Supporting information

Computational studies on the reactivity of substituted 1,2-dihydro-1,2-azaborines

Pedro J. Silva and Maria J. Ramos

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Geometries (computed at the B3LYP/6-31+G(d,p) level) of all species described in this paper, as well as their gas phase, ZPVE and solution energies (computed at the B3LYP/6-311+G(3d,2p) level, in CH_2Cl_2). Most-important resonance structures contributing to the computed electron densities of substituted benzenes and 1,2-azaborines, as predicted by Natural Resonance Theory.
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Nitration Computed energies

Table S1. Gas phase energies of Wheland intermediates and products of the nitration of substituted 1,2-azaborines (in Hartree)

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C4-bound, H^- transfer	C3-bound (cyclic)	C3-bound cyclic product	B-bound product	C3-bound product
Hydrogen	-235.7597429		-440.6191405		-440.6335220		-440.6479195	-440.2832739	-440.3883799	-440.3393156
Phenyl (on N)	-466.8705407		-671.7477907	-671.7100037	-671.7561721		-671.7710410	-671.3987442	-671.4969594	-671.4501231
Methyl (on N)	-275.0776366		-479.9514566		-479.9589179	-479.9651744	-479.9759532	-479.6046692	-479.7057187	-479.6577489
Vinyl (on N)	-313.1705806		-518.0420704	-518.0036723	-518.0509981		-518.0660943	-517.6993052	-517.7992025	-517.7497032
Chlorine (on N)	-695.3390424		-900.1936936		→C3-bound (cyclic)		-900.2219703	-899.8656700	-899.9646289	-899.9156780
Thiol (on N)	-633.9531831		-838.8172524	-838.7811066	→C3-bound (cyclic)		-838.8442854	-838.4809976	-838.5800958	-838.5310772
Hydroxy (on N)	-310.9510738		-515.8147597	-515.7721048	-515.8211439		-515.8418887	-515.4780162	-515.5782487	-515.5295592
Amino (on N)	-291.0925917	-495.9461693	-495.9700600		→C3-bound (cyclic)	-495.9814496	-495.9951882	-495.6253197	-495.7252949	-495.6765604
Ethynyl (on N)	-311.9048808		-516.7599047		-516.7723700		-516.7908745	-516.4324612	-516.5318954	-516.4817154
Formyl (on N)	-349.1188567		-553.9663691		-553.9792749		-553.9988522	C3-bound product	-553.7514508	-553.7016609
Phenyl (on B)	-466.8936002		-671.7787512		-671.7874579		-671.7861168	-671.4145555		-671.4693475
Methyl (on B)	-275.1020202		-479.9762587		-479.9868672	-479.9919325	-479.9943704	-479.6247136		-479.6829631
Vinyl (on B)	-313.1923651		-518.0705779		-518.0796757		-518.0822679	-517.7120041		-517.7717896
Chlorine (on B)	-695.4399711		-900.3019260		-900.3100617		-900.3177257	-899.9611923		-900.0125993
Thiol (on B)	-634.0161867		-838.8913340		-838.9015591	-838.9043826	-838.8974201	-838.5366114		-838.5951416
Hydroxy (on B)	-311.0683055		-515.9475334		-515.9587106		-515.9586556	C3-bound product		-515.6448233
Amino (on B)	-291.1822938		-496.0794208		-496.0925230	-496.0921481		C3-bound product		-495.7697165
Ethynyl (on B)	-311.9503400		-516.8198446		-516.8286368		-516.8348889	-516.4690627		-516.5257941
Formyl (on B)	-349.1202348		-553.9693536		→C3-bound (cyclic)		-554.0026869	-553.6467493		-553.7023382

Table S2. ZPVE (computed at 298.15 K) of Wheland intermediates and products of the nitration of substituted 1,2-azaborines (in kcal.mol^{-1})

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C4-bound, H^- transfer	C3-bound (cyclic)	C3-bound cyclic product	B-bound product	C3-bound product
Hydrogen	43.08		48.12		47.80		49.87	41.53	40.88	41.95
Phenyl (on N)	88.10		93.86	92.29	93.54		95.08	87.05	85.80	87.02
Methyl (on N)	58.76		63.50		63.46	63.35	65.72	57.48	55.85	57.77
Vinyl (on N)	60.60		65.50	64.65	65.23		67.72	59.66	58.64	59.40
Chlorine (on N)	34.90		39.39		→C3-bound (cyclic)		41.70	33.52	32.66	33.73
Thiol (on N)	40.11		44.33	43.92	→C3-bound (cyclic)		46.93	38.76	37.72	38.68
Hydroxy (on N)	43.82		49.29	47.35	48.66		50.55	42.38	41.76	42.62
Amino (on N)	51.86	57.03	57.52		→C3-bound (cyclic)	55.89	58.57	50.76	49.85	50.79
Ethynyl (on N)	46.14		50.44		50.86		52.95	44.82	43.92	44.87
Formyl (on N)	46.58		51.36		50.42		53.03	C3-bound product	44.72	45.62
Phenyl (on B)	89.89		95.06		93.82		95.45	87.70		87.87
Methyl (on B)	58.63		63.43		64.55	62.55	65.52	57.29		58.00
Vinyl (on B)	61.40		67.30		66.29		68.04	59.61		60.52
Chlorine (on B)	36.75		41.34		41.52		43.44	35.58		35.01
Thiol (on B)	41.65		46.66		47.37	46.45	48.20	40.27		41.28
Hydroxy (on B)	45.40		50.09		50.57		51.69	C3-bound product		44.13
Amino (on B)	52.45		59.53		59.26	58.35		C3-bound product		52.42
Ethynyl (on B)	47.48		52.30		52.11		53.99	45.90		46.06
Formyl (on B)	46.75		51.66		→C3-bound (cyclic)		53.64	45.36		46.21

Table S3. CPCM energies (including electrostatic, cavitation, dispersion an repulsion energies) of Wheland intermediates and products of the nitration of substituted 1,2-azaborines (in kcal.mol^{-1})

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C4-bound, H^- transfer	C3-bound (cyclic)	C3-bound cyclic product	B-bound product	C3-bound product
Hydrogen	-147944.17		-276547.03		-276558.66		-276562.09	-276290.69	-276352.88	-276326.56
Phenyl (on N)	-292968.71		-421575.07	-421551.42	-421582.65		-421587.23	-421318.12	-421375.35	-421350.99
Methyl (on N)	-172615.51		-301224.97		-301231.82	-301234.94	-301236.88	-300964.69	-301023.50	-300998.16
Vinyl (on N)	-196519.29		-325125.88	-325102.22	-325133.70		-325137.80	-324868.42	-324927.26	-324901.22
Chlorine (on N)	-436333.51		-564931.43		→C3-bound (cyclic)		-564946.96	-564681.49	-564739.91	-564712.95
Thiol (on N)	-397813.53		-526416.96	-526395.05	→C3-bound (cyclic)		-526430.88	-526162.41	-526220.93	-526194.40
Hydroxy (on N)	-195128.05		-323732.27	-323707.40	-323738.10		-323745.92	-323476.97	-323534.92	-323509.06
Amino (on N)	-182667.11	-311261.54	-311279.00		→C3-bound (cyclic)	-311288.38	-311291.17	-311018.42	-311076.60	-311051.03
Ethynyl (on N)	-195725.32		-324320.73		-324331.89		-324338.96	-324073.52	-324132.69	-324105.20
Formyl (on N)	-219080.35		-347674.75		-347685.45		-347691.71	C3-bound product	-347489.60	-347462.22
Phenyl (on B)	-292985.03		-421597.56		-421602.68		-421600.23	-421329.01		-421363.60
Methyl (on B)	-172631.24		-301242.94		-301249.92	-301253.44	-301250.82	-300977.26		-301014.20
Vinyl (on B)	-196534.10		-325146.06		-325152.24		-325150.62	-324877.98		-324915.62
Chlorine (on B)	-436399.11		-565003.38		-565008.37		-565011.04	-564744.71		-564776.80
Thiol (on B)	-397855.04		-526467.21		-526474.04	-526475.97	-526467.88	-526199.29		-526237.15
Hydroxy (on B)	-195203.86		-323819.67		-323826.53		-323822.16	C3-bound product		-323585.56
Amino (on B)	-182723.70		-311349.26		-311357.67	-311357.94		C3-bound product		-311110.73
Ethynyl (on B)	-195756.01		-324362.30		-324368.11		-324369.40	-324099.63		-324135.37
Formyl (on B)	-219082.99		-347680.73		→C3-bound (cyclic)		-347696.23	-347429.55		-347463.45

Chlorination Computed energies

Table S4. Gas phase energies of Wheland intermediates and products of the chlorination of substituted 1,2-azaborines (in Hartree)

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C4-bound, H^- transfer	C3-bound product	B-bound product
Hydrogen	-235.7597429		-695.6881170		-695.6983521	-695.7178698	-695.3889836	-695.4399699
Phenyl (on N)	-466.8705407		-926.8127561		-926.8220823		-926.4996735	-926.5474142
Methyl (on N)	-275.0776366	-734.9900396	-735.0170956		-735.0253303	-735.0416349	-734.7071553	-734.7567236
Vinyl (on N)	-313.1705806	-773.0821845	-773.1074761		-773.1181021	-773.1329302	-772.7994253	-772.8449694
Chlorine (on N)	-695.3390424		-1155.2603027		-1155.2704044		-1154.9668751	-1155.0151351
Thiol (on N)	-633.9531831	-1093.8590759	-1093.8830659		-1093.8928399	-1093.9090024	-1093.5817589	-1093.6303669
Hydroxy (on N)	-310.9510738	-770.8544971	-770.8809598		-770.8895464	-770.9045103	-770.5791565	-770.6306897
Amino (on N)	-291.0925917	-751.0103634	-751.0347564	-750.9992243	-751.0453421 (B-bound)			
Ethynyl (on N)	-311.9048808	-771.8091110	-771.8276552		-771.8395198	-771.8567462	-771.5328171	-771.5821258
Formyl (on N)	-349.1188567		-809.0327877		-809.0456386		-808.7465414	-808.7916730
Phenyl (on B)	-466.8936002		-926.8438905		-926.8506295			
Methyl (on B)	-275.1020202		-735.0422445		-735.0509614	-735.0698119		
Vinyl (on B)	-313.1923651		-773.1360613		-773.1436615	-773.1615655		
Chlorine (on B)	-695.4399711		-1155.3684213		-1155.3750529	-1155.3953780		
Thiol (on B)	-634.0161867		-1093.9574051		-1093.9639139			
Hydroxy (on B)	-311.0683055		-771.0137818		-771.0222028	-771.0413859		
Amino (on B)	-291.1822938		-751.1445418		-751.1516377	-751.1679455		
Ethynyl (on B)	-311.9503400		-771.8857924		-771.8929294			
Formyl (on B)	-349.1202348	-809.0191613	-809.0358912		-809.0458237	-809.0667313		

