

Supplementary Information

Harnessing Halogen Bond Donors for Enhanced Nitrogen Reduction: A Case Study on Metal-Free Boron Nitride Single Atom Catalysts

Venkata Surya Kumar Choutipalli^{*,a,b} and Venkatesan Subramanian^{*,a,b,c}

^aAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad-201 002, India.

^bCentre for High Computing, CSIR-Central Leather Research Institute, Adyar, Chennai-600 020, India.

^cDepartment of Chemistry, Indian Institute of Technology Madras, Adyar, Chennai-600 020, India.

*E-mail: subuchem@hotmail.com; subramanianv@iitm.ac.in; chvsk07@gmail.com

	Title	Page No.
Fig. S1	Optimized geometries of heteroatom doped BN nanosheets and their interaction with N ₂ molecule.	2
Fig. S2	Nitrogen activation at boron nitride nanomaterials of various diameters.	3
Fig. S3	Lewis acid-base pair formation on interaction of alkali metal ions with Si _B BN.	4
Fig. S4	MO correlation diagram for neutral B-Lewis acids assisted nitrogen activation. Significant stabilization of LUMO of N ₂ and HOMO of the activated N ₂ species are witnessed.	5
Fig. S5	Optimized geometries and FMO contours of Imidazolium based halogen bond donors (XB1-XB4) assisted N ₂ -Si _B BN system.	6
Fig. S6	Optimized geometries and FMO contours of triazole based halogen bond donors (XB5-XB8) assisted N ₂ -Si _B BN system.	7
Fig. S7	Optimized geometries and FMO contours of neutral Halogen bond donors (XB9 and XB10) assisted N ₂ -Si _B BN system	8
Table S1	Cohesive and Defect Formation Energies of Defective BN Sheet.	8
Table S2	Population Analysis and Nitrogen Interaction Energies of Various Si Doped Defective BN Nanomaterials.	9
Table S3	Geometric parameters, population analysis and overpotential details of Lewis acids assisted N ₂ -Si _B BN nanosheet.	10
Table S4	Geometrical and population analysis results of halogen bond donors augmented N ₂ -Si _B BN system.	11
Table S5	Energetics of elementary steps involved in nitrogen reduction reaction before and after the augmentation of XB4	12
Table S6	Cartesian coordinates of geometries of heteroatom doped BN sheet and their corresponding N ₂ activated systems optimized at ωB97X-D/6-31G(d) level of theory.	12

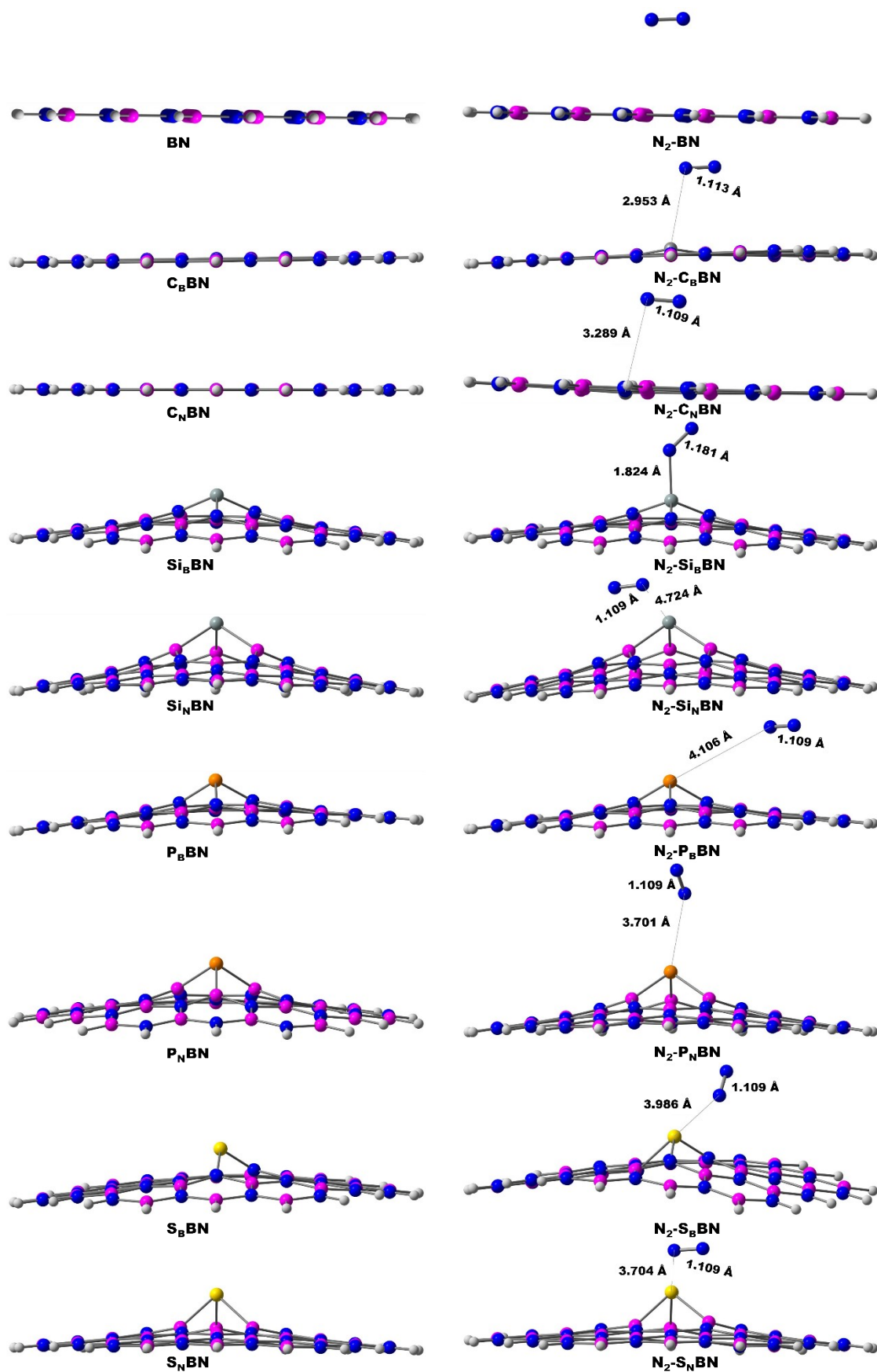


Fig. S1. Optimized geometries of heteroatom doped BN nanosheets and their interaction with N_2 molecule.

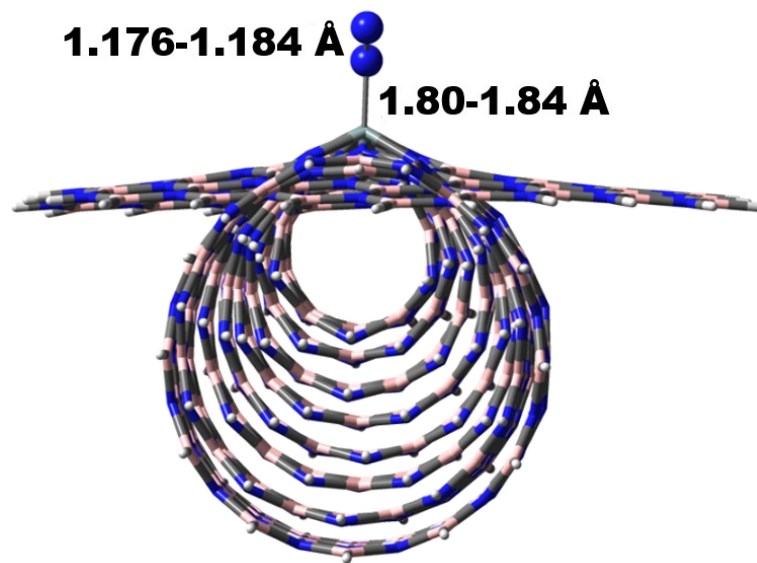


Fig. S2. Nitrogen activation at boron nitride nanomaterials of various diameters.

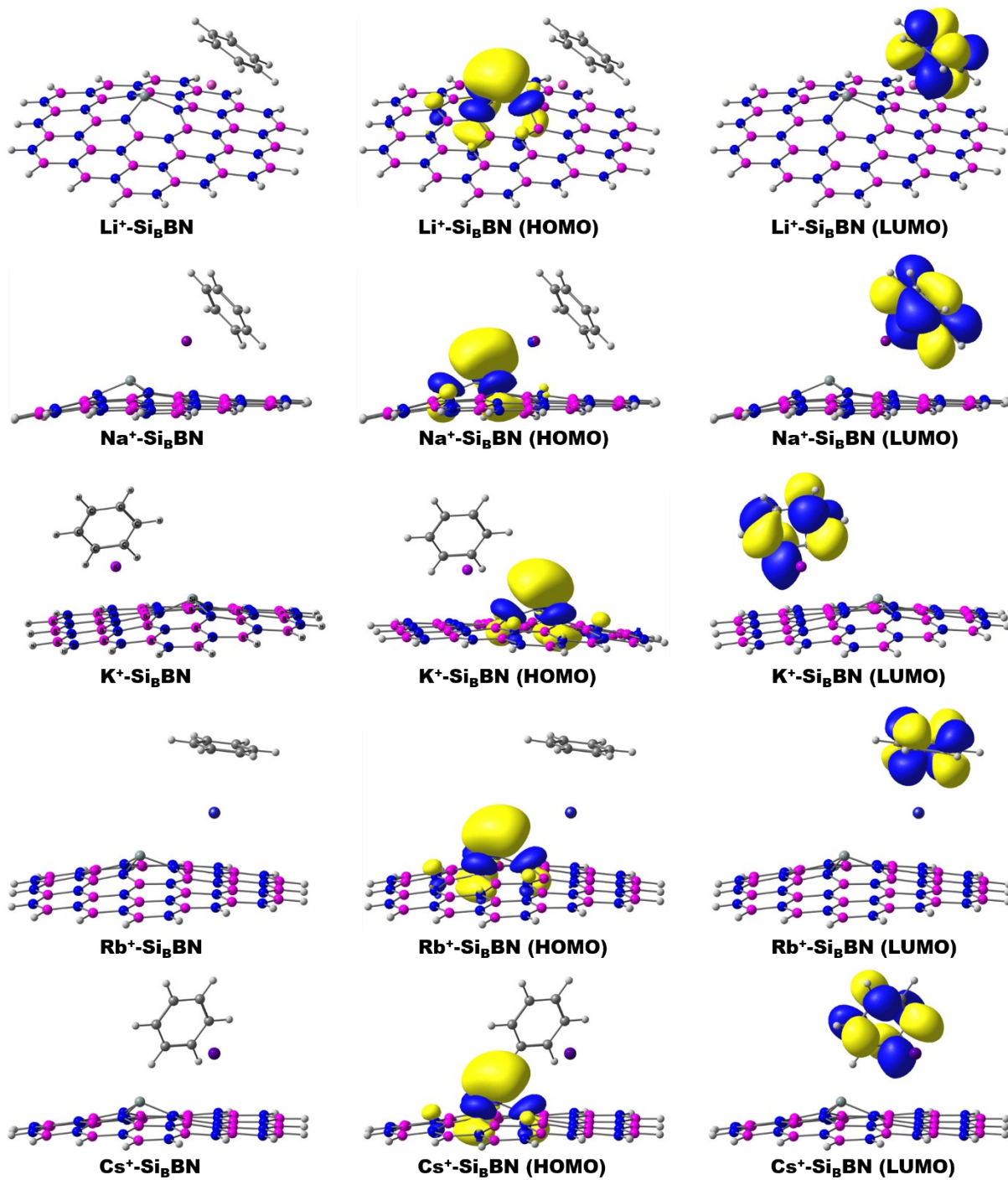


Fig. S3. Lewis acid-base pair formation on interaction of alkali metal ions with Si_BBN.

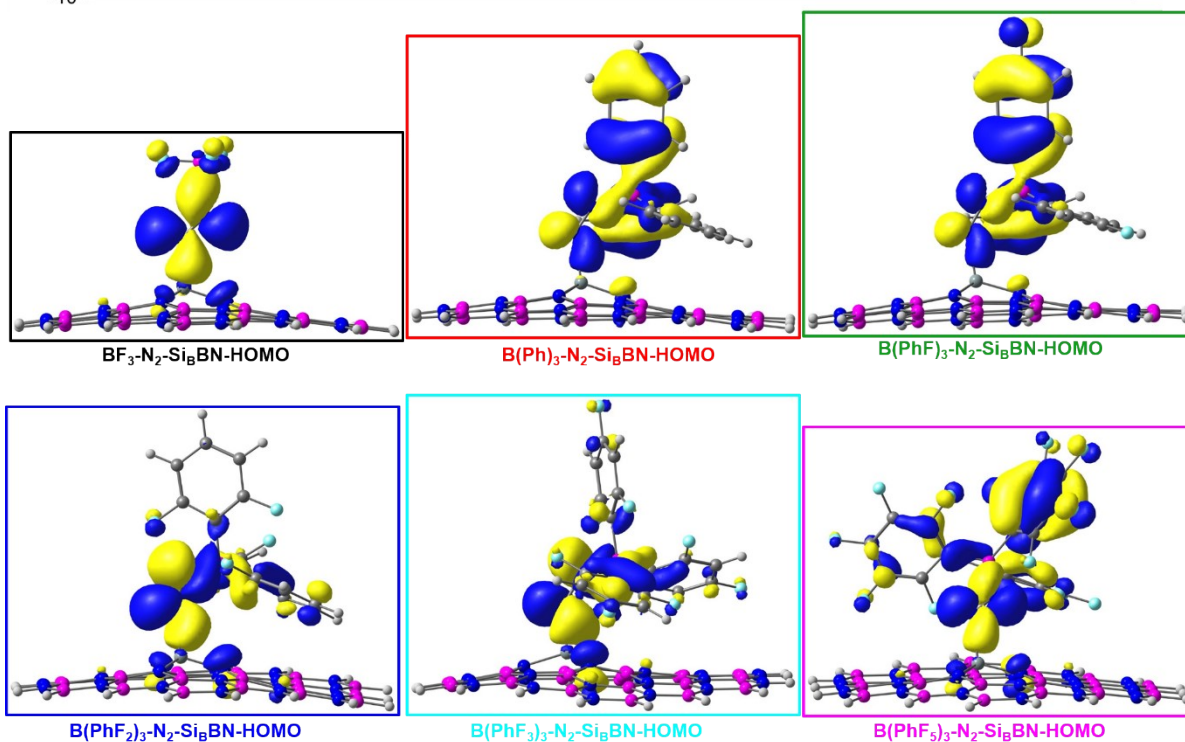
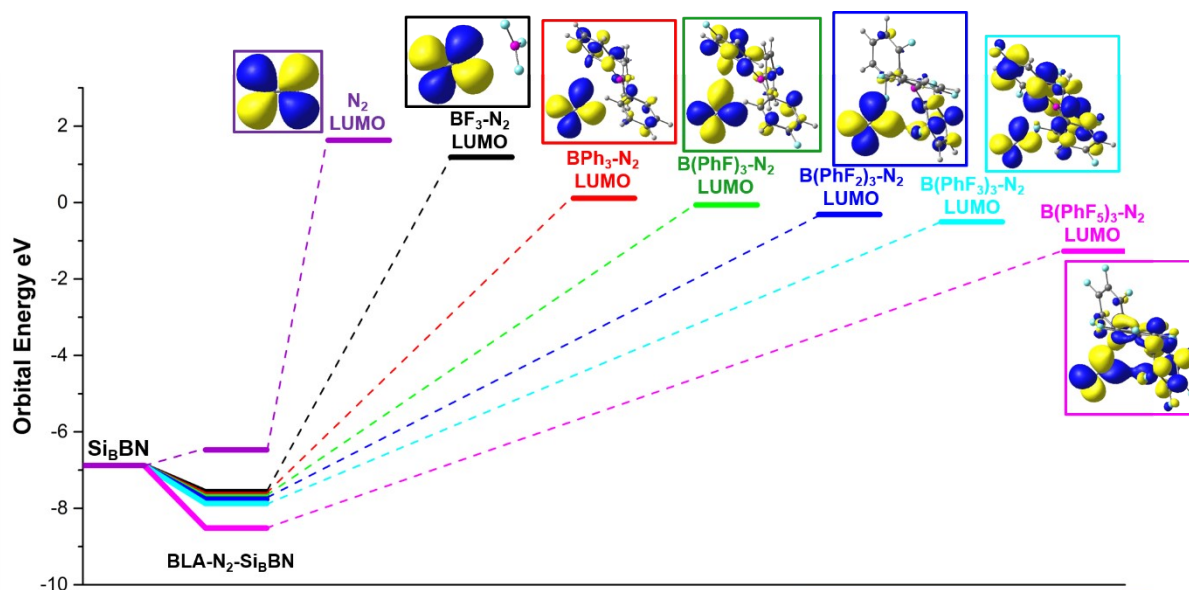


Fig. S4 MO correlation diagram for neutral B-Lewis acids assisted nitrogen activation. Significant stabilization of LUMO of N_2 and HOMO of the activated N_2 species are witnessed.

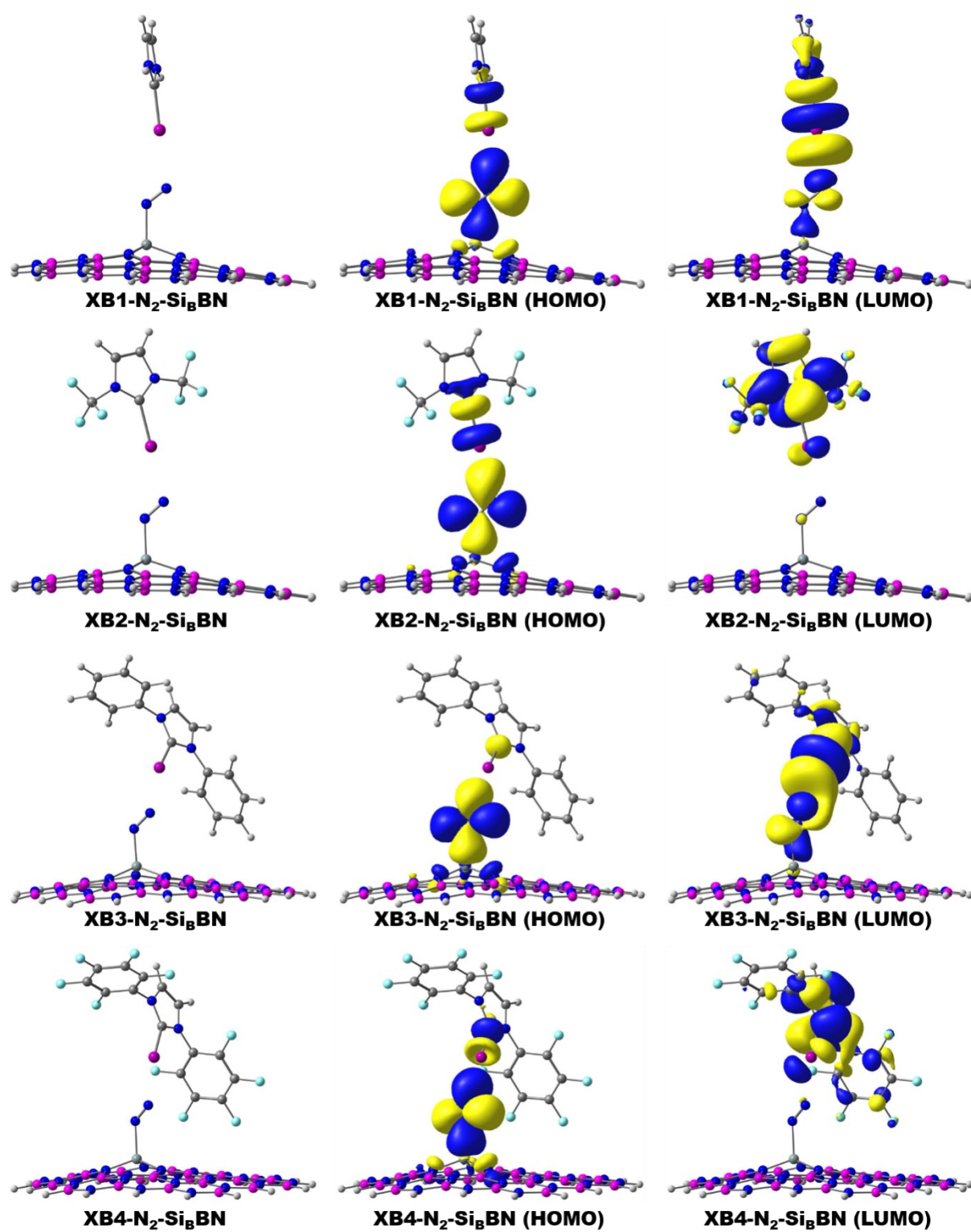


Fig. S5. Optimized geometries and FMO contours of Imidazolium based halogen bond donors (XB1-XB4) assisted N₂-Si_BBN system.

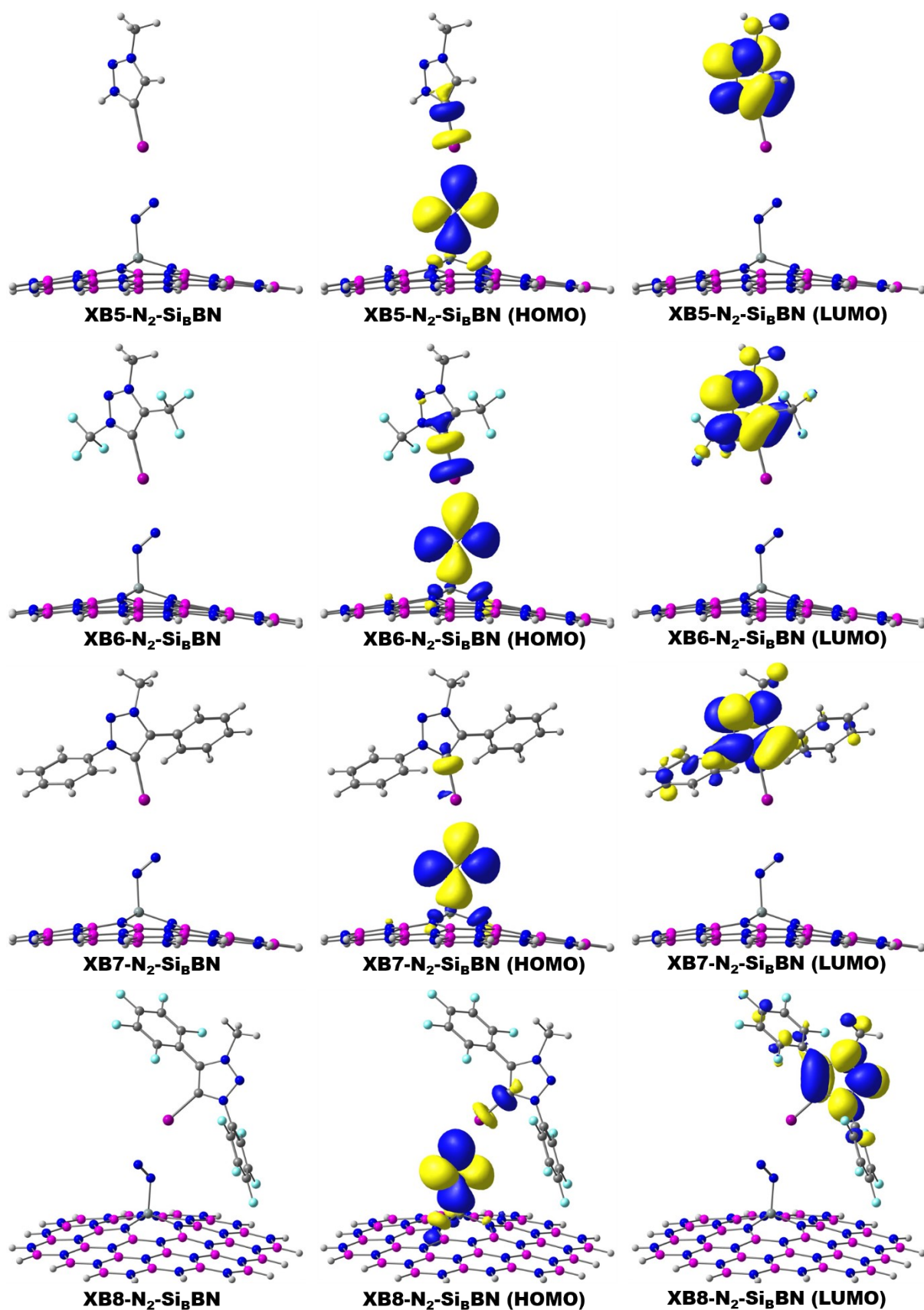


Fig. S6. Optimized geometries and FMO contours of triazole based halogen bond donors (XB5-XB8) assisted N₂-Si_BBN system.

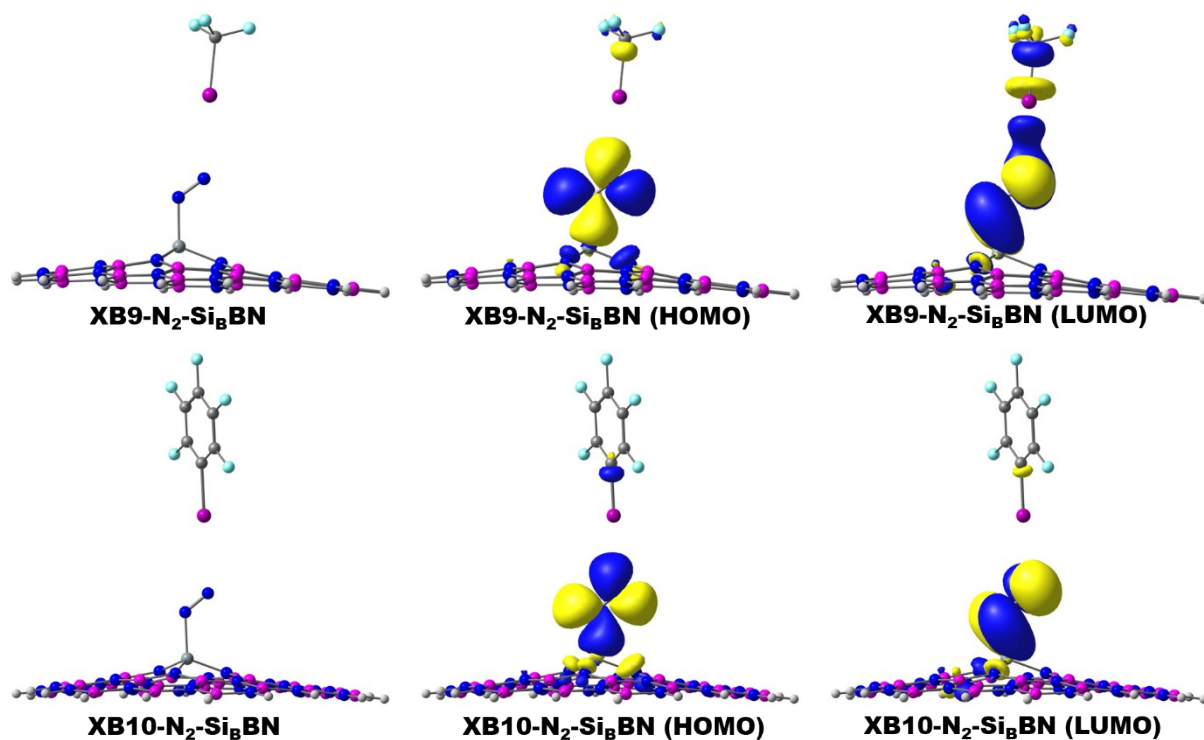


Fig. S7. Optimized geometries and FMO contours of neutral Halogen bond donors (XB9 and XB10) assisted N_2 - Si_B BN system.

Table S1. Cohesive and Defect Formation Energies of Defective BN Sheet.

S.No.	Defective BN	Cohesive Energy (E_{coh} , eV)	Defect Formation (E_{def} , eV)
1	C_B BN	-6.21	1.26
2	C_N BN	-6.19	2.72
3	Si_B BN	-6.17	3.75
4	Si_N BN	-6.09	9.66
5	P_B BN	-6.16	4.34
6	P_N BN	-6.13	6.67
7	S_B BN	-6.10	8.88
8	S_N BN	-6.11	8.49

Table S2. Population Analysis and Nitrogen Interaction Energies of Various Si Doped Defective BN Nanomaterials.

BN material	(Si _B BN)		N ₂ Activation (N ₂ -Si _B BN)		
	Spin density on Si _B	Charge on Si _B	ΔG _{N₂} (eV)	Charge (e)	
				Si _B	*N ₂
BN Sheet	0.793	0.557	0.22	0.790	-0.350
Si _B BNT(12,0)	0.792	0.605	0.27	0.834	-0.331
Si _B BNT(11,0)	0.792	0.612	0.27	0.839	-0.329
Si _B BNT(10,0)	0.792	0.623	0.28	0.842	-0.326
Si _B BNT(9,0)	0.792	0.635	0.29	0.860	-0.324
Si _B BNT(8,0)	0.792	0.653	0.30	0.877	-0.321
Si _B BNT(7,0)	0.791	0.680	0.31	0.920	-0.328
Si _B BNT(6,0)	0.790	0.716	0.34	0.948	-0.313
Si _B BNT(5,0)	0.787	0.750	0.36	1.009	-0.313
Si _B BNT(4,0)	0.777	0.766	0.43	1.029	-0.295

Table S3. Geometric parameters, population analysis and overpotential details of Lewis acids assisted N₂-Si_BBN nanosheet.

Structure	Charge			Bond Length			Spin Density		Potential req. (eV)	
	Si	*N ₂	Sheet	*N ₂	Si _B -N4	N5-LA	N4	N5	ΔG ₂	ΔG ₈
Si _B BN	0.557		-0.557							
N ₂ -Si _B BN	0.790	-0.350	0.350	1.181	1.824		0.171	0.709	0.26	2.38
Li ⁺ -N ₂ -Si _B BN	0.939	-0.361	0.845	1.175	1.864	2.212	0.246	0.605	-0.14	1.98
Na ⁺ -N ₂ -Si _B BN	0.886	-0.379	0.786	1.175	1.872	2.444	0.243	0.615	-0.11	2.06
K ⁺ -N ₂ -Si _B BN	0.856	-0.385	0.647	1.177	1.857	2.818	0.225	0.648	-0.06	2.05
Rb ⁺ -N ₂ -Si _B BN	0.813	-0.375	0.551	1.178	1.850	3.216	0.216	0.664	0.04	2.10
Cs ⁺ -N ₂ -Si _B BN	0.804	-0.376	0.535	1.177	1.854	3.005	0.221	0.658	0.05	2.18
BF ₃ -N ₂ -Si _B BN	0.800	-0.349	0.454	1.172	1.844	2.019	0.273	0.573	-0.23	2.11
BCL ₃ -N ₂ -Si _B BN	0.810	-0.341	0.421	1.169	1.874	1.649	0.368	0.467	-0.43	2.11
B(C ₆ H ₅) ₃ -N ₂ -Si _B BN	0.803	-0.324	0.453	1.167	1.860	1.675	0.300	0.504	-0.35	2.14
B(C ₆ H ₄ F) ₃ -N ₂ -Si _B BN	0.821	-0.330	0.458	1.166	1.865	1.689	0.307	0.497	-0.53	2.14
B(C ₆ H ₃ F ₂) ₃ -N ₂ -Si _B BN	0.830	-0.336	0.461	1.163	1.848	1.648	0.320	0.494	-0.30	1.96
B(C ₆ H ₃ F ₃) ₃ -N ₂ -Si _B BN	0.855	-0.344	0.469	1.173	1.879	1.596	0.313	0.536	-0.49	1.89
B(C ₆ F ₅) ₃ -N ₂ -Si _B BN	0.869	-0.344	0.475	1.169	1.876	1.630	0.351	0.490	-0.23	1.69

Table S4. Geometrical and population analysis results of halogen bond donors augmented N₂-Si_BBN system.

Structure	Charge (e)					Bond Length (Å)				Spin Density		E(2) of n-σ* kcal/mol	Potential req. (eV)	
	Si	*N ₂	BN Sheet	I	C _{Im/Tz}	*N ₂	Si _B -N4	N5-I	I-C	N4	N5		ΔG ₂	ΔG ₈
Si_BBN	0.557		-0.557											
N₂-Si_BBN	0.790	-0.35	0.350			1.181	1.824			0.171	0.709		0.26	2.38
XB1-N₂-Si_BBN	0.776	-0.342	0.501	0.445	0.055	1.170	1.877	2.709	2.129	0.266	0.532	19.80	0.03	0.36
XB2-N₂-Si_BBN	0.776	-0.318	0.550	0.431	0.121	1.163	1.891	2.618	2.201	0.288	0.451	31.86	-0.03	0.33
XB3-N₂-Si_BBN	0.774	-0.355	0.470	0.464	0.014	1.175	1.848	2.856	2.083	0.234	0.618	08.91	0.06	0.21
XB4-N₂-Si_BBN	0.769	-0.349	0.449	0.471	0.055	1.172	1.860	2.752	2.104	0.262	0.558	15.16	0.03	0.10
XB5-N₂-Si_BBN	0.775	-0.344	0.505	0.446	-0.166	1.171	1.870	2.736	2.122	0.260	0.550	17.25	0.06	0.35
XB6-N₂-Si_BBN	0.776	-0.331	0.523	0.464	-0.163	1.167	1.879	2.655	2.167	0.277	0.499	27.04	0.09	0.18
XB7-N₂-Si_BBN	0.775	-0.349	0.452	0.452	-0.256	1.174	1.856	2.827	2.098	0.242	0.597	12.15	0.02	0.24
XB8-N₂-Si_BBN	0.767	-0.348	0.435	0.474	-0.221	1.173	1.852	2.792	2.097	0.255	0.574	13.26	0.13	0.35
XB9-N₂-Si_BBN	0.781	-0.334	1.376	0.316	-0.691	1.178	1.832	3.089	2.101	0.199	0.665	04.59	0.28	0.51
XB10-N₂-Si_BBN	0.782	-0.335	1.373	0.172	0.546	1.179	1.833	3.130	2.184	0.194	0.670	04.33	0.23	0.54

Table S5: Energetics of elementary steps involved in nitrogen reduction reaction before and after the augmentation of XB4.

