -51.57 cm^{-1}

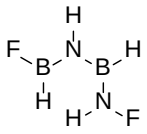
E = -361.5040421 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	2.420365	-0.483686	0.000000
2	1	0	2.081989	-1.628748	0.000000
3	1	0	3.572471	-0.186778	0.000000
4	5	0	0.000000	0.390112	0.000000
5	7	0	1.437518	0.522941	0.000000
6	1	0	1.753808	1.485882	0.000000
7	7	0	-0.626152	-0.869392	0.000000
8	1	0	-0.246498	-1.801501	0.000000
9	9	0	-2.015118	-0.938527	0.000000
10	9	0	-0.756344	1.496768	0.000000



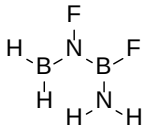
E = -361.3556247 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.895046	-0.562491	0.000000
2	7	0	1.375233	0.362661	0.000000
3	5	0	0.000000	0.584371	0.000000
4	1	0	-0.424982	1.683729	0.000000
5	5	0	-0.705167	-1.942122	0.000000
6	1	0	-1.621785	-2.689417	0.000000
7	9	0	-2.249448	-0.133647	0.000000
8	9	0	2.231345	1.462134	0.000000
9	1	0	1.940062	-0.472550	0.000000
10	1	0	0.434158	-2.290575	0.000000



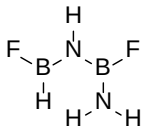
E = -361.5117659 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.397234	-0.868712	0.000000
2	1	0	-1.919700	0.201100	0.000000
3	5	0	1.042649	-0.033985	0.000000
4	1	0	2.186783	-0.340801	0.000000
5	7	0	0.000000	-1.035733	0.000000
6	1	0	0.327536	-1.994689	0.000000
7	7	0	0.727989	1.329351	0.000000
8	1	0	-0.140325	1.840757	0.000000
9	9	0	1.768501	2.261737	0.000000
10	9	0	-2.188200	-1.955982	0.000000



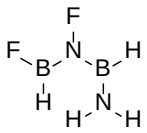
E = -361.5137831 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.228317	-1.599857	0.000000
2	1	0	2.292492	-1.067704	0.000000
3	1	0	1.079917	-2.773577	0.000000
4	5	0	0.000000	0.717350	0.000000
5	7	0	0.132136	-0.743185	0.000000
6	7	0	1.115844	1.556294	0.000000
7	1	0	1.007012	2.557729	0.000000
8	1	0	2.067787	1.231704	0.000000
9	9	0	-1.233051	1.236522	0.000000
10	9	0	-1.136355	-1.372899	0.000000



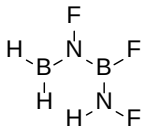
E = -361.6728135 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.344345	-1.935845	0.000000
2	1	0	0.973401	-2.722017	0.000000
3	7	0	0.000000	0.565115	0.000000
4	1	0	0.514357	1.439592	0.000000
5	5	0	0.824913	-0.620561	0.000000
6	5	0	-1.401322	0.664594	0.000000
7	9	0	2.166511	-0.424751	0.000000
8	9	0	-1.974094	1.882624	0.000000
9	1	0	-0.632518	-2.175889	0.000000
10	1	0	-2.115360	-0.287592	0.000000



E = -361.5144234 a.u.

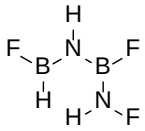
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.869610	0.828373	0.000000
2	1	0	0.384753	1.913650	0.000000
3	5	0	-1.447349	-0.416778	0.000000
4	1	0	-1.895093	-1.513268	0.000000
5	7	0	0.000000	-0.279792	0.000000
6	7	0	-2.281856	0.703898	0.000000
7	1	0	-3.283421	0.603165	0.000000
8	1	0	-1.967213	1.661236	0.000000
9	9	0	0.655194	-1.532896	0.000000
10	9	0	2.191769	0.678285	0.000000



imaginary frequency: -61.27 cm^{-1}

E = -460.6878667 a.u.

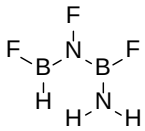
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.111365	2.294885	0.000000
2	1	0	-1.077258	2.365374	0.000000
3	1	0	0.828002	3.234939	0.000000
4	5	0	0.000000	-0.321272	0.000000
5	7	0	0.623849	1.001121	0.000000
6	7	0	-1.401537	-0.416507	0.000000
7	1	0	-2.128035	0.280058	0.000000
8	9	0	-1.976469	-1.681262	0.000000
9	9	0	0.750717	-1.412118	0.000000
10	9	0	2.032895	0.888853	0.000000



imaginary frequency: -72.75 cm^{-1}

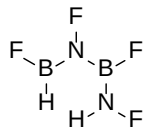
E = -460.8484369 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.730565	1.781578	0.000000
2	1	0	0.361807	2.254194	0.000000
3	5	0	0.000000	-0.685501	0.000000
4	7	0	-0.954973	0.392433	0.000000
5	1	0	-1.924029	0.090517	0.000000
6	7	0	1.388632	-0.450140	0.000000
7	1	0	1.924974	0.401456	0.000000
8	9	0	2.258372	-1.535353	0.000000
9	9	0	-0.446778	-1.948308	0.000000
10	9	0	-1.783321	2.614484	0.000000



E = -460.8511858 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.226342	0.997832	0.000000
2	1	0	-2.227151	0.357813	0.000000
3	5	0	0.324102	-1.119559	0.000000
4	7	0	0.000000	0.304636	0.000000
5	7	0	-0.663572	-2.108366	0.000000
6	1	0	-0.410021	-3.083419	0.000000
7	1	0	-1.653484	-1.930652	0.000000
8	9	0	1.618081	-1.459925	0.000000
9	9	0	1.144600	1.121459	0.000000
10	9	0	-1.268585	2.326355	0.000000



imaginary frequency: -80.99 cm^{-1}

E = -560.0246217 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.276219	1.356243	0.000000
2	1	0	2.218590	0.630951	0.000000
3	5	0	-0.430154	-0.635801	0.000000
4	7	0	0.000000	0.756757	0.000000
5	7	0	0.532176	-1.661735	0.000000
6	1	0	1.538592	-1.654213	0.000000
7	9	0	-1.087035	1.644561	0.000000
8	9	0	-1.723017	-0.922923	0.000000
9	9	0	0.086395	-2.978076	0.000000
10	9	0	1.422242	2.673760	0.000000