Table S5. ZPVE (computed at 298.15 K) of Wheland intermediates and products of the chlorination of substituted 1,2-azaborines (in kcal.mol-1)

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C4-bound, H^- transfer	C3-bound product	B-bound product
Hydrogen	43.078		42.215		42.557	41.991	35.818	36.754
Phenyl (on N)	88.1	87.221	87.303		87.852		80.921	81.617
Methyl (on N)	58.762	57.748	57.974		58.138	57.157	51.079	52.609
Vinyl (on N)	60.604	59.903	59.916		60.816	59.235	53.498	54.518
Chlorine (on N)	34.904		36.101		34.573		27.686	28.691
Thiol (on N)	40.106	39.354	39.116		39.202	38.473	32.83	33.714
Hydroxy (on N)	43.82	42.817	42.748		43.209	41.697	36.473	37.667
Amino (on N)	51.858	51.135	51.104	50.049	51.45 (B-bound)			
Ethynyl (on N)	46.141	45.162	45.247		45.804	45.091	38.908	39.816
Formyl (on N)	46.581		44.957		45.755		39.364	40.27
Phenyl (on B)	89.89		88.58		88.469			
Methyl (on B)	58.633		57.586		58.063	57.501		
Vinyl (on B)	61.397		60.962		60.78	60.657		
Chlorine (on B)	36.752		36.086		35.926	35.909		
Thiol (on B)	41.646		41.483		41.356			
Hydroxy (on B)	45.395		44.997		44.931	44.918		
Amino (on B)	52.453		53.105		52.771	52.855		
Ethynyl (on B)	47.481		46.754		46.731			
Formyl (on B)	46.754	45.484	45.329		46.037	45.133		

Table S6. CPCM energies (including electrostatic and cavitation energies) of Wheland intermediates and products of the chlorination of substituted 1,2-azaborines (in kcal.mol^{-1})

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C4-bound, H^- transfer	C3-bound product	B-bound product
Hydrogen			-436586.90		-436591.87	-436603.00	-436354.36	-436386.19
Phenyl (on N)			-581603.07		-581608.41		-581370.21	-581399.99
Methyl (on N)		-461242.30	-461260.15		-461264.20	-461273.88	-461024.23	-461055.01
Vinyl (on N)		-485143.45	-485159.70		-485165.44	-485174.41	-484926.29	-484954.64
Chlorine (on N)			-724967.47		-724973.59		-724740.97	-724771.40
Thiol (on N)		-686436.76	-686452.16		-686457.43	-686467.03	-686221.48	-686251.90
Hydroxy (on N)		-483751.34	-483768.26		-483772.61	-483781.69	-483535.86	-483567.32
Amino (on N)		-471297.08	-471313.96	-471292.17	-471323.65 (B-bound)			
Ethynyl (on N)		-484346.59	-484357.76		-484364.64	-484375.09	-484132.17	-484163.29
Formyl (on N)			-507709.92		-507717.64		-507486.81	-507515.47
Phenyl (on B)			-581625.12		-581628.76			
Methyl (on B)			-461277.57		-461282.90	-461292.71		
Vinyl (on B)			-485179.46		-485184.14	-485193.42		
Chlorine (on B)			-725038.99		-725042.91	-725053.83		
Thiol (on B)			-686501.87		-686505.69			
Hydroxy (on B)			-483855.39		-483860.15	-483869.70		
Amino (on B)			-471383.83		-471388.11	-471396.19		
Ethynyl (on B)			-484396.57		-484400.81			
Formyl (on B)		-507701.40	-507715.34		-507720.43	-507731.81		

Acylation Computed energies

Table S7. Gas phase energies of Wheland intermediates and products of the acylation of substituted 1,2-azaborines (in Hartree)

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C3-bound cyclic product
Hydrogen	-235.7597429	-349.4044809	-349.4227543		-349.4356515	-349.4319020
Phenyl (on N)	-466.8705407	-580.5263213	-580.5479742	-580.5119146	-580.5570471	-580.5527874
Methyl (on N)	-275.0776366		-388.7529817		-388.7605875	-388.7587337
Vinyl (on N)	-313.1705806	-426.8215956	-426.8430353		-426.8493225	-426.8490861
Chlorine (on N)	-695.3390424	-808.9793180	-808.9961883		-809.0061500	-809.0057449
Thiol (on N)	-633.9531831	-747.5993974	-747.6165502		-747.6240556	-747.6268095
Hydroxy (on N)	-310.9510738	-424.5974520	-424.6155822		-424.6229811	-424.6248388
Amino (on N)	-291.0925917	-404.7500668	-404.7673536		-404.7734058	-404.7770673
Ethynyl (on N)	-311.9048808	-425.5497446	-425.5637129		-425.5709074	-425.5742291
Formyl (on N)	-349.1188567	-462.7528657	-462.7672309		-462.7782238	-462.7837284
Phenyl (on B)	-466.8936002		-580.5780548		-580.5869173	-580.5707601
Methyl (on B)	-275.1020202		-388.7779663		-388.7876792	-388.7789668
Vinyl (on B)	-313.1923651		-426.8710569		-426.8797058	-426.8672463
Chlorine (on B)	-695.4399711	-809.0795240	-809.1019767		-809.1113746	-809.1033303
Thiol (on B)	-634.0161867	-747.6644825	-747.6893944		-747.6982415	-747.6831370
Hydroxy (on B)	-311.0683055	-424.7216427	-424.7460045		-424.7671160	
Amino (on B)	-291.1822938	-404.8436724	-404.8783424		-404.8880666	
Ethynyl (on B)	-311.9503400	-425.5957291	-425.6213484		-425.6268882	-425.6195882
Formyl (on B)	-349.1202348	-462.7570558	-462.7818808		-462.7883884	-462.7872346

Table S8. ZPVE (computed at 298.15 K) of Wheland intermediates and products of the acylation of substituted 1,2-azaborines (in kcal.mol^{-1})

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C3-bound cyclic product
Hydrogen	43.08	52.99	52.59		52.91	54.70
Phenyl (on N)	88.10	97.75	97.63	96.58	97.70	99.86
Methyl (on N)	58.76		68.20		68.26	70.69
Vinyl (on N)	60.60	70.28	70.25		70.16	72.71
Chlorine (on N)	34.90	44.28	45.26		44.68	46.59
Thiol (on N)	40.11	49.50	49.26		49.40	51.68
Hydroxy (on N)	43.82	53.52	53.35		52.84	55.43
Amino (on N)	51.86	62.47	61.36		61.48	63.57
Ethynyl (on N)	46.14	55.64	55.07		55.30	57.82
Formyl (on N)	46.58	55.28	55.57		55.58	57.93
Phenyl (on B)	89.89		98.55		99.25	100.85
Methyl (on B)	58.63		68.29		68.17	70.22
Vinyl (on B)	61.40		70.77		71.47	72.71
Chlorine (on B)	36.75	45.46	46.37		46.46	48.28
Thiol (on B)	41.65	50.64	51.60		52.77	52.31
Hydroxy (on B)	45.40	55.36	55.28		56.36	
Amino (on B)	52.45	61.92	64.13		63.65	
Ethynyl (on B)	47.48	56.33	56.91		56.90	58.79
Formyl (on B)	46.75	56.12	57.39		56.97	58.51

Table S9. CPCM energies (including electrostatic and cavitation energies) of Wheland intermediates and products of the acylation of substituted 1,2-azaborines (in kcal.mol^{-1})

Substituents	Reactant	C6-bound	C5-bound	C4-bound	C3-bound	C3-bound cyclic product
Hydrogen		-15.25	-15.25		-15.25	-14.96
Phenyl (on N)		-23.6	-24.17	-24.67	-24.33	-23.92
Methyl (on N)		to C4	-16.96		-17.17	-17
Vinyl (on N)		-18.26	-18.35		-18.47	-18.32
Chlorine (on N)		-16.47	-16.39		-16.57	-16.44
Thiol (on N)		-16.85	-17.16		-17.32	-17.03
Hydroxy (on N)		-16.4	-16.65		-16.68	-16.46
Amino (on N)		-16.88	-16.77		-16.79	-16.72
Ethynyl (on N)		-17.65	-17.65		-18.02	-17.68
Formyl (on N)		-17.73	-17.88		-18.19	-17.75
Phenyl (on B)		to C4	-24.59		-24.09	-24.06
Methyl (on B)		to C4	-17.45		-17.23	-17.29
Vinyl (on B)		to C4	-18.82		-18.42	-18.4
Chlorine (on B)		-17.05	-17.06		-16.91	-16.7
Thiol (on B)		-17.59	-17.51		-17.54	-17.27
Hydroxy (on B)		-16.78	-16.52		-16.45	to C3-bound
Amino (on B)		-17.84	-16.83		-16.74	to C3-bound
Ethynyl (on B)		-18.21	-18.15		-18.24	-17.82
Formyl (on B)		-18.44	-18.21		-17.81	-17.9

Mannich reactions Computed energies

Table S10. Gas phase energies of Wheland intermediates of the reaction of substituted 1,2-azaborines with methyleneiminium cation (in Hartree)