Step	Without XB4 (eV)		With XB4 (eV)	
	Distal	Alternating	Distal	Alternating
Step 1	0.23	0.23	-0.017	-0.017
Step 2	0.27	0.27	0.03	0.03
Step 3	-0.24	-0.32	-0.65	-0.45
Step 4	0.52	-1.00	-0.09	-1.09
Step 5	-0.98	0.50	-0.38	0.08
Step 6	-0.03	-2.15	-0.05	-1.99
Step 7	-2.28	-0.05	-2.26	0.02
Step 8	2.38	2.38	0.10	0.10

Table S6. Cartesian coordinates of geometries of heteroatom doped BN sheet and their corresponding N₂ activated systems optimized at ω B97X-D/6-31G(d) level of theory.

C _B BN				C _N BN			
N	5.119406000	-0.838255000	-0.000133000	N	5.083562000	1.303051000	-0.000014000
B	5.943020000	-2.025047000	0.000099000	B	6.307639000	0.536238000	0.000084000
B	5.744357000	0.450756000	-0.000270000	B	5.106950000	2.742883000	-0.000014000
B	5.553984000	2.927364000	-0.000158000	B	3.928158000	4.953647000	0.000047000
B	3.302135000	4.016241000	0.000060000	B	1.421040000	5.069688000	0.000028000
B	3.477828000	1.519249000	-0.000332000	B	2.598071000	2.826934000	-0.000126000
B	3.672357000	-0.958375000	-0.000227000	B	3.809884000	0.607467000	-0.000081000
B	3.888858000	-3.452249000	0.000246000	B	4.981547000	-1.603086000	0.000074000
B	1.629807000	-2.364190000	-0.000172000	B	2.480638000	-1.537116000	-0.000093000
B	1.240921000	2.589099000	-0.000239000	B	1.335529000	0.656134000	-0.000286000
B	-1.015408000	3.678225000	-0.000048000	B	0.090171000	2.977282000	-0.000214000
B	-0.615796000	-1.292737000	-0.000384000	B	-2.422209000	2.978878000	-0.000064000
B	-0.428995000	-3.791700000	-0.000121000	B	-0.043806000	-1.443389000	-0.000194000
B	-2.679274000	-2.714382000	-0.000257000	B	1.145677000	-3.650888000	-0.000049000
B	-2.880104000	-0.225990000	-0.000266000	B	-1.364621000	-3.575026000	-0.000058000
B	-3.070011000	2.263279000	-0.000099000	B	-2.569285000	-1.384407000	-0.000091000
B	-5.329555000	3.352952000	0.000216000	B	-3.766215000	0.836621000	-0.000022000
B	-5.139968000	0.853739000	0.000100000	B	-6.263743000	0.916645000	0.000232000
B	-4.943859000	-1.644631000	-0.000004000	B	-5.069655000	-1.299120000	0.000110000
B	-4.741327000	-4.142777000	-0.000065000	B	-3.876272000	-3.512838000	0.000061000
N	4.737836000	4.086905000	0.000116000	B	-2.672603000	-5.713843000	0.000035000
N	4.925883000	1.626454000	-0.000259000	N	2.715690000	5.698707000	0.000093000
N	5.318143000	-3.297931000	0.000368000	N	3.882614000	3.506260000	-0.000049000
N	3.066732000	-2.262636000	-0.000044000	N	6.229186000	-0.883613000	0.000132000
N	2.838090000	0.222667000	-0.000388000	N	3.751414000	-0.839173000	-0.000045000
N	2.675981000	2.713029000	-0.000182000	N	2.586698000	1.369726000	-0.000188000
N	0.420198000	3.779164000	-0.000012000	N	1.378249000	3.623847000	-0.000121000
N	0.824302000	-1.161262000	-0.000368000	N	-1.156351000	3.700525000	-0.000081000
N	1.004848000	-3.667579000	0.000014000	N	1.253850000	-0.780984000	-0.000214000
N	-1.237315000	-2.598876000	-0.000265000	N	2.425378000	-2.979045000	-0.000023000
N	-1.627716000	2.374069000	-0.000187000	N	-0.087564000	-2.889148000	-0.000112000
N	-3.889703000	3.463251000	0.000111000	N	-2.499096000	1.523612000	-0.000154000
N	-3.696313000	0.965363000	-0.000105000	N	-4.995430000	1.607962000	0.000106000
N	-3.500449000	-1.529914000	-0.000188000	N	-3.795498000	-0.610936000	-0.000016000

N	-3.301797000	-4.027364000	-0.000150000	N	-2.601358000	-2.827099000	-0.000034000
N	-5.525630000	-2.959715000	0.000088000	N	-1.400940000	-5.027240000	-0.000029000
N	-5.732017000	-0.449502000	0.000178000	N	-3.871467000	-4.951474000	0.000085000
N	-5.919790000	2.062184000	0.000323000	N	-5.079731000	-2.733107000	0.000128000
B	1.043593000	5.088470000	0.000258000	N	-6.271461000	-0.505363000	0.000215000
B	-1.217493000	6.175859000	0.000372000	B	-1.111444000	5.146303000	0.000079000
B	-3.270815000	4.759237000	0.000209000	B	-3.620959000	5.182221000	0.000214000
N	2.470696000	5.179673000	0.000344000	B	-4.931580000	3.046639000	0.000151000
N	0.199352000	6.252820000	0.000526000	N	0.175508000	5.790479000	0.000106000
N	-1.839684000	4.874130000	0.000181000	N	-2.365536000	5.852550000	0.000207000
B	1.824956000	-4.863744000	0.000308000	N	-3.663240000	3.734636000	0.000080000
B	-2.488223000	-5.211107000	-0.000109000	B	3.656463000	-3.740439000	0.000082000
N	3.248857000	-4.731087000	0.000485000	B	-0.174937000	-5.778618000	-0.000014000
N	-1.056675000	-5.101422000	0.000012000	N	4.904881000	-3.035003000	0.000132000
B	-0.239020000	-6.290378000	0.000272000	N	1.094197000	-5.102642000	-0.000007000
N	1.172481000	-6.145508000	0.000488000	B	2.322143000	-5.864727000	0.000077000
N	-1.442371000	-0.113216000	-0.000389000	N	3.564791000	-5.176058000	0.000132000
H	-6.016578000	4.334246000	0.000561000	N	-1.298945000	-0.703700000	-0.000225000
H	-3.949073000	5.745978000	0.000448000	H	-7.294141000	1.527864000	0.000335000
H	-1.881027000	7.173045000	0.000723000	H	-5.946966000	3.681832000	0.000254000
H	0.621250000	7.170253000	0.000796000	H	-4.637538000	5.816287000	0.000323000
H	2.903211000	6.092471000	0.000577000	H	-2.377180000	6.862414000	0.000309000
H	5.194328000	4.987456000	0.000322000	H	0.206115000	6.800818000	0.000217000
H	6.747512000	3.025795000	-0.000023000	H	2.788562000	6.706019000	0.000166000
H	6.937210000	0.545145000	-0.000169000	H	4.981479000	5.524660000	0.000073000
H	7.137135000	-1.934347000	0.000209000	H	6.159050000	3.315240000	0.000001000
H	5.909770000	-4.115966000	0.000602000	H	7.373341000	1.083548000	0.000118000
H	3.818521000	-5.565135000	0.000721000	H	7.098348000	-1.398008000	0.000203000
H	1.732254000	-6.985885000	0.000727000	H	5.763442000	-3.567744000	0.000210000
H	-0.739883000	-7.378378000	0.000423000	H	4.408484000	-5.730998000	0.000193000
H	-3.005016000	-6.291177000	0.000055000	H	2.295565000	-7.062332000	0.000099000
H	-5.267603000	-5.218813000	0.000083000	H	-0.210838000	-6.975487000	-0.000022000
H	-6.530326000	-3.060525000	0.000252000	H	-2.717804000	-6.910873000	0.000034000
H	-6.739113000	-0.528512000	0.000361000	H	-4.747036000	-5.454482000	0.000131000
H	-6.927930000	2.005151000	0.000549000	H	-5.968874000	-3.212955000	0.000205000
B	-0.810053000	1.180747000	-0.000411000	H	-7.170144000	-0.966153000	0.000302000
N	0.632922000	1.275507000	-0.000385000	B	-1.293454000	0.735725000	-0.000280000
C	1.431985000	0.112167000	-0.000559000	C	0.044116000	1.457320000	-0.000387000
Si_BBN				Si_NBN			
N	3.663874000	3.756326000	-0.140692000	N	1.405668000	-5.008340000	-0.233039000
B	5.106383000	3.749864000	-0.195595000	B	0.684086000	-6.239602000	-0.447610000
B	2.940194000	4.993867000	-0.246480000	B	2.837474000	-4.981835000	-0.304166000
B	0.782636000	6.246819000	-0.361689000	B	4.967932000	-3.748173000	-0.473200000
B	-1.395319000	5.018315000	-0.180287000	B	5.030576000	-1.266727000	-0.233927000
B	0.771868000	3.761492000	-0.023665000	B	2.870388000	-2.510741000	0.211552000
B	2.943014000	2.504500000	0.008625000	B	0.686104000	-3.779747000	0.039185000
B	5.097687000	1.245342000	-0.021518000	B	-1.481959000	-4.992752000	-0.238884000
B	2.926036000	-0.003433000	0.165504000	B	-1.494295000	-2.517663000	0.152902000
B	0.790492000	1.286421000	0.341980000	B	0.605640000	-1.467594000	0.858463000
B	-1.401238000	2.555972000	0.256852000	B	3.149415000	-0.003244000	0.721613000
B	-3.637044000	1.270882000	0.172595000	B	2.875557000	2.504846000	0.211635000
B	0.787473000	-1.288232000	0.342160000	B	-1.470918000	0.001518000	0.439302000
B	2.937064000	-2.511381000	0.008524000	B	-3.633980000	-1.244078000	0.054486000
B	0.762989000	-3.763259000	-0.023738000	B	-3.631409000	1.251541000	0.054438000
B	-1.407215000	-2.552670000	0.257230000	B	-1.489104000	2.520734000	0.152861000
B	-3.640038000	-1.262383000	0.172791000	B	0.693891000	3.778338000	0.039210000
B	-5.748358000	-2.500984000	-0.354259000	B	0.696932000	6.238192000	-0.447571000
B	-3.575409000	-3.744809000	-0.091141000	B	-1.471681000	4.995781000	-0.238966000

B	-1.407167000	-5.015005000	-0.180168000	B	-3.643347000	3.747796000	-0.189591000
B	0.767859000	-6.248550000	-0.362354000	B	-5.804129000	2.487803000	-0.215266000
N	-0.637940000	6.228478000	-0.351665000	N	5.667784000	-2.517312000	-0.534668000
N	1.502719000	5.004019000	-0.205238000	N	3.557234000	-3.744119000	-0.152985000
N	5.785064000	2.505574000	-0.121987000	N	-0.734097000	-6.207623000	-0.425495000
N	3.651197000	1.248068000	0.069383000	N	-0.760296000	-3.759980000	0.006759000
N	1.504088000	2.516862000	0.095246000	N	1.412382000	-2.575693000	0.385927000
N	-0.674944000	3.778688000	0.007775000	N	3.663479000	-1.276699000	0.257856000
N	-2.862249000	2.509805000	0.176184000	N	3.666109000	1.269169000	0.257909000
N	-0.630632000	1.376818000	0.557904000	N	-0.786935000	-1.299745000	0.495112000
N	1.484011000	-0.001708000	0.344097000	N	-2.928222000	-2.499771000	0.003253000
N	3.648239000	-1.256636000	0.069335000	N	-2.904901000	0.002986000	0.196735000
N	1.498149000	-2.520327000	0.095252000	N	1.417682000	2.572789000	0.385960000
N	-3.022119000	0.003526000	0.470126000	N	1.415986000	5.005456000	-0.232968000
N	-5.053782000	-1.251452000	-0.159613000	N	-0.752548000	3.761539000	0.006726000
N	-2.868147000	-2.503101000	0.176557000	N	-2.923067000	2.505778000	0.003179000
N	-0.683858000	-3.777080000	0.007978000	N	-5.079947000	1.247067000	-0.068438000
N	1.490838000	-5.007487000	-0.205596000	N	-5.077358000	3.704263000	-0.272470000
N	-0.652656000	-6.226896000	-0.351954000	N	-2.901510000	4.966312000	-0.291694000
N	-2.837920000	-4.970739000	-0.188938000	N	-0.721319000	6.209114000	-0.425550000
N	-5.003372000	-3.707021000	-0.277223000	B	5.033189000	1.256400000	-0.233855000
B	-3.566554000	3.753145000	-0.091703000	B	4.975687000	3.737982000	-0.472947000
B	-5.742429000	2.514421000	-0.354855000	B	2.847742000	4.976019000	-0.304013000
B	-5.748223000	0.006741000	-0.280982000	N	5.699807000	-0.005853000	-0.375040000
N	-2.826180000	4.977348000	-0.189450000	N	5.672990000	2.505675000	-0.534516000
N	-4.994565000	3.718696000	-0.278053000	N	3.564956000	3.736822000	-0.152837000
N	-5.050788000	1.263302000	-0.159917000	B	-3.651051000	-3.740316000	-0.189458000
B	5.094716000	-1.257404000	-0.021574000	B	-5.798256000	0.005952000	-0.102603000
B	2.928327000	-5.000713000	-0.247048000	N	-2.911724000	-4.960357000	-0.291545000
N	5.789373000	-0.006851000	-0.019075000	N	-5.082508000	-1.236641000	-0.068374000
N	3.654915000	-3.764923000	-0.140883000	B	-5.809243000	-2.475893000	-0.215126000
B	5.097436000	-3.761892000	-0.196017000	N	-5.084969000	-3.693844000	-0.272297000
N	5.779101000	-2.519250000	-0.122090000	N	-0.784255000	1.301367000	0.495100000
Si	-1.454038000	0.001781000	1.181897000	H	1.282527000	7.264914000	-0.641319000
N	-0.633778000	-1.375395000	0.558474000	H	3.448715000	5.988303000	-0.521301000
H	-6.924671000	-2.524159000	-0.578845000	H	5.543252000	4.764574000	-0.713706000
H	-6.923742000	0.008182000	-0.510345000	H	6.643428000	2.522660000	-0.812705000
H	-6.918665000	2.540484000	-0.579548000	H	6.655751000	-0.006838000	-0.702598000
H	-5.487688000	4.584920000	-0.440926000	H	6.638185000	-2.536298000	-0.812858000
H	-3.334396000	5.834179000	-0.358280000	H	5.533361000	-4.775935000	-0.713992000
H	-1.119402000	7.108056000	-0.470946000	H	3.436347000	-5.995344000	-0.521543000
H	1.371511000	7.280046000	-0.504920000	H	1.267549000	-7.267525000	-0.641408000
H	3.537355000	6.023416000	-0.377843000	H	-1.227185000	-7.074115000	-0.585934000
H	5.719099000	4.773163000	-0.305722000	H	-3.413264000	-5.823192000	-0.448073000
H	6.793485000	2.516485000	-0.173928000	H	-5.606967000	-4.550324000	-0.388477000
H	6.797161000	-0.008024000	-0.088870000	H	-7.003946000	-2.475932000	-0.299554000
H	6.787496000	-2.532523000	-0.173945000	H	-6.992486000	0.007172000	-0.185085000
H	5.707826000	-4.786566000	-0.306272000	H	-6.998829000	2.490276000	-0.299705000
H	3.523207000	-6.031560000	-0.378668000	H	-5.597597000	4.561807000	-0.388691000
H	1.354476000	-7.283032000	-0.505911000	H	-3.401274000	5.830168000	-0.448277000
H	-1.136191000	-7.105331000	-0.471353000	H	-1.212621000	7.076611000	-0.586038000
H	-3.348160000	-5.826364000	-0.357817000	B	0.608661000	1.466338000	0.858470000
H	-5.498557000	-4.572112000	-0.439928000	Si	1.508041000	-0.001564000	1.795601000
P_BBN				P_NBN			
N	3.654598000	3.755776000	-0.134909000	N	-1.410283000	5.009070000	-0.196426000
B	5.098175000	3.755346000	-0.166953000	B	-0.688718000	6.248878000	-0.359964000
B	2.931308000	4.993150000	-0.236650000	B	-2.843254000	4.988356000	-0.269517000
B	0.773182000	6.243620000	-0.330063000	B	-4.986078000	3.749127000	-0.412260000

B	-1.400531000	5.005708000	-0.155817000	B	-5.029420000	1.258482000	-0.206416000
B	0.765568000	3.751148000	-0.055917000	B	-2.864628000	2.506772000	0.142504000
B	2.934487000	2.500986000	-0.007992000	B	-0.686317000	3.772383000	0.026192000
B	5.099339000	1.252021000	-0.002405000	B	1.480680000	5.002335000	-0.181662000
B	2.930508000	0.000127000	0.146526000	B	1.490797000	2.515567000	0.122442000
B	0.777847000	1.267598000	0.259732000	B	-0.632801000	1.393715000	0.674268000
B	-1.403047000	2.527822000	0.192897000	B	-3.047181000	-0.000376000	0.559288000
B	-3.598546000	1.259070000	0.114829000	B	-2.863998000	-2.507478000	0.142494000
B	0.777956000	-1.267531000	0.259737000	B	1.477629000	0.000183000	0.339559000
B	2.934704000	-2.500732000	-0.007984000	B	3.640033000	1.249917000	0.030403000
B	0.765894000	-3.751083000	-0.055914000	B	3.640342000	-1.249016000	0.030406000
B	-1.402828000	-2.527945000	0.192895000	B	1.491420000	-2.515196000	0.122445000
B	-3.598436000	-1.259383000	0.114820000	B	-0.685378000	-3.772547000	0.026190000
B	-5.729257000	-2.499416000	-0.321101000	B	-0.687167000	-6.249045000	-0.359961000
B	-3.569831000	-3.751748000	-0.057017000	B	1.481919000	-5.001969000	-0.181651000
B	-1.400093000	-5.005830000	-0.155826000	B	3.651875000	-3.749096000	-0.151126000
B	0.773727000	-6.243554000	-0.330055000	B	5.813747000	-2.486711000	-0.197593000
N	-0.646354000	6.220660000	-0.304887000	N	-5.682169000	2.514055000	-0.451607000
N	1.494352000	4.998528000	-0.206848000	N	-3.563581000	3.747935000	-0.152879000
N	5.783099000	2.514683000	-0.089211000	N	0.729700000	6.220314000	-0.330270000
N	3.651838000	1.251655000	0.063412000	N	0.758784000	3.760292000	0.009688000
N	1.491567000	2.504655000	0.044481000	N	-1.412345000	2.548648000	0.291068000
N	-0.678377000	3.757820000	-0.023120000	N	-3.630111000	1.266010000	0.180260000
N	-2.856752000	2.505923000	0.158067000	N	-3.629790000	-1.266909000	0.180253000
N	-0.653193000	1.318438000	0.429135000	N	0.777953000	1.282384000	0.385719000
N	1.488470000	0.000064000	0.293795000	N	2.928089000	2.503505000	0.000471000
N	3.651947000	-1.251337000	0.063417000	N	2.914545000	0.000362000	0.145144000
N	1.491785000	-2.504525000	0.044486000	N	-1.411708000	-2.548990000	0.291057000
N	-2.939365000	-0.000129000	0.354246000	N	-1.409037000	-5.009413000	-0.196432000
N	-5.019371000	-1.249916000	-0.182871000	N	0.759718000	-3.760103000	0.009692000
N	-2.856534000	-2.506171000	0.158055000	N	2.928707000	-2.502780000	0.000478000
N	-0.678051000	-3.757878000	-0.023123000	N	5.089156000	-1.242948000	-0.080585000
N	1.494789000	-4.998398000	-0.206839000	N	5.086519000	-3.704460000	-0.227730000
N	-0.645811000	-6.220715000	-0.304889000	N	2.912188000	-4.971652000	-0.222477000
N	-2.830551000	-4.975791000	-0.135382000	N	0.731241000	-6.220133000	-0.330260000
N	-4.999435000	-3.711908000	-0.217676000	B	-5.029102000	-1.259736000	-0.206421000
B	-3.570158000	3.751438000	-0.056998000	B	-4.985135000	-3.750366000	-0.412278000
B	-5.729476000	2.498921000	-0.321079000	B	-2.842008000	-4.989054000	-0.269535000
B	-5.722336000	-0.000248000	-0.297089000	N	-5.706032000	-0.000711000	-0.314259000
N	-2.830986000	4.975546000	-0.135365000	N	-5.681536000	-2.515472000	-0.451620000
N	-4.999760000	3.711474000	-0.217647000	N	-3.562642000	-3.748813000	-0.152898000
N	-5.019481000	1.249483000	-0.182859000	B	3.650950000	3.750000000	-0.151139000
B	5.099448000	-1.251579000	-0.002397000	B	5.804859000	0.000715000	-0.116928000
B	2.931745000	-4.992897000	-0.236633000	N	2.910960000	4.972370000	-0.222492000
N	5.792435000	0.000252000	0.010479000	N	5.088848000	1.244205000	-0.080588000
N	3.654925000	-3.755459000	-0.134895000	B	5.813132000	2.488143000	-0.197603000
B	5.098502000	-3.754904000	-0.166931000	N	5.085606000	3.705714000	-0.227745000
N	5.783318000	-2.514181000	-0.089192000	N	0.778272000	-1.282187000	0.385716000
N	-0.653079000	-1.318496000	0.429145000	H	-1.271246000	-7.282348000	-0.519833000
H	-6.909909000	-2.514341000	-0.521222000	H	-3.439899000	-6.009764000	-0.453020000
H	-6.901779000	-0.000299000	-0.502551000	H	-5.564617000	-4.778429000	-0.615265000
H	-6.910130000	2.513743000	-0.521197000	H	-6.666151000	-2.534970000	-0.674580000
H	-5.506356000	4.575928000	-0.343823000	H	-6.682691000	-0.000833000	-0.573001000
H	-3.337244000	5.839764000	-0.267923000	H	-6.666789000	2.533300000	-0.674568000
H	-1.132092000	7.101546000	-0.393002000	H	-5.565826000	4.777041000	-0.615243000
H	1.359503000	7.280602000	-0.454584000	H	-3.441398000	6.008919000	-0.453000000
H	3.527487000	6.025208000	-0.350851000	H	-1.273054000	7.282037000	-0.519825000
H	5.707344000	4.782249000	-0.261738000	H	1.220118000	7.094291000	-0.454325000

H	6.792132000	2.531431000	-0.124836000	H	3.413141000	5.840219000	-0.346027000
H	6.801323000	0.000295000	-0.041188000	H	5.607125000	4.565429000	-0.320019000
H	6.792353000	-2.530841000	-0.124812000	H	7.008084000	2.493247000	-0.277707000
H	5.707760000	-4.781756000	-0.261703000	H	6.999277000	0.000862000	-0.197142000
H	3.528012000	-6.024904000	-0.350821000	H	7.008701000	-2.491523000	-0.277694000
H	1.360136000	-7.280486000	-0.454566000	H	5.608249000	-4.564046000	-0.319997000
H	-1.131472000	-7.101643000	-0.393006000	H	3.414584000	-5.839376000	-0.346010000
H	-3.336733000	-5.840053000	-0.267943000	H	1.221874000	-7.093989000	-0.454315000
H	-5.505955000	-4.576402000	-0.343858000	B	-0.632455000	-1.393863000	0.674271000
P	-1.441719000	-0.000061000	1.212234000	P	-1.484371000	-0.000181000	1.621372000
S_BBN				S_NBN			
N	-5.178303000	-1.008602000	-0.138930000	N	1.354881000	-5.014965000	-0.162147000
B	-6.357933000	-0.179020000	-0.145626000	B	0.617870000	-6.252043000	-0.268766000
B	-5.288936000	-2.439190000	-0.257427000	B	2.790160000	-5.032737000	-0.214613000
B	-4.224498000	-4.701951000	-0.359873000	B	4.959779000	-3.816151000	-0.314417000
B	-1.731168000	-4.922169000	-0.188803000	B	4.989187000	-1.312295000	-0.179440000
B	-2.798397000	-2.655044000	-0.114602000	B	2.829269000	-2.546095000	0.057539000
B	-3.866408000	-0.392669000	-0.023054000	B	0.644471000	-3.757159000	-0.014834000
B	-4.918202000	1.871649000	0.032146000	B	-1.536190000	-4.977261000	-0.140587000
B	-2.421118000	1.656006000	0.154464000	B	-1.511574000	-2.479816000	0.056568000
B	-1.377459000	-0.618148000	0.156493000	B	0.650790000	-1.309184000	0.399246000
B	-0.320328000	-2.863010000	0.088778000	B	2.920794000	-0.033530000	0.328834000
B	2.202710000	-3.074651000	0.152158000	B	2.887732000	2.480157000	0.057736000
B	0.063634000	1.461220000	0.285281000	B	-1.491377000	0.017172000	0.198283000
B	-0.994210000	3.708566000	0.006967000	B	-3.666318000	-1.206261000	0.007747000
B	1.499894000	3.508493000	-0.066958000	B	-3.637266000	1.290695000	0.006927000
B	2.620977000	1.299014000	0.237490000	B	-1.453450000	2.513840000	0.055499000
B	3.706418000	-1.001796000	0.169479000	B	0.731608000	3.741106000	-0.014813000
B	6.133294000	-1.206471000	-0.363492000	B	0.762909000	6.236126000	-0.266699000
B	5.084545000	1.059166000	-0.087307000	B	-1.420086000	5.011299000	-0.141280000
B	4.002950000	3.320099000	-0.221815000	B	-3.605441000	3.788015000	-0.113268000
B	2.901875000	5.560664000	-0.419773000	B	-5.793114000	2.561825000	-0.142099000
N	-3.044333000	-5.495404000	-0.329063000	N	5.651347000	-2.577223000	-0.342594000
N	-4.113375000	-3.266332000	-0.247953000	N	3.528698000	-3.804735000	-0.132294000
N	-6.203745000	1.230535000	-0.048928000	N	-0.799806000	-6.208051000	-0.241840000
N	-3.731325000	1.044831000	0.070302000	N	-0.798565000	-3.735468000	-0.019358000
N	-2.691681000	-1.216491000	-0.010459000	N	1.388423000	-2.526190000	0.157219000
N	-1.620086000	-3.489790000	-0.084105000	N	3.560950000	-1.303054000	0.082974000
N	0.896749000	-3.677284000	0.142695000	N	3.590463000	1.220656000	0.083339000
N	-0.254525000	-1.461188000	0.164011000	N	-0.779828000	-1.239789000	0.225666000
N	-1.234293000	0.834936000	0.276891000	N	-2.954686000	-2.460629000	-0.014555000
N	-2.296167000	3.098321000	0.092196000	N	-2.932368000	0.033887000	0.084566000
N	0.199599000	2.887558000	0.061276000	N	1.446818000	2.493264000	0.156555000
N	2.451852000	-1.665750000	0.461834000	N	1.471059000	4.982318000	-0.160681000
N	4.841121000	-1.824473000	-0.176673000	N	-0.711554000	3.752755000	-0.020013000
N	3.796450000	0.445265000	0.193369000	N	-2.896634000	2.528204000	-0.015765000
N	2.703639000	2.704796000	-0.039284000	N	-5.088217000	1.304500000	-0.065338000
N	1.607512000	4.944251000	-0.248865000	N	-5.042607000	3.766406000	-0.160437000
N	4.063024000	4.741804000	-0.409819000	N	-2.850658000	5.002156000	-0.161859000
N	5.164691000	2.483065000	-0.205887000	N	-0.655424000	6.224835000	-0.241246000
N	6.228822000	0.206874000	-0.271997000	B	5.018502000	1.196557000	-0.179017000
B	0.774776000	-5.109365000	-0.055468000	B	5.047322000	3.700520000	-0.312794000
B	3.265073000	-5.299634000	-0.282799000	B	2.906410000	4.967098000	-0.212377000
B	4.684130000	-3.253530000	-0.277991000	N	5.687873000	-0.065835000	-0.252131000
N	-0.526021000	-5.702492000	-0.154519000	N	5.709907000	2.445827000	-0.341684000
N	1.981398000	-5.889117000	-0.181988000	N	3.616334000	3.722340000	-0.131047000
N	3.390474000	-3.863501000	-0.143345000	B	-3.692661000	-3.703703000	-0.111270000
B	-3.485783000	3.925130000	0.041848000	B	-5.818152000	0.067371000	-0.089033000

B	0.421154000	5.757008000	-0.267239000	N	-2.966190000	-4.934974000	-0.160083000
N	-4.769573000	3.296316000	0.064689000	N	-5.117195000	-1.186345000	-0.064285000
N	-0.871490000	5.150178000	-0.132265000	B	-5.851178000	-2.427024000	-0.139721000
B	-2.057335000	5.976272000	-0.148402000	N	-5.128953000	-3.648778000	-0.157589000
N	-3.326275000	5.353073000	-0.043361000	N	-0.750750000	1.257138000	0.224409000
N	1.315120000	0.739940000	0.528579000	H	1.359505000	7.268820000	-0.376317000
H	7.102335000	-1.870247000	-0.593642000	H	3.509177000	5.993532000	-0.339609000
H	5.643912000	-3.933779000	-0.497024000	H	5.662157000	4.718481000	-0.453511000
H	4.234206000	-5.975311000	-0.479001000	H	6.708050000	2.442994000	-0.494664000
H	1.914389000	-6.889581000	-0.302008000	H	6.682800000	-0.077351000	-0.426718000
H	-0.590875000	-6.703368000	-0.276207000	H	6.649269000	-2.597412000	-0.495703000
H	-3.150466000	-6.496698000	-0.404983000	H	5.551030000	-4.847839000	-0.456120000
H	-5.297426000	-5.223421000	-0.477661000	H	3.369474000	-6.072388000	-0.343583000
H	-6.370689000	-2.942920000	-0.366270000	H	1.190854000	-7.297833000	-0.380442000
H	-7.449605000	-0.664785000	-0.236502000	H	-1.299553000	-7.081696000	-0.323115000
H	-7.039909000	1.796282000	-0.066653000	H	-3.478362000	-5.802089000	-0.239493000
H	-5.597115000	3.874372000	0.026599000	H	-5.657183000	-4.507321000	-0.216951000
H	-4.145095000	5.943326000	-0.069683000	H	-7.047735000	-2.428025000	-0.192549000
H	-1.968904000	7.166185000	-0.253987000	H	-7.014198000	0.081385000	-0.142529000
H	0.516192000	6.942852000	-0.401147000	H	-6.989324000	2.590865000	-0.195603000
H	3.000045000	6.744274000	-0.572428000	H	-5.550712000	4.636938000	-0.220933000
H	4.958123000	5.192764000	-0.532315000	H	-3.342605000	5.880840000	-0.241821000
H	6.066906000	2.903816000	-0.378330000	H	-1.134863000	7.109785000	-0.322376000
H	7.132997000	0.625360000	-0.436998000	B	0.681344000	1.293114000	0.397403000
S	1.374243000	-0.726973000	1.361065000	S	1.455768000	-0.016725000	1.569987000
N₂-C_BBN				N₂-C_NBN			
N	4.671104000	-2.085462000	-0.194432000	N	1.653677000	-4.976009000	-0.093578000
B	6.009380000	-1.541231000	-0.203527000	B	2.959027000	-5.592940000	-0.051188000
B	4.491697000	-3.505983000	-0.222731000	B	0.454040000	-5.772468000	-0.080609000
B	2.984552000	-5.478376000	-0.231040000	B	-2.042432000	-5.972834000	-0.074335000
B	0.505241000	-5.166971000	-0.158323000	B	-3.492323000	-3.925324000	-0.123131000
B	2.010452000	-3.167105000	-0.142121000	B	-0.970012000	-3.706696000	-0.161541000
B	3.524201000	-1.196685000	-0.142944000	B	1.552329000	-3.529280000	-0.139960000
B	5.067029000	0.773943000	-0.166003000	B	4.045024000	-3.323102000	-0.088227000
B	2.579843000	1.090107000	-0.142812000	B	2.640716000	-1.253636000	-0.159793000
B	-0.441905000	-2.846278000	-0.096738000	B	0.176584000	-1.473609000	-0.233386000
B	-2.927381000	-2.529438000	-0.086968000	B	-2.449056000	-1.676818000	-0.210080000
B	0.114447000	1.415594000	-0.094492000	B	-3.805661000	0.436751000	-0.164853000
B	1.631420000	3.407329000	-0.198853000	B	1.200838000	0.820806000	-0.200411000
B	-0.840497000	3.732393000	-0.124538000	B	3.700130000	1.010262000	-0.134054000
B	-2.363937000	1.758567000	-0.028637000	B	2.282294000	3.081875000	-0.132646000
B	-3.878685000	-0.224418000	-0.024037000	B	-0.211615000	2.914106000	-0.159059000
B	-6.366549000	0.093015000	0.028622000	B	-2.727079000	2.723573000	-0.141624000
B	-4.846164000	2.085263000	0.022936000	B	-4.141528000	4.781995000	-0.054008000
B	-3.320674000	4.072443000	-0.036677000	B	-1.632380000	4.972362000	-0.086991000
B	-1.790565000	6.054081000	-0.148497000	B	0.874727000	5.162082000	-0.089415000
N	1.669586000	-6.007829000	-0.203689000	B	3.376875000	5.336689000	-0.069578000
N	3.165130000	-4.045455000	-0.205398000	N	-3.323817000	-5.354131000	-0.083614000
N	6.180849000	-0.134303000	-0.179112000	N	-0.848778000	-5.153863000	-0.110256000
N	3.729497000	0.224366000	-0.127922000	N	4.112192000	-4.761234000	-0.053585000
N	2.179828000	-1.730807000	-0.107183000	N	2.738618000	-2.699792000	-0.134183000
N	0.690899000	-3.733189000	-0.114351000	N	0.250922000	-2.911036000	-0.187211000
N	-1.778767000	-3.396101000	-0.115279000	N	-2.298548000	-3.109647000	-0.173439000
N	1.249475000	0.516632000	-0.102758000	N	-3.730212000	-1.017735000	-0.175315000
N	2.765423000	2.521856000	-0.200002000	N	1.342460000	-0.629349000	-0.209907000
N	0.304333000	2.847976000	-0.147275000	N	3.824730000	-0.429520000	-0.132117000
N	-2.729380000	-1.102590000	-0.059197000	N	2.393893000	1.637295000	-0.162556000
N	-5.219626000	-0.783765000	-0.012064000	N	-2.621851000	1.286689000	-0.189670000