Substituents	Reactant	C3-bound	C5-bound
Hydrogen	-235.7597429	-330.7892421	
Phenyl (on N)	-466.8705407	-561.9086285	-561.9024610
Methyl (on N)	-275.0776366	-370.1129744	-370.1080251
Vinyl (on N)	-313.1705806	-408.2039655	-408.1980930
Chlorine (on N)	-695.3390424	-790.3604100	
Thiol (on N)	-633.9531831	-728.9801247	-728.9747272
Hydroxy (on N)	-310.9510738	-405.9772897	-405.9746825
Amino (on N)	-291.0925917	-386.1287791	-386.1252733
Ethynyl (on N)	-311.9048808	-406.9282249	
Formyl (on N)	-349.1188567	-444.1364004	
Phenyl (on B)	-466.8936002	-561.9354699	-561.9312785
Methyl (on B)	-275.1020202	-370.1397154	-370.1330053
Vinyl (on B)	-313.1923651	-408.2310983	-408.2269138
Chlorine (on B)	-695.4399711	-790.4671536	-790.4604344
Thiol (on B)	-634.0161867	-729.0531100	-729.0486476
Hydroxy (on B)	-311.0683055	-406.1154253	-406.1108414
Amino (on B)	-291.1822938	-386.2371217	-386.2315425
Ethynyl (on B)	-311.9503400	-406.9833290	-406.9765674
Formyl (on B)			

Table S11. ZPVE (computed at 298.15 K) of Wheland intermediates of the reaction of substituted 1,2-azaborines with methyleneiminium cation (in kcal.mol^{-1})

Substituents	Reactant	C3-bound	C5-bound
Hydrogen	43.08	75.18	
Phenyl (on N)	88.10	120.21	120.59
Methyl (on N)	58.76	90.99	91.05
Vinyl (on N)	60.60	92.44	92.35
Chlorine (on N)	34.90	66.91	
Thiol (on N)	40.11	71.35	71.71
Hydroxy (on N)	43.82	74.93	75.58
Amino (on N)	51.86	83.74	83.61
Ethynyl (on N)	46.14	77.81	
Formyl (on N)	46.58	77.93	
Phenyl (on B)	89.89	121.54	121.05
Methyl (on B)	58.63	90.50	89.42
Vinyl (on B)	61.40	94.18	93.55
Chlorine (on B)	36.75	68.87	68.46
Thiol (on B)	41.65	74.25	73.97
Hydroxy (on B)	45.40	78.08	77.98
Amino (on B)	52.45	85.82	85.56
Ethynyl (on B)	47.48	79.49	79.27
Formyl (on B)			

Table S12. CPCM energies (including electrostatic, cavitation, dispersion an repulsion energies) of Wheland intermediates of the reaction of substituted 1,2-azaborines with methyleneiminium cation (in kcal.mol^{-1})

Substituents	Reactant	C3-bound	C5-bound
Hydrogen	-147944.17	-207618.44	
Phenyl (on N)	-292968.71	-352642.66	-352638.81
Methyl (on N)	-172615.51	-232291.10	-232288.62
Vinyl (on N)	-196519.29	-256193.08	-256189.74
Chlorine (on N)	-436333.51	-496001.63	
Thiol (on N)	-397813.53	-457484.47	-457481.31
Hydroxy (on N)	-195128.05	-254799.30	-254797.62
Amino (on N)	-182667.11	-242343.07	-242341.74
Ethynyl (on N)	-195725.32	-255393.43	
Formyl (on N)	-219080.35	-278747.22	
Phenyl (on B)	-292985.03	-352660.89	-352659.85
Methyl (on B)	-172631.24	-232309.19	-232305.93
Vinyl (on B)	-196534.10	-256210.68	-256209.32
Chlorine (on B)	-436399.11	-496070.94	-496067.75
Thiol (on B)	-397855.04	-457532.58	-457530.42
Hydroxy (on B)	-195203.86	-254887.19	-254885.04
Amino (on B)	-182723.70	-242411.49	-242409.12
Ethynyl (on B)	-195756.01	-255429.30	-255426.23
Formyl (on B)			

Reactions of substituted benzenes: nitration

Table S13. Gas phase energies of Wheland intermediates of the nitration of substituted benzenes (in Hartree)

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	-232.3242369	-437.1649547	-437.1649547	-437.1649547
Phenyl	-463.4482454	-668.3149670	-668.2986989	-668.3216932
Methyl	-271.6543528	-476.5074182	-476.5028468	-476.5119506
Vinyl	-309.7483501	-514.6059652	-514.5943118	-514.6124833
Chlorine	-691.9514522	-896.7901579	-896.7822821	-896.7964674
Thiol	-630.5441050	-835.4030299	-835.3840047	-835.4116563
Hydrox	-307.5769077	-512.4444584	-512.4189065	-512.4455733
Amino	-287.7041163	-492.5931157	-492.5557691	-492.5992915
Ethynyl	-308.4937206	-513.3413386	-513.3313853	-513.3458549
Formyl	-345.6884558	-550.5145998	-550.5165273	-550.5157206
N-bound 1,2-azaborine	-466.8705407	-671.7302634	-671.7135138	-671.7382220
B-bound 1,2-azaborine	-466.8936002	-671.7636917	-671.7511368	-671.7671117

Table S14 . ZPVE (computed at 298.15 K) of Wheland intermediates of the nitration of substituted benzenes (in kcal.mol^{-1})

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	44.83	48.71	48.71	48.71
Phenyl	90.37	95.49	94.53	96.58
Methyl	60.29	64.96	64.35	65.03
Vinyl	62.68	67.74	66.79	67.35
Chlorine	37.49	42.14	41.37	41.86
Thiol	42.02	47.80	46.45	48.61
Hydrox	46.44	52.36	50.61	51.50
Amino	54.06	60.10	57.69	59.59
Ethynyl	48.51	53.11	52.52	53.87
Formyl	48.58	52.16	52.42	51.95
N-bound 1,2-azaborine	88.10	93.47	92.37	94.37
B-bound 1,2-azaborine	89.89	93.87	93.11	93.85

Table S15. CPCM energies (including electrostatic, cavitation, dispersion an repulsion energies)of Wheland intermediates of the nitration of substituted benzenes (in kcal.mol^{-1})

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	-145788.26	-274374.06	-274374.06	-274374.06
Phenyl	-290822.08	-419420.26	-419413.56	-419426.06
Methyl	-170467.73	-299063.72	-299062.03	-299067.65
Vinyl	-194372.43	-322969.83	-322964.07	-322975.07
Chlorine	-434209.26	-562796.22	-562794.04	-562801.61
Thiol	-395675.66	-524274.96	-524264.94	-524281.90
Hydrox	-193012.33	-321617.61	-321603.27	-321620.96
Amino	-180541.29	-309160.32	-309136.98	-309166.45
Ethynyl	-193586.28	-322176.94	-322173.06	-322180.57
Formyl	-216928.20	-345505.25	-345512.21	-345505.44
N-bound 1,2-azaborine	-292968.71	-421562.84	-421556.37	-421569.86
B-bound 1,2-azaborine	-292985.03	-421584.55	-421579.15	-421588.07

Reactions of substituted benzenes: chlorination

Table S16. Gas phase energies of Wheland intermediates of the chlorination of substituted benzenes (in Hartree)

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	-232.3242369	-692.2294010	-692.2294010	-692.2294010
Phenyl	-463.4482454	-923.3786414	-923.3615799	-923.3842689
Methyl	-271.6543528	-731.5729922	-731.5660550	-731.5754657
Vinyl	-309.7483501	-769.6708413	-769.6573384	-769.6755835
Chlorine	-691.9514522	-1151.8553758	-1151.8459608	-1151.8603404
Thiol	-630.5441050	-1090.4684767	-1090.4471506	-1090.4752792
Hydrox	-307.5769077	-767.5025049	-767.4819029	-767.5097905
Amino	-287.7041163	-747.6562039	-747.6183084	-747.6629372
Ethynyl	-308.4937206	-768.4059666	-768.3948532	-768.4091667
Formyl	-345.6884558	-805.5775012	-805.5803621	-805.5781613
N-bound 1,2-azaborine	-466.8705407	-926.7957302	-926.7753705	-926.8010776
B-bound 1,2-azaborine	-466.8936002	-926.8262289	-926.8138554	-926.8293134

Table S17 . ZPVE (computed at 298.15 K) of Wheland intermediates of the chlorination of substituted benzenes (in kcal.mol^{-1})

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	44.83	43.40	43.40	43.40
Phenyl	90.37	90.09	88.80	90.80
Methyl	60.29	59.28	58.80	58.71
Vinyl	62.68	61.75	61.24	61.94
Chlorine	37.49	36.27	35.82	36.37
Thiol	42.02	41.99	40.87	42.18
Hydrox	46.44	45.83	45.00	46.06
Amino	54.06	54.17	52.00	54.22
Ethynyl	48.51	47.25	46.95	47.29
Formyl	48.58	46.80	46.80	46.52
N-bound 1,2-azaborine	88.10	87.77	85.87	87.61
B-bound 1,2-azaborine	89.89	88.25	87.32	88.11

Table S18. CPCM energies (including electrostatic and cavitation energies)of Wheland intermediates of the chlorination of substituted benzenes (in kcal.mol^{-1})

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	-145788.26	-434430.49	-434430.49	-434430.49
Phenyl	-290822.08	-579470.99	-579463.25	-579475.30
Methyl	-170467.73	-459115.09	-459111.62	-459117.26
Vinyl	-194372.43	-483020.84	-483013.80	-483024.31
Chlorine	-434209.26	-722848.42	-722844.21	-722851.57
Thiol	-395675.66	-684326.56	-684314.53	-684331.51
Hydrox	-193012.33	-481665.38	-481652.96	-481670.49
Amino	-180541.29	-469210.01	-469186.21	-469215.67
Ethynyl	-193586.28	-482228.18	-482223.17	-482230.25
Formyl	-216928.20	-505559.90	-505562.56	-505560.18
N-bound 1,2-azaborine	-292968.71	-581615.42	-581605.34	-581619.20
B-bound 1,2-azaborine	-292985.03	-581634.42	-581628.77	-581637.03

Reactions of substituted benzenes: acylation

Table S19. Gas phase energies of Wheland intermediates of the acylation of substituted benzenes (in Hartree)