N	-3.696641000	1.204666000	-0.003367000	N	-4.039179000	3.341853000	-0.097241000
N	-2.173450000	3.188726000	-0.057684000	N	-1.524299000	3.528994000	-0.134161000
N	-0.647630000	5.171573000	-0.171621000	N	0.985227000	3.719366000	-0.130181000
N	-3.091743000	5.491400000	-0.076496000	N	3.485036000	3.896139000	-0.100587000
N	-4.631806000	3.500469000	0.018415000	N	2.088030000	5.934435000	-0.065489000
N	-6.158000000	1.496825000	0.048332000	N	-0.430858000	5.754587000	-0.073420000
B	-1.971286000	-4.833270000	-0.144105000	N	-2.948596000	5.555827000	-0.054077000
B	-4.459236000	-4.512563000	-0.122437000	B	-4.922814000	-1.835168000	-0.125857000
B	-5.407403000	-2.207053000	-0.046035000	B	-6.306710000	0.257656000	-0.082842000
N	-0.825692000	-5.688496000	-0.162542000	B	-5.216081000	2.512081000	-0.087368000
N	-3.313767000	-5.348892000	-0.152763000	N	-4.771023000	-3.265828000	-0.112565000
N	-4.270152000	-3.082573000	-0.086530000	N	-6.193729000	-1.160716000	-0.090189000
B	4.104024000	3.078842000	-0.227786000	N	-5.110997000	1.073721000	-0.116476000
B	0.678236000	5.719368000	-0.239906000	B	5.129629000	-1.054885000	-0.092633000
N	5.226748000	2.193592000	-0.201070000	B	4.779055000	3.269530000	-0.089562000
N	1.818010000	4.846484000	-0.249066000	N	5.209171000	-2.486401000	-0.076084000
B	3.150623000	5.397769000	-0.298070000	N	4.894621000	1.836520000	-0.102239000
N	4.255253000	4.507686000	-0.283676000	B	6.198383000	1.214043000	-0.073109000
N	-1.219256000	0.879611000	-0.033584000	N	6.288916000	-0.203707000	-0.069363000
H	-7.476780000	-0.356060000	0.044503000	N	-0.099668000	1.478027000	-0.210609000
H	-6.513458000	-2.665285000	-0.040584000	H	-5.211649000	5.319402000	-0.018043000
H	-5.559179000	-4.986430000	-0.126245000	H	-6.297842000	3.024752000	-0.049129000
H	-3.460007000	-6.347771000	-0.175129000	H	-7.388112000	0.772193000	-0.045516000
H	-0.961128000	-6.689053000	-0.189951000	H	-7.049599000	-1.695978000	-0.060213000
H	1.562019000	-7.011368000	-0.228627000	H	-5.604652000	-3.836292000	-0.076585000
H	3.931927000	-6.209573000	-0.274833000	H	-4.132592000	-5.958100000	-0.052238000
H	5.439637000	-4.235218000	-0.260316000	H	-1.954230000	-7.166957000	-0.032637000
H	6.959537000	-2.269595000	-0.231886000	H	0.540281000	-6.966313000	-0.039216000
H	7.122731000	0.228930000	-0.195293000	H	3.072676000	-6.784928000	-0.012065000
H	6.158522000	2.582616000	-0.226830000	H	5.013983000	-5.214799000	-0.021320000
H	5.182566000	4.906350000	-0.311569000	H	6.120461000	-2.921661000	-0.044426000
H	3.323214000	6.581815000	-0.349357000	H	7.210849000	-0.615017000	-0.044851000
H	0.833959000	6.905460000	-0.288575000	H	7.192338000	1.882297000	-0.049836000
H	-1.644483000	7.242157000	-0.190980000	H	5.767335000	3.945287000	-0.065846000
H	-3.878403000	6.124323000	-0.063440000	H	4.360276000	6.020423000	-0.045841000
H	-5.432749000	4.115911000	0.032656000	H	2.038932000	6.942722000	-0.040312000
H	-6.971988000	2.093831000	0.071744000	H	-0.506402000	6.761604000	-0.041357000
B	-1.393483000	-0.548219000	-0.051320000	H	-3.044731000	6.560630000	-0.021765000
N	-0.233396000	-1.413313000	-0.061324000	B	-1.308737000	0.697005000	-0.234663000
C	1.068550000	-0.873952000	0.098938000	C	-1.194551000	-0.818423000	-0.266787000
N	1.635662000	-0.498281000	2.973009000	N	-0.657998000	-0.444415000	2.956086000
N	1.984062000	0.548776000	2.989525000	N	0.235472000	0.198647000	2.905818000
N₂-Si_BBN				N₂-Si_NBN			
N	3.980458000	3.495195000	-0.192389000	N	3.434402000	-4.020197000	-0.250502000
B	5.419943000	3.385645000	-0.224834000	B	3.279360000	-5.438001000	-0.471591000
B	3.348661000	4.782514000	-0.295481000	B	4.734442000	-3.416366000	-0.279117000
B	1.287282000	6.188532000	-0.429825000	B	6.189659000	-1.427044000	-0.393306000
B	-0.976398000	5.119211000	-0.293992000	B	5.238341000	0.867747000	-0.176533000
B	1.094705000	3.708218000	-0.117352000	B	3.749476000	-1.143920000	0.210902000
B	3.171286000	2.296980000	-0.065406000	B	2.271192000	-3.188191000	-0.014802000
B	5.229977000	0.886248000	-0.072976000	B	0.788682000	-5.175907000	-0.336872000
B	2.973311000	-0.205613000	0.073622000	B	-0.235341000	-2.916624000	0.014319000
B	0.935784000	1.234761000	0.221484000	B	1.235034000	-1.104679000	0.765199000
B	-1.164548000	2.663304000	0.117213000	B	2.973109000	1.263016000	0.694526000
B	-3.489593000	1.540322000	-0.003094000	B	1.728726000	3.445907000	0.133462000
B	0.748908000	-1.337362000	0.209160000	B	-1.238889000	-0.601842000	0.250037000
B	2.807811000	-2.710078000	-0.078486000	B	-2.703179000	-2.617280000	-0.157084000
B	0.548847000	-3.805278000	-0.141795000	B	-3.708315000	-0.333156000	-0.201712000

B	-1.535136000	-2.444323000	0.087897000	B	-2.263485000	1.694040000	-0.074222000
B	-3.672579000	-0.995346000	-0.021648000	B	-0.772815000	3.726070000	-0.139090000
B	-5.857275000	-2.077371000	-0.561303000	B	-1.746936000	5.974738000	-0.669032000
B	-3.778952000	-3.475123000	-0.285287000	B	-3.235495000	3.963017000	-0.499927000
B	-1.704729000	-4.899727000	-0.331860000	B	-4.720446000	1.945025000	-0.475363000
B	0.380437000	-6.285522000	-0.467534000	B	-6.188763000	-0.080464000	-0.516662000
N	-0.131202000	6.272313000	-0.441922000	N	6.335910000	-0.018306000	-0.442267000
N	1.914504000	4.895591000	-0.276089000	N	4.887723000	-1.993857000	-0.117117000
N	6.006276000	2.095170000	-0.153921000	N	1.969843000	-5.983812000	-0.487753000
N	3.785638000	0.992029000	-0.005018000	N	0.942500000	-3.755951000	-0.090204000
N	1.734911000	2.412663000	-0.000267000	N	2.436983000	-1.793188000	0.337891000
N	-0.348332000	3.829092000	-0.107407000	N	3.974603000	0.305403000	0.268541000
N	-2.623328000	2.716535000	0.011712000	N	2.948837000	2.635432000	0.229083000
N	-0.480135000	1.428987000	0.418067000	N	-0.091321000	-1.514713000	0.351740000
N	1.530651000	-0.100893000	0.223546000	N	-1.548951000	-3.480462000	-0.171135000
N	3.604010000	-1.507259000	-0.011569000	N	-2.543397000	-1.180501000	-0.026650000
N	1.370068000	-2.617052000	-0.016164000	N	0.362936000	2.917533000	0.253229000
N	-2.970295000	0.226235000	0.285707000	N	-0.598936000	5.139664000	-0.408380000
N	-5.077701000	-0.878908000	-0.358070000	N	-2.086717000	3.125474000	-0.218672000
N	-2.986882000	-2.284780000	-0.015328000	N	-3.564757000	1.099705000	-0.255788000
N	-0.896523000	-3.715623000	-0.138089000	N	-5.028611000	-0.923088000	-0.344361000
N	1.188445000	-5.098072000	-0.305728000	N	-6.013245000	1.325613000	-0.578302000
N	-1.035376000	-6.162762000	-0.482221000	N	-4.530094000	3.358317000	-0.583836000
N	-3.128487000	-4.749996000	-0.369982000	N	-3.032621000	5.375016000	-0.688920000
N	-5.198351000	-3.332751000	-0.485799000	B	4.222761000	3.177078000	-0.211844000
B	-3.234758000	4.010953000	-0.246974000	B	3.176538000	5.423428000	-0.491650000
B	-5.494831000	2.933240000	-0.526943000	B	0.723722000	5.693017000	-0.425887000
B	-5.680222000	0.427714000	-0.471400000	N	5.347200000	2.291838000	-0.309772000
N	-2.406441000	5.178738000	-0.325604000	N	4.314617000	4.578782000	-0.506948000
N	-4.660101000	4.078695000	-0.442641000	N	1.874810000	4.851303000	-0.225671000
N	-4.896457000	1.632490000	-0.339090000	B	-1.702683000	-4.908360000	-0.359485000
B	5.048443000	-1.610769000	-0.079741000	B	-5.183381000	-2.349247000	-0.371349000
B	2.623852000	-5.193359000	-0.325193000	N	-0.530003000	-5.725058000	-0.426004000
N	5.829749000	-0.412241000	-0.067423000	N	-4.027586000	-3.196525000	-0.307210000
N	3.435526000	-4.011534000	-0.213552000	B	-4.186905000	-4.624984000	-0.448849000
B	4.875619000	-4.110345000	-0.248998000	N	-3.030477000	-5.445945000	-0.474144000
N	5.642068000	-2.918216000	-0.169195000	N	-1.136835000	0.863924000	0.302236000
Si	-1.407623000	0.109078000	0.928837000	H	-1.617097000	7.149223000	-0.865299000
N	-0.681427000	-1.322174000	0.388374000	H	0.873761000	6.861561000	-0.638544000
H	-7.030757000	-2.015460000	-0.790986000	H	3.291866000	6.592062000	-0.726263000
H	-6.851301000	0.515180000	-0.704474000	H	5.205973000	4.987447000	-0.747859000
H	-6.665336000	3.046826000	-0.752197000	H	6.233440000	2.676973000	-0.605334000
H	-5.090096000	4.979466000	-0.596824000	H	7.239905000	0.356965000	-0.690261000
H	-2.850203000	6.072076000	-0.486706000	H	7.128486000	-2.137854000	-0.610902000
H	-0.546145000	7.185475000	-0.558483000	H	5.699316000	-4.098598000	-0.470695000
H	1.951086000	7.177727000	-0.552403000	H	4.235332000	-6.139775000	-0.639537000
H	4.020033000	5.767604000	-0.405527000	H	1.874673000	-6.975830000	-0.650596000
H	6.106524000	4.362911000	-0.313156000	H	-0.635458000	-6.717912000	-0.579726000
H	7.013706000	2.034713000	-0.188612000	H	-3.159167000	-6.441047000	-0.586679000
H	6.835940000	-0.485322000	-0.120002000	H	-5.276794000	-5.110108000	-0.555996000
H	6.647612000	-3.003470000	-0.206358000	H	-6.274192000	-2.831904000	-0.473097000
H	5.414616000	-5.175042000	-0.350199000	H	-7.281060000	-0.561321000	-0.617854000
H	3.146913000	-6.263586000	-0.445602000	H	-6.833251000	1.899258000	-0.712796000
H	0.895320000	-7.359121000	-0.596754000	H	-5.332161000	3.946107000	-0.761838000
H	-1.577767000	-7.005839000	-0.604064000	H	-3.826652000	5.969070000	-0.879334000
H	-3.696649000	-5.568281000	-0.539145000	B	0.053630000	1.578840000	0.714568000
H	-5.753983000	-4.159893000	-0.651029000	Si	1.430520000	0.601466000	1.709417000
N	-1.555244000	0.208960000	2.744355000	N	-2.962919000	-0.321527000	3.180435000

N	-1.202027000	-0.603317000	3.526068000	N	-2.955952000	0.774533000	3.067282000
	N₂-P_BBN				N₂-PNBN		
N	-5.234046000	1.372088000	-0.026536000	N	1.663499000	-4.868242000	-0.492767000
B	-5.932918000	2.635501000	-0.024229000	B	1.040275000	-6.163674000	-0.627340000
B	-5.969876000	0.140084000	-0.101874000	B	3.083839000	-4.727293000	-0.642387000
B	-6.022986000	-2.353678000	-0.196644000	B	5.106764000	-3.312939000	-0.882890000
B	-3.882555000	-3.656705000	-0.102940000	B	4.953367000	-0.827800000	-0.664695000
B	-3.829077000	-1.153984000	-0.009579000	B	2.920379000	-2.253973000	-0.213747000
B	-3.783348000	1.349302000	0.038356000	B	0.851988000	-3.697658000	-0.220477000
B	-3.737947000	3.848457000	0.048226000	B	-1.212439000	-5.106144000	-0.313184000
B	-1.588608000	2.556420000	0.094564000	B	-1.414458000	-2.630357000	0.009868000
B	-1.650631000	0.059108000	0.210545000	B	0.634973000	-1.333149000	0.444267000
B	-1.699912000	-2.459263000	0.152519000	B	2.915387000	0.258295000	0.205427000
B	0.467225000	-3.767875000	-0.012453000	B	2.499373000	2.740967000	-0.186986000
B	0.564571000	1.286163000	0.100699000	B	-1.600535000	-0.123296000	0.239200000
B	0.588306000	3.770013000	-0.163733000	B	-3.664384000	-1.550852000	0.058806000
B	2.725979000	2.475826000	-0.320769000	B	-3.874405000	0.939519000	0.070986000
B	2.714841000	-0.013386000	-0.070345000	B	-1.837082000	2.381374000	0.031877000
B	2.667948000	-2.549099000	-0.119803000	B	0.217900000	3.816621000	-0.184898000
B	4.766443000	-3.817152000	-0.624756000	B	-0.010064000	6.284693000	-0.557030000
B	4.824583000	-1.318587000	-0.394111000	B	-2.053577000	4.859525000	-0.263738000
B	4.864989000	1.187128000	-0.516082000	B	-4.105703000	3.429598000	-0.101220000
B	4.890243000	3.688573000	-0.685810000	B	-6.153293000	1.991055000	-0.001157000
N	-5.315519000	-3.584785000	-0.197276000	N	5.695444000	-2.024268000	-0.948310000
N	-5.278417000	-1.119885000	-0.102165000	N	3.704024000	-3.431755000	-0.552474000
N	-5.176268000	3.835341000	0.025596000	N	-0.371461000	-6.255533000	-0.516883000
N	-3.035158000	2.581940000	0.078898000	N	-0.587558000	-3.808142000	-0.154245000
N	-3.086712000	0.084957000	0.059251000	N	1.486588000	-2.417521000	0.011591000
N	-3.135129000	-2.420588000	-0.003611000	N	3.580085000	-0.953724000	-0.210933000
N	-0.979697000	-3.721233000	0.092980000	N	3.368319000	1.569887000	-0.195571000
N	-0.995249000	-1.217103000	0.353615000	N	-0.793953000	-1.341837000	0.237745000
N	-0.884951000	1.294682000	0.207158000	N	-2.852184000	-2.739619000	-0.024547000
N	-0.847031000	3.793375000	-0.021871000	N	-3.040970000	-0.244592000	0.132900000
N	1.290671000	2.508939000	-0.150357000	N	1.058166000	2.658476000	0.033998000
N	1.259404000	-2.579899000	0.182548000	N	0.821845000	5.110352000	-0.439014000
N	3.335750000	-3.799652000	-0.431712000	N	-1.219709000	3.682776000	-0.120722000
N	3.399336000	-1.295396000	-0.123021000	N	-3.272916000	2.248251000	-0.001648000
N	3.430052000	1.214825000	-0.327181000	N	-5.321509000	0.811782000	0.058711000
N	3.458375000	3.717380000	-0.500196000	N	-5.533533000	3.265102000	-0.080434000
N	5.557099000	2.434849000	-0.691683000	N	-3.476240000	4.709378000	-0.217566000
N	5.531988000	-0.078800000	-0.511732000	N	-1.417360000	6.136283000	-0.451232000
N	5.476626000	-2.589980000	-0.562962000	B	4.742565000	1.681664000	-0.649687000
B	-1.732969000	-4.949166000	-0.083219000	B	4.478699000	4.160756000	-0.831607000
B	0.395628000	-6.236279000	-0.422767000	B	2.246274000	5.212498000	-0.580878000
B	2.578665000	-5.020948000	-0.500991000	N	5.515863000	0.483983000	-0.799196000
N	-3.163920000	-4.894106000	-0.105562000	N	5.274072000	2.989223000	-0.915249000
N	-1.013373000	-6.182531000	-0.262704000	N	3.074978000	4.037951000	-0.506924000
N	1.150541000	-5.009187000	-0.328651000	B	-3.475180000	-4.042537000	-0.139263000
B	-1.549237000	5.060194000	-0.050354000	B	-5.931091000	-0.488016000	0.067693000
B	2.758393000	4.972751000	-0.491856000	N	-2.640111000	-5.197459000	-0.267477000
N	-2.978019000	5.060909000	0.030180000	N	-5.112411000	-1.667238000	0.044979000
N	1.331804000	5.007441000	-0.322566000	B	-5.734866000	-2.968362000	-0.030705000
B	0.632391000	6.270584000	-0.315970000	N	-4.910392000	-4.119654000	-0.121439000
N	-0.779514000	6.269565000	-0.169924000	N	-1.009102000	1.212947000	0.248358000
N	1.307329000	0.058062000	0.232009000	H	0.477541000	7.363114000	-0.741142000
H	5.342978000	-4.845769000	-0.833749000	H	2.747499000	6.280538000	-0.784108000
H	3.140695000	-6.055889000	-0.716338000	H	4.961638000	5.234709000	-1.049601000
H	0.945147000	-7.279428000	-0.633020000	H	6.242125000	3.093235000	-1.182992000

H	-1.528558000	-7.045772000	-0.358775000	H	6.475731000	0.566092000	-1.103871000
H	-3.679517000	-5.756238000	-0.213385000	H	6.666152000	-1.961578000	-1.219164000
H	-5.853682000	-4.436653000	-0.263357000	H	5.758914000	-4.288174000	-1.123053000
H	-7.217931000	-2.341184000	-0.277089000	H	3.754455000	-5.693016000	-0.867697000
H	-7.165060000	0.163761000	-0.169372000	H	1.699508000	-7.142830000	-0.830231000
H	-7.129258000	2.673317000	-0.068411000	H	-0.793150000	-7.167118000	-0.620660000
H	-5.680742000	4.710051000	0.014494000	H	-3.073787000	-6.104473000	-0.365997000
H	-3.467971000	5.943965000	0.003331000	H	-5.362321000	-5.020384000	-0.184512000
H	-1.253498000	7.161186000	-0.179596000	H	-6.927655000	-3.076050000	-0.024787000
H	1.228931000	7.302274000	-0.435955000	H	-7.123876000	-0.589453000	0.076490000
H	3.365396000	5.995538000	-0.629777000	H	-7.347123000	1.895837000	0.008251000
H	5.506191000	4.705080000	-0.833360000	H	-6.130491000	4.077853000	-0.131279000
H	6.558780000	2.435249000	-0.819521000	H	-4.056423000	5.531852000	-0.304249000
H	6.529143000	-0.103587000	-0.672191000	H	-1.986224000	6.965644000	-0.542287000
H	6.472977000	-2.616103000	-0.725424000	B	0.401475000	1.442333000	0.455581000
P	0.575687000	-1.262982000	1.064071000	P	1.418341000	0.126829000	1.347909000
N	3.927071000	0.321213000	2.828811000	N	3.996423000	-0.160977000	3.988071000
N	5.011242000	0.125437000	2.843992000	N	3.407458000	0.066674000	4.876443000
N2-SBBN				N2-SNBN			
N	-3.168885000	-4.234909000	-0.279086000	N	1.403111000	-4.938259000	-0.337670000
B	-4.598973000	-4.441913000	-0.250900000	B	0.729022000	-6.213183000	-0.411070000
B	-2.291948000	-5.357315000	-0.438700000	B	2.831493000	-4.864154000	-0.484166000
B	-0.003712000	-6.314548000	-0.545328000	B	4.908636000	-3.520874000	-0.747831000
B	1.988179000	-4.821508000	-0.290036000	B	4.798265000	-1.017083000	-0.619258000
B	-0.308004000	-3.835488000	-0.283592000	B	2.744759000	-2.371385000	-0.222225000
B	-2.621802000	-2.898404000	-0.139744000	B	0.634155000	-3.728240000	-0.131326000
B	-4.946483000	-1.978366000	0.016794000	B	-1.482945000	-5.057333000	-0.162509000
B	-2.966392000	-0.449881000	0.127107000	B	-1.575914000	-2.562534000	0.045335000
B	-0.627405000	-1.370896000	0.020663000	B	0.523143000	-1.318886000	0.367807000
B	1.680718000	-2.339009000	-0.027368000	B	2.683662000	0.160512000	-0.011784000
B	3.682121000	-0.882314000	0.181188000	B	2.577108000	2.668573000	-0.148981000
B	-1.019234000	1.081893000	0.244411000	B	-1.656124000	-0.049823000	0.156429000
B	-3.311629000	2.025821000	0.034334000	B	-3.779164000	-1.385598000	0.060035000
B	-1.333371000	3.525771000	-0.190022000	B	-3.869401000	1.110351000	0.034693000
B	0.979916000	2.588432000	-0.008608000	B	-1.746717000	2.442701000	-0.007742000
B	3.330079000	1.590253000	-0.023663000	B	0.359332000	3.803264000	-0.108703000
B	5.232872000	3.013747000	-0.827267000	B	0.243851000	6.299631000	-0.305346000
B	2.935869000	3.984234000	-0.650274000	B	-1.861302000	4.945443000	-0.156874000
B	0.640717000	4.975009000	-0.663890000	B	-3.971654000	3.603563000	-0.076602000
B	-1.667547000	5.956845000	-0.693404000	B	-6.093603000	2.269305000	-0.021514000
N	1.397242000	-6.115786000	-0.471721000	N	5.519752000	-2.244789000	-0.824925000
N	-0.870115000	-5.166575000	-0.436990000	N	3.494954000	-3.591574000	-0.462870000
N	-5.450336000	-3.319123000	-0.095774000	N	-0.686459000	-6.245479000	-0.306166000
N	-3.509764000	-1.778520000	0.013633000	N	-0.804748000	-3.779518000	-0.061225000
N	-1.183884000	-2.692931000	-0.160453000	N	1.316905000	-2.458886000	0.029516000
N	1.122746000	-3.654683000	-0.225020000	N	3.383339000	-1.084637000	-0.296168000
N	3.098953000	-2.199232000	0.131636000	N	3.327617000	1.443238000	-0.201748000
N	0.821194000	-1.164597000	0.032579000	N	-0.897000000	-1.288342000	0.207805000
N	-1.532002000	-0.261148000	0.211387000	N	-3.015499000	-2.609491000	0.018960000
N	-3.851231000	0.692299000	0.127253000	N	-3.099343000	-0.111130000	0.093324000
N	-1.883111000	2.216379000	0.035328000	N	1.145254000	2.598848000	0.009175000
N	2.876157000	0.278497000	0.422226000	N	1.024978000	5.088157000	-0.242603000
N	4.727805000	1.728718000	-0.404579000	N	-1.082391000	3.726044000	-0.082094000
N	2.408842000	2.705307000	-0.216230000	N	-3.192971000	2.381690000	-0.018525000
N	0.092914000	3.681581000	-0.310771000	N	-5.321266000	1.050229000	0.023825000
N	-2.219106000	4.660597000	-0.377915000	N	-5.406846000	3.508960000	-0.068962000
N	-0.262725000	6.079599000	-0.846885000	N	-3.288978000	4.857347000	-0.139351000
N	2.051057000	5.095839000	-0.819450000	N	-1.170877000	6.203178000	-0.249171000

N	4.342437000	4.107027000	-0.907150000	B	4.738544000	1.490158000	-0.518772000
B	3.974431000	-3.346792000	-0.013336000	B	4.661173000	3.998146000	-0.541170000
B	5.973094000	-1.841667000	-0.125890000	B	2.458645000	5.155879000	-0.333002000
B	5.621757000	0.615687000	-0.321227000	N	5.444868000	0.256760000	-0.690990000
N	3.397185000	-4.642109000	-0.173033000	N	5.373730000	2.774062000	-0.646132000
N	5.394803000	-3.134713000	-0.036725000	N	3.237636000	3.951442000	-0.312203000
N	5.102015000	-0.694012000	-0.064894000	B	-3.695702000	-3.887757000	-0.046871000
B	-5.287072000	0.498587000	0.118470000	B	-5.991421000	-0.218931000	0.042364000
B	-3.642086000	4.484273000	-0.283374000	N	-2.912549000	-5.083511000	-0.121685000
N	-5.801892000	-0.837013000	0.118133000	N	-5.229870000	-1.437303000	0.046753000
N	-4.194043000	3.172239000	-0.079919000	B	-5.907951000	-2.711156000	0.008759000
B	-5.624094000	2.980868000	-0.031719000	N	-5.132618000	-3.899719000	-0.036086000
N	-6.134106000	1.659977000	0.086499000	N	-0.971268000	1.219393000	0.105794000
N	0.375810000	1.340597000	0.452511000	H	0.776473000	7.367809000	-0.406579000
H	6.380448000	3.154531000	-1.129598000	H	2.999907000	6.218064000	-0.446332000
H	6.788611000	0.768403000	-0.541248000	H	5.229130000	5.046090000	-0.660695000
H	7.153934000	-1.704244000	-0.268913000	H	6.364994000	2.820341000	-0.832893000
H	6.010730000	-3.931608000	-0.112377000	H	6.431590000	0.286516000	-0.904994000
H	4.003916000	-5.444486000	-0.263778000	H	6.507112000	-2.206946000	-1.033342000
H	1.991825000	-6.929579000	-0.529691000	H	5.547211000	-4.518009000	-0.926607000
H	-0.455979000	-7.414292000	-0.684489000	H	3.463577000	-5.867486000	-0.646571000
H	-2.746255000	-6.457666000	-0.564949000	H	1.349377000	-7.226358000	-0.560481000
H	-5.057218000	-5.542856000	-0.360037000	H	-1.141660000	-7.144633000	-0.369477000
H	-6.446916000	-3.481037000	-0.087773000	H	-3.386110000	-5.973662000	-0.184415000
H	-6.802529000	-0.974902000	0.107247000	H	-5.623798000	-4.781337000	-0.070138000
H	-7.137134000	1.543707000	0.094749000	H	-7.104168000	-2.767606000	0.009587000
H	-6.367346000	3.916739000	-0.108252000	H	-7.187706000	-0.263957000	0.043643000
H	-4.368211000	5.427540000	-0.411517000	H	-7.290734000	2.235308000	-0.021595000
H	-2.379927000	6.906674000	-0.852910000	H	-5.959248000	4.353515000	-0.102915000
H	0.106115000	6.989739000	-1.081400000	H	-3.831511000	5.708067000	-0.187221000
H	2.434440000	5.989287000	-1.094366000	H	-1.703705000	7.059462000	-0.298186000
H	4.716477000	4.996596000	-1.204831000	B	0.474050000	1.335248000	0.213610000
S	1.328169000	0.243039000	1.259233000	S	1.342946000	0.070796000	1.380353000
N	1.941914000	1.947141000	2.744231000	N	4.963207000	0.140573000	2.672767000
N	1.192173000	2.112731000	3.570222000	N	4.634821000	-0.906867000	2.768818000

Table S6. Cartesian coordinates of important intermediates of nitrogen reduction catalyzed by Si_BBN calculated at the ω B97X-D/6-31G(d) level of theory.

HN₂-Si_BBN				H₂N₂-Si_BBN			
N	4.238133000	3.187335000	-0.174423000	N	-3.925149000	-3.596481000	-0.174620000
B	5.664779000	2.967898000	-0.200625000	B	-5.366853000	-3.527679000	-0.187634000
B	3.707224000	4.520031000	-0.275536000	B	-3.258029000	-4.863830000	-0.294827000
B	1.760532000	6.079482000	-0.423232000	B	-1.159170000	-6.207557000	-0.464722000
B	-0.578977000	5.185351000	-0.305568000	B	1.072303000	-5.071088000	-0.346973000
B	1.376646000	3.620578000	-0.116498000	B	-1.034068000	-3.723846000	-0.138376000
B	3.338391000	2.054704000	-0.057558000	B	-3.147124000	-2.375794000	-0.050555000
B	5.282458000	0.489888000	-0.070163000	B	-5.245635000	-1.025189000	-0.022865000
B	2.948230000	-0.425529000	0.069505000	B	-3.017735000	0.128850000	0.099149000
B	1.025534000	1.167528000	0.221189000	B	-0.935870000	-1.250427000	0.217275000
B	-0.956062000	2.751168000	0.108588000	B	1.192831000	-2.608376000	0.079213000
B	-3.358482000	1.810753000	-0.014527000	B	3.483384000	-1.425557000	-0.063633000
B	0.644219000	-1.383979000	0.210456000	B	-0.820670000	1.317926000	0.215827000
B	2.592164000	-2.908676000	-0.100095000	B	-2.924598000	2.634732000	-0.049541000
B	0.256033000	-3.827994000	-0.158878000	B	-0.700806000	3.790175000	-0.143546000
B	-1.717298000	-2.312016000	0.091171000	B	1.419238000	2.481615000	0.066298000
B	-3.735490000	-0.699956000	-0.023201000	B	3.594421000	1.102530000	-0.077004000

B	-5.997693000	-1.614270000	-0.559355000	B	5.741931000	2.249600000	-0.655881000
B	-4.033063000	-3.166395000	-0.282928000	B	3.628199000	3.582935000	-0.345416000
B	-2.075115000	-4.745969000	-0.344606000	B	1.515552000	4.944556000	-0.367173000
B	-0.102331000	-6.285103000	-0.506557000	B	-0.606632000	6.274477000	-0.477544000
N	0.352965000	6.270720000	-0.448028000	N	0.261065000	-6.249114000	-0.493264000
N	2.286359000	4.741982000	-0.267442000	N	-1.821475000	-4.935500000	-0.294596000
N	6.149759000	1.635283000	-0.138454000	N	-5.989343000	-2.255218000	-0.100365000
N	3.850414000	0.705563000	-0.002247000	N	-3.799374000	-1.090421000	0.025353000
N	1.915486000	2.279239000	0.001639000	N	-1.708752000	-2.450082000	-0.005323000
N	-0.052031000	3.851257000	-0.115438000	N	0.411417000	-3.801652000	-0.146944000
N	-2.405547000	2.917144000	-0.003397000	N	2.655278000	-2.627650000	-0.039684000
N	-0.370016000	1.468381000	0.412341000	N	0.483815000	-1.398603000	0.393771000
N	1.517673000	-0.212012000	0.224384000	N	-1.574259000	0.064830000	0.231059000
N	3.477636000	-1.771582000	-0.026081000	N	-3.688357000	1.412271000	0.026465000
N	1.165442000	-2.706890000	-0.025479000	N	-1.485070000	2.581182000	-0.005684000
N	-2.941367000	0.462195000	0.278827000	N	2.938443000	-0.133109000	0.260842000
N	-5.127650000	-0.479883000	-0.362155000	N	5.000987000	1.030146000	-0.437989000
N	-3.151048000	-2.041155000	-0.011323000	N	2.876661000	2.372525000	-0.060008000
N	-1.178006000	-3.628130000	-0.143955000	N	0.745679000	3.739358000	-0.158507000
N	0.794261000	-5.163971000	-0.338239000	N	-1.378131000	5.066537000	-0.300130000
N	-1.504538000	-6.054836000	-0.509865000	N	0.811344000	6.189729000	-0.512612000
N	-3.482620000	-4.487850000	-0.371542000	N	2.942817000	4.839120000	-0.422886000
N	-5.437175000	-2.916934000	-0.480477000	N	5.049721000	3.484844000	-0.566105000
B	-2.915414000	4.253325000	-0.266759000	B	3.297409000	-3.901536000	-0.316839000
B	-5.250843000	3.351640000	-0.547488000	B	5.521664000	-2.763025000	-0.629828000
B	-5.628251000	0.869261000	-0.480605000	B	5.637592000	-0.256681000	-0.571315000
N	-1.999813000	5.354164000	-0.345925000	N	2.503717000	-5.092546000	-0.392533000
N	-4.330990000	4.429932000	-0.467107000	N	4.722812000	-3.931542000	-0.531699000
N	-4.754094000	2.009643000	-0.354163000	N	4.890471000	-1.481297000	-0.425022000
B	4.910003000	-1.984888000	-0.100790000	B	-5.134742000	1.475351000	-0.021888000
B	2.218168000	-5.368260000	-0.368792000	B	-2.815214000	5.122403000	-0.298474000
N	5.780931000	-0.851002000	-0.077387000	N	-5.882752000	0.255715000	-0.002387000
N	3.117619000	-4.253061000	-0.251119000	N	-3.591597000	3.919232000	-0.174516000
B	4.545974000	-4.461759000	-0.295726000	B	-5.033763000	3.978349000	-0.188815000
N	5.401306000	-3.333059000	-0.206758000	N	-5.766654000	2.766163000	-0.099537000
Si	-1.398478000	0.230922000	0.947550000	Si	1.378105000	-0.068437000	0.979490000
N	-0.779207000	-1.264429000	0.417103000	N	0.608087000	1.339140000	0.387515000
H	-7.163434000	-1.463744000	-0.787524000	H	6.913195000	2.221674000	-0.905799000
H	-6.789639000	1.044082000	-0.713385000	H	6.807052000	-0.310086000	-0.825209000
H	-6.409299000	3.552520000	-0.774638000	H	6.691385000	-2.841997000	-0.876110000
H	-4.690831000	5.360475000	-0.624207000	H	5.172883000	-4.819695000	-0.700940000
H	-2.373870000	6.278585000	-0.508444000	H	2.969954000	-5.971375000	-0.568970000
H	0.009068000	7.212947000	-0.565010000	H	0.702133000	-7.148381000	-0.620963000
H	2.500653000	7.014151000	-0.536604000	H	-1.794031000	-7.216135000	-0.586844000
H	4.454868000	5.449807000	-0.374517000	H	-3.901857000	-5.867826000	-0.403453000
H	6.426644000	3.888696000	-0.276917000	H	-6.026547000	-4.523970000	-0.274087000
H	7.149701000	1.497796000	-0.170263000	H	-6.998396000	-2.223131000	-0.122164000
H	6.778535000	-1.000362000	-0.132707000	H	-6.891150000	0.300377000	-0.042265000
H	6.397277000	-3.494377000	-0.249902000	H	-6.774554000	2.823293000	-0.122745000
H	5.001854000	-5.563158000	-0.410825000	H	-5.603043000	5.028501000	-0.280065000
H	2.657875000	-6.473740000	-0.501780000	H	-3.368847000	6.178448000	-0.410994000
H	0.329596000	-7.392839000	-0.649042000	H	-1.151484000	7.334198000	-0.601980000
H	-2.110856000	-6.852263000	-0.637734000	H	1.329767000	7.045894000	-0.646354000
H	-4.113356000	-5.258324000	-0.543621000	H	3.483677000	5.672646000	-0.605972000
H	-6.055284000	-3.698926000	-0.643600000	H	5.575845000	4.328414000	-0.744001000
N	-1.518812000	0.291868000	2.740218000	N	1.468437000	-0.108228000	2.715500000
N	-1.185238000	-0.660238000	3.465053000	N	2.644805000	0.161349000	3.274038000
H	-0.836327000	-1.476002000	2.897981000	H	3.507409000	0.053227000	2.742500000

				H	2.712553000	-0.015394000	4.268046000
		H₃N₂-Si_BBN			H₃NHN-Si_BBN		
N	4.426419000	2.990608000	-0.142313000	N	2.138367000	4.859508000	-0.239838000
B	5.841317000	2.708936000	-0.144212000	B	3.478211000	5.397601000	-0.240812000
B	3.953168000	4.343149000	-0.258614000	B	1.007300000	5.729851000	-0.405436000
B	2.075155000	5.980031000	-0.445701000	B	-1.457715000	6.072960000	-0.621432000
B	-0.299362000	5.179577000	-0.353031000	B	-3.017608000	4.116836000	-0.467481000
B	1.584220000	3.541093000	-0.125969000	B	-0.542616000	3.771956000	-0.222674000
B	3.474426000	1.897496000	-0.033063000	B	1.937738000	3.429144000	-0.082183000
B	5.348828000	0.250644000	-0.006314000	B	4.406005000	3.077730000	0.009366000
B	2.972587000	-0.560545000	0.096512000	B	2.859510000	1.101246000	0.135802000
B	1.118917000	1.110475000	0.223452000	B	0.392901000	1.489305000	0.195984000
B	-0.781758000	2.760821000	0.084559000	B	-2.106283000	1.836314000	0.009122000
B	-3.218795000	1.924225000	-0.079951000	B	-3.685651000	-0.199670000	-0.124810000
B	0.617976000	-1.407102000	0.198451000	B	1.356119000	-0.896751000	0.247325000
B	2.510020000	-3.021999000	-0.074066000	B	3.823264000	-1.215996000	0.040317000
B	0.143547000	-3.836093000	-0.174652000	B	2.286659000	-3.193801000	-0.086005000
B	-1.755240000	-2.225575000	0.046601000	B	-0.189183000	-2.888253000	0.068418000
B	-3.703993000	-0.549417000	-0.100038000	B	-2.734746000	-2.539837000	-0.119659000
B	-6.001857000	-1.371855000	-0.669577000	B	-4.207775000	-4.484295000	-0.682442000
B	-4.110776000	-3.002207000	-0.339832000	B	-1.730254000	-4.811483000	-0.363804000
B	-2.217907000	-4.653431000	-0.384062000	B	0.758433000	-5.166881000	-0.345154000
B	-0.314972000	-6.278809000	-0.523950000	B	3.244221000	-5.491647000	-0.389368000
N	0.676715000	6.227705000	-0.492244000	N	-2.767756000	5.520564000	-0.648215000
N	2.543366000	4.625153000	-0.272311000	N	-0.329396000	5.196910000	-0.411657000
N	6.267830000	1.357068000	-0.066126000	N	4.571261000	4.503470000	-0.102483000
N	3.928982000	0.528728000	0.036300000	N	3.063205000	2.534517000	0.038235000
N	2.064556000	2.182737000	0.004644000	N	0.597933000	2.898226000	-0.049637000
N	0.166606000	3.829418000	-0.144039000	N	-1.890995000	3.242391000	-0.237853000
N	-2.225617000	2.993209000	-0.057794000	N	-3.444007000	1.243398000	-0.108572000
N	-0.257220000	1.465329000	0.404604000	N	-0.964556000	1.037789000	0.353905000
N	1.556185000	-0.285747000	0.225237000	N	1.518179000	0.558889000	0.247474000
N	3.447713000	-1.929195000	0.013326000	N	4.005871000	0.214681000	0.105312000
N	1.094212000	-2.757054000	-0.028661000	N	2.492165000	-1.767232000	0.053367000
N	-2.875271000	0.564614000	0.245806000	N	-2.645154000	-1.137832000	0.178751000
N	-5.088218000	-0.276301000	-0.463556000	N	-4.044851000	-3.064741000	-0.474160000
N	-3.190593000	-1.916945000	-0.051595000	N	-1.555607000	-3.397630000	-0.082963000
N	-1.280282000	-3.574688000	-0.179979000	N	0.951957000	-3.750305000	-0.134650000
N	0.624704000	-5.198948000	-0.342368000	N	3.438414000	-4.071798000	-0.209061000
N	-1.706067000	-5.987812000	-0.543578000	N	1.921193000	-6.004812000	-0.463739000
N	-3.617586000	-4.345379000	-0.416816000	N	-0.581625000	-5.666629000	-0.426500000
N	-5.503912000	-2.697081000	-0.556135000	N	-3.061768000	-5.315850000	-0.594669000
B	-2.670106000	4.344972000	-0.343214000	B	-4.557422000	2.129038000	-0.398135000
B	-5.035848000	3.548687000	-0.669790000	B	-6.108408000	0.160377000	-0.651860000
B	-5.523564000	1.092232000	-0.605067000	B	-5.163215000	-2.166421000	-0.591867000
N	-1.711908000	5.409087000	-0.414776000	N	-4.330276000	3.540417000	-0.500548000
N	-4.074820000	4.586195000	-0.571296000	N	-5.870038000	1.558598000	-0.575946000
N	-4.602854000	2.188611000	-0.454500000	N	-4.998198000	-0.737556000	-0.450214000
B	4.868417000	-2.204855000	-0.033459000	B	5.347500000	0.760229000	0.085014000
B	2.037949000	-5.465291000	-0.345700000	B	4.767384000	-3.524303000	-0.164352000
N	5.789723000	-1.111076000	0.001971000	N	5.518232000	2.181042000	0.080663000
N	2.981516000	-4.391035000	-0.211558000	N	4.968371000	-2.106096000	-0.042819000
B	4.398928000	-4.662803000	-0.227538000	B	6.303554000	-1.558722000	-0.017553000
N	5.303233000	-3.574513000	-0.124956000	N	6.461838000	-0.150120000	0.057397000
Si	-1.342780000	0.297936000	1.025604000	Si	-1.229850000	-0.545049000	0.952156000
N	-0.796527000	-1.212637000	0.363048000	N	0.064799000	-1.512562000	0.397761000
H	-7.156367000	-1.174425000	-0.923159000	H	-5.284181000	-4.951461000	-0.924836000
H	-6.672318000	1.316399000	-0.863208000	H	-6.252045000	-2.607559000	-0.826926000

H	-6.180715000	3.796166000	-0.924445000	H	-7.208359000	-0.259144000	-0.873638000
H	-4.386468000	5.530381000	-0.748349000	H	-6.651202000	2.174254000	-0.752036000
H	-2.044834000	6.345414000	-0.596956000	H	-5.118156000	4.142536000	-0.694756000
H	0.371770000	7.181336000	-0.623278000	H	-3.539835000	6.152629000	-0.803317000
H	2.853589000	6.884568000	-0.555333000	H	-1.295957000	7.249676000	-0.777217000
H	4.741127000	5.240775000	-0.351594000	H	1.178004000	6.906698000	-0.547483000
H	6.644580000	3.595548000	-0.213381000	H	3.665726000	6.574633000	-0.361643000
H	7.261069000	1.175810000	-0.081311000	H	5.502513000	4.893808000	-0.115246000
H	6.780473000	-1.304326000	-0.036227000	H	6.454211000	2.560362000	0.056902000
H	6.291641000	-3.779590000	-0.149103000	H	7.402221000	0.217825000	0.060418000
H	4.807405000	-5.784617000	-0.330316000	H	7.261173000	-2.277167000	-0.063338000
H	2.430691000	-6.590294000	-0.468528000	H	5.713551000	-4.254982000	-0.237024000
H	0.068147000	-7.405804000	-0.661346000	H	4.183521000	-6.229631000	-0.481206000
H	-2.346128000	-6.756632000	-0.680814000	H	1.809923000	-6.999647000	-0.596038000
H	-4.273744000	-5.089886000	-0.606754000	H	-0.722682000	-6.651102000	-0.604640000
H	-6.148473000	-3.453756000	-0.735363000	H	-3.188134000	-6.303296000	-0.765025000
N	-1.481506000	0.427872000	2.706621000	N	-1.321523000	-0.496750000	2.695149000
N	-2.702483000	-0.150419000	3.191408000	N	-4.301118000	0.315177000	2.984120000
H	-3.530642000	0.064627000	2.607799000	H	-4.866729000	-0.348802000	2.460978000
H	-2.890258000	0.228127000	4.122974000	H	-2.284657000	-0.254873000	2.995292000
H	-2.676286000	-1.175228000	3.292816000	H	-4.363468000	1.197429000	2.483112000
				H	-4.751584000	0.446223000	3.885608000
		HHN₂-Si₆BN				H₂HN₂-Si₆BN	
N	4.062372000	3.404421000	-0.176213000	N	2.663105000	4.573105000	-0.215270000
B	5.498565000	3.260324000	-0.205097000	B	4.058924000	4.937730000	-0.233114000
B	3.463674000	4.707505000	-0.274287000	B	1.648330000	5.583713000	-0.344207000
B	1.439244000	6.162286000	-0.424279000	B	-0.754757000	6.239735000	-0.525617000
B	-0.849237000	5.145110000	-0.313353000	B	-2.545891000	4.489132000	-0.407487000
B	1.183461000	3.685970000	-0.119243000	B	-0.134950000	3.833282000	-0.180509000
B	3.222164000	2.225627000	-0.062982000	B	2.283778000	3.176593000	-0.083258000
B	5.247436000	0.765636000	-0.084843000	B	4.690823000	2.515026000	-0.051832000
B	2.964140000	-0.270121000	0.050387000	B	2.909545000	0.748550000	0.080593000
B	0.955258000	1.217114000	0.213172000	B	0.506118000	1.443435000	0.190105000
B	-1.099796000	2.690240000	0.097140000	B	-1.928978000	2.105266000	0.033235000
B	-3.448947000	1.635047000	-0.033418000	B	-3.749411000	0.294597000	-0.081358000
B	0.713994000	-1.345148000	0.182979000	B	1.174566000	-1.044724000	0.217725000
B	2.737179000	-2.768014000	-0.126252000	B	3.574684000	-1.671818000	-0.055212000
B	0.451481000	-3.806038000	-0.178536000	B	1.799047000	-3.441559000	-0.136112000
B	-1.594396000	-2.392165000	0.084771000	B	-0.614531000	-2.828182000	0.089485000
B	-3.695495000	-0.887456000	-0.019554000	B	-3.100109000	-2.146646000	-0.051304000
B	-5.908039000	-1.920261000	-0.557430000	B	-4.811047000	-3.893017000	-0.596304000
B	-3.864682000	-3.365334000	-0.279169000	B	-2.396056000	-4.534947000	-0.297701000
B	-1.829276000	-4.842299000	-0.347864000	B	0.027511000	-5.207951000	-0.338691000
B	0.218576000	-6.279502000	-0.515433000	B	2.450789000	-5.841983000	-0.458227000
N	0.023508000	6.278767000	-0.452071000	N	-2.121774000	5.856084000	-0.558230000
N	2.033157000	4.854690000	-0.266776000	N	0.256923000	5.224316000	-0.343088000
N	6.053872000	1.955432000	-0.148856000	N	5.033690000	3.910083000	-0.138205000
N	3.806548000	0.906497000	-0.015110000	N	3.291432000	2.144926000	-0.001026000
N	1.788980000	2.375166000	-0.001077000	N	0.889733000	2.818357000	-0.037214000
N	-0.255509000	3.840029000	-0.121707000	N	-1.535756000	3.478209000	-0.193294000
N	-2.556998000	2.790589000	-0.012704000	N	-3.324068000	1.689264000	-0.099477000
N	-0.456445000	1.438476000	0.406073000	N	-0.893058000	1.162698000	0.354084000
N	1.525756000	-0.130931000	0.204301000	N	1.513223000	0.378199000	0.217584000
N	3.562957000	-1.586567000	-0.050350000	N	3.935288000	-0.276129000	0.014376000
N	1.302866000	-2.639713000	-0.053474000	N	2.186169000	-2.052352000	-0.005380000
N	-2.965502000	0.318443000	0.283115000	N	-2.832502000	-0.765812000	0.239300000
N	-5.097890000	-0.741404000	-0.363172000	N	-4.465392000	-2.507589000	-0.398565000
N	-3.042109000	-2.195378000	-0.013082000	N	-2.037545000	-3.154162000	-0.023322000

N	-0.990363000	-3.679590000	-0.156131000	N	0.404543000	-3.827179000	-0.139379000
N	1.057478000	-5.113406000	-0.356165000	N	2.827216000	-4.457401000	-0.289719000
N	-1.193566000	-6.121211000	-0.512485000	N	1.072354000	-6.185690000	-0.487129000
N	-3.248480000	-4.657121000	-0.368749000	N	-1.366416000	-5.531836000	-0.376320000
N	-5.281606000	-3.191024000	-0.472811000	N	-3.782229000	-4.867851000	-0.505456000
B	-3.133841000	4.097341000	-0.284249000	B	-4.318476000	2.707360000	-0.375531000
B	-5.416901000	3.075187000	-0.581365000	B	-6.100769000	0.949883000	-0.637828000
B	-5.666745000	0.577254000	-0.498820000	B	-5.461171000	-1.472599000	-0.536341000
N	-2.276905000	5.243687000	-0.357698000	N	-3.917226000	4.082354000	-0.463105000
N	-4.555520000	4.200536000	-0.493581000	N	-5.688978000	2.306815000	-0.576405000
N	-4.852534000	1.762289000	-0.379693000	N	-5.114065000	-0.079828000	-0.419983000
B	5.003940000	-1.725373000	-0.124401000	B	5.334202000	0.096470000	-0.035618000
B	2.489769000	-5.243940000	-0.390328000	B	4.215163000	-4.080320000	-0.287752000
N	5.815070000	-0.547446000	-0.098234000	N	5.682738000	1.483781000	-0.024287000
N	3.331423000	-4.083732000	-0.276245000	N	4.595804000	-2.698949000	-0.172535000
B	4.768398000	-4.217908000	-0.321103000	B	5.989454000	-2.323280000	-0.183382000
N	5.564537000	-3.046253000	-0.232617000	N	6.324415000	-0.946428000	-0.103795000
Si	-1.415340000	0.139594000	0.965652000	Si	-1.330645000	-0.369064000	0.969642000
N	-0.708410000	-1.297579000	0.395113000	N	-0.175255000	-1.499978000	0.417786000
H	-7.079829000	-1.829823000	-0.787451000	H	-5.939388000	-4.218640000	-0.834248000
H	-6.834783000	0.691602000	-0.736813000	H	-6.595441000	-1.777646000	-0.773895000
H	-6.582503000	3.216380000	-0.817344000	H	-7.243484000	0.670723000	-0.867677000
H	-4.960820000	5.110772000	-0.658661000	H	-6.387244000	3.015277000	-0.750262000
H	-2.695335000	6.147595000	-0.527095000	H	-4.624719000	4.780873000	-0.642351000
H	-0.369803000	7.201065000	-0.571538000	H	-2.810796000	6.580947000	-0.697124000
H	2.128009000	7.135651000	-0.536686000	H	-0.447326000	7.390562000	-0.656000000
H	4.160525000	5.676306000	-0.371116000	H	1.965863000	6.732565000	-0.462530000
H	6.209602000	4.221286000	-0.279115000	H	4.391949000	6.084403000	-0.331332000
H	7.059577000	1.870943000	-0.182326000	H	6.006178000	4.180526000	-0.164368000
H	6.819050000	-0.644635000	-0.153708000	H	6.658102000	1.743224000	-0.066224000
H	6.567492000	-3.155885000	-0.275408000	H	7.303057000	-0.698584000	-0.124955000
H	5.280574000	-5.294496000	-0.435994000	H	6.848062000	-3.155370000	-0.259843000
H	2.985428000	-6.325784000	-0.522908000	H	5.060249000	-4.923186000	-0.387725000
H	0.705609000	-7.364676000	-0.655902000	H	3.287878000	-6.691039000	-0.576114000
H	-1.758791000	-6.949334000	-0.633028000	H	0.833255000	-7.158397000	-0.615111000
H	-3.839238000	-5.459541000	-0.536404000	H	-1.637502000	-6.489006000	-0.553050000
H	-5.857060000	-4.005336000	-0.633653000	H	-4.035442000	-5.830800000	-0.674365000
N	-1.550570000	0.009046000	2.706022000	N	-1.343794000	-0.401488000	2.688763000
N	-0.754754000	-0.693237000	3.555523000	N	-2.321185000	0.441901000	3.267823000
H	-0.186242000	-1.297458000	2.948103000	H	-1.908686000	0.973681000	4.027851000
H	-2.175621000	0.621318000	3.217670000	H	-1.029230000	-1.194933000	3.236071000
				H	-3.101980000	-0.098903000	3.629730000
H₂H₂N₂-Si_BBN				H₃NH₂N-Si_BBN			
N	3.255471000	4.199680000	-0.189233000	N	0.350072000	5.252162000	-0.263653000
B	4.692143000	4.382785000	-0.219454000	B	1.428224000	6.212031000	-0.276402000
B	2.381400000	5.334965000	-0.316025000	B	-1.009690000	5.690413000	-0.414648000
B	0.081191000	6.298321000	-0.505064000	B	-3.446130000	5.181366000	-0.614912000
B	-1.928191000	4.804400000	-0.399461000	B	-4.248668000	2.809634000	-0.483895000
B	0.384300000	3.838692000	-0.145733000	B	-1.803204000	3.321919000	-0.240992000
B	2.708501000	2.869897000	-0.055978000	B	0.645930000	3.836621000	-0.116413000
B	5.007638000	1.897268000	-0.044152000	B	3.088897000	4.342505000	-0.056813000
B	3.017456000	0.377024000	0.097760000	B	2.303401000	1.959662000	0.086901000
B	0.733320000	1.388103000	0.213595000	B	-0.153194000	1.482688000	0.156235000
B	-1.634046000	2.374463000	0.054837000	B	-2.611026000	0.963956000	-0.036854000
B	-3.692896000	0.802391000	-0.091846000	B	-3.410106000	-1.477982000	-0.149608000
B	1.069014000	-1.181238000	0.213755000	B	1.567650000	-0.427177000	0.238123000
B	3.356061000	-2.113417000	-0.045099000	B	3.994259000	0.104389000	-0.021089000
B	1.356306000	-3.642922000	-0.131729000	B	3.218046000	-2.280088000	-0.074239000

B	-0.967846000	-2.741845000	0.071949000	B	0.786984000	-2.826639000	0.142243000
B	-3.365679000	-1.748101000	-0.060553000	B	-1.730702000	-3.353136000	-0.047443000
B	-5.278066000	-3.244554000	-0.611485000	B	-2.448022000	-5.691022000	-0.594769000
B	-2.959521000	-4.195983000	-0.319356000	B	-0.016154000	-5.161931000	-0.230319000
B	-0.635213000	-5.172676000	-0.352931000	B	2.446639000	-4.660506000	-0.242508000
B	1.689268000	-6.102455000	-0.465873000	B	4.892775000	-4.123957000	-0.369761000
N	-1.326478000	6.094235000	-0.548323000	N	-4.491029000	4.218245000	-0.643594000
N	0.949885000	5.155978000	-0.310525000	N	-2.086836000	4.737224000	-0.415566000
N	5.521150000	3.234562000	-0.132008000	N	2.761199000	5.740524000	-0.158577000
N	3.564432000	1.710379000	0.020760000	N	2.009711000	3.377267000	-0.010209000
N	1.270271000	2.694151000	0.002762000	N	-0.433966000	2.883140000	-0.080533000
N	-1.058525000	3.664507000	-0.160563000	N	-2.892051000	2.367857000	-0.253276000
N	-3.066344000	2.114173000	-0.089380000	N	-3.673673000	-0.037554000	-0.155969000
N	-0.710097000	1.299670000	0.397663000	N	-1.270273000	0.593261000	0.302698000
N	1.568807000	0.189370000	0.243540000	N	1.226226000	0.997189000	0.219979000
N	3.886658000	-0.774226000	0.027206000	N	3.682218000	1.513371000	0.036905000
N	1.919862000	-2.310056000	0.008659000	N	2.930228000	-0.864401000	0.033464000
N	-2.933880000	-0.393892000	0.263128000	N	-2.127278000	-1.996505000	0.215621000
N	-4.754285000	-1.908030000	-0.400311000	N	-2.773206000	-4.295954000	-0.424866000
N	-2.423508000	-2.861348000	-0.029445000	N	-0.329110000	-3.765457000	0.014458000
N	-0.084401000	-3.844607000	-0.137829000	N	2.152169000	-3.256628000	-0.066504000
N	2.237768000	-4.774418000	-0.286190000	N	4.596902000	-2.717460000	-0.221479000
N	0.275477000	-6.265864000	-0.500275000	N	3.822846000	-5.057892000	-0.379820000
N	-2.061663000	-5.304628000	-0.400168000	N	1.354550000	-5.584268000	-0.276375000
N	-4.375129000	-4.335500000	-0.525564000	N	-1.094297000	-6.091976000	-0.452109000
B	-3.922720000	3.263997000	-0.391972000	B	-5.017136000	0.415682000	-0.462931000
B	-5.922142000	1.749942000	-0.669892000	B	-5.787917000	-1.960471000	-0.769831000
B	-5.605733000	-0.746503000	-0.547714000	B	-4.120871000	-3.828362000	-0.619527000
N	-3.339245000	4.565393000	-0.474589000	N	-5.285952000	1.823490000	-0.538067000
N	-5.326310000	3.034607000	-0.609454000	N	-6.048218000	-0.564700000	-0.684971000
N	-5.077145000	0.594042000	-0.427878000	N	-4.447880000	-2.426292000	-0.522506000
B	5.330127000	-0.586966000	-0.034202000	B	4.759447000	2.480213000	-0.015123000
B	3.668471000	-4.582759000	-0.285075000	B	5.660215000	-1.750498000	-0.237595000
N	5.850071000	0.743314000	-0.025408000	N	4.439883000	3.875111000	-0.012025000
N	4.223520000	-3.261803000	-0.165320000	N	5.371002000	-0.345686000	-0.134277000
B	5.660085000	-3.072715000	-0.184998000	B	6.441321000	0.621752000	-0.155545000
N	6.167929000	-1.750488000	-0.107360000	N	6.114839000	2.001219000	-0.079912000
Si	-1.355440000	-0.187435000	0.767183000	Si	-0.985827000	-0.966030000	0.986170000
N	-0.349680000	-1.464829000	0.399785000	N	0.569338000	-1.437712000	0.444058000
H	-6.435511000	-3.417894000	-0.847064000	H	-3.297123000	-6.494686000	-0.857610000
H	-6.764860000	-0.900513000	-0.788267000	H	-4.983757000	-4.613770000	-0.891812000
H	-7.084314000	1.615261000	-0.908337000	H	-6.668621000	-2.726321000	-1.040185000
H	-5.924006000	3.827139000	-0.799891000	H	-6.987788000	-0.253050000	-0.885287000
H	-3.947378000	5.348801000	-0.670923000	H	-6.229438000	2.122974000	-0.740927000
H	-1.908679000	6.905617000	-0.701625000	H	-5.432131000	4.550820000	-0.796633000
H	0.539337000	7.393692000	-0.636407000	H	-3.692209000	6.344772000	-0.760221000
H	2.842004000	6.430520000	-0.435921000	H	-1.247011000	6.856642000	-0.548494000
H	5.166753000	5.474682000	-0.320849000	H	1.205399000	7.383604000	-0.390302000
H	6.520515000	3.378728000	-0.168226000	H	3.505185000	6.422920000	-0.182685000
H	6.851091000	0.873120000	-0.076181000	H	5.191440000	4.548755000	-0.055124000
H	7.171286000	-1.635401000	-0.136822000	H	6.874094000	2.666370000	-0.108290000
H	6.397762000	-4.009124000	-0.266080000	H	7.583813000	0.271223000	-0.239753000
H	4.392434000	-5.527025000	-0.388673000	H	6.795607000	-2.116317000	-0.344989000
H	2.410680000	-7.046566000	-0.587185000	H	6.024174000	-4.499506000	-0.490019000
H	-0.080357000	-7.201225000	-0.639138000	H	4.052138000	-6.034744000	-0.493149000
H	-2.451005000	-6.219139000	-0.585488000	H	1.550403000	-6.562844000	-0.433916000
H	-4.752079000	-5.256914000	-0.700429000	H	-0.878172000	-7.067332000	-0.599880000
N	-1.478382000	-0.269759000	2.702699000	N	-1.088690000	-1.062812000	2.689030000

N	-2.590822000	0.500355000	3.181096000	N	-3.698157000	0.509904000	3.072204000
H	-2.706003000	0.340645000	4.178915000	H	-4.313302000	0.024384000	2.424911000
H	-1.479318000	-1.249690000	3.011458000	H	-1.911944000	-0.614861000	3.102116000
H	-3.417883000	0.161084000	2.695458000	H	-3.496627000	1.410317000	2.644025000
H	-0.628302000	0.162948000	3.072281000	H	-0.248695000	-0.887192000	3.224802000
				H	-4.232680000	0.694278000	3.916707000
		H₂N-Si₈BN				H₃N-Si₈BN	
N	3.730346000	3.732758000	-0.159427000	N	4.415398000	2.818932000	-0.226388000
B	5.173026000	3.717217000	-0.199612000	B	5.816783000	2.482018000	-0.290021000
B	3.017279000	4.975878000	-0.268220000	B	3.997262000	4.191713000	-0.314970000
B	0.871251000	6.243410000	-0.408616000	B	2.186936000	5.906839000	-0.422109000
B	-1.316067000	5.026820000	-0.264159000	B	-0.214491000	5.204720000	-0.256441000
B	0.838143000	3.756350000	-0.080179000	B	1.603506000	3.487642000	-0.099954000
B	2.998040000	2.485022000	-0.026027000	B	3.423377000	1.765920000	-0.088061000
B	5.146113000	1.212437000	-0.042451000	B	5.231621000	0.045746000	-0.149371000
B	2.963843000	-0.021744000	0.115982000	B	2.829556000	-0.670482000	0.044968000
B	0.828621000	1.279608000	0.274582000	B	1.042881000	1.075204000	0.264925000
B	-1.343949000	2.559021000	0.164177000	B	-0.785685000	2.803550000	0.182030000
B	-3.587943000	1.298744000	0.046447000	B	-3.242672000	2.060817000	0.047090000
B	0.815449000	-1.291170000	0.267549000	B	0.448886000	-1.428053000	0.264092000
B	2.959844000	-2.529402000	-0.049448000	B	2.264048000	-3.112565000	-0.106686000
B	0.777643000	-3.765574000	-0.093551000	B	-0.134844000	-3.835208000	-0.102193000
B	-1.383215000	-2.535553000	0.176687000	B	-1.961216000	-2.152892000	0.194482000
B	-3.607896000	-1.228257000	0.067255000	B	-3.824541000	-0.388116000	0.059446000
B	-5.720182000	-2.456841000	-0.475365000	B	-6.167866000	-1.114659000	-0.452411000
B	-3.556806000	-3.711146000	-0.190869000	B	-4.346016000	-2.822779000	-0.154046000
B	-1.399806000	-5.000052000	-0.257651000	B	-2.531375000	-4.555805000	-0.233851000
B	0.766474000	-6.251579000	-0.426814000	B	-0.701395000	-6.257913000	-0.431937000
N	-0.548987000	6.233602000	-0.419172000	N	0.800802000	6.212580000	-0.418135000
N	1.580093000	4.995472000	-0.245819000	N	2.602185000	4.531064000	-0.272063000
N	5.843392000	2.468432000	-0.127199000	N	6.191460000	1.113990000	-0.238691000
N	3.699287000	1.224746000	0.035063000	N	3.825968000	0.379907000	-0.044222000
N	1.558512000	2.506392000	0.044088000	N	2.028062000	2.106989000	0.013216000
N	-0.607778000	3.781688000	-0.068644000	N	0.201997000	3.833313000	-0.069276000
N	-2.805194000	2.532426000	0.062133000	N	-2.214079000	3.099988000	0.078570000
N	-0.592401000	1.372945000	0.477886000	N	-0.308501000	1.488449000	0.515526000
N	1.521634000	-0.010128000	0.280805000	N	1.432583000	-0.339374000	0.246756000
N	3.679288000	-1.279589000	0.021437000	N	3.247114000	-2.055832000	-0.057107000
N	1.521421000	-2.528308000	0.026075000	N	0.864847000	-2.791912000	0.007052000
N	-2.988467000	0.035447000	0.367875000	N	-2.922881000	0.692636000	0.331156000
N	-5.019151000	-1.211226000	-0.281227000	N	-5.201583000	-0.059715000	-0.280326000
N	-2.843005000	-2.474092000	0.074222000	N	-3.371719000	-1.777921000	0.099600000
N	-0.668373000	-3.767907000	-0.066965000	N	-1.542272000	-3.516664000	-0.056762000
N	1.498220000	-5.015637000	-0.269758000	N	0.287894000	-5.214664000	-0.287717000
N	-0.653522000	-6.218884000	-0.422240000	N	-2.077407000	-5.911203000	-0.404408000
N	-2.829415000	-4.944669000	-0.277185000	N	-3.913651000	-4.189079000	-0.232376000
N	-4.983727000	-3.666775000	-0.387068000	N	-5.726608000	-2.460598000	-0.347478000
B	-3.496348000	3.779560000	-0.215043000	B	-2.614513000	4.468629000	-0.190594000
B	-5.677559000	2.557183000	-0.510526000	B	-5.008691000	3.757027000	-0.488694000
B	-5.703327000	0.049569000	-0.422347000	B	-5.587570000	1.321639000	-0.417342000
N	-2.746665000	4.999106000	-0.296570000	N	-1.614769000	5.495399000	-0.271225000
N	-4.921950000	3.756308000	-0.423137000	N	-4.009859000	4.762331000	-0.395668000
N	-4.998464000	1.302126000	-0.303786000	N	-4.620426000	2.382719000	-0.296651000
B	5.125959000	-1.290088000	-0.057744000	B	4.652812000	-2.388121000	-0.168074000
B	2.935454000	-5.018596000	-0.305520000	B	1.686154000	-5.535652000	-0.354276000
N	5.829493000	-0.044389000	-0.042092000	N	5.617354000	-1.331592000	-0.166209000
N	3.670538000	-3.787777000	-0.195496000	N	2.676489000	-4.497182000	-0.264713000
B	5.113008000	-3.794121000	-0.241590000	B	4.079056000	-4.824461000	-0.346501000

N	5.802641000	-2.556178000	-0.159104000	N	5.029336000	-3.772063000	-0.282222000
Si	-1.434948000	-0.000158000	1.083723000	Si	-1.430907000	0.340928000	1.175601000
N	-0.601084000	-1.366872000	0.485264000	N	-0.943173000	-1.190447000	0.518858000
H	-6.895160000	-2.473554000	-0.708876000	H	-7.318467000	-0.869110000	-0.681193000
H	-6.876524000	0.057702000	-0.664762000	H	-6.731365000	1.590719000	-0.653672000
H	-6.850711000	2.592432000	-0.750928000	H	-6.147029000	4.049080000	-0.724131000
H	-5.405628000	4.626168000	-0.594522000	H	-4.291490000	5.718005000	-0.560524000
H	-3.244900000	5.860125000	-0.473330000	H	-1.913035000	6.445518000	-0.441715000
H	-1.024049000	7.115879000	-0.543864000	H	0.531030000	7.178655000	-0.534809000
H	1.468884000	7.273417000	-0.539543000	H	2.999909000	6.777366000	-0.552627000
H	3.623509000	6.001889000	-0.386440000	H	4.818648000	5.055757000	-0.430603000
H	5.793557000	4.737308000	-0.296382000	H	6.650296000	3.337295000	-0.385362000
H	6.852280000	2.472928000	-0.169821000	H	7.174886000	0.892698000	-0.298351000
H	6.837751000	-0.051996000	-0.104069000	H	6.596890000	-1.563738000	-0.250485000
H	6.811218000	-2.575959000	-0.204790000	H	6.006839000	-4.015333000	-0.352664000
H	5.717706000	-4.822395000	-0.351060000	H	4.438047000	-5.960771000	-0.469218000
H	3.524317000	-6.053433000	-0.434430000	H	2.030668000	-6.674392000	-0.492471000
H	1.346141000	-7.290814000	-0.565897000	H	-0.367106000	-7.399089000	-0.579444000
H	-1.143691000	-7.093425000	-0.543018000	H	-2.752955000	-6.652996000	-0.518095000
H	-3.345895000	-5.796443000	-0.446216000	H	-4.607591000	-4.905252000	-0.394135000
H	-5.482468000	-4.529979000	-0.548557000	H	-6.409263000	-3.189171000	-0.498695000
N	-1.598581000	-0.131929000	2.790614000	N	0.271692000	-0.054442000	3.112859000
H	-2.217830000	0.503060000	3.277585000	H	0.294984000	0.792044000	3.674219000
H	-0.781179000	-0.343787000	3.348063000	H	-0.093128000	-0.802886000	3.695089000
				H	1.228155000	-0.290454000	2.859266000

Table S7. Cartesian coordinates of optimized geometries of Lewis acid assisted N₂ activated systems calculated at the ω B97X-D/6-31G(d) level of theory.