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	-232.3242369	-345.9707987	-345.9707987	-345.9707987
Phenyl	-463.4482454	-577.1157500	-577.1017861	-577.1199256
Methyl	-271.6543528	-385.3133410	-385.3068061	-385.3144700
Vinyl	-309.7483501	-423.4093577	-423.3975189	-423.4129238
Chlorine	-691.9514522	-805.5974697	-805.5881240	-805.5996900
Thiol	-630.5441050	-744.2064884	-744.1880745	-744.2118053
Hydrox	-307.5769077	-421.2433990	-421.2225219	-421.2468966
Amino	-287.7041163	-401.3878055	-401.3588428	-401.3974280
Ethynyl	-308.4937206	-422.1476197	-422.1363581	-422.1478667
Formyl	-345.6884558	-459.3275320	-459.3215864	-459.3204889

Table S20 . ZPVE (computed at 298.15 K) of Wheland intermediates of the acylation of substituted benzenes (in kcal.mol^{-1})

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	44.83	54.12	54.12	54.12
Phenyl	90.37	100.08	102.26	101.24
Methyl	60.29	70.08	69.08	69.89
Vinyl	62.68	72.65	71.85	73.58
Chlorine	37.49	47.19	46.46	47.79
Thiol	42.02	52.63	51.33	53.50
Hydrox	46.44	56.67	55.56	56.56
Amino	54.06	64.57	62.77	65.56
Ethynyl	48.51	58.10	57.66	58.03
Formyl	48.58	58.64	57.45	58.28

Table S21. CPCM energies (including electrostatic and cavitation energies) of Wheland intermediates of the acylation of substituted benzenes (in kcal.mol^{-1})

Substituents	Reactant	*Orto-*	*Meta-*	*Para-*
Hydrogen	-145788.26	-217150.77	-217150.77	-217150.77
Phenyl	-290822.08	-362189.73	-362182.29	-362193.16
Methyl	-170467.73	-241835.38	-241832.13	-241836.69
Vinyl	-194372.43	-265739.97	-265733.48	-265742.79
Chlorine	-434209.26	-505569.89	-505565.48	-505571.64
Thiol	-395675.66	-467045.75	-467035.40	-467049.42
Hydrox	-193012.33	-264385.71	-264373.33	-264388.69
Amino	-180541.29	-251925.95	-251906.36	-251932.09
Ethynyl	-193586.28	-264949.41	-264943.98	-264949.74
Formyl	-216928.20	-288283.44	-288283.03	-288281.63

Reactions of substituted benzenes: Mannich reactions

Table S22. Gas phase energies of Wheland intermediates of the reaction of methyleneiminium cation with substituted benzenes (in Hartree)

Substituents	Reactant	*Orto-*	*Para-*
Vinyl	-309.7483501		-404.7691923
Thiol	-630.5441050		-725.5682771
Hydrox	-307.5769077		-402.6042269
Amino	-287.7041163	-382.7548166	-382.7527759

Table S23 . ZPVE (computed at 298.15 K) of Wheland intermediates of the reaction of methyleneiminium cation with substituted benzenes (in kcal.mol^{1})

Substituents	Reactant	*Orto-*	*Para-*
Vinyl	62.68		95.84
Thiol	42.02		75.18
Hydrox	46.44		79.24
Amino	54.06	88.49	87.40

Table S24. CPCM energies (including electrostatic, cavitation, dispersion and repulsion energies)of Wheland intermediates of the reaction of methyleneiminium cation with substituted benzenes (in kcal.mol^{1})

Substituents	Reactant	*Orto-*	*Para-*
Vinyl	-194372.43		-254037.37
Thiol	-395675.66		-455343.87
Hydroxy	-193012.33		-252683.50
Amino	-180541.29	-240226.37	-240225.31

Table S25 Additional molecules - Computed energies

	Gas phase (Hartree)	CPCM energy (kcal.mol^{-1})	ZPVE (kcal.mol^{-1})
NO_2^+	-204.7905166	-128577.8	-6.156
$FeCl_3$ (S=5/2)	-1504.1843168	-943881.04	-19.317
$FeCl_4^-$ (S=5/2)	-1964.6024166	-1232834.3	-20.335
Cl_2	-920.4245908	-577569.4	-12.986
Br_2	-26.730174565	-16767.2	-14.706
Br^-	-13.4633275	-8503.15	-10.6
$H_2C=NH_2^+$	-95.011349197	-59682.60	19.631
HCOCl	-574.1977267	-360318.09	-4.027
HCO^+	-113.588755611	-7134.63	-3.273

Note: All solution energies in this table include electrostatic and cavitation effects. Values for Br_2, Br^-, NO_2^+ and $H_2C=NH_2^+$ also include dispersion and repulsion energies.

Table S26 Natural population charges on N-substituted 1,2-azaborines

	N1	B2	C3	C4	C5	C6
Hydrogen	-0.72115	0.47331	-0.50358	-0.15184	-0.29576	0.04629
Phenyl	-0.61198	0.49028	-0.50867	-0.1477	-0.28697	0.05112
Methyl	-0.5853	0.48389	-0.5037	-0.15444	-0.28562	0.05215
Vinyl	-0.59444	0.5106	-0.51205	-0.14282	-0.28676	0.05783
Chloro	-0.56565	0.49324	-0.49753	-0.14929	-0.27905	0.04015
Thiol	-0.71658	0.50974	-0.50623	-0.14452	-0.28661	0.04767
Hydroxy	-0.24589	0.41556	-0.49992	-0.15697	-0.28137	0.03402
Amino	-0.42756	0.49081	-0.49963	-0.15565	-0.28582	0.03346
Ethynyl	-0.61799	0.52711	-0.5089	-0.14091	-0.27948	0.06294
Formyl	-0.6465	0.53853	-0.507	-0.13206	-0.27803	0.04947

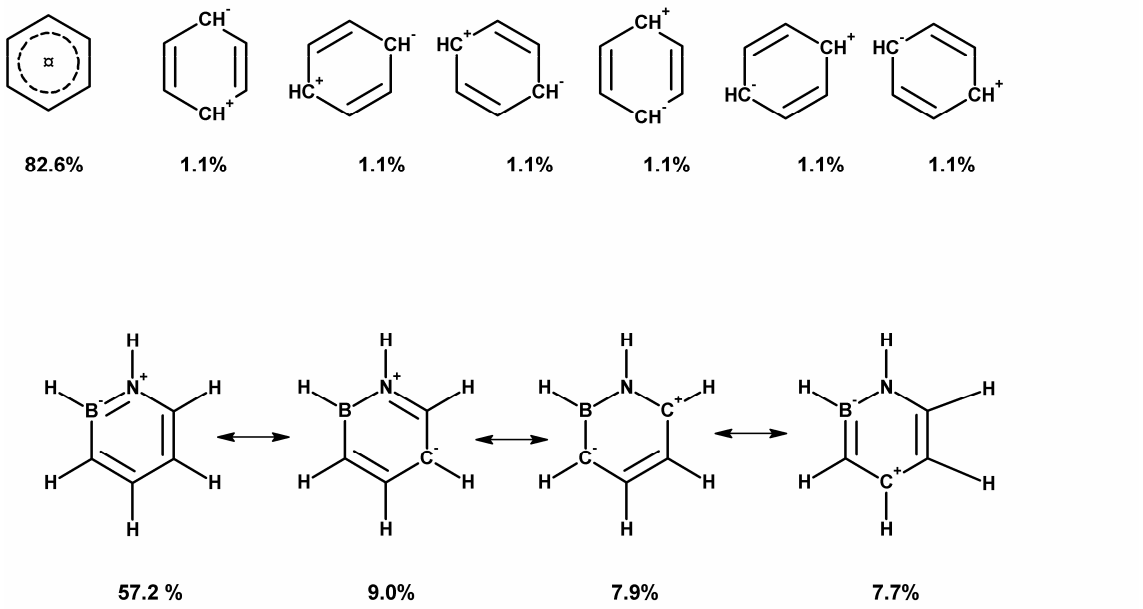
Table S27 Natural population charges on B-substituted 1,2-azaborines

	N1	B2	C3	C4	C5	C6
Hydrogen	-0.72115	0.47331	-0.50358	-0.15184	-0.29576	0.04629
Phenyl	-0.72343	0.67021	-0.49667	-0.14857	-0.29855	0.05347
Methyl	-0.7389	0.71263	-0.51224	-0.15183	-0.30093	0.04825
Vinyl	-0.71775	0.64136	-0.49354	-0.14799	-0.29926	0.05559
Chloro	-0.75665	0.62669	-0.53438	-0.1399	-0.2971	0.05468
Thiol	-0.75811	0.51916	-0.5211	-0.14517	-0.30257	0.05304
Hydroxy	-0.77348	0.89563	-0.52004	-0.15715	-0.31053	0.04793
Amino	-0.75618	0.78499	-0.51057	-0.1595	-0.32233	0.05408
Ethynyl	-0.70215	0.58095	-0.47344	-0.14763	-0.29314	0.05378
Formyl	-0.70555	0.54034	-0.46829	-0.14741	-0.2767	0.04767