Li⁺-N₂-Si₈BN				Na⁺-N₂-Si₈BN			
N	-5.870552000	0.700935000	0.386434000	N	1.376299000	4.912047000	-0.935122000
B	-6.727838000	1.862245000	0.494769000	B	2.684904000	5.463840000	-1.202601000
B	-6.439889000	-0.620730000	0.389548000	B	0.226888000	5.781982000	-0.852169000
B	-6.178096000	-3.101839000	0.196314000	B	-2.235290000	6.114661000	-0.566113000
B	-3.900883000	-4.114160000	-0.071906000	B	-3.735737000	4.145470000	-0.162888000
B	-4.158880000	-1.621611000	0.170676000	B	-1.254641000	3.815229000	-0.408838000
B	-4.441797000	0.877495000	0.263743000	B	1.215775000	3.487406000	-0.773815000
B	-4.721795000	3.358692000	0.283944000	B	3.659621000	3.151318000	-1.189329000
B	-2.428304000	2.369957000	0.053360000	B	2.179971000	1.164388000	-0.803760000
B	-2.165259000	-0.114440000	0.178340000	B	-0.242161000	1.539205000	-0.250995000
B	-1.886447000	-2.651769000	0.024470000	B	-2.750537000	1.868666000	0.076124000
B	0.441442000	-3.676313000	-0.471488000	B	-4.317847000	-0.187175000	0.255058000
B	-0.128809000	1.432908000	-0.186300000	B	0.712732000	-0.850961000	-0.502594000
B	-0.475707000	3.886065000	-0.415585000	B	3.128119000	-1.157989000	-1.101185000
B	1.789114000	2.892381000	-0.857568000	B	1.599952000	-3.164633000	-0.908991000
B	2.168971000	0.432275000	-0.654913000	B	-0.822104000	-2.881689000	-0.343729000
B	2.473914000	-2.160056000	-0.752326000	B	-3.357309000	-2.546190000	0.045979000
B	4.612519000	-3.103802000	-1.631419000	B	-4.888642000	-4.488050000	-0.258924000
B	4.342919000	-0.605554000	-1.401532000	B	-2.394568000	-4.808624000	-0.421173000
B	4.014117000	1.895092000	-1.495752000	B	0.064584000	-5.155139000	-0.864905000
B	3.683187000	4.378895000	-1.549523000	B	2.506512000	-5.454610000	-1.360027000
N	-5.324916000	-4.227697000	0.021913000	N	-3.521440000	5.551075000	-0.352491000
N	-5.591619000	-1.779581000	0.258679000	N	-1.080336000	5.236610000	-0.602385000
N	-6.132159000	3.150347000	0.447446000	N	3.789595000	4.571584000	-1.304865000
N	-3.851091000	2.195037000	0.214367000	N	2.350511000	2.590557000	-0.894302000

N	-3.584244000	-0.286608000	0.192734000	N	-0.088563000	2.941199000	-0.484194000
N	-3.309929000	-2.792236000	0.032271000	N	-2.574565000	3.271411000	-0.169749000
N	-0.987850000	-3.780419000	-0.231841000	N	-4.064298000	1.251211000	0.216069000
N	-1.358484000	-1.319006000	0.257645000	N	-1.540478000	1.068534000	0.153927000
N	-1.541836000	1.204993000	0.064736000	N	0.884943000	0.599602000	-0.426410000
N	-1.871840000	3.694403000	-0.124832000	N	3.298451000	0.274424000	-1.055127000
N	0.400794000	2.731378000	-0.489763000	N	1.826729000	-1.720612000	-0.794617000
N	1.138299000	-2.411343000	-0.294710000	N	-3.225189000	-1.138604000	0.368125000
N	3.251842000	-3.290001000	-1.187168000	N	-4.695431000	-3.067156000	-0.061175000
N	3.027807000	-0.778857000	-0.755763000	N	-2.176234000	-3.382976000	-0.181864000
N	2.665840000	1.730817000	-0.991867000	N	0.284961000	-3.725290000	-0.708823000
N	2.318134000	4.211739000	-1.113392000	N	2.717958000	-4.022198000	-1.226460000
N	4.496998000	3.218239000	-1.734206000	N	1.199915000	-5.976457000	-1.176778000
N	4.806458000	0.712139000	-1.692710000	N	-1.264535000	-5.649723000	-0.697355000
N	5.125818000	-1.774578000	-1.679108000	N	-3.737338000	-5.312216000	-0.391533000
B	-1.604858000	-5.096314000	-0.405275000	B	-5.226465000	2.136784000	0.151023000
B	0.627014000	-6.104723000	-1.013751000	B	-6.783890000	0.154783000	0.145410000
B	2.635171000	-4.608395000	-1.226373000	B	-5.827166000	-2.169081000	0.029512000
N	-3.019796000	-5.229709000	-0.261548000	N	-5.021944000	3.549656000	0.028719000
N	-0.757003000	-6.213084000	-0.735216000	N	-6.538646000	1.552496000	0.187908000
N	1.246087000	-4.794400000	-0.904575000	N	-5.644431000	-0.740463000	0.146410000
B	-2.743701000	4.858618000	-0.055896000	B	4.612674000	0.834821000	-1.342028000
B	1.458610000	5.368945000	-0.977123000	B	4.024673000	-3.467101000	-1.457848000
N	-4.137081000	4.660532000	0.180834000	N	4.768850000	2.253129000	-1.339158000
N	0.076129000	5.205832000	-0.633820000	N	4.233552000	-2.040090000	-1.386761000
B	-0.789084000	6.365892000	-0.528216000	B	5.543780000	-1.482675000	-1.648360000
N	-2.159958000	6.160425000	-0.235600000	N	5.700966000	-0.071611000	-1.586146000
Si	0.290998000	-1.149903000	0.436850000	Si	-1.687560000	-0.533861000	0.639070000
N	0.830595000	0.337901000	-0.146897000	N	-0.522762000	-1.478409000	-0.139430000
H	5.291334000	-4.029371000	-1.958023000	H	-5.985437000	-4.957579000	-0.312728000
H	3.301564000	-5.543277000	-1.554438000	H	-6.932687000	-2.617770000	-0.024092000
H	1.272887000	-7.057707000	-1.332469000	H	-7.898025000	-0.273796000	0.103723000
H	-1.175927000	-7.127375000	-0.835097000	H	-7.344960000	2.161247000	0.166801000
H	-3.426457000	-6.149423000	-0.364450000	H	-5.836771000	4.147428000	0.003723000
H	-5.760837000	-5.137571000	-0.029772000	H	-4.309457000	6.183311000	-0.341367000
H	-7.360796000	-3.247863000	0.284941000	H	-2.103160000	7.292168000	-0.720469000
H	-7.621867000	-0.760472000	0.494983000	H	0.367375000	6.959094000	-0.998466000
H	-7.910036000	1.738296000	0.619751000	H	2.840820000	6.640299000	-1.337155000
H	-6.746776000	3.949498000	0.512335000	H	4.693636000	4.975083000	-1.506992000
H	-4.742861000	5.468279000	0.224101000	H	5.676540000	2.641802000	-1.556671000
H	-2.751340000	6.977601000	-0.178080000	H	6.616962000	0.302620000	-1.792660000
H	-0.349960000	7.465872000	-0.688271000	H	6.471575000	-2.192000000	-1.897257000
H	1.911319000	6.459340000	-1.159254000	H	4.944213000	-4.186143000	-1.709135000
H	4.134800000	5.464614000	-1.757601000	H	3.421484000	-6.176110000	-1.622486000
H	5.434223000	3.361550000	-2.083834000	H	1.079993000	-6.974072000	-1.284070000
H	5.712997000	0.811913000	-2.129751000	H	-1.432198000	-6.636440000	-0.840380000
H	6.049476000	-1.658527000	-2.073474000	H	-3.894893000	-6.298884000	-0.542849000
C	4.650400000	1.498862000	2.691422000	C	3.277834000	0.400222000	4.244065000
C	5.442771000	1.279007000	1.560995000	C	3.465865000	1.372173000	3.256945000
C	6.117682000	0.064632000	1.407668000	C	4.270611000	1.096030000	2.149505000
C	6.000923000	-0.929380000	2.384745000	C	4.886064000	-0.153055000	2.025608000
C	5.215438000	-0.703433000	3.519112000	C	4.699163000	-1.124646000	3.011983000
C	4.542128000	0.510224000	3.672294000	C	3.894980000	-0.847077000	4.122271000
H	4.124305000	2.440857000	2.807873000	H	2.658137000	0.616769000	5.108281000
H	5.527588000	2.049159000	0.801624000	H	2.994258000	2.344867000	3.356818000
H	6.724704000	-0.110224000	0.526314000	H	4.423995000	1.850196000	1.383621000
H	6.523767000	-1.872822000	2.264117000	H	5.512201000	-0.362640000	1.163574000
H	5.121677000	-1.474276000	4.276694000	H	5.190223000	-2.089023000	2.923264000

H	3.921314000	0.677356000	4.545765000	H	3.760502000	-1.596376000	4.896307000
Li	3.697537000	-0.561532000	1.418306000	N	-1.262473000	-0.547440000	2.462655000
N	1.948081000	-1.060108000	2.509957000	N	-0.159806000	-0.685804000	2.847071000
N	0.813207000	-1.210008000	2.245530000	Na	2.084132000	-0.765133000	1.880391000
K⁺-N₂-Si_BBN				Rb⁺-N₂-Si_BBN			
N	0.828819000	-5.318609000	-0.625720000	N	-1.576058000	5.251934000	-0.629169000
B	-0.132813000	-6.376560000	-0.840967000	B	-0.748230000	6.413432000	-0.865063000
B	2.226779000	-5.633670000	-0.468184000	B	-2.993452000	5.406060000	-0.414152000
B	4.598214000	-4.906531000	-0.151472000	B	-5.253751000	4.413241000	-0.013361000
B	5.149630000	-2.471973000	0.085033000	B	-5.518202000	1.929299000	0.206231000
B	2.759474000	-3.206456000	-0.181817000	B	-3.238369000	2.931335000	-0.144747000
B	0.387102000	-3.944849000	-0.579025000	B	-0.980943000	3.936118000	-0.617474000
B	-1.967423000	-4.672004000	-1.004710000	B	1.260515000	4.928636000	-1.111225000
B	-1.438139000	-2.229430000	-0.785898000	B	1.018828000	2.439958000	-0.903922000
B	0.899235000	-1.539144000	-0.198049000	B	-1.203791000	1.484237000	-0.252000000
B	3.310933000	-0.789577000	0.150182000	B	-3.501240000	0.464594000	0.170356000
B	3.901847000	1.730102000	0.103717000	B	-3.807065000	-2.104725000	0.107169000
B	-0.956889000	0.209443000	-0.574129000	B	0.825125000	-0.040479000	-0.702105000
B	-3.253224000	-0.538339000	-1.213440000	B	3.001757000	0.969109000	-1.391664000
B	-2.689825000	1.916775000	-1.210433000	B	2.716146000	-1.531870000	-1.411716000
B	-0.381271000	2.699025000	-0.598365000	B	0.530217000	-2.575559000	-0.750409000
B	2.066683000	3.459715000	-0.278907000	B	-1.804330000	-3.611111000	-0.364735000
B	2.671141000	5.829300000	-0.759087000	B	-2.156731000	-6.026181000	-0.871594000
B	0.265407000	5.090767000	-0.879696000	B	0.146906000	-5.021792000	-1.048395000
B	-2.118189000	4.372146000	-1.281990000	B	2.421323000	-4.034584000	-1.506388000
B	-4.462985000	3.604640000	-1.755177000	B	4.657977000	-3.004688000	-2.008592000
N	5.535213000	-3.850966000	0.013897000	N	-6.059063000	3.256885000	0.173980000
N	3.189198000	-4.583919000	-0.260431000	N	-3.823341000	4.252547000	-0.185043000
N	-1.500315000	-6.025752000	-1.011067000	N	0.643379000	6.221163000	-1.087907000
N	-1.008321000	-3.603611000	-0.770149000	N	0.436428000	3.756609000	-0.860919000
N	1.345183000	-2.892358000	-0.331087000	N	-1.804764000	2.780028000	-0.351066000
N	3.734226000	-2.152785000	0.012644000	N	-4.080768000	1.772799000	0.070483000
N	4.258228000	0.320449000	0.209734000	N	-4.315458000	-0.745772000	0.248967000
N	1.876792000	-0.551659000	0.195705000	N	-2.050111000	0.389013000	0.157959000
N	-0.495952000	-1.161849000	-0.465442000	N	0.215137000	1.270039000	-0.567014000
N	-2.820033000	-1.903302000	-1.087115000	N	2.420821000	2.275735000	-1.243561000
N	-2.302731000	0.535040000	-0.988894000	N	2.183770000	-0.206211000	-1.165573000
N	2.512513000	2.151430000	0.136380000	N	-2.379620000	-2.367679000	0.086850000
N	3.073003000	4.475034000	-0.452973000	N	-2.696263000	-4.731101000	-0.525899000
N	0.643449000	3.724698000	-0.526209000	N	-0.369311000	-3.712615000	-0.660347000
N	-1.738757000	2.992516000	-1.004587000	N	1.896117000	-2.710409000	-1.209256000
N	-4.064450000	2.226332000	-1.533042000	N	4.113240000	-1.683060000	-1.758813000
N	-3.489404000	4.630465000	-1.621076000	N	3.808422000	-4.135464000	-1.868357000
N	-1.112933000	5.377584000	-1.173594000	N	1.540427000	-5.149565000	-1.383136000
N	1.282934000	6.097882000	-0.929571000	N	-0.752770000	-6.136182000	-1.087249000
B	5.681788000	-0.013676000	0.210698000	B	-5.765674000	-0.574491000	0.311442000
B	6.294286000	2.423866000	0.009740000	B	-6.108528000	-3.062306000	0.086326000
B	4.473158000	4.130601000	-0.302881000	B	-4.120458000	-4.547807000	-0.325077000
N	6.076264000	-1.389397000	0.219137000	N	-6.311712000	0.747761000	0.360787000
N	6.639830000	1.058458000	0.179508000	N	-6.598184000	-1.747407000	0.297574000
N	4.888129000	2.769175000	-0.065958000	N	-4.676699000	-3.245868000	-0.047557000
B	-3.786083000	-2.973629000	-1.290120000	B	3.252843000	3.450228000	-1.459744000
B	-5.029126000	1.161606000	-1.689047000	B	4.949228000	-0.514196000	-1.918314000
N	-3.341904000	-4.324729000	-1.217256000	N	2.659030000	4.741524000	-1.366939000
N	-4.627907000	-0.207405000	-1.524175000	N	4.400425000	0.798745000	-1.729667000
B	-5.598066000	-1.273628000	-1.688822000	B	5.238961000	1.970029000	-1.905206000
N	-5.157968000	-2.611918000	-1.536393000	N	4.651868000	3.248994000	-1.739556000
Si	1.359733000	1.004078000	0.557638000	Si	-1.348494000	-1.101224000	0.488945000

N	-0.114276000	1.328572000	-0.218361000	N	0.123634000	-1.250904000	-0.341241000
N	1.077779000	1.131564000	2.389628000	N	-1.012369000	-1.205332000	2.309600000
N	0.060582000	1.465775000	2.879480000	N	0.043747000	-1.433939000	2.778612000
H	3.479102000	6.702079000	-0.866030000	H	-2.865081000	-6.981996000	-0.973782000
H	5.297378000	4.989581000	-0.400440000	H	-4.846656000	-5.491842000	-0.413960000
H	7.136367000	3.267435000	-0.071955000	H	-6.854444000	-3.992899000	0.017776000
H	7.624508000	0.833169000	0.208067000	H	-7.600008000	-1.635070000	0.367393000
H	7.064261000	-1.602248000	0.238684000	H	-7.315622000	0.847860000	0.423833000
H	6.511943000	-4.101720000	0.075201000	H	-7.054174000	3.395111000	0.280225000
H	4.966099000	-6.042083000	-0.208170000	H	-5.749351000	5.500315000	-0.036310000
H	2.586476000	-6.771841000	-0.517189000	H	-3.480732000	6.496527000	-0.432160000
H	0.211228000	-7.520160000	-0.876480000	H	-1.220665000	7.510609000	-0.873123000
H	-2.156783000	-6.777263000	-1.169044000	H	1.204616000	7.043679000	-1.258695000
H	-4.009935000	-5.067163000	-1.372332000	H	3.233326000	5.556674000	-1.532258000
H	-5.842874000	-3.343593000	-1.666439000	H	5.245632000	4.054936000	-1.878859000
H	-6.741687000	-1.024764000	-1.929360000	H	6.398860000	1.851788000	-2.166431000
H	-6.166376000	1.426373000	-1.940821000	H	6.104588000	-0.650049000	-2.189560000
H	-5.594265000	3.868369000	-2.033099000	H	5.806340000	-3.140140000	-2.307783000
H	-3.787005000	5.578664000	-1.805294000	H	4.206425000	-5.042323000	-2.070477000
H	-1.359125000	6.331493000	-1.401257000	H	1.885747000	-6.067247000	-1.630454000
H	1.025195000	7.047387000	-1.160251000	H	-0.398728000	-7.046477000	-1.346650000
C	-2.843225000	-1.415487000	2.423432000	C	2.607325000	1.840807000	2.241388000
C	-4.148015000	-1.081586000	2.054319000	C	3.956353000	1.712749000	1.905541000
C	-4.913394000	-0.248450000	2.872116000	C	4.837786000	1.089296000	2.790861000
C	-4.376405000	0.244248000	4.064857000	C	4.369581000	0.598107000	4.012460000
C	-3.071980000	-0.092323000	4.434561000	C	3.019076000	0.724774000	4.345440000
C	-2.304736000	-0.920443000	3.612085000	C	2.137579000	1.345005000	3.458085000
H	-2.254959000	-2.076303000	1.794986000	H	1.926996000	2.347330000	1.565445000
H	-4.574920000	-1.488686000	1.143358000	H	4.323382000	2.119936000	0.968159000
H	-5.935326000	-0.006711000	2.595048000	H	5.892150000	1.009732000	2.542010000
H	-4.981957000	0.868518000	4.715594000	H	5.061407000	0.140925000	4.714363000
H	-2.657083000	0.278313000	5.367001000	H	2.656170000	0.356159000	5.300345000
H	-1.292611000	-1.183925000	3.902742000	H	1.089568000	1.452030000	3.720100000
K	-2.564523000	1.821190000	1.916603000	Rb	2.896161000	-1.638680000	1.854837000
Cs⁺-N₂-Si_BBN				BF₃-N₂-Si_BBN			
N	0.548993000	5.100649000	-1.288161000	N	4.730112000	2.686535000	-0.257886000
B	1.771363000	5.800830000	-1.610617000	B	6.121088000	2.303549000	-0.180952000
B	-0.686315000	5.829840000	-1.127786000	B	4.363631000	4.072343000	-0.372363000
B	-3.145774000	5.872392000	-0.672259000	B	2.622172000	5.848260000	-0.629193000
B	-4.374369000	3.740613000	-0.182265000	B	0.193002000	5.230608000	-0.701114000
B	-1.895095000	3.704201000	-0.594978000	B	1.940403000	3.447270000	-0.401248000
B	0.565773000	3.666794000	-1.124044000	B	3.702623000	1.663557000	-0.227230000
B	3.017005000	3.621690000	-1.616022000	B	5.448896000	-0.115658000	-0.114912000
B	1.788662000	1.472265000	-1.207629000	B	3.022885000	-0.757580000	-0.168016000
B	-0.619582000	1.557354000	-0.531836000	B	1.293939000	1.045289000	-0.141823000
B	-3.114543000	1.594110000	-0.025674000	B	-0.488459000	2.854922000	-0.367023000
B	-4.418994000	-0.629760000	0.207747000	B	-2.973138000	2.196406000	-0.672965000
B	0.591597000	-0.691651000	-0.857366000	B	0.621571000	-1.445729000	-0.221731000
B	2.982902000	-0.711755000	-1.575415000	B	2.394691000	-3.183557000	-0.384702000
B	1.709206000	-2.879923000	-1.364282000	B	-0.022303000	-3.826856000	-0.632407000
B	-0.673733000	-2.887338000	-0.602195000	B	-1.823774000	-2.097402000	-0.525648000
B	-3.204698000	-2.854852000	-0.082782000	B	-3.636646000	-0.264718000	-0.751288000
B	-4.512536000	-4.964415000	-0.308935000	B	-5.944360000	-0.905996000	-1.445321000
B	-2.010987000	-4.989314000	-0.611851000	B	-4.191142000	-2.676967000	-1.064139000
B	0.441890000	-5.044368000	-1.191205000	B	-2.425368000	-4.470578000	-0.999661000
B	2.884884000	-5.056869000	-1.771652000	B	-0.635541000	-6.226097000	-1.018681000
N	-4.339788000	5.162012000	-0.374694000	N	1.250603000	6.201221000	-0.752703000
N	-1.901549000	5.136409000	-0.792434000	N	2.979306000	4.457048000	-0.463366000

N	2.970708000	5.046101000	-1.750740000	N	6.443569000	0.923527000	-0.102746000
N	1.790442000	2.910604000	-1.298103000	N	4.049409000	0.264119000	-0.156015000
N	-0.644582000	2.972555000	-0.754658000	N	2.312768000	2.051338000	-0.270621000
N	-3.122700000	3.009175000	-0.271502000	N	0.549091000	3.841676000	-0.499716000
N	-4.338729000	0.828218000	0.182545000	N	-1.899578000	3.181475000	-0.574775000
N	-1.817918000	0.941398000	-0.025110000	N	-0.072563000	1.507097000	-0.049754000
N	0.582905000	0.761890000	-0.811422000	N	1.617269000	-0.379652000	-0.125700000
N	3.002440000	0.724562000	-1.483876000	N	3.396790000	-2.154814000	-0.235508000
N	1.755255000	-1.425587000	-1.301310000	N	0.999045000	-2.817650000	-0.425121000
N	-3.218523000	-1.444017000	0.231215000	N	-2.737020000	0.801812000	-0.375292000
N	-4.476606000	-3.531832000	-0.114721000	N	-4.964938000	0.121925000	-1.174943000
N	-1.947018000	-3.549996000	-0.374650000	N	-3.205982000	-1.659342000	-0.723124000
N	0.495467000	-3.597723000	-1.059296000	N	-1.421787000	-3.462752000	-0.729013000
N	2.924495000	-3.607069000	-1.667367000	N	0.369778000	-5.215437000	-0.777084000
N	1.656008000	-5.728259000	-1.545655000	N	-1.998033000	-5.835532000	-1.129165000
N	-0.804335000	-5.695139000	-0.946841000	N	-3.788570000	-4.050641000	-1.130205000
N	-3.281151000	-5.648266000	-0.514271000	N	-5.540588000	-2.263852000	-1.350375000
B	-5.596854000	1.571295000	0.202978000	B	-2.233155000	4.572696000	-0.849079000
B	-6.910958000	-0.578864000	0.267497000	B	-4.632040000	3.947405000	-1.306593000
B	-5.698407000	-2.773163000	0.056377000	B	-5.297140000	1.521413000	-1.305401000
N	-5.567606000	2.999204000	0.088122000	N	-1.193686000	5.559598000	-0.842477000
N	-6.828126000	0.837768000	0.314166000	N	-3.601489000	4.910398000	-1.144735000
N	-5.677795000	-1.334080000	0.177067000	N	-4.308104000	2.554048000	-1.101097000
B	4.244368000	1.436721000	-1.743338000	B	4.796882000	-2.532456000	-0.196895000
B	4.157546000	-2.901813000	-1.897838000	B	1.758976000	-5.583513000	-0.694530000
N	4.228241000	2.863636000	-1.757656000	N	5.787582000	-1.505178000	-0.098825000
N	4.197300000	-1.463070000	-1.815398000	N	2.770025000	-4.579371000	-0.500539000
B	5.446117000	-0.754198000	-2.021351000	B	4.164080000	-4.951743000	-0.430857000
N	5.437600000	0.662555000	-1.959144000	N	5.134819000	-3.928625000	-0.270811000
Si	-1.747668000	-0.666246000	0.469336000	Si	-1.266174000	0.384226000	0.331552000
N	-0.514101000	-1.468499000	-0.370515000	N	-0.792601000	-1.159676000	-0.145548000
N	-1.361620000	-0.660092000	2.278618000	H	-7.067816000	-0.622087000	-1.744706000
N	-0.350509000	-1.036521000	2.752106000	H	-6.411072000	1.830724000	-1.614242000
H	-5.547356000	-5.560573000	-0.298358000	H	-5.740307000	4.281847000	-1.610150000
H	-6.744713000	-3.349110000	0.072553000	H	-3.840852000	5.877656000	-1.310353000
H	-7.968300000	-1.134085000	0.298465000	H	-1.446578000	6.522866000	-1.013601000
H	-7.699222000	1.348342000	0.354774000	H	1.027952000	7.178669000	-0.874829000
H	-6.446622000	3.497433000	0.120657000	H	3.469243000	6.693352000	-0.669456000
H	-5.194281000	5.696820000	-0.307026000	H	5.215956000	4.912155000	-0.400271000
H	-3.165737000	7.056941000	-0.827835000	H	6.985218000	3.132261000	-0.187710000
H	-0.696154000	7.014744000	-1.277760000	H	7.420709000	0.672153000	-0.059724000
H	1.780527000	6.986556000	-1.753727000	H	6.762397000	-1.769173000	-0.074220000
H	3.813950000	5.553725000	-1.978853000	H	6.105307000	-4.205377000	-0.233615000
H	5.084361000	3.357808000	-1.969503000	H	4.495678000	-6.099223000	-0.513090000
H	6.311605000	1.139922000	-2.131378000	H	2.074893000	-6.733154000	-0.798975000
H	6.459990000	-1.353362000	-2.222532000	H	-0.327063000	-7.377052000	-1.134257000
H	5.160366000	-3.509172000	-2.126503000	H	-2.680219000	-6.559488000	-1.303076000
H	3.877567000	-5.667176000	-2.035275000	H	-4.489537000	-4.745597000	-1.346505000
H	1.652451000	-6.734574000	-1.638522000	H	-6.233208000	-2.968876000	-1.558982000
H	-0.861295000	-6.695938000	-1.078532000	N	-1.518809000	0.485810000	2.155349000
H	-3.330218000	-6.646363000	-0.664487000	N	-1.397200000	-0.367307000	2.950426000
C	1.888183000	2.237031000	2.193050000	B	-1.721542000	-0.167936000	4.933902000
C	3.252412000	2.273356000	1.900387000	F	-1.868515000	1.162332000	4.990842000
C	4.179109000	1.835206000	2.847418000	F	-0.567134000	-0.689386000	5.364940000
C	3.741277000	1.360008000	4.085548000	F	-2.824345000	-0.924062000	5.006994000
C	2.375939000	1.316240000	4.372726000				
C	1.449426000	1.756000000	3.426322000				
H	1.168459000	2.598534000	1.465957000				

H	3.594073000	2.655158000	0.943045000			
H	5.242247000	1.885449000	2.629996000			
H	4.463836000	1.041473000	4.831462000			
H	2.033229000	0.954447000	5.337547000			
H	0.388407000	1.728613000	3.652750000			
Cs	2.732716000	-1.387644000	1.905256000			
BCl₃-N₂-Si_BBN				B(C₆H₅)₃-N₂-Si_BBN		
N	-5.499261000	-0.791704000	-0.182645000	N	5.183071000	-2.227181000
B	-6.640202000	0.089121000	-0.072887000	B	5.548652000	-3.617460000
B	-5.682765000	-2.217275000	-0.224039000	B	6.179666000	-1.241780000
B	-4.746701000	-4.526927000	-0.444531000	B	6.827024000	1.134000000
B	-2.271668000	-4.871549000	-0.651195000	B	5.077665000	2.930374000
B	-3.208497000	-2.550048000	-0.389349000	B	4.423330000	0.539147000
B	-4.166440000	-0.227523000	-0.257240000	B	3.795082000	-1.833780000
B	-5.112650000	2.080531000	-0.190386000	B	3.155231000	-4.192157000
B	-2.630558000	1.762647000	-0.373544000	B	1.397712000	-2.407921000
B	-1.703778000	-0.554679000	-0.303415000	B	2.029533000	-0.098130000
B	-0.737116000	-2.916504000	-0.484398000	B	2.675099000	2.317614000
B	1.797321000	-3.251595000	-0.915391000	B	0.896280000	4.192546000
B	-0.154954000	1.497861000	-0.559726000	B	-0.399543000	-0.681676000
B	-1.152282000	3.765795000	-0.743020000	B	-0.949198000	-2.983772000
B	1.318049000	3.445074000	-1.096880000	B	-2.660426000	-1.155603000
B	2.347340000	1.171291000	-0.975636000	B	-2.146546000	1.165477000
B	3.332556000	-1.218111000	-1.152454000	B	-1.498035000	3.620789000
B	5.670752000	-1.516719000	-1.956859000	B	-3.088090000	5.450401000
B	4.731748000	0.797490000	-1.602401000	B	-3.738964000	3.037288000
B	3.772228000	3.127350000	-1.560097000	B	-4.340719000	0.680825000
B	2.769482000	5.425072000	-1.594833000	B	-4.923617000	-1.675674000
N	-3.615323000	-5.373998000	-0.603193000	N	6.443448000	2.496382000
N	-4.549149000	-3.097595000	-0.348862000	N	5.813936000	0.141240000
N	-6.419557000	1.491031000	-0.073110000	N	4.534007000	-4.559847000
N	-3.960213000	1.200826000	-0.261585000	N	2.787850000	-2.798040000
N	-3.025836000	-1.111717000	-0.329849000	N	3.421873000	-0.456576000
N	-2.071957000	-3.442864000	-0.517942000	N	4.059484000	1.930649000
N	0.439502000	-3.752570000	-0.722891000	N	2.259058000	3.718915000
N	-0.604206000	-1.496366000	-0.234580000	N	1.702140000	1.257252000
N	-1.466542000	0.884412000	-0.365094000	N	0.999314000	-1.035363000
N	-2.457044000	3.192854000	-0.508661000	N	0.409109000	-3.382489000
N	0.002319000	2.900461000	-0.813931000	N	-1.331482000	-1.603113000
N	2.118476000	-1.857893000	-0.687647000	N	-0.208972000	3.268407000
N	4.392788000	-2.092340000	-1.597851000	N	-1.775951000	5.034754000
N	3.451885000	0.235421000	-1.185832000	N	-2.447271000	2.597248000
N	2.474914000	2.578581000	-1.221957000	N	-3.029027000	0.240554000
N	1.468326000	4.872946000	-1.288439000	N	-3.613173000	-2.118871000
N	3.881459000	4.548373000	-1.728436000	N	-5.250413000	-0.295746000
N	4.869332000	2.218605000	-1.716818000	N	-4.663530000	2.071339000
N	5.810070000	-0.104700000	-1.913639000	N	-4.036509000	4.448361000
B	0.213453000	-5.178226000	-0.931223000	B	3.305373000	4.719925000
B	2.643488000	-5.516149000	-1.516498000	B	1.632596000	6.575288000
B	4.168263000	-3.517816000	-1.668182000	B	-0.746671000	6.003488000
N	-1.116790000	-5.700535000	-0.827692000	N	4.666466000	4.297125000
N	1.338275000	-6.013610000	-1.261436000	N	2.940131000	6.112529000
N	2.877039000	-4.096398000	-1.370918000	N	0.590331000	5.597977000
B	-3.611064000	4.070609000	-0.441185000	B	0.779127000	-4.774714000
B	0.321957000	5.738574000	-1.182496000	B	-3.257606000	-3.510956000
N	-4.906482000	3.494321000	-0.249866000	N	2.141735000	-5.153006000
N	-0.982553000	5.194268000	-0.915747000	N	-1.938050000	-3.950880000
B	-2.131987000	6.065267000	-0.822124000	B	-1.573239000	-5.344542000

N	-3.405866000	5.486980000	-0.581444000	N	-0.238787000	-5.723557000	-2.243483000
Si	0.936573000	-0.883855000	-0.007690000	Si	0.082439000	1.652223000	-0.043167000
N	1.053159000	0.701532000	-0.531848000	N	-0.901369000	0.636836000	-0.942595000
H	6.585236000	-2.213673000	-2.287354000	H	-3.365004000	6.611477000	-1.649877000
H	5.063445000	-4.235039000	-2.007191000	H	-0.996129000	7.170196000	-0.921350000
H	3.524480000	-6.253577000	-1.849909000	H	1.403986000	7.747156000	-0.328007000
H	1.189758000	-7.005251000	-1.384208000	H	3.660287000	6.809277000	0.188110000
H	-1.251017000	-6.694550000	-0.950888000	H	5.375538000	5.004745000	0.379376000
H	-3.781773000	-6.367574000	-0.674334000	H	7.171796000	3.171087000	0.401739000
H	-5.847555000	-4.994108000	-0.397687000	H	7.977293000	0.818558000	0.180565000
H	-6.785410000	-2.677612000	-0.161658000	H	7.324009000	-1.570429000	-0.246389000
H	-7.748426000	-0.354943000	0.013088000	H	6.684654000	-3.969017000	-0.694104000
H	-7.228243000	2.092183000	-0.004972000	H	4.806481000	-5.527775000	-1.239616000
H	-5.709049000	4.106159000	-0.202591000	H	2.401267000	-6.124749000	-1.745553000
H	-4.199054000	6.109579000	-0.525253000	H	0.002181000	-6.700452000	-2.329535000
H	-2.013564000	7.249318000	-0.952100000	H	-2.377481000	-6.165990000	-2.883871000
H	0.455758000	6.918605000	-1.328786000	H	-4.065837000	-4.309603000	-3.192757000
H	2.910766000	6.604079000	-1.744880000	H	-5.727468000	-2.459857000	-3.569373000
H	4.777648000	4.960460000	-1.945168000	H	-6.172154000	-0.011041000	-3.357878000
H	5.770255000	2.592408000	-1.981191000	H	-5.563935000	2.392440000	-2.724911000
H	6.705149000	0.279770000	-2.181126000	H	-4.939203000	4.756134000	-2.220625000
N	1.233868000	-0.931688000	1.842553000	N	-0.143836000	1.574758000	1.801423000
N	1.442893000	-0.016039000	2.538582000	N	-0.603810000	0.851737000	2.593633000
B	1.708087000	0.171411000	4.156070000	B	-1.417945000	-0.611363000	2.663796000
Cl	1.648275000	-1.477685000	4.932903000	C	-1.831565000	-0.797812000	4.219444000
Cl	3.361929000	0.950238000	4.190920000	C	-3.144336000	-1.066782000	4.620468000
Cl	0.333006000	1.273842000	4.644936000	C	-0.854786000	-0.742100000	5.224195000
				C	-3.471350000	-1.269575000	5.960987000
				C	-1.170026000	-0.928234000	6.564908000
				C	-2.486059000	-1.196179000	6.938677000
				C	-2.718112000	-0.381201000	1.714473000
				C	-3.327923000	-1.415619000	0.991416000
				C	-3.411602000	0.840058000	1.756070000
				C	-4.581046000	-1.262278000	0.400788000
				C	-4.641888000	1.019466000	1.130702000
				C	-5.245540000	-0.043441000	0.466093000
				C	-0.266731000	-1.690324000	2.261564000
				C	1.108962000	-1.413414000	2.228254000
				C	-0.628418000	-3.036339000	2.084803000
				C	2.061846000	-2.405395000	2.009398000
				C	0.311680000	-4.029837000	1.827103000
				C	1.667475000	-3.719473000	1.788732000
				H	-4.500873000	-1.479911000	6.239220000
				H	-2.736884000	-1.349693000	7.984808000
				H	-0.390309000	-0.872842000	7.320099000
				H	-0.017280000	-5.054330000	1.674837000
				H	2.407189000	-4.490646000	1.593681000
				H	3.117286000	-2.144978000	2.001004000
				H	-5.028527000	-2.098806000	-0.128165000
				H	-6.214683000	0.079986000	-0.008061000
				H	-5.137794000	1.984976000	1.182570000
				H	-3.931651000	-1.119194000	3.872938000
				H	0.182059000	-0.555624000	4.948421000
				H	-1.668293000	-3.329482000	2.191819000
				H	1.473325000	-0.401927000	2.392183000
				H	-2.999966000	1.674597000	2.320574000
				H	-2.828779000	-2.372440000	0.886487000
B(C₆H₄F)₃-N₂-Si_BBN				B(C₆H₃F₂)₃-N₂-Si_BBN			