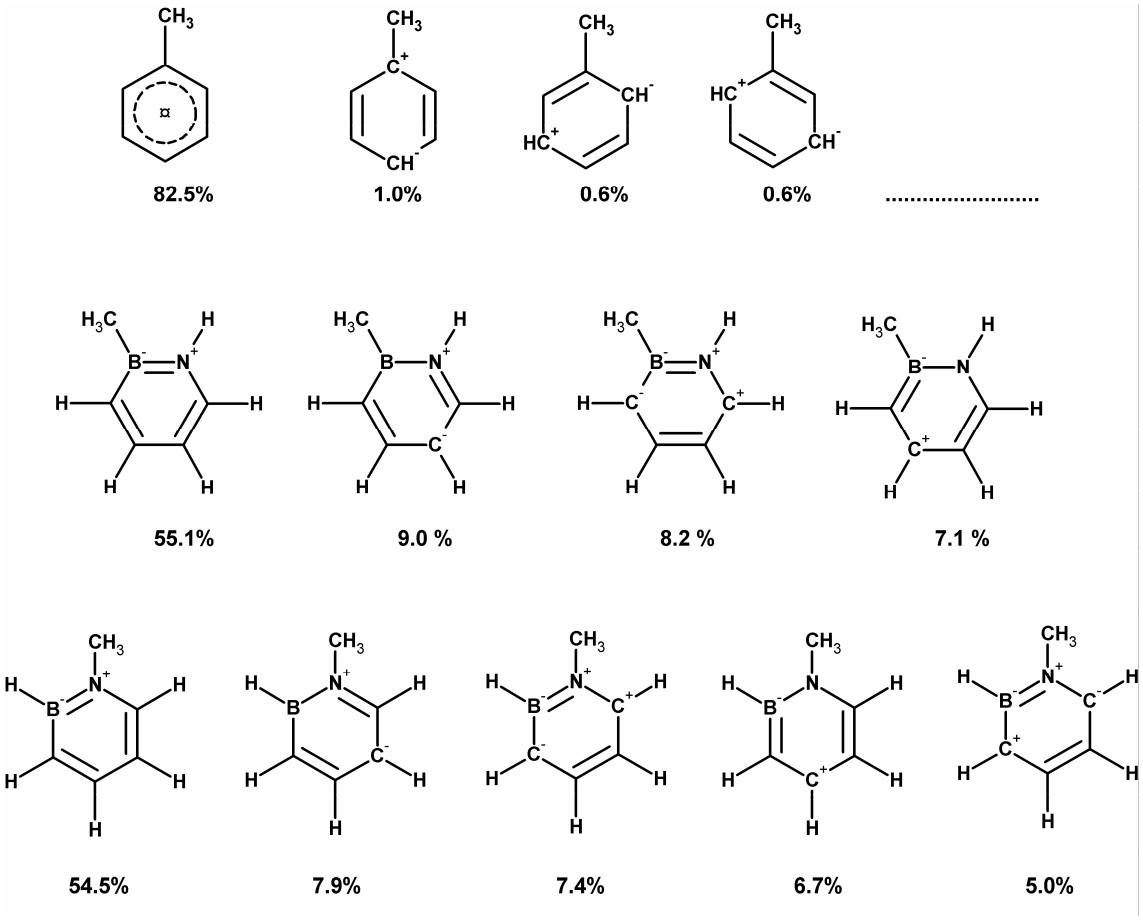
Table S28 Electrostatic potential ranges in Figures 1 and 2, Main Text (kcal.mol^{-1})

	Red			Blue		
Substituent	**N-substituted**	**Benzene**	**B-substituted**	**N-substituted**	**Benzene**	**B-substituted**
Hydrogen	88	93		151	140	
Phenyl	27	51	2	149	129	147
Methyl	78	88	61	147	134	151
Vinyl	69	55	56	152	141	148
Chloro	84	84	61	153	137	154
Thiol	77	65	72	151	149	148
Hydroxyl	50	51	34	158	174	161
Amino	65	83	70	156	146	149
Ethynyl	70	76	63	155	122	150
Formyl	22	18	-49	166	161	193

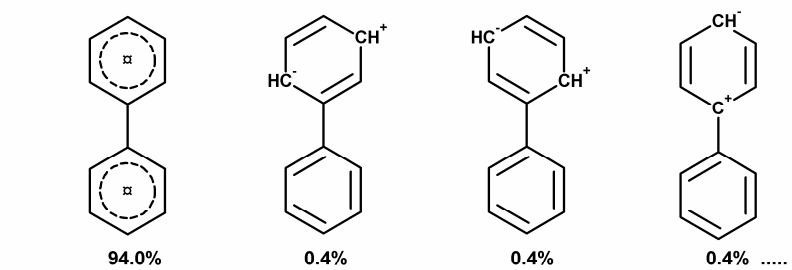
Most-important contributing resonance structures for benzene and 1,2-azaborine derivatives (as computed by Natural Resonance Theory)

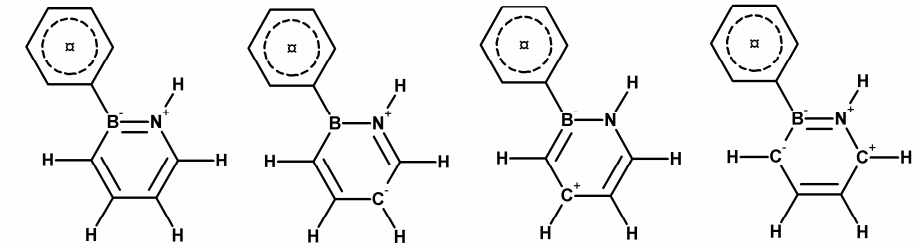


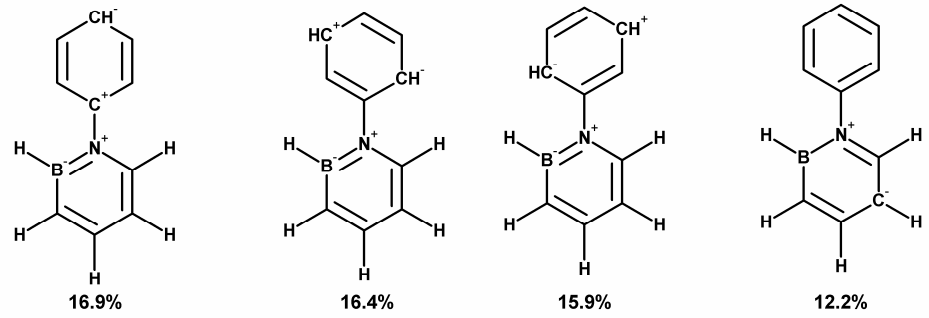
Methyl-substituted molecules

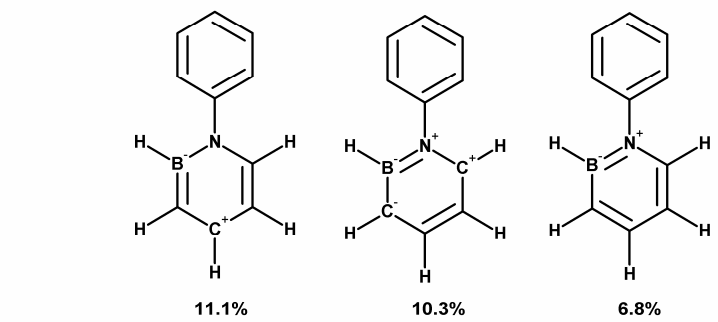


Phenyl-substituted molecules

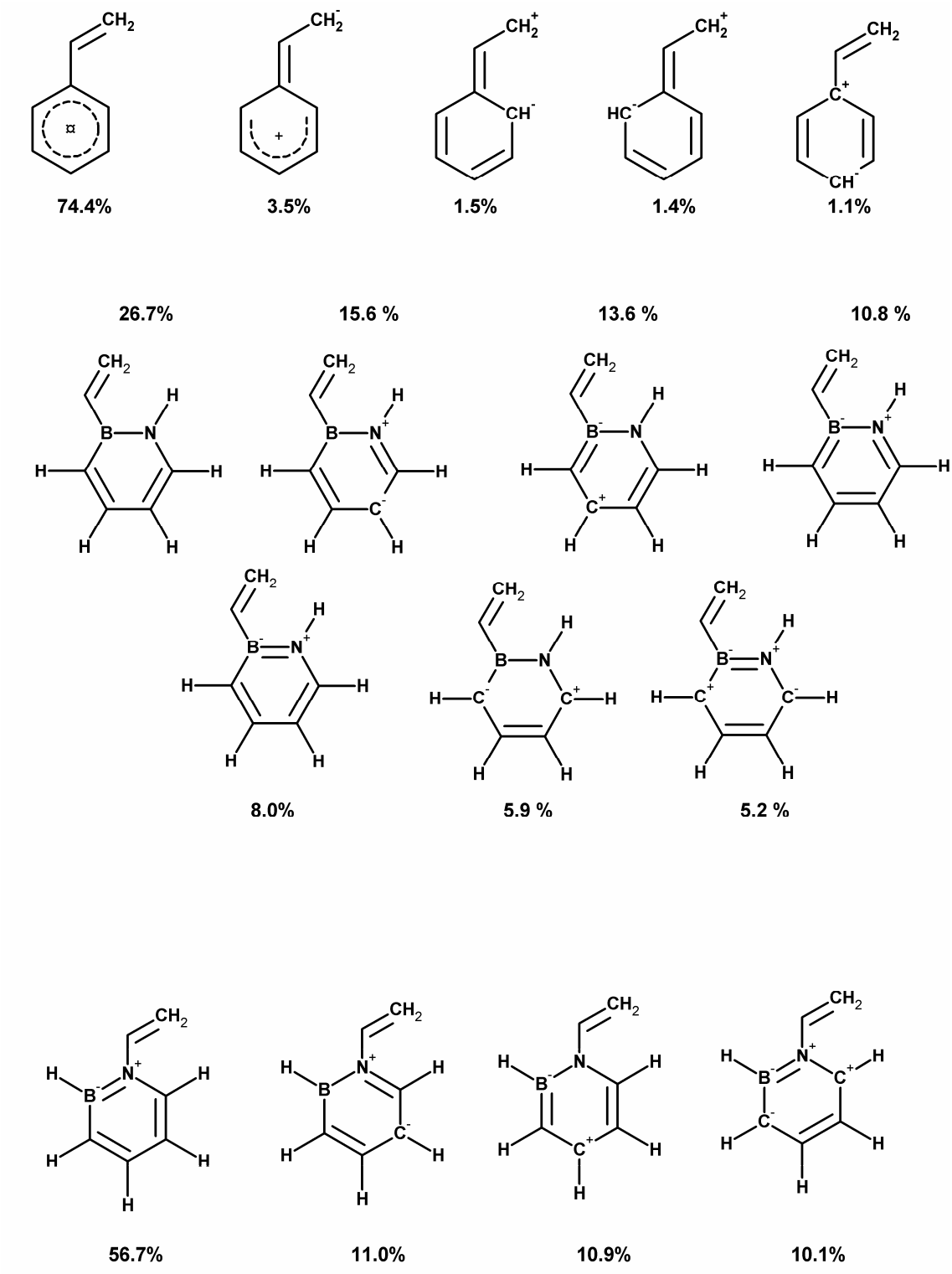




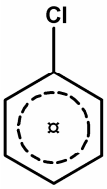




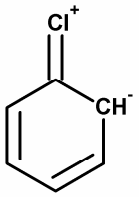
Vinyl-substituted molecules



Chlorine-substituted molecules



81.2%



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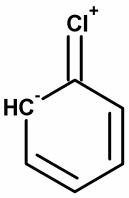

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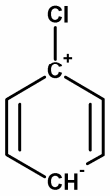

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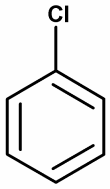

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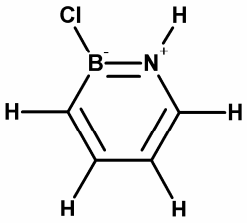

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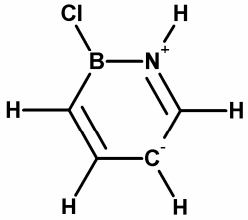

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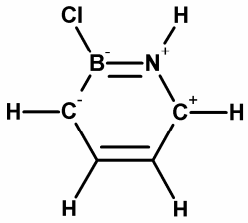

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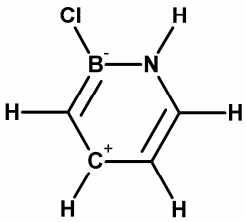

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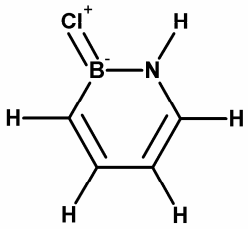

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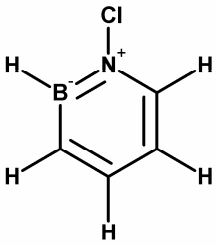

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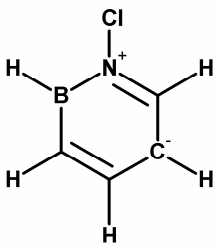

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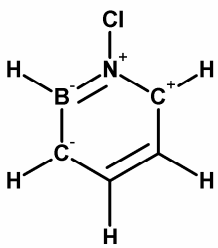

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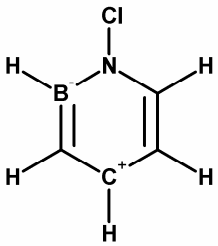
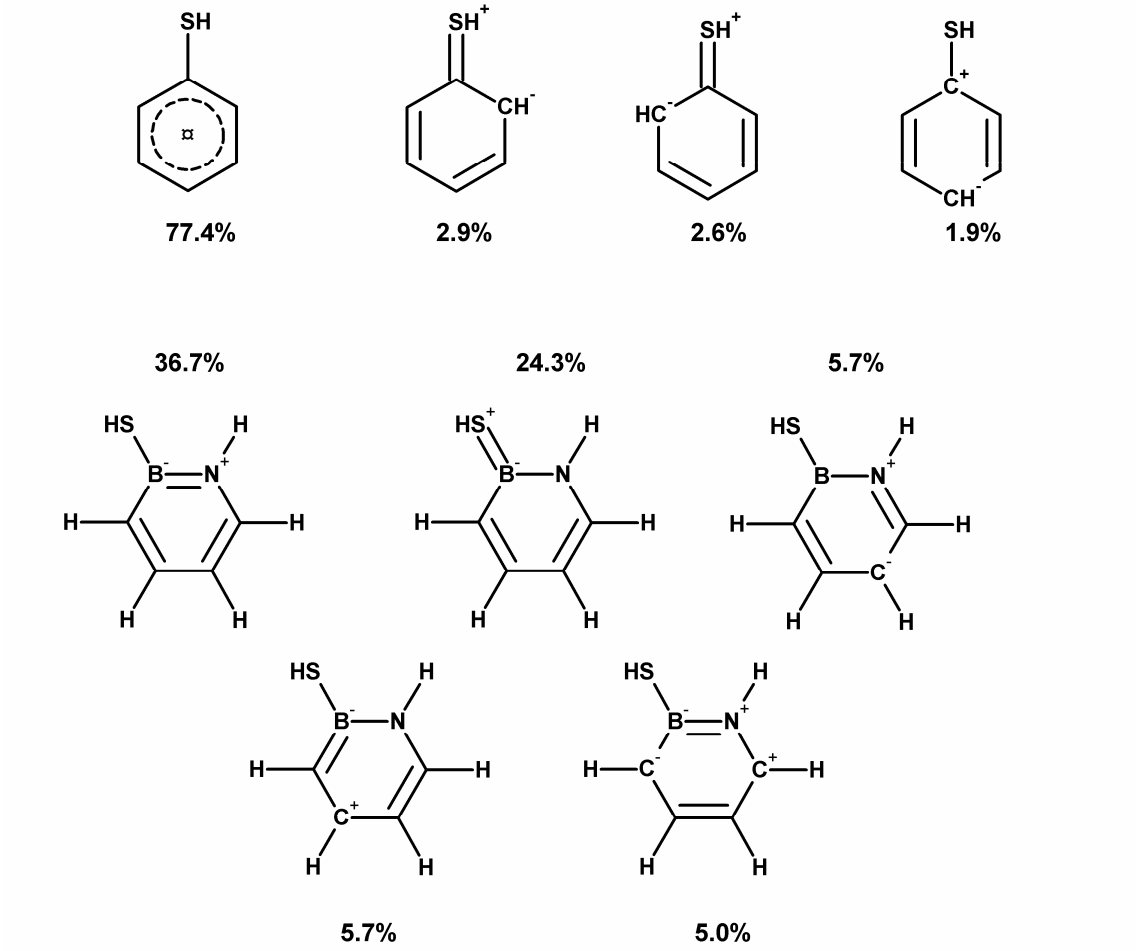
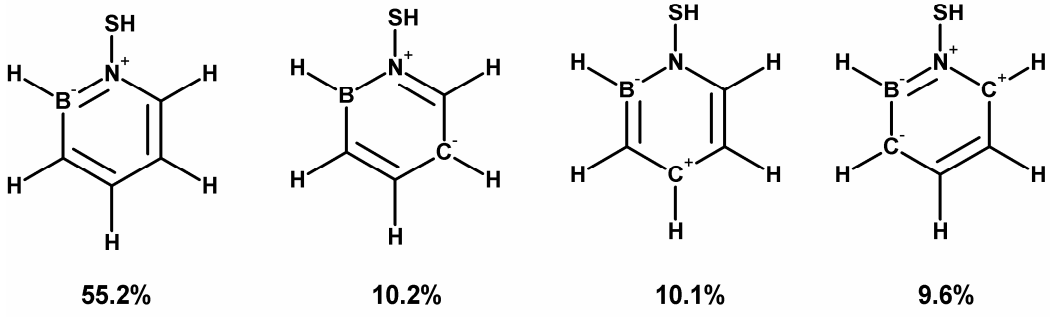