N	5.499438000	-1.543574000	-0.719754000	N	3.552971000	2.057365000	3.013860000
B	6.023467000	-2.869592000	-0.966451000	B	3.914112000	3.441635000	3.209696000
B	6.371073000	-0.486903000	-0.288371000	B	4.531243000	1.014634000	3.167499000
B	6.742456000	1.904558000	0.348497000	B	5.161196000	-1.408582000	3.121581000
B	4.813835000	3.505991000	0.418245000	B	3.461135000	-3.150911000	2.507234000
B	4.433412000	1.093901000	-0.189671000	B	2.816812000	-0.712319000	2.587763000
B	4.084523000	-1.289023000	-0.911337000	B	2.191236000	1.724000000	2.642988000
B	3.727437000	-3.657408000	-1.601579000	B	1.549648000	4.132460000	2.715201000
B	1.783838000	-2.073260000	-1.541473000	B	-0.138291000	2.427749000	2.006543000
B	2.135650000	0.235384000	-0.674863000	B	0.545785000	0.037533000	1.896004000
B	2.502228000	2.669823000	0.004013000	B	1.191527000	-2.434506000	1.810119000
B	0.550558000	4.365210000	-0.155345000	B	-0.525394000	-4.197817000	0.998518000
B	-0.189495000	-0.550218000	-1.454773000	B	-1.808554000	0.789927000	1.140313000
B	-0.454706000	-2.836929000	-2.380538000	B	-2.498598000	3.142763000	1.503869000
B	-2.339730000	-1.185158000	-2.553815000	B	-4.191417000	1.432327000	0.768761000
B	-2.109355000	1.120571000	-1.628594000	B	-3.531281000	-0.952960000	0.411949000
B	-1.740105000	3.596171000	-0.977742000	B	-2.886838000	-3.464124000	0.338984000
B	-3.497012000	5.282821000	-1.508978000	B	-4.670972000	-5.174326000	0.033893000
B	-3.873896000	2.841568000	-2.019043000	B	-5.237356000	-2.714782000	-0.037241000
B	-4.191007000	0.485530000	-2.837421000	B	-5.917154000	-0.292168000	0.144516000
B	-4.488320000	-1.866410000	-3.646712000	B	-6.572480000	2.116266000	0.399762000
N	6.211595000	3.207860000	0.557175000	N	4.790701000	-2.766098000	2.893550000
N	5.851912000	0.834790000	-0.039463000	N	4.170502000	-0.368171000	2.975923000
N	5.135887000	-3.879973000	-1.412015000	N	2.909394000	4.436817000	3.074296000
N	3.198710000	-2.326877000	-1.371178000	N	1.192152000	2.751578000	2.470295000
N	3.555960000	0.023533000	-0.615091000	N	1.829273000	0.341432000	2.453498000
N	3.916646000	2.425327000	0.068221000	N	2.476074000	-2.105716000	2.352877000
N	1.940277000	4.015627000	0.128431000	N	0.790064000	-3.806641000	1.495078000
N	1.650622000	1.522077000	-0.214667000	N	0.284999000	-1.343694000	1.569302000
N	1.227383000	-0.773749000	-1.197353000	N	-0.465333000	1.058352000	1.642432000
N	0.924365000	-3.111735000	-2.067474000	N	-1.153589000	3.458001000	1.919830000
N	-0.990957000	-1.519188000	-2.145029000	N	-2.840818000	1.785191000	1.155739000
N	-0.441137000	3.342645000	-0.396862000	N	-1.477460000	-3.210087000	0.533043000
N	-2.161784000	4.979507000	-1.044517000	N	-3.291159000	-4.853458000	0.323348000
N	-2.561238000	2.506366000	-1.484220000	N	-3.842361000	-2.368561000	0.197316000
N	-2.861190000	0.154123000	-2.374909000	N	-4.547943000	0.061206000	0.449621000
N	-3.157970000	-2.200710000	-3.189883000	N	-5.210234000	2.463858000	0.735302000
N	-4.959453000	-0.536614000	-3.488936000	N	-6.896686000	0.758417000	0.123152000
N	-4.669136000	1.819296000	-2.626008000	N	-6.217979000	-1.671081000	-0.112369000
N	-4.319938000	4.210531000	-1.940726000	N	-5.587269000	-4.106946000	-0.164795000
B	2.867801000	5.105128000	0.402748000	B	1.747404000	-4.861179000	1.792758000
B	1.025601000	6.799563000	0.096430000	B	0.010223000	-6.613569000	1.253957000
B	-1.253539000	6.027396000	-0.643420000	B	-2.317117000	-5.890329000	0.586875000
N	4.256158000	4.812519000	0.606196000	N	3.059197000	-4.505763000	2.252093000
N	2.359386000	6.452001000	0.438244000	N	1.327790000	-6.230058000	1.624156000
N	0.103564000	5.738493000	-0.238476000	N	-0.953776000	-5.577681000	0.952792000
B	1.451539000	-4.442855000	-2.288689000	B	-0.806285000	4.832205000	2.219623000
B	-2.653869000	-3.539694000	-3.341099000	B	-4.861962000	3.826977000	1.046929000
N	2.835168000	-4.690335000	-2.030160000	N	0.537606000	5.141063000	2.599943000
N	-1.313470000	-3.866068000	-2.936173000	N	-3.517821000	4.172449000	1.425517000
B	-0.797090000	-5.203686000	-3.112064000	B	-3.168987000	5.540748000	1.729908000
N	0.555951000	-5.462500000	-2.770392000	N	-1.830955000	5.837430000	2.102502000
Si	-0.008895000	1.747478000	-0.081000000	Si	-0.935849000	-1.626160000	0.459503000
N	-0.843223000	0.686188000	-1.073031000	N	-2.175425000	-0.516101000	0.633729000
H	-3.897600000	6.410524000	-1.533435000	H	-5.035849000	-6.312267000	-0.034210000
H	-1.624655000	7.164854000	-0.669531000	H	-2.654814000	-7.036675000	0.521884000
H	0.677068000	7.944449000	0.082265000	H	-0.291802000	-7.769985000	1.186917000
H	2.995312000	7.207998000	0.649142000	H	1.983913000	-6.970827000	1.827150000

H	4.881042000	5.577944000	0.817971000	H	3.730512000	-5.245344000	2.405376000
H	6.857122000	3.939308000	0.818317000	H	5.506894000	-3.469401000	3.004022000
H	7.913985000	1.702060000	0.489395000	H	6.287560000	-1.140537000	3.427326000
H	7.538813000	-0.700710000	-0.135469000	H	5.657700000	1.294931000	3.460834000
H	7.186259000	-3.103995000	-0.801672000	H	5.038099000	3.746636000	3.489974000
H	5.514690000	-4.803806000	-1.562064000	H	3.177844000	5.397436000	3.232034000
H	3.202950000	-5.619272000	-2.178830000	H	0.781415000	6.101759000	2.795295000
H	0.905552000	-6.398908000	-2.914661000	H	-1.606121000	6.799737000	2.310552000
H	-1.495642000	-6.076985000	-3.540780000	H	-3.990397000	6.410109000	1.668464000
H	-3.355231000	-4.388004000	-3.812441000	H	-5.701962000	4.678560000	0.997235000
H	-5.184972000	-2.699804000	-4.150923000	H	-7.423601000	2.957766000	0.362331000
H	-5.904517000	-0.337040000	-3.782884000	H	-7.857818000	0.544330000	-0.100737000
H	-5.591815000	2.059036000	-2.960624000	H	-7.177647000	-1.928675000	-0.296503000
H	-5.239380000	4.443012000	-2.288704000	H	-6.549487000	-4.352953000	-0.349197000
N	-0.344559000	1.577427000	1.746066000	N	-0.008477000	-1.351920000	-1.124747000
N	-0.765380000	0.780303000	2.486848000	N	0.155910000	-0.287326000	-1.583031000
B	-1.367604000	-0.797284000	2.434215000	B	1.293888000	0.425305000	-2.522113000
C	-1.817159000	-1.135227000	3.953148000	C	1.549313000	1.835023000	-1.735435000
C	-3.135522000	-1.452591000	4.298829000	C	2.799561000	2.389772000	-1.460799000
C	-0.870308000	-1.146382000	4.988528000	C	0.485846000	2.665831000	-1.378708000
C	-3.504423000	-1.761497000	5.607238000	C	2.997025000	3.631462000	-0.870743000
C	-1.209667000	-1.437317000	6.304108000	C	0.612127000	3.927479000	-0.818992000
C	-2.531917000	-1.743718000	6.590892000	C	1.889292000	4.407637000	-0.557801000
C	-2.641970000	-0.677635000	1.430953000	C	2.492555000	-0.672950000	-2.489673000
C	-3.090364000	-1.737264000	0.630536000	C	2.930706000	-1.450421000	-3.558786000
C	-3.478127000	0.450728000	1.485629000	C	3.125275000	-0.989329000	-1.287592000
C	-4.313785000	-1.705550000	-0.035579000	C	3.910396000	-2.433948000	-3.460564000
C	-4.684270000	0.529632000	0.796232000	C	4.097734000	-1.954525000	-1.109296000
C	-5.093278000	-0.567157000	0.057785000	C	4.494573000	-2.683345000	-2.227078000
C	-0.046268000	-1.657960000	2.021098000	C	0.609702000	0.750898000	-3.951383000
C	1.269694000	-1.180724000	2.131452000	C	-0.688625000	0.461533000	-4.351282000
C	-0.177972000	-3.016945000	1.690502000	C	1.342695000	1.472917000	-4.891218000
C	2.384766000	-1.983316000	1.904428000	C	-1.239699000	0.843917000	-5.567036000
C	0.915778000	-3.834942000	1.421704000	C	0.860385000	1.885219000	-6.121481000
C	2.187183000	-3.300286000	1.536530000	C	-0.451654000	1.563713000	-6.455442000
F	-2.874498000	-2.034757000	7.859613000	F	3.907443000	1.703803000	-1.785837000
F	-6.266900000	-0.513390000	-0.601139000	F	-0.777784000	2.226059000	-1.589886000
F	3.257036000	-4.080901000	1.286122000	F	2.384520000	-1.276723000	-4.774035000
H	-4.528472000	-2.008882000	5.866780000	F	2.738630000	-0.303414000	-0.182590000
H	-0.471769000	-1.439088000	7.099421000	F	-1.490695000	-0.240216000	-3.516363000
H	0.790642000	-4.877654000	1.149851000	F	2.614968000	1.788840000	-4.580684000
H	3.392566000	-1.593336000	2.001962000	H	4.009165000	3.972489000	-0.685608000
H	-4.650481000	-2.542108000	-0.637779000	H	2.018055000	5.383437000	-0.101446000
H	-5.309644000	1.414834000	0.841841000	H	-0.277996000	4.503263000	-0.594957000
H	0.171240000	-0.927497000	4.762165000	H	1.505463000	2.444113000	-6.789547000
H	-3.904204000	-1.462536000	3.531408000	H	-0.860069000	1.875506000	-7.411407000
H	-1.160374000	-3.476783000	1.676262000	H	-2.265843000	0.577817000	-5.793246000
H	1.463166000	-0.150420000	2.416532000	H	4.191411000	-2.985741000	-4.350358000
H	-3.201490000	1.299093000	2.107678000	H	5.258659000	-3.448426000	-2.133688000
H	-2.484281000	-2.627645000	0.512514000	H	4.528571000	-2.113040000	-0.126337000
B(C₆H₃F₃)₃-N₂-Si_BBN				B(C₆F₅)₃-N₂-Si_BBN			
N	1.343012000	-4.276277000	-2.787997000	N	1.280248000	-3.151896000	-3.747577000
B	0.452110000	-5.340021000	-3.185840000	B	0.565832000	-4.348080000	-4.134569000
B	2.747809000	-4.531219000	-2.610430000	B	2.715942000	-3.087828000	-3.837882000
B	5.027951000	-3.767219000	-1.917896000	B	4.866211000	-1.826310000	-3.565315000
B	5.390143000	-1.416812000	-1.117962000	B	4.864758000	0.478232000	-2.579773000
B	3.083909000	-2.199478000	-1.764715000	B	2.695345000	-0.754071000	-2.941158000
B	0.791286000	-2.978497000	-2.448844000	B	0.534649000	-2.001222000	-3.283503000

B	-1.516508000	-3.788125000	-2.951712000	B	-1.621214000	-3.188842000	-3.696069000
B	-1.166473000	-1.407184000	-2.275888000	B	-1.647645000	-0.908073000	-2.665387000
B	1.110988000	-0.686664000	-1.557739000	B	0.519922000	0.231762000	-2.227586000
B	3.442199000	0.111275000	-0.880066000	B	2.722498000	1.465786000	-1.809524000
B	3.831433000	2.601325000	-0.270031000	B	2.712533000	3.759393000	-0.599940000
B	-0.860272000	0.977035000	-1.628220000	B	-1.720732000	1.275123000	-1.462448000
B	-3.097483000	0.200459000	-2.356262000	B	-3.846310000	0.202556000	-2.151535000
B	-2.700710000	2.637351000	-1.870880000	B	-3.872732000	2.460258000	-1.033873000
B	-0.469716000	3.442135000	-1.092633000	B	-1.743688000	3.574679000	-0.339583000
B	1.886984000	4.260355000	-0.393199000	B	0.488159000	4.821220000	0.105421000
B	2.333529000	6.707846000	-0.282356000	B	0.426168000	7.214511000	0.789352000
B	0.000698000	5.862055000	-0.746291000	B	-1.719636000	5.913095000	0.516836000
B	-2.304621000	5.085754000	-1.425387000	B	-3.904076000	4.762830000	-0.010165000
B	-4.591710000	4.267416000	-2.057443000	B	-6.052354000	3.617715000	-0.618687000
N	5.875607000	-2.731370000	-1.430141000	N	5.545704000	-0.641603000	-3.163005000
N	3.621703000	-3.499750000	-2.108167000	N	3.424594000	-1.889145000	-3.464223000
N	-0.945513000	-5.083804000	-3.221015000	N	-0.854643000	-4.330254000	-4.113658000
N	-0.621315000	-2.711727000	-2.580689000	N	-0.907784000	-2.021605000	-3.214894000
N	1.670761000	-1.942949000	-1.958791000	N	1.245309000	-0.812087000	-2.882313000
N	3.973206000	-1.165937000	-1.262383000	N	3.421991000	0.420268000	-2.490127000
N	4.294728000	1.231267000	-0.475172000	N	3.389720000	2.641622000	-1.249452000
N	2.011897000	0.261862000	-0.939860000	N	1.295116000	1.318667000	-1.677630000
N	-0.293342000	-0.357444000	-1.775972000	N	-0.930349000	0.211645000	-2.072959000
N	-2.571621000	-1.136217000	-2.483367000	N	-3.092473000	-0.903132000	-2.691727000
N	-2.208815000	1.282091000	-2.005158000	N	-3.147655000	1.321303000	-1.562062000
N	2.419865000	2.922366000	-0.230512000	N	1.314827000	3.674810000	-0.214457000
N	2.828973000	5.349045000	-0.255560000	N	1.186954000	6.060298000	0.362023000
N	0.477241000	4.486865000	-0.698831000	N	-0.968933000	4.724396000	0.131398000
N	-1.817475000	3.726628000	-1.494254000	N	-3.172272000	3.601170000	-0.468249000
N	-4.100773000	2.909472000	-2.136758000	N	-5.319368000	2.469854000	-1.103448000
N	-3.690569000	5.318261000	-1.724542000	N	-5.336730000	4.731142000	-0.093402000
N	-1.375381000	6.117818000	-1.061112000	N	-3.152628000	5.877764000	0.491163000
N	0.944078000	6.920797000	-0.489180000	N	-0.985779000	7.095872000	0.888607000
B	5.729352000	0.985300000	-0.423260000	B	4.827146000	2.746774000	-1.467651000
B	6.164457000	3.439912000	-0.031104000	B	4.809407000	5.096198000	-0.539951000
B	4.236144000	5.063663000	-0.085519000	B	2.621505000	6.130474000	0.185560000
N	6.225305000	-0.336440000	-0.676338000	N	5.522142000	1.656491000	-2.085652000
N	6.605262000	2.093911000	-0.140358000	N	5.487835000	3.961841000	-1.061069000
N	4.747319000	3.7111755000	-0.128266000	N	3.381256000	5.007834000	-0.317827000
B	-3.468645000	-2.220641000	-2.826039000	B	-3.805340000	-2.042016000	-3.240728000
B	-4.990527000	1.827711000	-2.486165000	B	-6.018778000	1.342062000	-1.669593000
N	-2.920637000	-3.527109000	-3.036029000	N	-3.050822000	-3.156693000	-3.723460000
N	-4.501898000	0.480408000	-2.585330000	N	-5.293936000	0.215133000	-2.191199000
B	-5.403570000	-0.614902000	-2.863358000	B	-5.996920000	-0.913241000	-2.761374000
N	-4.871201000	-1.927943000	-2.962865000	N	-5.241870000	-1.997973000	-3.276881000
Si	1.332124000	1.646737000	-0.282838000	Si	0.556374000	2.206693000	-0.472058000
N	-0.065864000	2.062423000	-1.102193000	N	-1.085206000	2.354169000	-0.734851000
H	3.077802000	7.633408000	-0.134329000	H	0.972305000	8.247355000	1.047530000
H	5.001674000	5.970661000	0.066933000	H	3.189329000	7.152906000	0.437392000
H	6.950286000	4.327466000	0.133774000	H	5.405429000	6.102515000	-0.286989000
H	7.600279000	1.928466000	-0.085177000	H	6.483879000	4.047693000	-1.206599000
H	7.221565000	-0.493377000	-0.6111703000	H	6.525601000	1.723898000	-2.184917000
H	6.856519000	-2.944768000	-1.319944000	H	6.553239000	-0.638406000	-3.230245000
H	5.484216000	-4.844802000	-2.170372000	H	5.484761000	-2.758221000	-3.992065000
H	3.198078000	-5.603484000	-2.889670000	H	3.326869000	-4.037294000	-4.234537000
H	0.877832000	-6.425061000	-3.460020000	H	1.157349000	-5.327887000	-4.483839000
H	-1.552576000	-5.843310000	-3.494505000	H	-1.336632000	-5.172859000	-4.392048000
H	-3.544184000	-4.283564000	-3.280009000	H	-3.546769000	-3.977539000	-4.040644000

H	-5.515573000	-2.677044000	-3.171355000	H	-5.749707000	-2.782447000	-3.659592000
H	-6.573691000	-0.418555000	-3.020819000	H	-7.193336000	-0.928763000	-2.803369000
H	-6.148393000	2.057007000	-2.685118000	H	-7.214713000	1.350648000	-1.712268000
H	-5.744975000	4.509027000	-2.270593000	H	-7.248214000	3.639936000	-0.665344000
H	-4.065746000	6.254540000	-1.674335000	H	-5.876541000	5.520854000	0.230436000
H	-1.697892000	7.075525000	-1.051540000	H	-3.655600000	6.704408000	0.782795000
H	0.622433000	7.878137000	-0.511660000	H	-1.498452000	7.918433000	1.173342000
N	0.831152000	1.107853000	1.446992000	N	0.852008000	1.051027000	0.976220000
N	-0.065775000	0.351710000	1.448885000	N	0.131681000	0.170063000	1.247086000
B	-0.826873000	-0.823495000	2.216021000	B	0.314195000	-1.286453000	1.956578000
C	-2.389033000	-0.676769000	1.802335000	C	-0.422641000	-2.282000000	0.882456000
C	-3.293832000	-1.702039000	2.071701000	C	0.118508000	-3.453453000	0.359729000
C	-2.980719000	0.438054000	1.218706000	C	-1.761844000	-2.059091000	0.558235000
C	-4.629532000	-1.706038000	1.704129000	C	-0.612060000	-4.348096000	-0.416109000
C	-4.308562000	0.526621000	0.825887000	C	-2.539536000	-2.955157000	-0.160082000
C	-5.107540000	-0.577384000	1.057715000	C	-1.956688000	-4.113752000	-0.651868000
C	0.006941000	-2.071284000	1.545509000	C	1.925059000	-1.429269000	2.132362000
C	1.374365000	-2.216602000	1.803493000	C	2.607347000	-1.482257000	3.343544000
C	-0.500460000	-3.084295000	0.730647000	C	2.743525000	-1.403790000	1.005317000
C	2.175669000	-3.260972000	1.370019000	C	3.997994000	-1.521238000	3.429457000
C	0.217651000	-4.190382000	0.298242000	C	4.125148000	-1.431561000	1.040830000
C	1.556101000	-4.255901000	0.634894000	C	4.761838000	-1.492436000	2.273930000
C	-0.627600000	-0.645728000	3.816106000	C	-0.559234000	-1.282460000	3.321622000
C	-0.828659000	0.588833000	4.429975000	C	-1.210554000	-0.189743000	3.875022000
C	-0.340290000	-1.675308000	4.710043000	C	-0.731646000	-2.488210000	3.994871000
C	-0.738542000	0.832478000	5.791382000	C	-1.993047000	-0.274008000	5.020994000
C	-0.235274000	-1.518683000	6.085618000	C	-1.498445000	-2.617276000	5.142250000
C	-0.435821000	-0.250126000	6.600365000	C	-2.138358000	-1.496844000	5.657833000
F	-6.383820000	-0.549805000	0.650618000	F	-2.678422000	-4.989371000	-1.346939000
F	-2.833377000	-2.788643000	2.714045000	F	-0.033239000	-5.440812000	-0.911639000
F	-2.232952000	1.542631000	0.993109000	F	1.383423000	-3.803108000	0.610627000
F	1.987629000	-1.265788000	2.532541000	F	-2.379460000	-0.942626000	0.979392000
F	2.282299000	-5.297834000	0.206778000	F	-3.833115000	-2.713242000	-0.379579000
F	-1.767382000	-3.021090000	0.288337000	F	1.958410000	-1.483739000	4.512011000
F	-0.338872000	-0.063452000	7.923389000	F	4.597020000	-1.571664000	4.617516000
F	-1.137924000	1.640951000	3.645952000	F	6.088834000	-1.518510000	2.341671000
F	-0.152370000	-2.919105000	4.240877000	F	4.843308000	-1.395978000	-0.083828000
H	-5.266425000	-2.556258000	1.911637000	F	2.174963000	-1.333472000	-0.211803000
H	-4.694484000	1.424432000	0.360549000	F	-2.881448000	-1.596976000	6.755976000
H	-0.007589000	-2.360694000	6.726814000	F	-2.601224000	0.807297000	5.507413000
H	-0.902046000	1.821190000	6.200454000	F	-1.109638000	1.026219000	3.310820000
H	3.230176000	-3.300011000	1.611398000	F	-1.626602000	-3.795053000	5.750340000
H	-0.254215000	-4.950529000	-0.311232000	F	-0.119143000	-3.589476000	3.537529000

Table S8. Cartesian coordinates of optimized geometries of halogen bond donors augmented N₂-Si_BBN systems calculated at the ω B97X-D/6-31G(d) level of theory.

XB1-N ₂ -Si _B BN				XB2-N ₂ -Si _B BN			
N	-3.890840000	3.937158000	-1.502762000	N	3.623314000	-1.814887000	-4.594090000
B	-4.920631000	4.009477000	-2.515971000	B	4.301444000	-1.139023000	-5.679148000
B	-3.455367000	5.130183000	-0.828154000	B	3.225457000	-3.189827000	-4.733640000
B	-2.045557000	6.261165000	0.898922000	B	2.231661000	-5.275134000	-3.773777000
B	-0.446366000	4.926700000	2.293804000	B	1.314766000	-5.279176000	-1.440219000
B	-1.832576000	3.791418000	0.527407000	B	2.274810000	-3.167909000	-2.419229000
B	-3.316480000	2.654072000	-1.155563000	B	3.365698000	-1.104486000	-3.359653000

B	-4.826733000	1.513972000	-2.783534000	B	4.514505000	0.921116000	-4.257690000
B	-3.238527000	0.151124000	-1.397242000	B	3.574645000	0.956462000	-1.930733000
B	-1.645785000	1.328903000	0.126415000	B	2.320819000	-1.039803000	-1.104764000
B	-0.175654000	2.484154000	1.870067000	B	1.261796000	-3.158190000	-0.132590000
B	1.262353000	1.069936000	3.497044000	B	0.526691000	-3.218527000	2.353038000
B	-1.697978000	-1.250632000	-0.017119000	B	2.659918000	1.039879000	0.393229000
B	-3.392027000	-2.359184000	-1.462322000	B	4.037555000	2.933080000	-0.443721000
B	-1.974158000	-3.733835000	0.094896000	B	3.267890000	2.900228000	1.951426000
B	-0.298927000	-2.648000000	1.600686000	B	1.935311000	0.983598000	2.847444000
B	1.191289000	-1.482002000	3.369709000	B	0.861334000	-1.158395000	3.835145000
B	2.183305000	-2.838703000	5.212983000	B	0.563216000	-1.348196000	6.302644000
B	0.874818000	-3.957634000	3.371405000	B	1.450039000	0.782958000	5.287108000
B	-0.667049000	-5.109926000	1.746292000	B	2.626211000	2.819709000	4.384147000
B	-2.267902000	-6.221516000	0.169391000	B	3.883418000	4.789826000	3.478214000
N	-1.065561000	6.167036000	1.925538000	N	1.622574000	-5.941827000	-2.674018000
N	-2.439114000	5.062270000	0.191143000	N	2.570593000	-3.874167000	-3.646689000
N	-5.347010000	2.806427000	-3.136718000	N	4.716885000	0.204436000	-5.486753000
N	-3.772353000	1.438526000	-1.786468000	N	3.797261000	0.260913000	-3.179476000
N	-2.267754000	2.589833000	-0.161942000	N	2.659013000	-1.773439000	-2.289127000
N	-0.819048000	3.730552000	1.564088000	N	1.620186000	-3.865822000	-1.327289000
N	0.758115000	2.341956000	2.987497000	N	0.707772000	-3.833036000	1.041438000
N	-0.515065000	1.351467000	1.032638000	N	1.496810000	-1.727002000	-0.128337000
N	-2.130741000	0.076868000	-0.449301000	N	2.786224000	0.325097000	-0.874985000
N	-3.807520000	-1.062459000	-1.941837000	N	4.135357000	2.273468000	-1.724213000
N	-2.358361000	-2.446428000	-0.455614000	N	3.325114000	2.286207000	0.636099000
N	1.035602000	-0.168176000	2.778010000	N	0.697814000	-1.790382000	2.540331000
N	1.906893000	-1.546497000	4.623109000	N	0.523394000	-1.956668000	4.989445000
N	0.630136000	-2.668455000	2.731172000	N	1.360275000	0.208035000	3.947011000
N	-0.982488000	-3.826805000	1.149868000	N	2.611151000	2.230289000	3.059098000
N	-2.609331000	-4.936445000	-0.401008000	N	3.899105000	4.184670000	2.163886000
N	-1.317284000	-6.277925000	1.226220000	N	3.254463000	4.097598000	4.550354000
N	0.278220000	-5.137992000	2.822562000	N	2.012304000	2.088718000	5.452880000
N	1.697685000	-3.997111000	4.551415000	N	0.983688000	0.003956000	6.403631000
B	1.068384000	3.544092000	3.755539000	B	0.477003000	-5.271642000	0.936370000
B	2.329788000	2.180336000	5.458929000	B	-0.085601000	-5.400256000	3.391380000
B	2.322875000	-0.328376000	5.279611000	B	0.162931000	-3.346621000	4.825111000
N	0.519593000	4.801203000	3.343972000	N	0.720812000	-5.931203000	-0.310891000
N	1.903559000	3.423088000	4.921155000	N	0.025761000	-5.984552000	2.102150000
N	1.980167000	0.970258000	4.746619000	N	0.195975000	-3.987058000	3.529219000
B	-4.856174000	-0.985196000	-2.944477000	B	4.857352000	2.930159000	-2.801269000
B	-3.599866000	-4.851906000	-1.444037000	B	4.568431000	4.849247000	1.074189000
N	-5.309611000	0.302617000	-3.369513000	N	4.992700000	2.252603000	-4.052963000
N	-3.992784000	-3.573418000	-1.973311000	N	4.639923000	4.230237000	-0.222099000
B	-5.006699000	-3.491735000	-3.001472000	B	5.332279000	4.891835000	-1.306505000
N	-5.400610000	-2.209076000	-3.465091000	N	5.411253000	4.234156000	-2.561980000
Si	0.352057000	-0.069189000	1.246499000	Si	0.923070000	-0.847122000	1.173966000
N	-0.587594000	-1.415625000	0.897880000	N	1.864681000	0.503254000	1.481205000
H	2.801510000	-2.928637000	6.232311000	H	0.251991000	-1.968738000	7.275674000
H	2.942624000	-0.396824000	6.299565000	H	-0.147875000	-3.986963000	5.785297000
H	2.957730000	2.134322000	6.475202000	H	-0.402010000	-6.057668000	4.338226000
H	2.132923000	4.255843000	5.445304000	H	-0.148374000	-6.977156000	2.028980000
H	0.754486000	5.623827000	3.882208000	H	0.543423000	-6.924639000	-0.368447000
H	-0.818658000	7.015742000	2.414462000	H	1.411184000	-6.923522000	-2.783155000
H	-2.540002000	7.316404000	0.630573000	H	2.463707000	-5.867092000	-4.786312000
H	-3.942979000	6.184875000	-1.109825000	H	3.442195000	-3.770919000	-5.755553000
H	-5.403758000	5.059655000	-2.822754000	H	4.506509000	-1.699354000	-6.715410000
H	-6.076927000	2.872831000	-3.831789000	H	5.202478000	0.656281000	-6.248617000
H	-6.048155000	0.355836000	-4.057142000	H	5.500371000	2.706717000	-4.799396000