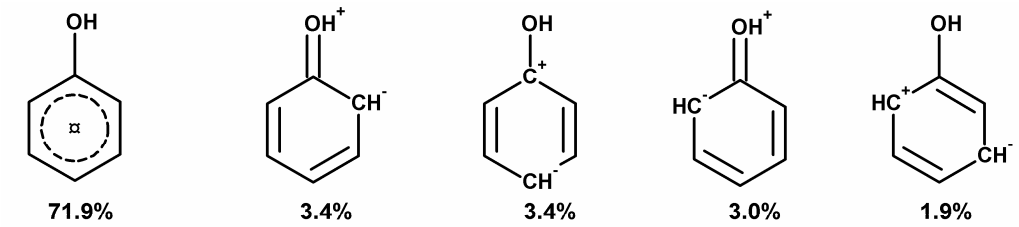
9.0%

Thiol-substituted molecules

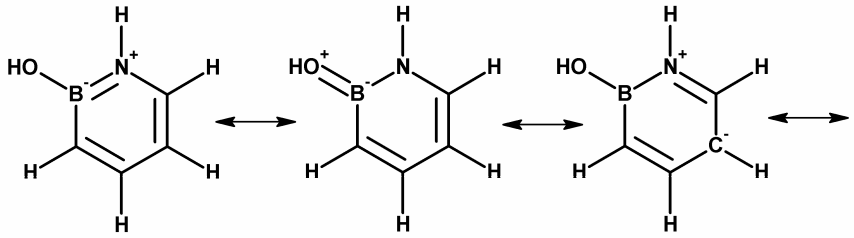




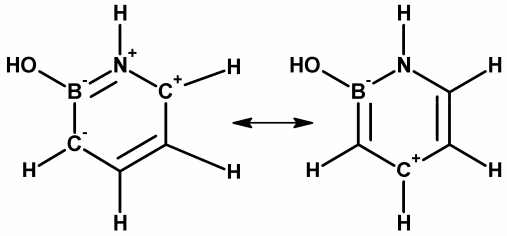
Hydroxyl-substituted molecules



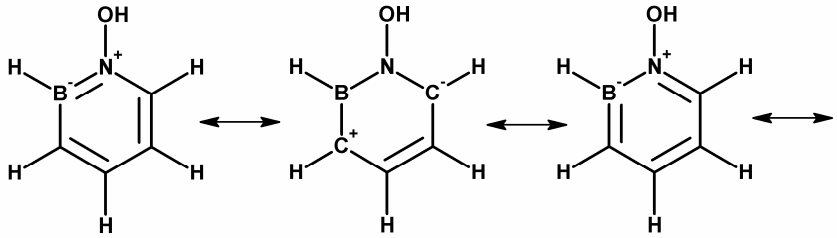
71.9% 3.4% 3.4% 3.0% 1.9%



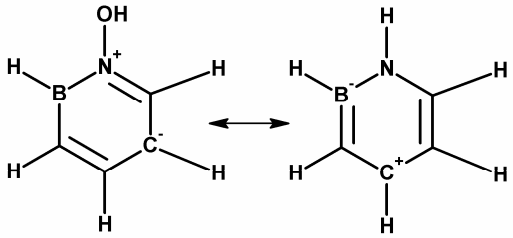
53.2 % 8.3% 8.3%



6.7% 5.1%

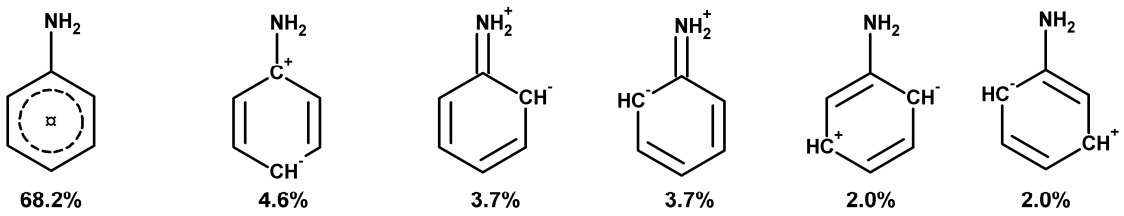


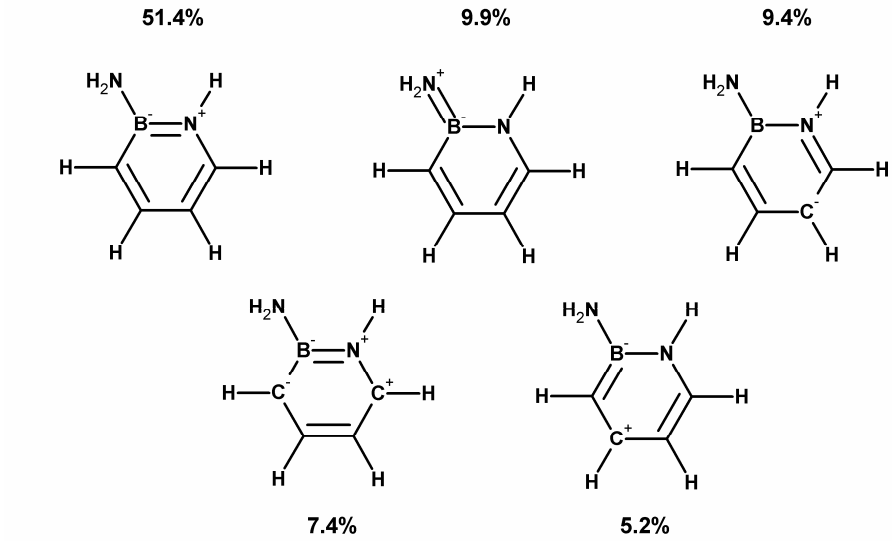
31.2 % 11.5% 11.2%

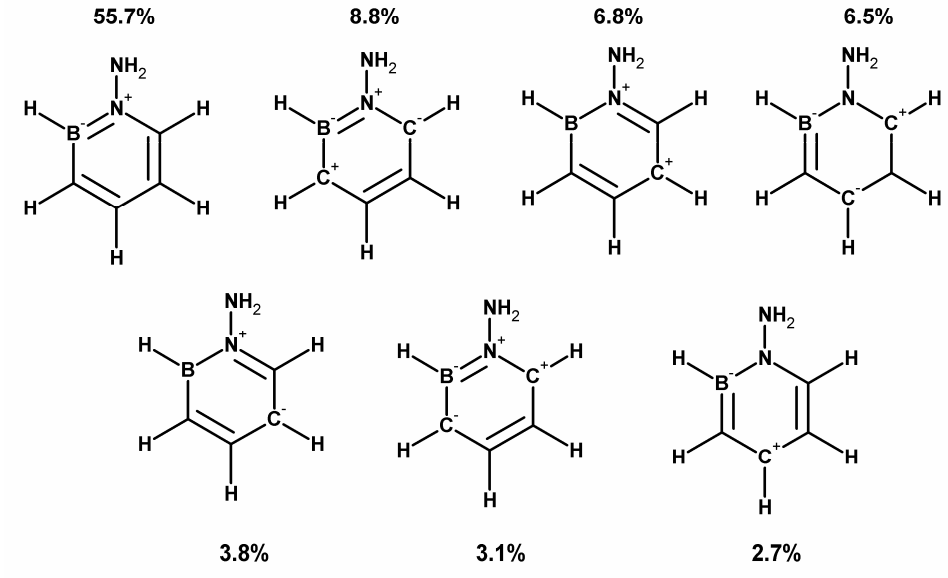


9.9% 7.9%

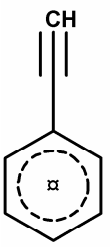
Amino-substituted molecules







Ethynyl-substituted molecules



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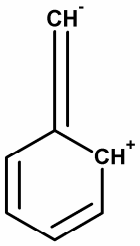

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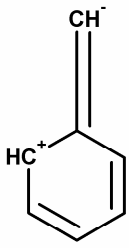

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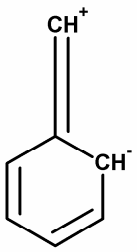

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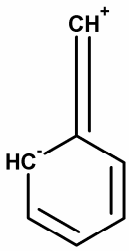

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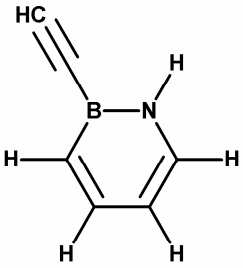

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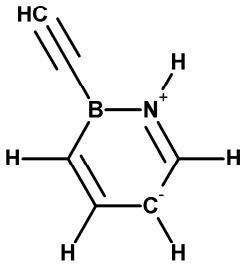

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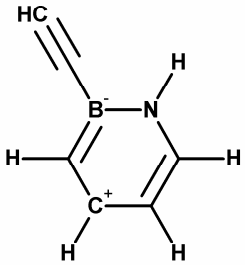

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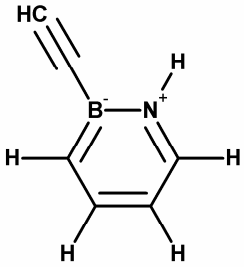

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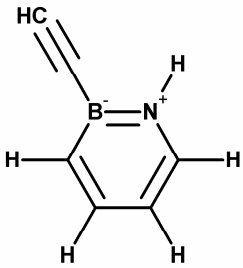

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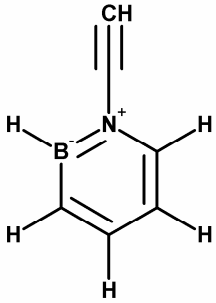

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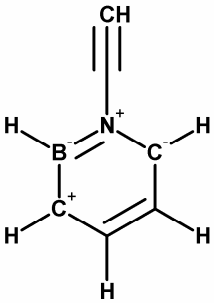

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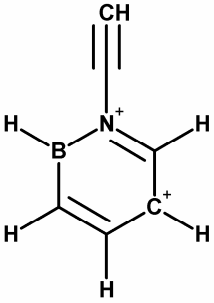

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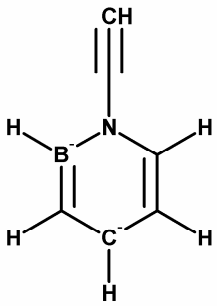
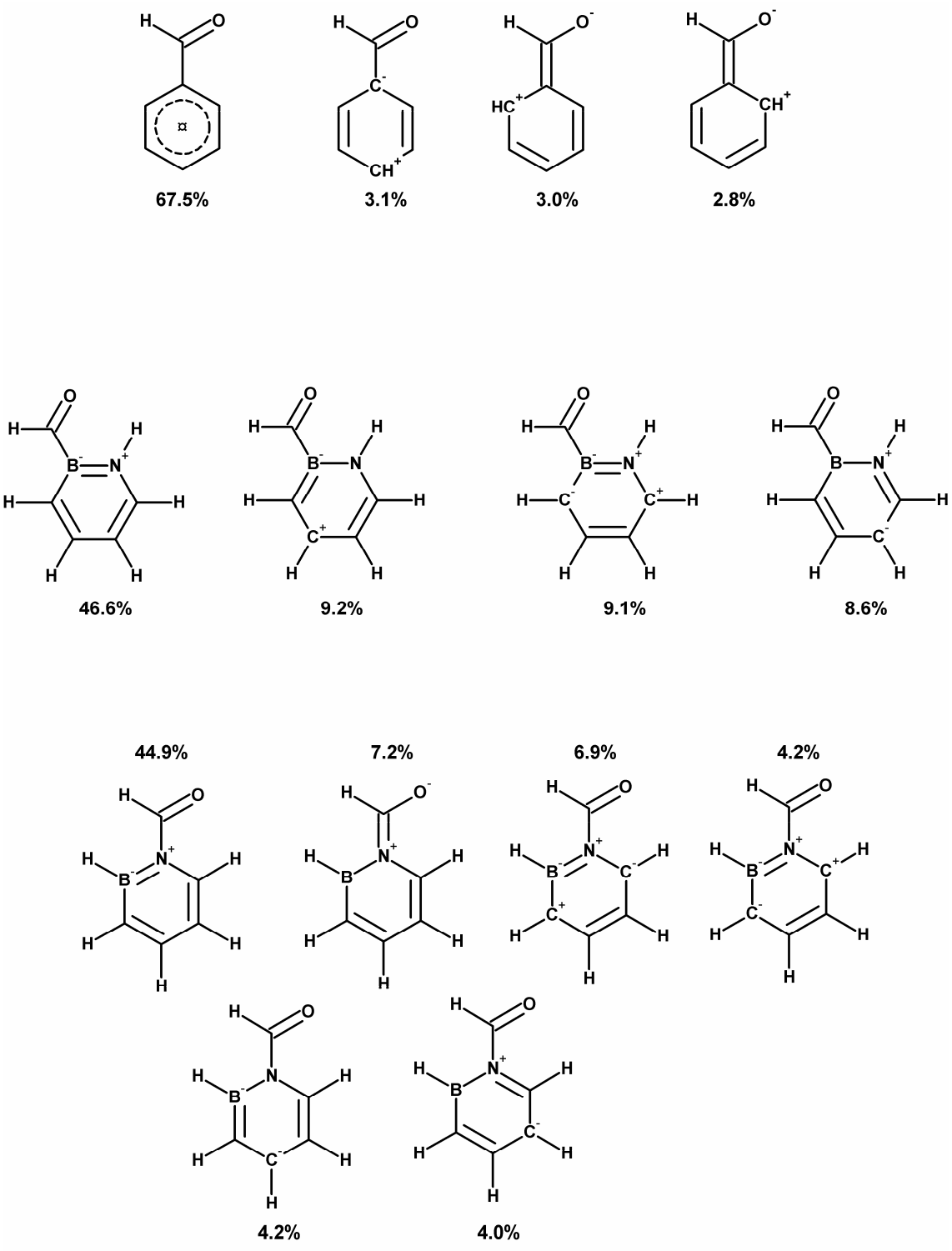