N	2.617221000	2.863724000	0.262690000	N	1.912818000	3.212336000	1.598814000
N	4.316553000	4.411073000	-0.619158000	N	2.431423000	5.617986000	1.625455000
N	4.066538000	2.107258000	-1.669514000	N	2.932901000	4.261679000	-0.467663000
N	4.214958000	-0.286976000	-2.495455000	N	3.862129000	2.947157000	-2.429965000
N	4.381512000	-2.669988000	-3.251664000	N	4.807749000	1.618734000	-4.333059000
N	5.687416000	-0.903405000	-4.387242000	N	4.868407000	4.091199000	-4.380081000
N	5.567505000	1.484028000	-3.563548000	N	3.961374000	5.416623000	-2.426609000
N	5.628037000	3.807314000	-2.611688000	N	3.253512000	6.733483000	-0.408018000
B	1.313280000	4.088558000	3.654658000	B	1.275434000	1.935279000	5.159879000
B	2.764046000	5.852066000	2.587525000	B	1.414821000	4.452685000	5.144316000
B	3.974846000	5.325721000	0.445645000	B	2.043698000	5.641164000	3.017113000
N	0.550266000	3.629265000	4.778976000	N	1.168610000	0.708213000	5.892769000
N	1.879878000	5.409335000	3.608094000	N	1.166625000	3.217996000	5.801600000
N	3.044794000	4.955023000	1.488885000	N	1.720888000	4.425430000	3.730867000
B	1.544786000	-5.312335000	0.217762000	B	4.366605000	-3.334932000	-2.786003000
B	4.032415000	-4.056332000	-3.097086000	B	5.125328000	0.350470000	-4.936601000
N	0.770939000	-5.713840000	1.356604000	N	4.184479000	-4.532422000	-2.023933000
N	3.168238000	-4.474702000	-2.022418000	N	4.838443000	-0.878488000	-4.243888000
B	2.871306000	-5.875174000	-1.836769000	B	5.186154000	-2.147939000	-4.841504000
N	2.064520000	-6.256754000	-0.729491000	N	4.928973000	-3.336646000	-4.107470000
Si	1.717648000	1.453112000	0.086551000	Si	1.723963000	1.788607000	0.729576000
N	2.590461000	0.271789000	-0.737734000	N	2.730826000	1.741818000	-0.613451000
H	5.822929000	5.843004000	-1.609111000	H	2.795933000	7.887666000	1.501556000
H	4.490091000	6.403883000	0.479282000	H	2.010103000	6.685457000	3.597615000
H	3.264215000	6.936637000	2.639697000	H	1.372279000	5.485974000	5.743697000
H	1.712498000	6.040949000	4.378724000	H	0.979500000	3.253190000	6.793888000
H	0.389480000	4.273530000	5.541033000	H	0.990719000	0.760133000	6.886448000
H	-0.811871000	2.413136000	6.834299000	H	1.176202000	-1.790976000	7.037926000
H	-1.562738000	0.057168000	7.193848000	H	1.680472000	-4.060121000	6.122426000
H	-1.573543000	-2.277452000	6.281156000	H	2.400230000	-5.371988000	4.113748000
H	-1.454979000	-4.650266000	5.461176000	H	3.211733000	-6.695233000	2.135957000
H	-0.614480000	-6.160637000	3.653150000	H	3.942319000	-6.582773000	-0.253461000
H	0.615344000	-6.699884000	1.515271000	H	4.480575000	-5.411740000	-2.424315000
H	1.889986000	-7.242860000	-0.596818000	H	5.197096000	-4.213701000	-4.530893000
H	3.292390000	-6.698840000	-2.594427000	H	5.684097000	-2.198701000	-5.927528000
H	4.465263000	-4.869616000	-3.859090000	H	5.637997000	0.316949000	-6.016064000
H	5.752076000	-3.077815000	-5.051686000	H	5.678350000	2.823379000	-6.086264000
H	6.346624000	-0.652040000	-5.110229000	H	5.131242000	4.934855000	-4.869489000
H	6.267151000	1.758448000	-4.239469000	H	4.255424000	6.277671000	-2.866891000
H	6.331053000	4.065819000	-3.289810000	H	3.547880000	7.586951000	-0.861798000
N	0.145459000	1.884615000	-0.784505000	N	-0.064461000	1.678981000	0.228178000
N	-0.265584000	1.437695000	-1.791468000	N	-0.538629000	1.611572000	-0.841523000
C	-4.916818000	-0.049545000	-1.425403000	C	-4.479406000	-1.162279000	-0.565856000
C	-7.103044000	-0.381003000	-1.211441000	C	-6.484436000	-2.127610000	-0.380219000
H	-8.148674000	-0.123560000	-1.264901000	H	-7.561854000	-2.164051000	-0.363046000
C	-6.473315000	-1.516419000	-0.824077000	C	-5.551458000	-3.092547000	-0.226601000
H	-6.853092000	-2.461147000	-0.469501000	H	-5.640567000	-4.151894000	-0.047380000
N	-6.121937000	0.520738000	-1.583181000	N	-5.801816000	-0.936613000	-0.588697000
N	-5.115460000	-1.295227000	-0.963595000	N	-4.313413000	-2.476729000	-0.342733000
I	-3.054477000	0.818599000	-1.770178000	I	-2.918649000	0.229705000	-0.800238000
C	-6.369584000	1.862150000	-2.048698000	C	-6.408891000	0.333383000	-0.794188000
C	-6.554132000	2.079685000	-3.408932000	C	-6.704301000	0.760191000	-2.086321000
C	-6.426040000	2.894503000	-1.119641000	C	-6.697355000	1.148201000	0.297476000
C	-6.799761000	3.376542000	-3.848791000	C	-7.286137000	2.003652000	-2.290650000
H	-6.501473000	1.250814000	-4.107679000	C	-7.279297000	2.392795000	0.101064000
C	-6.671690000	4.186293000	-1.573444000	C	-7.571915000	2.815058000	-1.194329000
H	-6.273848000	2.689387000	-0.064774000	C	-3.051795000	-3.129692000	-0.256064000
C	-6.857899000	4.425065000	-2.933303000	C	-2.351716000	-3.141706000	0.947811000

H	-6.945277000	3.565883000	-4.906812000	C	-2.505483000	-3.723577000	-1.390890000
H	-6.716160000	5.004800000	-0.863110000	C	-1.104374000	-3.746806000	1.021344000
H	-7.048173000	5.434683000	-3.282179000	C	-1.261055000	-4.333392000	-1.324367000
C	-4.083388000	-2.254075000	-0.656552000	C	-0.569443000	-4.348152000	-0.115209000
C	-3.731504000	-2.459566000	0.672888000	F	-2.873856000	-2.559242000	2.015668000
C	-3.466778000	-2.935057000	-1.699689000	F	-0.435447000	-3.757441000	2.161410000
C	-2.728251000	-3.378958000	0.961548000	F	0.603848000	-4.942729000	-0.052872000
H	-4.226107000	-1.903178000	1.462984000	F	-0.734079000	-4.902242000	-2.394062000
C	-2.460416000	-3.845712000	-1.396754000	F	-3.175741000	-3.692681000	-2.532381000
H	-3.764178000	-2.748375000	-2.726686000	F	-6.405377000	0.731885000	1.520205000
C	-2.095060000	-4.067620000	-0.071354000	F	-7.553960000	3.172979000	1.131198000
H	-2.436403000	-3.554183000	1.991666000	F	-8.124163000	3.995399000	-1.384768000
H	-1.961613000	-4.381488000	-2.197326000	F	-7.568139000	2.417356000	-3.513118000
H	-1.312110000	-4.782191000	0.159744000	F	-6.419397000	-0.022178000	-3.115729000
XB5-N₂-Si₃BN				XB6-N₂-Si₃BN			
N	-3.810394000	3.922938000	-2.122169000	N	-3.883506000	4.270456000	-2.347267000
B	-4.670827000	3.983848000	-3.283201000	B	-4.481621000	4.483795000	-3.647289000
B	-3.474132000	5.124543000	-1.407587000	B	-3.613201000	5.387547000	-1.483237000
B	-2.352641000	6.273398000	0.508671000	B	-2.831562000	6.302323000	0.709119000
B	-1.007806000	4.951066000	2.160343000	B	-1.958161000	4.759240000	2.481407000
B	-2.097506000	3.798185000	0.207694000	B	-2.699469000	3.840663000	0.258649000
B	-3.308131000	2.642301000	-1.669187000	B	-3.577902000	2.923391000	-1.912804000
B	-4.566087000	1.482723000	-3.485954000	B	-4.518600000	2.001802000	-4.032613000
B	-3.211817000	0.135486000	-1.856845000	B	-3.613924000	0.435977000	-2.291149000
B	-1.858014000	1.330775000	-0.130002000	B	-2.566923000	1.391531000	-0.234121000
B	-0.674946000	2.504432000	1.807157000	B	-1.728461000	2.325062000	1.994835000
B	0.496520000	1.109427000	3.649442000	B	-1.047378000	0.709586000	3.903806000
B	-1.893384000	-1.250332000	-0.248365000	B	-2.733443000	-1.163757000	-0.584181000
B	-3.373343000	-2.374509000	-1.902801000	B	-3.913920000	-2.044102000	-2.589037000
B	-2.197816000	-3.730895000	-0.141719000	B	-3.195523000	-3.615858000	-0.761271000
B	-0.748706000	-2.628193000	1.572000000	B	-2.062490000	-2.759563000	1.296993000
B	0.458607000	-1.442510000	3.532601000	B	-1.214762000	-1.818532000	3.557192000
B	1.208239000	-2.782718000	5.497995000	B	-0.992076000	-3.351180000	5.511639000
B	0.161974000	-3.919267000	3.505180000	B	-1.648622000	-4.255938000	3.251650000
B	-1.140894000	-5.088038000	1.693987000	B	-2.611118000	-5.184655000	1.117308000
B	-2.518510000	-6.215645000	-0.070966000	B	-3.661910000	-6.068295000	-0.980053000
N	-1.555427000	6.188520000	1.683665000	N	-2.304996000	6.068592000	2.010006000
N	-2.634782000	5.066899000	-0.237765000	N	-3.040363000	5.178242000	-0.177194000
N	-5.012452000	2.772057000	-3.938140000	N	-4.772190000	3.352699000	-4.453523000
N	-3.673060000	1.418680000	-2.341752000	N	-3.882594000	1.783863000	-2.744115000
N	-2.425192000	2.588978000	-0.525555000	N	-2.953555000	2.716860000	-0.624679000
N	-1.261755000	3.747908000	1.392739000	N	-2.131023000	3.638082000	1.578651000
N	0.072245000	2.375498000	3.059021000	N	-1.261074000	2.044709000	3.352608000
N	-0.878064000	1.364388000	0.936727000	N	-1.828978000	1.268876000	1.007612000
N	-2.255104000	0.071932000	-0.756193000	N	-2.906369000	0.216677000	-1.032337000
N	-3.705660000	-1.084202000	-2.458378000	N	-4.051389000	-0.693819000	-3.081184000
N	-2.491587000	-2.450549000	-0.759919000	N	-3.285189000	-2.273057000	-1.306980000
N	0.374189000	-0.134374000	2.918085000	N	-1.083770000	-0.465167000	3.055486000
N	0.997423000	-1.495203000	4.872515000	N	-0.980318000	-2.009321000	4.969504000
N	0.003361000	-2.636302000	2.827616000	N	-1.584551000	-2.917402000	2.671220000
N	-1.364466000	-3.812366000	1.042929000	N	-2.624748000	-3.849413000	0.552322000
N	-2.768249000	-4.938054000	-0.702023000	N	-3.708343000	-4.730469000	-1.529016000
N	-1.720282000	-6.261078000	1.105550000	N	-3.121563000	-6.262933000	0.321494000
N	-0.352914000	-5.105579000	2.890515000	N	-2.088854000	-5.350822000	2.441203000
N	0.819312000	-3.947416000	4.785461000	N	-1.283639000	-4.427494000	4.633195000
B	0.260935000	3.584709000	3.853764000	B	-1.167109000	3.174390000	4.272579000
B	1.274558000	2.240838000	5.731081000	B	-0.672198000	1.620152000	6.194881000
B	1.313741000	-0.269786000	5.569768000	B	-0.751415000	-0.866566000	5.823666000

B	3.735648000	-1.832440000	1.487602000	B	3.858055000	-1.391252000	-1.796708000
B	2.731843000	0.453399000	1.389497000	B	2.812713000	-1.103223000	0.455829000
B	1.942305000	2.872918000	1.197797000	B	1.977003000	-0.766727000	2.845679000
B	1.306194000	3.850134000	-1.114568000	B	1.796668000	1.621209000	3.833995000
B	2.899423000	-1.021210000	-0.724276000	B	3.465417000	0.939656000	-0.985029000
B	4.038161000	-3.229929000	-0.581941000	B	4.606151000	0.582162000	-3.166500000
B	3.367205000	-2.303137000	-2.820368000	B	4.385275000	2.905111000	-2.228115000
B	2.278161000	-0.060112000	-3.004097000	B	3.298016000	3.294120000	-0.011154000
B	1.475135000	2.392958000	-3.202672000	B	2.464223000	3.638410000	2.416100000
B	1.284198000	3.437735000	-5.460485000	B	2.711600000	5.877072000	3.486266000
B	1.907258000	1.005596000	-5.231268000	B	3.355580000	5.541960000	1.071279000
B	2.829638000	-1.332643000	-5.077565000	B	4.293160000	5.218958000	-1.244485000
B	3.836425000	-3.621550000	-4.900029000	B	5.292060000	4.854875000	-3.515012000
N	2.504916000	4.579729000	4.535021000	N	1.818254000	-4.153965000	4.541251000
N	3.194447000	2.214095000	4.745550000	N	2.617683000	-4.482808000	2.225645000
N	4.835957000	-2.455537000	5.083975000	N	4.315473000	-5.129044000	-2.389974000
N	3.989984000	-1.629706000	2.898396000	N	3.834250000	-2.825168000	-1.592516000
N	3.108580000	0.699771000	2.753657000	N	2.908465000	-2.516658000	0.704107000
N	2.334032000	3.094934000	2.562154000	N	2.084866000	-2.183062000	3.067043000
N	1.505253000	3.965814000	0.327443000	N	1.677531000	0.167665000	3.930581000
N	2.022066000	1.514212000	0.707327000	N	2.207086000	-0.298408000	1.494962000
N	3.058119000	-0.799416000	0.712236000	N	3.312929000	-0.501233000	-0.777102000
N	4.160282000	-3.058512000	0.846491000	N	4.431513000	-0.843134000	-3.005765000
N	3.440770000	-2.181100000	-1.375959000	N	4.159266000	1.473895000	-2.121347000
N	1.333464000	2.562404000	-1.773035000	N	2.018650000	2.267602000	2.559341000
N	1.264070000	3.567572000	-4.020031000	N	2.386213000	4.470801000	3.594602000
N	1.830084000	1.099446000	-3.777698000	N	2.979614000	4.133379000	1.144030000
N	2.828567000	-1.228968000	-3.632381000	N	3.997222000	3.802358000	-1.156928000
N	3.865872000	-3.504163000	-3.458651000	N	5.029539000	3.435370000	-3.411101000
N	3.325923000	-2.541058000	-5.671358000	N	4.927006000	5.706144000	-2.435642000
N	2.335774000	-0.220607000	-5.834260000	N	3.935638000	6.051583000	-0.134774000
N	1.565268000	2.162575000	-6.017426000	N	3.146456000	6.371646000	2.228676000
B	1.423117000	5.297696000	0.915331000	B	1.414935000	-0.397415000	5.249490000
B	0.958930000	6.309985000	-1.346309000	B	1.405439000	1.902942000	6.280424000
B	1.042147000	4.849529000	-3.392755000	B	1.987335000	3.895596000	4.858028000
N	1.692576000	5.468177000	2.311908000	N	1.378109000	-1.821541000	5.407441000
N	1.086896000	6.409559000	0.064303000	N	1.219313000	0.496566000	6.359304000
N	1.098315000	5.006963000	-1.957510000	N	1.727586000	2.479324000	4.994121000
B	4.770853000	-4.114877000	1.634039000	B	4.901550000	-1.731767000	-4.054383000
B	4.417880000	-4.568793000	-2.660989000	B	5.428311000	2.549573000	-4.474494000
N	4.936954000	-3.918872000	3.040951000	N	4.790635000	-3.145093000	-3.860225000
N	4.506325000	-4.437366000	-1.231457000	N	5.222307000	1.130083000	-4.356194000
B	5.084692000	-5.498554000	-0.438169000	B	5.648798000	0.242538000	-5.414841000
N	5.189950000	-5.316578000	0.965770000	N	5.467300000	-1.155500000	-5.242361000
Si	1.365731000	1.183743000	-0.805814000	Si	1.911322000	1.327204000	1.170423000
N	2.207444000	-0.063946000	-1.559606000	N	2.936705000	1.892291000	-0.034285000
H	1.068861000	4.380316000	-6.164540000	H	2.618264000	6.603059000	4.431543000
H	0.826641000	5.806613000	-4.076938000	H	1.891322000	4.601211000	5.818226000
H	0.740488000	7.280603000	-2.010444000	H	1.300279000	2.589473000	7.253485000
H	1.016344000	7.331525000	0.471320000	H	1.023763000	0.107535000	7.271018000
H	1.619433000	6.396899000	2.703804000	H	1.190448000	-2.194775000	6.327842000
H	2.392396000	5.483959000	4.970621000	H	1.585781000	-4.560683000	5.436141000
H	3.249426000	3.702713000	6.496725000	H	2.302422000	-6.212644000	3.704744000
H	3.973456000	1.309368000	6.691746000	H	3.146485000	-6.532730000	1.370801000
H	4.789115000	-1.064028000	6.885074000	H	3.982916000	-6.880092000	-0.975218000
H	5.248296000	-3.188095000	5.644012000	H	4.646938000	-5.756449000	-3.108940000
H	5.371221000	-4.650483000	3.586077000	H	5.135586000	-3.762918000	-4.581659000
H	5.611487000	-6.060658000	1.503271000	H	5.786675000	-1.762922000	-5.983563000

H	5.469853000	-6.507337000	-0.953074000	H	6.146551000	0.675321000	-6.412381000
H	4.812350000	-5.565261000	-3.191661000	H	5.939187000	2.996276000	-5.458776000
H	4.241588000	-4.610082000	-5.437957000	H	5.812748000	5.307274000	-4.491855000
H	3.329376000	-2.641810000	-6.676348000	H	5.132013000	6.690902000	-2.528093000
H	2.370798000	-0.271260000	-6.843083000	H	4.173987000	7.033073000	-0.173027000
H	1.601798000	2.095737000	-7.024868000	H	3.390863000	7.350680000	2.177468000
N	-0.408073000	0.726615000	-0.503993000	N	0.137821000	1.376414000	0.636146000
N	-0.936901000	-0.295680000	-0.737592000	N	-0.355214000	1.794483000	-0.342777000
C	-5.707389000	-0.818141000	0.371027000	C	-4.491222000	-0.739077000	-0.567753000
N	-6.599554000	0.207166000	0.493286000	N	-4.365808000	-2.084807000	-0.383859000
I	-3.676118000	-0.615911000	-0.115162000	I	-2.852512000	0.569617000	-0.594199000
C	-6.434159000	-1.957145000	0.660981000	C	-5.849889000	-0.532219000	-0.658146000
N	-7.801931000	-0.202890000	0.835238000	N	-5.525973000	-2.713376000	-0.349693000
N	-7.690845000	-1.502863000	0.938484000	N	-6.409206000	-1.771611000	-0.518558000
C	-6.052241000	-3.375979000	0.712469000	C	-6.613798000	0.695056000	-0.888367000
C	-5.063851000	-3.795788000	1.607406000	C	-6.446164000	1.413022000	-2.074173000
C	-6.674606000	-4.301461000	-0.131560000	C	-7.489884000	1.197797000	0.074427000
C	-4.707276000	-5.138493000	1.659830000	C	-7.127370000	2.601717000	-2.294382000
H	-4.581077000	-3.075473000	2.260905000	C	-8.186022000	2.378976000	-0.130363000
C	-6.312668000	-5.642153000	-0.073727000	C	-7.996398000	3.082406000	-1.318273000
H	-7.421816000	-3.971275000	-0.848007000	C	-3.151704000	-2.822753000	-0.287332000
C	-5.331179000	-6.060240000	0.822361000	C	-2.503493000	-2.947917000	0.938080000
H	-3.942391000	-5.464632000	2.356530000	C	-2.583396000	-3.338839000	-1.448719000
H	-6.790570000	-6.358481000	-0.733667000	C	-1.281220000	-3.602828000	1.006381000
H	-5.050229000	-7.107531000	0.866002000	C	-1.363426000	-3.994637000	-1.385966000
C	-8.863846000	-2.283564000	1.325325000	C	-0.720701000	-4.125358000	-0.156773000
H	-9.323794000	-2.720590000	0.438091000	F	-5.629952000	0.951521000	-3.012297000
H	-8.545206000	-3.072335000	2.006737000	F	-7.662162000	0.527256000	1.213130000
H	-9.561676000	-1.607388000	1.816541000	F	-6.962081000	3.270658000	-3.421627000
C	-6.374001000	1.618537000	0.311527000	F	-8.650184000	4.207284000	-1.521268000
C	-6.068863000	2.091778000	-0.958673000	F	-9.014999000	2.839576000	0.790337000
C	-6.471755000	2.453581000	1.417114000	F	-3.204781000	-3.183965000	-2.606476000
C	-5.848644000	3.454811000	-1.120140000	F	-3.047552000	-2.428746000	2.025975000
H	-6.009974000	1.410271000	-1.800962000	F	-0.654693000	-3.729939000	2.163070000
C	-6.252934000	3.815187000	1.237699000	F	0.433606000	-4.755746000	-0.102399000
H	-6.710146000	2.044588000	2.393101000	F	-0.810347000	-4.491623000	-2.477324000
C	-5.939942000	4.312251000	-0.025460000	C	-7.830915000	-2.113769000	-0.527088000
H	-5.610516000	3.846859000	-2.102872000	H	-8.295221000	-1.712483000	0.373946000
H	-6.323553000	4.486477000	2.086690000	H	-8.287236000	-1.678642000	-1.417028000
H	-5.767796000	5.375046000	-0.159157000	H	-7.908438000	-3.199255000	-0.550309000
XB9-N₂-Si_BBN				XB10-N₂-Si_BBN			
N	-5.077873000	0.439517000	-2.675569000	N	4.486141000	-3.626466000	-2.684136000
B	-5.895785000	-0.515880000	-3.386028000	B	5.091222000	-3.634902000	-3.995595000
B	-5.294990000	1.851021000	-2.846322000	B	4.435469000	-4.831526000	-1.900898000
B	-4.745972000	4.222238000	-2.271988000	B	3.843600000	-6.029851000	0.211337000
B	-2.901455000	4.730622000	-0.650812000	B	2.721967000	-4.798464000	2.085435000
B	-3.423485000	2.348388000	-1.260605000	B	3.270095000	-3.603781000	-0.057142000
B	-4.033144000	-0.032130000	-1.786287000	B	3.938240000	-2.391999000	-2.154188000
B	-4.665655000	-2.398510000	-2.266902000	B	4.652415000	-1.171457000	-4.210703000
B	-2.795051000	-1.912375000	-0.664874000	B	3.510718000	0.078136000	-2.356344000
B	-2.091554000	0.458961000	-0.306879000	B	2.685960000	-1.191104000	-0.367265000
B	-1.509789000	2.870859000	0.260950000	B	2.064186000	-2.410340000	1.779356000
B	0.239693000	3.381781000	2.096207000	B	1.154508000	-1.082690000	3.804486000
B	-0.928884000	-1.477731000	0.938734000	B	2.394480000	1.367350000	-0.529524000
B	-1.750110000	-3.805858000	0.619903000	B	3.349557000	2.585169000	-2.480317000
B	-0.006460000	-3.315058000	2.361067000	B	2.397654000	3.868224000	-0.541693000
B	0.797060000	-0.979288000	2.739347000	B	1.486506000	2.674011000	1.455686000
B	1.382688000	1.469586000	3.327906000	B	0.868360000	1.441924000	3.643463000

B	2.731133000	1.941599000	5.374602000	B	0.404038000	2.772425000	5.703839000
B	2.295050000	-0.435487000	4.659513000	B	0.830069000	3.933687000	3.508239000
B	1.652092000	-2.823630000	4.185232000	B	1.560423000	5.168186000	1.439912000
B	0.942732000	-5.185941000	3.732335000	B	2.381873000	6.374606000	-0.598650000
N	-3.961232000	5.145635000	-1.528213000	N	3.290766000	-5.991046000	1.520391000
N	-4.490085000	2.806328000	-2.131079000	N	3.846254000	-4.825155000	-0.587913000
N	-5.668891000	-1.900672000	-3.170271000	N	5.149532000	-2.419148000	-4.726294000
N	-3.819019000	-1.444585000	-1.576958000	N	4.016597000	-1.162675000	-2.907354000
N	-3.194919000	0.924723000	-1.105108000	N	3.309085000	-2.393505000	-0.855538000
N	-2.619968000	3.315466000	-0.540570000	N	2.692903000	-3.601839000	1.271619000
N	-0.743551000	3.795054000	1.097892000	N	1.584846000	-2.320603000	3.159200000
N	-1.201468000	1.461287000	0.229023000	N	1.957046000	-1.289219000	0.875485000
N	-1.889876000	-0.963047000	-0.035846000	N	2.804828000	0.077692000	-1.083848000
N	-2.679489000	-3.327448000	-0.376593000	N	3.721640000	1.321008000	-3.070498000
N	-0.908700000	-2.865467000	1.318621000	N	2.725695000	2.607873000	-1.179792000
N	0.683830000	2.011329000	2.186727000	N	0.976043000	0.132414000	3.046227000
N	1.920037000	2.420669000	4.279369000	N	0.636400000	1.494005000	5.072343000
N	1.516800000	0.027943000	3.520115000	N	1.013796000	2.653112000	2.840726000
N	0.802952000	-2.371388000	3.104754000	N	1.824277000	3.903550000	0.788004000
N	0.065197000	-4.729083000	2.678232000	N	2.676452000	5.111230000	-1.236551000
N	1.701850000	-4.232291000	4.464855000	N	1.840609000	6.377339000	0.716023000
N	2.394364000	-1.842209000	4.919086000	N	1.039827000	5.146954000	2.774024000
N	2.925835000	0.541248000	5.509896000	N	0.467628000	3.942829000	4.902130000
B	-1.095627000	5.205932000	1.037984000	B	1.692244000	-3.512400000	3.988097000
B	0.468118000	5.717200000	2.947002000	B	0.977491000	-2.210757000	6.024028000
B	1.649120000	3.829319000	4.114230000	B	0.630177000	0.272072000	5.841387000
N	-2.110391000	5.640326000	0.122516000	N	2.187812000	-4.728330000	3.412232000
N	-0.427321000	6.125149000	1.922810000	N	1.320803000	-3.427403000	5.377025000
N	0.788279000	4.313210000	3.060699000	N	0.921206000	-1.004208000	5.231888000
B	-3.524870000	-4.279954000	-1.069716000	B	4.355220000	1.309470000	-4.374854000
B	-0.739715000	-5.671711000	1.946462000	B	3.258784000	5.084873000	-2.552346000
N	-4.477212000	-3.795265000	-2.021325000	N	4.771581000	0.058827000	-4.930772000
N	-1.649810000	-5.219941000	0.928229000	N	3.598527000	3.834064000	-3.175462000
B	-2.468248000	-6.167195000	0.207870000	B	4.198745000	3.813499000	-4.488946000
N	-3.376447000	-5.678950000	-0.768309000	N	4.550869000	2.561015000	-5.057075000
Si	0.236366000	0.946922000	0.950766000	Si	1.018271000	0.029090000	1.358870000
N	0.024800000	-0.607262000	1.580270000	N	1.664273000	1.450885000	0.711582000
H	3.224096000	2.705077000	6.153709000	H	0.169290000	2.847190000	6.875156000
H	2.126041000	4.611288000	4.884657000	H	0.404608000	0.322046000	7.015655000
H	0.938947000	6.518751000	3.701125000	H	0.747167000	-2.186911000	7.198344000
H	-0.655642000	7.107658000	1.870205000	H	1.374723000	-4.258264000	5.948813000
H	-2.324807000	6.626786000	0.077280000	H	2.235388000	-5.551160000	3.996815000
H	-4.164513000	6.128720000	-1.638140000	H	3.307914000	-6.843095000	2.062148000
H	-5.610492000	4.614418000	-3.001489000	H	4.307646000	-7.046009000	-0.219368000
H	-6.155075000	2.234032000	-3.585275000	H	4.894673000	-5.845113000	-2.341656000
H	-6.749496000	-0.149507000	-4.141373000	H	5.539951000	-4.644256000	-4.457504000
H	-6.254886000	-2.554949000	-3.668736000	H	5.583842000	-2.439923000	-5.637800000
H	-5.068179000	-4.458953000	-2.501971000	H	5.216927000	0.052266000	-5.837605000
H	-3.947839000	-6.353415000	-1.256713000	H	4.978787000	2.564338000	-5.971844000
H	-2.385317000	-7.340877000	0.429537000	H	4.400397000	4.832019000	-5.085126000
H	-0.655055000	-6.840248000	2.191243000	H	3.468955000	6.112782000	-3.128317000
H	1.027980000	-6.351907000	3.990715000	H	2.595780000	7.407775000	-1.164570000
H	2.303035000	-4.576412000	5.199698000	H	1.650420000	7.272639000	1.142674000
H	2.960711000	-2.146921000	5.698508000	H	0.885728000	6.026766000	3.246562000
H	3.481355000	0.223525000	6.291366000	H	0.321248000	4.829848000	5.362565000
N	1.543559000	1.008763000	-0.333027000	N	-0.699404000	-0.283430000	0.800652000
N	2.168106000	0.086236000	-0.719680000	N	-1.334998000	0.403124000	0.083509000
I	4.287953000	-0.099887000	-3.015376000	C	-8.078692000	-1.498838000	-2.315419000

C	5.751330000	-0.290262000	-4.626567000	C	-9.048608000	-0.742064000	-1.671885000
F	6.890514000	0.309543000	-4.296783000	C	-8.671786000	0.206699000	-0.730967000
F	5.292525000	0.266799000	-5.742588000	C	-7.325561000	0.393187000	-0.440073000
F	6.008137000	-1.570689000	-4.872764000	C	-6.338482000	-0.354428000	-1.074440000
				C	-6.736520000	-1.300452000	-2.013580000
				F	-5.842715000	-2.047263000	-2.653734000
				F	-8.436440000	-2.408585000	-3.217315000
				F	-7.011352000	1.312087000	0.467401000
				F	-9.598926000	0.933088000	-0.113040000
				F	-10.332735000	-0.925076000	-1.955246000
				I	-4.305643000	-0.061418000	-0.628346000

Table S9. Cartesian coordinates of optimized geometries of intermediates involved in NRR by C_BBN calculated at the ω B97X-D/6-31G(d) level of theory.

HN ₂ -C _B BN				H ₂ N ₂ -C _B BN			
N	-5.103465000	-0.214992000	-0.297312000	N	-4.992344000	1.063311000	-0.374593000
B	-6.069434000	-1.287456000	-0.333158000	B	-6.198235000	0.271184000	-0.368553000
B	-5.561797000	1.140433000	-0.377034000	B	-5.087964000	2.484898000	-0.528538000
B	-5.084870000	3.573115000	-0.329489000	B	-4.013428000	4.720004000	-0.518555000
B	-2.734044000	4.387039000	-0.111257000	B	-1.547329000	4.925763000	-0.177032000
B	-3.197833000	1.929163000	-0.119570000	B	-2.608979000	2.658904000	-0.213257000
B	-3.692396000	-0.505668000	-0.125197000	B	-3.700739000	0.435448000	-0.152542000
B	-4.223765000	-2.953688000	-0.104691000	B	-4.837898000	-1.794356000	-0.021552000
B	-1.854633000	-2.142984000	-0.015693000	B	-2.341410000	-1.608391000	0.049006000
B	-0.866687000	2.718036000	-0.017369000	B	-0.162580000	2.845067000	-0.000404000
B	1.504701000	3.523914000	-0.075995000	B	2.334285000	3.030833000	-0.007043000
B	0.512968000	-1.347926000	0.006236000	B	0.142459000	-1.431599000	-0.013902000
B	0.019906000	-3.806014000	-0.097441000	B	-0.952462000	-3.690781000	-0.063948000
B	2.385037000	-3.012387000	-0.090920000	B	1.534386000	-3.515623000	-0.156846000
B	2.890085000	-0.571885000	-0.021340000	B	2.638799000	-1.280546000	-0.080325000
B	3.374384000	1.873084000	-0.067888000	B	3.725449000	0.962991000	-0.054695000
B	5.749168000	2.681722000	-0.099376000	B	6.227707000	1.146846000	-0.094834000
B	5.261811000	0.224708000	-0.069500000	B	5.135070000	-1.106958000	-0.147707000
B	4.764379000	-2.230444000	-0.087807000	B	4.033327000	-3.356257000	-0.217686000
B	4.255922000	-4.682333000	-0.162482000	B	2.922646000	-5.601153000	-0.295833000
N	-4.146382000	4.628726000	-0.218355000	N	-2.846792000	5.510744000	-0.363623000
N	-4.612812000	2.207589000	-0.290422000	N	-3.902041000	3.281889000	-0.448744000
N	-5.616308000	-2.626288000	-0.213378000	N	-6.102511000	-1.130175000	-0.165156000
N	-3.261947000	-1.872740000	-0.035747000	N	-3.635727000	-0.991355000	0.016838000
N	-2.722545000	0.561214000	-0.055128000	N	-2.493771000	1.221883000	-0.120384000
N	-2.270381000	3.019027000	-0.048835000	N	-1.444066000	3.487557000	-0.091334000
N	0.092735000	3.797816000	-0.068170000	N	1.038169000	3.652531000	-0.017090000
N	-0.907122000	-1.041285000	0.072565000	N	-1.147140000	-0.787009000	0.104006000
N	-1.388380000	-3.508456000	-0.075986000	N	-2.238679000	-3.050910000	0.007550000
N	0.965722000	-2.718627000	-0.072002000	N	0.236539000	-2.876189000	-0.092092000
N	1.955088000	2.154050000	-0.064901000	N	2.424946000	1.592353000	-0.022846000
N	4.332972000	2.963546000	-0.092699000	N	4.929721000	1.776655000	-0.052993000
N	3.841537000	0.509705000	-0.047776000	N	3.834291000	-0.474381000	-0.090346000
N	3.344619000	-1.940180000	-0.059610000	N	2.734071000	-2.719675000	-0.149952000
N	2.840984000	-4.389908000	-0.142490000	N	1.628108000	-4.964283000	-0.220330000
N	5.179708000	-3.606011000	-0.131707000	N	4.087774000	-4.791515000	-0.292727000
N	5.691169000	-1.140936000	-0.075545000	N	5.205650000	-2.536209000	-0.206881000
N	6.180658000	1.329308000	-0.088218000	N	6.303830000	-0.270227000	-0.144029000
B	-0.365319000	5.174682000	-0.083126000	B	0.939491000	5.098697000	-0.036550000

B	2.010265000	5.978665000	-0.107407000	B	3.441084000	5.279834000	0.013382000
B	3.874703000	4.324692000	-0.106659000	B	4.829716000	3.209274000	-0.015977000
N	-1.769218000	5.440975000	-0.087553000	N	-0.352216000	5.707702000	-0.094985000
N	0.614382000	6.227422000	-0.099559000	N	2.152834000	5.872248000	-0.005029000
N	2.468234000	4.609843000	-0.098781000	N	3.541302000	3.840130000	0.003156000
B	-2.346669000	-4.599907000	-0.097811000	B	-3.441100000	-3.863234000	0.027006000
B	1.890221000	-5.464666000	-0.170963000	B	0.437585000	-5.766173000	-0.197161000
N	-3.743002000	-4.298913000	-0.085040000	N	-4.715388000	-3.217798000	0.057417000
N	0.482910000	-5.179922000	-0.145444000	N	-0.850680000	-5.138528000	-0.108058000
B	-0.470875000	-6.262909000	-0.165434000	B	-2.046447000	-5.945919000	-0.070432000
N	-1.853604000	-5.949196000	-0.136966000	N	-3.304269000	-5.295107000	0.006171000
N	1.474396000	-0.285890000	0.033185000	N	1.344721000	-0.649796000	-0.001475000
H	6.549533000	3.572492000	-0.115879000	H	7.227544000	1.806641000	-0.090921000
H	4.667774000	5.221265000	-0.124728000	H	5.823738000	3.876983000	-0.006209000
H	2.792494000	6.885359000	-0.121747000	H	4.425769000	5.961995000	0.031937000
H	0.306198000	7.188976000	-0.104689000	H	2.096928000	6.880431000	-0.005583000
H	-2.087230000	6.399089000	-0.118785000	H	-0.418988000	6.714450000	-0.140221000
H	-4.491707000	5.576633000	-0.256372000	H	-2.941578000	6.513980000	-0.423850000
H	-6.252419000	3.806573000	-0.456754000	H	-5.077962000	5.238883000	-0.699918000
H	-6.727114000	1.374177000	-0.513828000	H	-6.152897000	3.000852000	-0.709653000
H	-7.235935000	-1.052428000	-0.464037000	H	-7.266874000	0.787333000	-0.531115000
H	-6.303538000	-3.364796000	-0.253996000	H	-6.954787000	-1.671004000	-0.182413000
H	-4.408316000	-5.057996000	-0.123133000	H	-5.551880000	-3.783566000	0.037685000
H	-2.511363000	-6.715299000	-0.150373000	H	-4.133250000	-5.871298000	0.024865000
H	-0.103970000	-7.401829000	-0.206232000	H	-1.979036000	-7.141174000	-0.104694000
H	2.269757000	-6.598834000	-0.216599000	H	0.519213000	-6.959470000	-0.249914000
H	4.643987000	-5.814279000	-0.206760000	H	3.013185000	-6.793828000	-0.360034000
H	6.164323000	-3.829183000	-0.149908000	H	4.983714000	-5.254126000	-0.346511000
H	6.681186000	-1.341072000	-0.093971000	H	6.112654000	-2.978706000	-0.252090000
H	7.174691000	1.152090000	-0.097659000	H	7.220572000	-0.692033000	-0.178964000
B	0.999139000	1.071570000	0.000032000	B	1.223027000	0.784854000	0.021487000
N	-0.420354000	1.337181000	0.023005000	N	-0.078670000	1.401124000	0.060830000
C	-1.364499000	0.294574000	0.404599000	C	-1.275675000	0.639582000	0.449608000
N	-1.485144000	0.504403000	1.936829000	N	-1.448971000	0.835182000	1.907297000
N	-1.191022000	-0.399913000	2.710755000	N	-0.635605000	0.055668000	2.637391000
H	-0.877182000	-1.254015000	2.191506000	H	-0.486079000	-0.899392000	2.312622000
				H	-0.849849000	0.116790000	3.623884000
		H₃N₂-C_BBN				H₃NHN-C_BBN	
N	2.589803000	-4.395091000	-0.430626000	N	-3.587251000	3.576412000	-0.394842000
B	3.988329000	-4.744501000	-0.466706000	B	-5.023363000	3.533451000	-0.523366000
B	1.604034000	-5.426817000	-0.555368000	B	-2.923245000	4.847190000	-0.376527000
B	-0.768708000	-6.149363000	-0.481042000	B	-0.838029000	6.179477000	-0.181505000
B	-2.581219000	-4.468213000	-0.120369000	B	1.368578000	5.023823000	0.011763000
B	-0.192030000	-3.719652000	-0.196131000	B	-0.731297000	3.673190000	-0.070052000
B	2.183143000	-3.018038000	-0.190900000	B	-2.830029000	2.347594000	-0.221772000
B	4.595024000	-2.347744000	-0.106566000	B	-4.959804000	1.043506000	-0.338575000
B	2.773221000	-0.635980000	0.038710000	B	-2.742441000	-0.117057000	-0.149006000
B	-1.981871000	-2.041429000	0.034893000	B	1.442112000	2.514504000	0.006644000
B	-3.809004000	-0.327186000	-0.027818000	B	3.661348000	1.357067000	-0.084368000
B	0.974145000	1.067875000	-0.004278000	B	-0.551294000	-1.281265000	-0.032944000
B	3.375609000	1.795581000	-0.031124000	B	-2.663053000	-2.623503000	-0.195328000
B	1.565875000	3.509548000	-0.119127000	B	-0.462600000	-3.789694000	-0.089589000
B	-0.830340000	2.810582000	-0.087894000	B	1.650152000	-2.467449000	-0.005866000
B	-3.221840000	2.095514000	-0.111773000	B	3.754624000	-1.133494000	-0.072287000
B	-5.046868000	3.815154000	-0.209633000	B	5.978566000	-2.296528000	-0.109907000
B	-2.645642000	4.532640000	-0.203935000	B	3.863909000	-3.636909000	-0.032118000
B	-0.242292000	5.242313000	-0.209808000	B	1.743855000	-4.971199000	-0.025837000
B	2.163212000	5.944621000	-0.227018000	B	-0.380710000	-6.298317000	-0.105468000

N	-2.138348000	-5.823096000	-0.301254000	N	0.571305000	6.219701000	-0.041697000
N	0.215443000	-5.096116000	-0.437734000	N	-1.502672000	4.897038000	-0.216746000
N	4.959871000	-3.726385000	-0.281496000	N	-5.682057000	2.276910000	-0.475357000
N	3.195148000	-2.004821000	-0.044963000	N	-3.522588000	1.090330000	-0.215557000
N	0.788362000	-2.667786000	-0.135333000	N	-1.397073000	2.388477000	-0.060275000
N	-1.592197000	-3.419755000	-0.053393000	N	0.695767000	3.745595000	0.028291000
N	-3.392061000	-1.701181000	0.010795000	N	2.888102000	2.569286000	-0.050265000
N	1.364039000	-0.308249000	0.102698000	N	-1.305179000	-0.051085000	-0.026594000
N	3.772426000	0.415957000	0.013650000	N	-3.418916000	-1.397946000	-0.223897000
N	1.971339000	2.124299000	-0.059817000	N	-1.228365000	-2.562239000	-0.112573000
N	-2.809089000	0.712225000	-0.055671000	N	2.980859000	0.087054000	-0.075601000
N	-4.635389000	2.433430000	-0.141059000	N	5.206671000	-1.077077000	-0.112533000
N	-2.233970000	3.146349000	-0.129216000	N	3.091289000	-2.413049000	-0.029499000
N	0.165492000	3.855024000	-0.133805000	N	0.974551000	-3.744616000	-0.029132000
N	2.568974000	4.561202000	-0.154998000	N	-1.145778000	-5.072804000	-0.130694000
N	0.778057000	6.254284000	-0.254317000	N	1.034611000	-6.223076000	-0.048157000
N	-1.639793000	5.550918000	-0.235690000	N	3.172024000	-4.890966000	-0.007115000
N	-4.052295000	4.827933000	-0.240953000	N	5.297847000	-3.541822000	-0.065079000
B	-4.391308000	-2.752397000	0.000986000	B	3.569561000	3.848160000	-0.033203000
B	-6.215699000	-1.029180000	-0.014947000	B	5.788830000	2.683500000	-0.126791000
B	-5.625256000	1.392331000	-0.103282000	B	5.875833000	0.193240000	-0.145957000
N	-3.967112000	-4.115457000	-0.027791000	N	2.797289000	5.050248000	0.021815000
N	-5.782412000	-2.378384000	0.012069000	N	5.007700000	3.865889000	-0.077174000
N	-5.221344000	0.017595000	-0.041791000	N	5.113651000	1.408573000	-0.125455000
B	5.182340000	0.076397000	0.007759000	B	-4.864424000	-1.454720000	-0.302174000
B	3.965649000	4.225639000	-0.118239000	B	-2.577125000	-5.124623000	-0.208783000
N	5.566637000	-1.298784000	-0.012509000	N	-5.608938000	-0.232836000	-0.311779000
N	4.374021000	2.852376000	-0.050447000	N	-3.341401000	-3.907979000	-0.240307000
B	5.777391000	2.514443000	-0.020872000	B	-4.779746000	-3.961374000	-0.325926000
N	6.146823000	1.146419000	0.015079000	N	-5.504999000	-2.741352000	-0.348398000
N	-0.422552000	1.430716000	0.008300000	N	0.882473000	-1.248129000	0.026647000
H	-6.208618000	4.105778000	-0.239736000	H	7.175467000	-2.261701000	-0.146178000
H	-6.788954000	1.674352000	-0.122684000	H	7.071814000	0.237966000	-0.187972000
H	-7.383935000	-0.763449000	-0.018792000	H	6.984653000	2.744715000	-0.167394000
H	-6.487995000	-3.100738000	0.017957000	H	5.491911000	4.751935000	-0.071502000
H	-4.663187000	-4.846299000	-0.066560000	H	3.273568000	5.940845000	0.013683000
H	-2.814482000	-6.571280000	-0.346876000	H	1.022315000	7.122930000	-0.036758000
H	-0.437141000	-7.286390000	-0.663542000	H	-1.468691000	7.193877000	-0.272736000
H	1.939857000	-6.560670000	-0.745143000	H	-3.553651000	5.857907000	-0.493739000
H	4.329546000	-5.879206000	-0.646045000	H	-5.652496000	4.543117000	-0.661229000
H	5.934250000	-3.987232000	-0.321005000	H	-6.687034000	2.263856000	-0.570648000
H	6.548249000	-1.533952000	-0.047772000	H	-6.614766000	-0.273263000	-0.396485000
H	7.131724000	0.923781000	0.023068000	H	-6.511641000	-2.792106000	-0.409741000
H	6.612537000	3.373354000	-0.029026000	H	-5.354085000	-5.011264000	-0.373693000
H	4.788002000	5.095656000	-0.143785000	H	-3.138258000	-6.181689000	-0.248238000
H	2.979402000	6.820515000	-0.264457000	H	-0.932244000	-7.361368000	-0.135685000
H	0.513779000	7.227264000	-0.310108000	H	1.552665000	-7.089777000	-0.039926000
H	-1.925557000	6.518245000	-0.291933000	H	3.710173000	-5.745850000	-0.010128000
H	-4.359360000	5.788355000	-0.294094000	H	5.854568000	-4.384122000	-0.067208000
B	-1.397871000	0.367247000	-0.003277000	B	1.533687000	0.036276000	-0.010021000
N	-0.977116000	-1.000070000	0.100224000	N	0.750409000	1.245760000	0.005852000
C	0.413885000	-1.401420000	0.497667000	C	-0.660790000	1.200591000	0.413202000
N	0.499607000	-1.698943000	1.892291000	N	-0.702862000	1.298932000	1.862914000
N	0.144242000	-0.501029000	2.602116000	N	-3.296035000	-0.196766000	2.825846000
H	-0.819360000	-0.168236000	2.415240000	H	-3.080172000	-1.180308000	2.687685000
H	0.211638000	-0.727372000	3.592917000	H	-3.392928000	-0.050096000	3.827082000
H	0.769912000	0.304028000	2.414649000	H	-4.209880000	-0.042240000	2.408222000
				H	-1.639068000	0.959625000	2.149732000

HHN₂-C_BBN				H₂HN₂-C_BBN			
N	-5.070363000	0.656243000	-0.296661000	N	-5.112740000	-0.051484000	-0.371098000
B	-6.210540000	-0.231374000	-0.264266000	B	-6.115491000	-1.091655000	-0.392358000
B	-5.278685000	2.059284000	-0.491847000	B	-5.514680000	1.313756000	-0.518302000
B	-4.379139000	4.370816000	-0.575843000	B	-4.950195000	3.731145000	-0.491949000
B	-1.935561000	4.780936000	-0.245408000	B	-2.587111000	4.465994000	-0.139249000
B	-2.816253000	2.437916000	-0.222797000	B	-3.133134000	2.022332000	-0.197819000
B	-3.732819000	0.130113000	-0.092758000	B	-3.715454000	-0.391425000	-0.154239000
B	-4.678907000	-2.181059000	0.040373000	B	-4.331314000	-2.812293000	-0.077211000
B	-2.202484000	-1.793787000	0.058875000	B	-1.932047000	-2.082230000	0.009325000
B	-0.387742000	2.815944000	-0.024576000	B	-0.778371000	2.729602000	0.004365000
B	2.085594000	3.203206000	-0.009547000	B	1.618004000	3.457768000	-0.029532000
B	0.258502000	-1.418901000	-0.017524000	B	0.447649000	-1.370741000	-0.014209000
B	-0.652448000	-3.754316000	-0.098881000	B	-0.124626000	-3.812564000	-0.051255000
B	1.812174000	-3.380801000	-0.185436000	B	2.261937000	-3.102348000	-0.129669000
B	2.736264000	-1.068253000	-0.057131000	B	2.851524000	-0.681327000	-0.111621000
B	3.638790000	1.254177000	-0.010385000	B	3.425552000	1.744014000	-0.096106000
B	6.118156000	1.638714000	-0.013135000	B	5.827432000	2.471435000	-0.156714000
B	5.210826000	-0.695417000	-0.090253000	B	5.252041000	0.032840000	-0.182980000
B	4.291723000	-3.023390000	-0.212652000	B	4.667189000	-2.403352000	-0.205520000
B	3.362511000	-5.345846000	-0.356298000	B	4.074217000	-4.837103000	-0.220216000
N	-3.276950000	5.253220000	-0.448668000	N	-3.982814000	4.754493000	-0.320795000
N	-4.155077000	2.947978000	-0.461125000	N	-4.529508000	2.351753000	-0.431415000
N	-5.996952000	-1.618037000	-0.063013000	N	-5.713345000	-2.439006000	-0.215974000
N	-3.544835000	-1.282510000	0.057995000	N	-3.336025000	-1.766741000	-0.029705000
N	-2.591215000	1.020059000	-0.065645000	N	-2.712583000	0.649284000	-0.087344000
N	-1.719262000	3.355135000	-0.113231000	N	-2.173625000	3.082095000	-0.051064000
N	0.741491000	3.717040000	-0.051183000	N	0.215042000	3.782403000	-0.017203000
N	-1.077892000	-0.876538000	0.082054000	N	-0.951378000	-1.020959000	0.029641000
N	-1.985587000	-3.220212000	-0.005936000	N	-1.521742000	-3.469574000	-0.019655000
N	0.467474000	-2.847074000	-0.120732000	N	0.858481000	-2.761009000	-0.076305000
N	2.289846000	1.777853000	0.001491000	N	2.017366000	2.075719000	-0.046554000
N	4.772324000	2.162773000	0.003952000	N	4.422391000	2.803196000	-0.107093000
N	3.862509000	-0.168476000	-0.045531000	N	3.845174000	0.367893000	-0.129442000
N	2.945193000	-2.492413000	-0.150494000	N	3.261883000	-2.064614000	-0.149905000
N	2.021126000	-4.814976000	-0.280140000	N	2.672700000	-4.497271000	-0.160701000
N	4.460284000	-4.447099000	-0.319794000	N	5.035804000	-3.792926000	-0.242330000
N	5.395056000	-2.112910000	-0.167400000	N	5.633481000	-1.345959000	-0.220599000
N	6.308176000	0.232888000	-0.060818000	N	6.210565000	1.105982000	-0.194897000
B	0.529188000	5.150704000	-0.103770000	B	-0.194924000	5.172826000	-0.028720000
B	3.006245000	5.533811000	-0.024130000	B	2.206867000	5.894906000	-0.017727000
B	4.557568000	3.582157000	0.018896000	B	4.013607000	4.177906000	-0.070056000
N	-0.807337000	5.653867000	-0.185577000	N	-1.590012000	5.486899000	-0.060878000
N	1.673954000	6.019278000	-0.078618000	N	0.819349000	6.192246000	-0.012042000
N	3.221269000	4.107626000	0.002222000	N	2.617353000	4.512622000	-0.032519000
B	-3.117208000	-4.127977000	0.025542000	B	-2.516082000	-4.523388000	-0.008015000
B	0.897737000	-5.709096000	-0.278547000	B	1.685028000	-5.538657000	-0.126521000
N	-4.439605000	-3.588644000	0.093683000	N	-3.903056000	-4.174234000	-0.008645000
N	-0.436020000	-5.187647000	-0.173443000	N	0.290246000	-5.205946000	-0.068828000
B	-1.562397000	-6.089147000	-0.136582000	B	-0.701016000	-6.253400000	-0.039420000
N	-2.866868000	-5.542689000	-0.026274000	N	-2.072112000	-5.891933000	-0.004058000
N	1.394303000	-0.542190000	0.018040000	N	1.455135000	-0.346129000	-0.053258000
H	7.059862000	2.378538000	0.006577000	H	6.657940000	3.335022000	-0.165257000
H	5.492174000	4.330118000	0.036264000	H	4.836330000	5.048113000	-0.072501000
H	3.930245000	6.295410000	-0.006718000	H	3.018461000	6.775891000	-0.012976000
H	1.537378000	7.019484000	-0.102592000	H	0.544761000	7.163891000	-0.010035000
H	-0.952093000	6.650870000	-0.258063000	H	-1.873598000	6.455177000	-0.108141000
H	-3.449953000	6.243753000	-0.540004000	H	-4.292307000	5.713678000	-0.379925000

H	-5.480722000	4.799105000	-0.767187000	H	-6.100735000	4.007580000	-0.677073000
H	-6.381548000	2.488678000	-0.667316000	H	-6.665398000	1.588522000	-0.700264000
H	-7.318256000	0.200316000	-0.406569000	H	-7.270699000	-0.819354000	-0.555123000
H	-6.802686000	-2.226395000	-0.061581000	H	-6.424761000	-3.154679000	-0.247116000
H	-5.226878000	-4.221426000	0.087797000	H	-4.594568000	-4.909984000	-0.033254000
H	-3.645994000	-6.184608000	-0.002545000	H	-2.756250000	-6.634397000	0.011761000
H	-1.400839000	-7.274036000	-0.199633000	H	-0.375674000	-7.406565000	-0.046684000
H	1.073035000	-6.890335000	-0.362138000	H	2.025385000	-6.686839000	-0.147364000
H	3.547158000	-6.525497000	-0.449435000	H	4.423886000	-5.982745000	-0.250578000
H	5.390305000	-4.836945000	-0.371609000	H	6.011206000	-4.050445000	-0.283389000
H	6.334690000	-2.482033000	-0.204590000	H	6.615095000	-1.581224000	-0.258833000
H	7.256279000	-0.114001000	-0.080297000	H	7.197045000	0.893678000	-0.231078000
B	1.159146000	0.875835000	0.041452000	B	1.022686000	1.018582000	-0.003429000
N	-0.194156000	1.384870000	0.073265000	N	-0.386158000	1.341254000	0.076796000
C	-1.317955000	0.516462000	0.450445000	C	-1.383789000	0.312732000	0.436924000
N	-1.486440000	0.548969000	1.936834000	N	-1.580211000	0.268528000	1.902430000
N	-0.562088000	0.109364000	2.800856000	N	-0.359014000	0.064007000	2.582864000
H	-0.105741000	-0.686003000	2.340273000	H	-0.553372000	-0.450060000	3.433688000
H	-1.896411000	1.424749000	2.247074000	H	-2.031054000	1.140570000	2.180362000
				H	0.100085000	0.940529000	2.821999000
		H₂H₂N₂-C_BBN				H₃NH₂N-C_BBN	
N	-2.733701000	-4.401729000	-0.055596000	N	4.618150000	-2.038700000	-0.256520000
B	-2.373780000	-5.799688000	-0.005666000	B	5.945595000	-1.488576000	-0.378426000
B	-4.117621000	-4.034119000	-0.042355000	B	4.453533000	-3.461354000	-0.219611000
B	-5.871431000	-2.279287000	-0.094564000	B	2.969337000	-5.445618000	-0.135354000
B	-5.229147000	0.135312000	-0.175409000	B	0.489729000	-5.151819000	-0.080580000
B	-3.449584000	-1.622492000	-0.179269000	B	1.976007000	-3.135422000	-0.045018000
B	-1.699473000	-3.385029000	-0.147079000	B	3.458425000	-1.160365000	-0.165585000
B	0.045824000	-5.178472000	-0.099076000	B	4.983007000	0.817122000	-0.389473000
B	0.692753000	-2.755218000	-0.199322000	B	2.495855000	1.107103000	-0.204696000
B	-2.798880000	0.762446000	-0.208066000	B	-0.470885000	-2.832325000	-0.060422000
B	-2.151720000	3.178613000	-0.097382000	B	-2.956737000	-2.536619000	-0.163729000
B	1.350046000	-0.358340000	-0.221409000	B	0.042855000	1.419508000	-0.010320000
B	3.118333000	-2.128209000	-0.199231000	B	1.528586000	3.420878000	-0.259023000
B	3.770833000	0.271583000	-0.226757000	B	-0.935088000	3.730493000	-0.047978000
B	2.017114000	2.046672000	-0.209782000	B	-2.435030000	1.744080000	0.077705000
B	0.257678000	3.811715000	-0.102544000	B	-3.931082000	-0.246796000	-0.022456000
B	0.908051000	6.233702000	0.002501000	B	-6.422878000	0.048505000	-0.012266000
B	2.676166000	4.462468000	-0.112999000	B	-4.920664000	2.049612000	0.123006000
B	4.439782000	2.684958000	-0.185454000	B	-3.412994000	4.050106000	0.120276000
B	6.201238000	0.902578000	-0.211710000	B	-1.903631000	6.045484000	-0.026918000
N	-6.220254000	-0.906832000	-0.145585000	N	1.660273000	-5.986595000	-0.088723000
N	-4.475134000	-2.649116000	-0.098679000	N	3.136235000	-4.011411000	-0.135575000
N	-1.002979000	-6.159510000	-0.032932000	N	6.106777000	-0.079217000	-0.417415000
N	-0.319515000	-3.781237000	-0.167235000	N	3.660240000	0.260033000	-0.239379000
N	-2.048455000	-1.982902000	-0.217574000	N	2.135205000	-1.703146000	-0.001813000
N	-3.833633000	-0.240781000	-0.217998000	N	0.664417000	-3.718396000	-0.005674000
N	-3.167117000	2.159121000	-0.136166000	N	-1.801537000	-3.395489000	-0.170123000
N	0.303009000	-1.365390000	-0.261234000	N	1.186768000	0.536962000	-0.038745000
N	2.087759000	-3.134792000	-0.164555000	N	2.670082000	2.543302000	-0.319044000
N	2.745950000	-0.742460000	-0.246455000	N	0.214407000	2.855617000	-0.113282000
N	-0.765980000	2.792018000	-0.132804000	N	-2.773927000	-1.111856000	-0.069893000
N	-0.114843000	5.215767000	-0.028231000	N	-5.268245000	-0.815678000	-0.077530000
N	1.649958000	3.442781000	-0.144324000	N	-3.764599000	1.180842000	0.074320000
N	3.411401000	1.667728000	-0.208065000	N	-2.259554000	3.177951000	0.066666000
N	5.174699000	-0.111957000	-0.218075000	N	-0.755727000	5.172551000	-0.107779000
N	5.816919000	2.268829000	-0.197585000	N	-3.195921000	5.472496000	0.097447000
N	4.050363000	4.061938000	-0.146691000	N	-4.718762000	3.466381000	0.181747000

N	2.271407000	5.840685000	-0.043574000	N	-6.228160000	1.450287000	0.099407000
B	-4.563960000	2.542495000	-0.110164000	B	-1.983348000	-4.831433000	-0.224055000
B	-3.911808000	4.961610000	0.005587000	B	-4.470009000	-4.527626000	-0.343010000
B	-1.499971000	5.591282000	0.013778000	B	-5.440692000	-2.235549000	-0.201531000
N	-5.567500000	1.523635000	-0.150502000	N	-0.834600000	-5.681954000	-0.163381000
N	-4.895785000	3.940639000	-0.040807000	N	-3.318440000	-5.356299000	-0.331279000
N	-2.520590000	4.582814000	-0.025055000	N	-4.294778000	-3.099532000	-0.244241000
B	2.459373000	-4.534273000	-0.120994000	B	3.994236000	3.110584000	-0.467504000
B	5.539353000	-1.500020000	-0.201260000	B	0.557757000	5.727632000	-0.266197000
N	1.431017000	-5.528595000	-0.090179000	N	5.127810000	2.236487000	-0.481213000
N	4.520936000	-2.511950000	-0.182667000	N	1.701434000	4.861598000	-0.347665000
B	4.887244000	-3.905570000	-0.139719000	B	3.018927000	5.420420000	-0.519207000
N	3.855468000	-4.879544000	-0.108520000	N	4.129617000	4.537947000	-0.575986000
N	0.994905000	1.035538000	-0.266050000	N	-1.285207000	0.877911000	0.070493000
H	0.614815000	7.393452000	0.069079000	H	-7.529572000	-0.408644000	-0.054100000
H	-1.803690000	6.747754000	0.081702000	H	-6.541917000	-2.701767000	-0.267614000
H	-4.232085000	6.114288000	0.069978000	H	-5.564041000	-5.008422000	-0.429062000
H	-5.866131000	4.219111000	-0.021448000	H	-3.455175000	-6.355184000	-0.386565000
H	-6.540598000	1.792575000	-0.122090000	H	-0.961422000	-6.682573000	-0.216363000
H	-7.200264000	-0.665014000	-0.129609000	H	1.559677000	-6.990757000	-0.116049000
H	-6.721727000	-3.121555000	-0.046950000	H	3.923602000	-6.168737000	-0.177859000
H	-4.965937000	-4.876431000	0.015485000	H	5.409008000	-4.181295000	-0.265278000
H	-3.221689000	-6.643408000	0.057904000	H	6.900955000	-2.208933000	-0.436662000
H	-0.769315000	-7.140861000	0.007613000	H	7.041111000	0.290033000	-0.517334000
H	1.691513000	-6.503650000	-0.051332000	H	6.050803000	2.631553000	-0.591543000
H	4.124529000	-5.852348000	-0.081565000	H	5.047672000	4.941912000	-0.692036000
H	6.037989000	-4.238962000	-0.127431000	H	3.178851000	6.604064000	-0.611134000
H	6.694804000	-1.816040000	-0.195185000	H	0.703654000	6.914419000	-0.334113000
H	7.360477000	0.598703000	-0.213382000	H	-1.768234000	7.235245000	-0.068748000
H	6.548493000	2.964752000	-0.190163000	H	-3.986741000	6.098730000	0.141703000
H	4.767540000	4.773145000	-0.128764000	H	-5.525161000	4.074059000	0.210809000
H	2.972740000	6.566700000	-0.020293000	H	-7.047870000	2.038644000	0.136194000
B	-0.394652000	1.393625000	-0.211586000	B	-1.440280000	-0.550269000	0.015954000
N	-1.411404000	0.363928000	-0.270378000	N	-0.277614000	-1.407585000	0.008664000
C	-1.053938000	-0.995418000	-0.477743000	C	1.009056000	-0.840726000	0.449399000
N	-0.123546000	-0.252207000	2.733615000	N	0.944401000	-0.747068000	1.898738000
N	1.295084000	-0.263687000	2.612954000	N	3.666999000	0.464647000	2.861073000
H	1.738227000	-0.919616000	3.253126000	H	3.684816000	1.380269000	2.419326000
H	-0.429284000	-0.504870000	3.671381000	H	3.848109000	0.606785000	3.851169000
H	1.631303000	0.666807000	2.835264000	H	4.456653000	-0.048384000	2.478531000
H	-0.475955000	-0.952844000	2.089428000	H	1.826721000	-0.369409000	2.264024000
				H	0.821292000	-1.680637000	2.285347000
H₂N-C_BBN				H₃N-C_BBN			
N	-4.752692000	-1.939804000	-0.174518000	N	-5.015439000	1.221103000	-0.019721000
B	-5.295881000	-3.275057000	-0.261827000	B	-6.239354000	0.453161000	-0.013452000
B	-5.646631000	-0.822325000	-0.204284000	B	-5.085139000	2.649806000	0.047433000
B	-6.019993000	1.627311000	-0.113823000	B	-3.946193000	4.854970000	0.052151000
B	-4.075293000	3.187660000	0.021921000	B	-1.453196000	4.982947000	-0.077742000
B	-3.681301000	0.713431000	0.029746000	B	-2.585292000	2.750134000	-0.092132000
B	-3.319808000	-1.736569000	-0.024236000	B	-3.732716000	0.547216000	-0.119058000
B	-2.987948000	-4.218267000	-0.121650000	B	-4.911857000	-1.660661000	-0.148709000
B	-1.030448000	-2.651578000	-0.001224000	B	-2.405837000	-1.539058000	-0.181170000
B	-1.749079000	2.244141000	0.034733000	B	-0.115124000	2.862534000	-0.148429000
B	0.206145000	3.802779000	-0.116361000	B	2.386426000	2.981735000	-0.093789000
B	0.918231000	-1.113217000	0.082505000	B	0.080864000	-1.428461000	-0.157503000
B	1.292925000	-3.586165000	-0.078813000	B	-1.069214000	-3.654785000	-0.090000000
B	3.247812000	-2.042731000	0.012803000	B	1.420150000	-3.543527000	-0.056740000
B	2.891933000	0.423564000	0.064610000	B	2.578108000	-1.336202000	-0.120981000

B	2.522759000	2.885252000	-0.064823000	B	3.724651000	0.878382000	-0.085965000
B	4.483298000	4.449326000	-0.161571000	B	6.230140000	0.999851000	-0.024189000
B	4.855890000	1.976762000	-0.004156000	B	5.079484000	-1.225924000	-0.047191000
B	5.220233000	-0.500320000	0.053827000	B	3.921904000	-3.446912000	-0.023151000
B	5.575594000	-2.979960000	0.005985000	B	2.757735000	-5.664419000	0.046358000
N	-5.489813000	2.938394000	-0.018275000	N	-2.745848000	5.606779000	-0.007082000
N	-5.114355000	0.502527000	-0.103112000	N	-3.873498000	3.412606000	0.012432000
N	-4.412416000	-4.382161000	-0.210794000	N	-6.165634000	-0.960037000	-0.094266000
N	-2.452096000	-2.879926000	0.005372000	N	-3.689924000	-0.886536000	-0.178112000
N	-2.773070000	-0.406501000	0.098793000	N	-2.501462000	1.307027000	-0.155118000
N	-3.175836000	2.055956000	0.091725000	N	-1.385905000	3.538771000	-0.132097000
N	-1.216483000	3.585275000	-0.078635000	N	1.104049000	3.636990000	-0.105220000
N	-0.515047000	-1.308584000	0.100928000	N	-1.197071000	-0.744203000	-0.213441000
N	-0.132966000	-3.783303000	-0.100580000	N	-2.341795000	-2.981656000	-0.131835000
N	1.816026000	-2.246962000	-0.003546000	N	0.139001000	-2.872672000	-0.097655000
N	1.092401000	2.669842000	-0.052572000	N	2.439297000	1.543246000	-0.110046000
N	3.055353000	4.234953000	-0.155878000	N	4.947662000	1.663467000	-0.053665000
N	3.423980000	1.764418000	0.009446000	N	3.795205000	-0.559388000	-0.092438000
N	3.787756000	-0.708475000	0.056516000	N	2.639596000	-2.777459000	-0.074379000
N	4.146493000	-3.184886000	-0.021613000	N	1.479044000	-4.995025000	-0.000386000
N	6.079195000	-1.653780000	0.048934000	N	3.942697000	-4.883946000	0.030628000
N	5.723760000	0.839603000	0.047451000	N	5.115357000	-2.656385000	-0.026472000
N	5.347030000	3.326505000	-0.077104000	N	6.269631000	-0.418409000	-0.022953000
B	-2.111432000	4.724968000	-0.106380000	B	1.043410000	5.085738000	-0.083624000
B	-0.151009000	6.279783000	-0.270094000	B	3.548465000	5.202243000	-0.048299000
B	2.163604000	5.356498000	-0.238248000	B	4.884349000	3.097054000	-0.043949000
N	-3.522496000	4.503828000	-0.029052000	N	-0.234233000	5.728532000	-0.082197000
N	-1.548814000	6.044153000	-0.210338000	N	2.274626000	5.827556000	-0.059974000
N	0.743047000	5.149480000	-0.214408000	N	3.611230000	3.761500000	-0.062952000
B	-0.663657000	-5.130118000	-0.172908000	B	-3.562811000	-3.763517000	-0.128176000
B	3.615516000	-4.516308000	-0.095579000	B	0.268377000	-5.765587000	0.010542000
N	-2.081029000	-5.320720000	-0.171744000	N	-4.822746000	-3.086526000	-0.157845000
N	2.195287000	-4.723855000	-0.132683000	N	-1.005743000	-5.104971000	-0.039672000
B	1.663928000	-6.062029000	-0.216848000	B	-2.221604000	-5.880438000	-0.038540000
N	0.255847000	-6.233655000	-0.240064000	N	-3.464450000	-5.197039000	-0.088212000
N	1.466540000	0.214474000	0.110583000	N	1.301196000	-0.671152000	-0.197250000
H	4.934561000	5.556375000	-0.238996000	H	7.245613000	1.634863000	0.000883000
H	2.604751000	6.466289000	-0.325488000	H	5.893634000	3.740789000	-0.018583000
H	0.275665000	7.395221000	-0.361820000	H	4.549393000	5.859671000	-0.025758000
H	-2.164205000	6.844117000	-0.240016000	H	2.244734000	6.836806000	-0.048599000
H	-4.146259000	5.297023000	-0.073144000	H	-0.274985000	6.737294000	-0.051489000
H	-6.134757000	3.714479000	-0.050897000	H	-2.814430000	6.613421000	0.028574000
H	-7.201630000	1.454729000	-0.205133000	H	-5.005527000	5.407147000	0.135561000
H	-6.826012000	-0.994012000	-0.313442000	H	-6.144158000	3.200403000	0.131938000
H	-6.475821000	-3.445092000	-0.376914000	H	-7.300455000	1.003233000	0.061581000
H	-4.806186000	-5.308305000	-0.290927000	H	-7.030173000	-1.481289000	-0.079642000
H	-2.450269000	-6.257635000	-0.249156000	H	-5.672605000	-3.632076000	-0.140989000
H	-0.104174000	-7.175522000	-0.293171000	H	-4.308228000	-5.751596000	-0.086089000
H	2.394567000	-7.010065000	-0.263959000	H	-2.186438000	-7.076843000	0.004772000
H	4.358226000	-5.455055000	-0.128044000	H	0.319780000	-6.960805000	0.061434000
H	6.327215000	-3.912673000	-0.010706000	H	2.819709000	-6.859643000	0.099272000
H	7.081263000	-1.529941000	0.057678000	H	4.827512000	-5.368983000	0.067886000
H	6.723159000	0.986467000	0.037191000	H	6.010798000	-3.122508000	0.010349000
H	6.342451000	3.495565000	-0.087223000	H	7.174901000	-0.864867000	0.004428000
B	0.559137000	1.327474000	0.064004000	B	1.223123000	0.761196000	-0.163189000
N	-0.869281000	1.103335000	0.099644000	N	-0.072122000	1.415348000	-0.193227000
C	-1.373101000	-0.202995000	0.547785000	C	-1.259118000	0.661806000	-0.411613000
N	-1.277024000	-0.189587000	2.010425000	N	-0.475041000	0.038447000	2.780522000

H	-1.637839000	-1.070410000	2.372279000	H	-1.324589000	-0.407765000	2.445373000
H	-1.873809000	0.551087000	2.374322000	H	-0.405587000	0.914468000	2.268714000
				H	-0.632197000	0.278298000	3.755974000