6.9%

Formyl-substituted molecules



Atom Coordinates (Reactants)

NO_2^+

N	-0.000009961	0.000002492	0.000000000
O	-1.129042450	-0.000001091	0.000000000
O	1.129051171	-0.000001091	0.000000000

Cl_2

Cl	0.000000000	0.000000000	0.0000000
Cl	0.000000000	0.000000000	2.0442525

Br_2

Cl	0.000000000	0.000000000	0.0000000
Cl	0.000000000	0.000000000	2.3135595

Methyleneiminium cation

C	0.682259460	0.000003001	-0.000006385
H	1.221031575	-0.945038676	0.000006106
H	1.221065591	0.945030231	0.000006395
N	-0.596991394	0.000000820	0.000014533
H	-1.135371246	-0.867855215	-0.000069043
H	-1.135467257	0.867816541	-0.000069360

Formyl chloride

C	0.703134384	-0.460366934	0.000000000
O	1.624016952	0.290124558	0.000000000
H	0.754860865	-1.556929557	0.000000000
Cl	-1.005877667	0.070148133	0.000000000

Formyl cation

C	0.635175638	-2.401966057	-1.643567908
O	-0.365353781	-2.845437838	-1.845645826
H	1.624091715	-1.963690293	-1.443893206

$FeCl_4^-$ *(S=5/2)*

Fe	-0.109486660	0.041607595	0.093934840
Cl	1.472859038	1.030885553	1.329214219
Cl	-1.769860747	-0.652501188	1.424595192
Cl	-0.912041490	1.502985535	-1.399491938
Cl	0.768599119	-1.714492330	-0.979901855

$FeCl_3$ (S=5/2)

Fe	0.416173285	0.564086492	0.335796466
Cl	1.268612605	0.144628219	-1.594422461
Cl	1.342725543	-0.214706782	2.114287427
Cl	-1.362482191	1.764707825	0.487107876

Benzene

C	-0.461296991	1.322485038	0.000000000
C	-1.350598600	0.243348096	0.000000000
C	0.917818363	1.091907879	0.000000000
C	-0.860529303	-1.066296450	0.000000000
C	1.407910536	-0.217790469	0.000000000
C	0.518681941	-1.296893332	0.000000000
H	1.608823748	1.930221643	0.000000000
H	-1.551338006	-1.904783609	0.000000000
H	2.479479096	-0.396606868	0.000000000
H	0.899176306	-2.314483604	0.000000000
H	-0.841906871	2.340041914	0.000000000
H	-2.422121959	0.422465387	0.000000000

Benzene$^{\bullet+}$

C	-0.456868951	1.310570002	0.000000000
C	-1.383199035	0.218210320	0.000000000
C	0.959572728	1.093307804	0.000000000
C	-0.902244499	-1.067735463	0.000000000
C	1.440524571	-0.192592344	0.000000000
C	0.514248983	-1.284990746	0.000000000
H	1.629423719	1.946777122	0.000000000
H	-1.572163062	-1.921149123	0.000000000
H	2.506024671	-0.396964607	0.000000000
H	0.894426153	-2.303328155	0.000000000
H	-0.837455731	2.328758707	0.000000000
H	-2.448713193	0.422655997	0.000000000

Phenylbenzene

C	-1.344843079	-0.068028972	-0.610415442
C	-0.820760128	1.076926577	0.016008744
C	-1.734438711	-1.180882486	0.136753161
C	-0.699247873	1.068738991	1.417029416
C	-1.607601376	-1.174294225	1.528532847
C	-1.087221689	-0.044169234	2.165107618
H	-2.129135801	-2.057089753	-0.369948274
H	-0.321386653	1.950858322	1.925600820
H	-1.910051721	-2.039972061	2.110515566
H	-0.992071097	-0.023887326	3.247145506
H	-1.423910614	-0.095004274	-1.693264503
C	-0.407927900	2.262614746	-0.780853125
C	0.753296714	2.985848680	-0.454810632

C	-1.168576916	2.692485646	-1.882880223
C	1.139737520	4.099284946	-1.202910456
C	-0.782477636	3.804964247	-2.632392718
C	0.374003580	4.513897603	-2.296079437
H	1.371199315	2.658169813	0.376109632
H	-2.083631129	2.166269179	-2.138541047
H	2.045411633	4.637197654	-0.937077628
H	-1.390883023	4.123115191	-3.474358667
H	0.674935200	5.379546696	-2.878885132

Phenylbenzene$^{\bullet+}$

C	-1.544311646	0.015269611	-0.596343646
C	-0.814263228	1.093047175	0.004005044
C	-1.918509327	-1.087103228	0.144938124
C	-0.495487498	0.989443924	1.397917308
C	-1.600880829	-1.155382098	1.516586622
C	-0.891593668	-0.107200422	2.136508789
H	-2.451778880	-1.905065166	-0.327578657
H	0.026300988	1.797315828	1.895670241
H	-1.904305566	-2.020638283	2.098041235
H	-0.663202236	-0.160610139	3.195608572
H	-1.773553947	0.038833746	-1.654533019
C	-0.414850141	2.246290570	-0.769399748
C	0.635052402	3.112874797	-0.320019760
C	-1.054626814	2.561108897	-2.013108786
C	1.021852417	4.205666544	-1.069253216
C	-0.675981267	3.668077455	-2.745337663
C	0.367471975	4.495345576	-2.283455462
H	1.164984932	2.891947758	0.598230636
H	-1.874939630	1.950875504	-2.370142946
H	1.833338589	4.839320968	-0.727677210
H	-1.184204395	3.905971194	-3.673666830
H	0.668671279	5.360629522	-2.866034835

Methylbenzene (Toluene)

C	-1.360534823	-0.315863559	-1.053387040
C	-1.433313702	0.952675657	-0.462370272
C	-1.553757763	-1.476736331	-0.296996801
C	-1.706043296	1.028145284	0.913170482
C	-1.823997807	-1.386576283	1.069719144
C	-1.899518616	-0.126735850	1.673001433
H	-1.492536051	-2.449146255	-0.777859898
H	-1.767584463	2.002679847	1.392594093
H	-1.974451762	-2.286075229	1.659612367
H	-2.109137739	-0.044460805	2.735979392
H	-1.150392319	-0.397752533	-2.117121132
C	-1.224506848	2.210197858	-1.275317644
H	-0.377134304	2.793486821	-0.896194589
H	-1.025647509	1.977491986	-2.325434520

H	-2.106823697	2.859915601	-1.238444310

Methylbenzene$^{\bullet+}$ (Toluene$^{\bullet+}$)

C	-1.355433388	-0.348539203	-1.084424724
C	-1.431580891	0.948306008	-0.471611354
C	-1.546781996	-1.481223642	-0.332565897
C	-1.711867834	1.041293444	0.944851435
C	-1.822329220	-1.365424075	1.064785332
C	-1.902462166	-0.092304794	1.694046452
H	-1.491523693	-2.465670290	-0.785486236
H	-1.768305776	2.025243859	1.400958010
H	-1.972793918	-2.265599110	1.654223295
H	-2.112765665	-0.029878863	2.756430151
H	-1.144950051	-0.414887970	-2.146995964
C	-1.228978421	2.183284768	-1.258643801
H	-0.402021102	2.772046024	-0.829783243
H	-1.027422689	1.993428910	-2.312838536
H	-2.110583532	2.838054759	-1.167854241

Styrene (vinylbenzene)

C	-1.305914876	-0.226799053	-0.669184690
C	-1.569872034	1.089202374	-0.242655690
C	-0.933022367	-1.212688612	0.241626249
C	-1.445044565	1.375086531	1.128899120
C	-0.812598390	-0.910815304	1.603599587
C	-1.070753779	0.388880710	2.043646504
H	-0.734710968	-2.221271341	-0.110043948
H	-1.644168559	2.384974356	1.479089925
H	-0.520800100	-1.681664228	2.310779388
H	-0.981881492	0.636330278	3.097632425
H	-1.391765748	-0.482533568	-1.720746929
C	-1.968000326	2.170940138	-1.160780520
H	-2.139693103	3.132430737	-0.677551523
C	-2.135976158	2.098947724	-2.489744522
H	-1.986652931	1.183544671	-3.054993470
H	-2.433549777	2.973813915	-3.058514405

Styrene$^{\bullet+}$ (vinylbenzene$^{\bullet+}$)

C	-1.306000879	-0.239950660	-0.693764132
C	-1.572418191	1.099885557	-0.242548048
C	-0.937829094	-1.213469283	0.207039065
C	-1.446023746	1.395426034	1.157333187
C	-0.819966603	-0.894573284	1.580252749
C	-1.076036161	0.414017140	2.050359993
H	-0.736660440	-2.224781971	-0.129517271
H	-1.646370483	2.405781497	1.500588987
H	-0.527774116	-1.668068080	2.284555382
H	-0.980576360	0.637028402	3.107549350

H	-1.393657569	-0.487855156	-1.745154590
C	-1.958378062	2.156063052	-1.118753369
H	-2.134964440	3.125881098	-0.658559003
C	-2.125903498	2.060833174	-2.484282159
H	-1.973640800	1.140092404	-3.037781343
H	-2.423221592	2.932330264	-3.058783500

Chlorobenzene

C	-0.756708519	-0.031524759	-1.074410096
C	-1.959113242	-0.048894408	-0.366451440
C	0.446280242	0.009562487	-0.364511845
C	-1.981410875	-0.025807147	1.028614577
C	0.444181492	0.032997348	1.032848659
C	-0.770029789	0.015222863	1.724323401
H	1.385478457	0.023177268	-0.909594972
H	-2.927878473	-0.039699040	1.557897627
H	1.382048958	0.064754935	1.578711861
H	-0.780758943	0.033263373	2.810142739
Cl	-3.479722055	-0.100777379	-1.252018863
H	-0.763842172	-0.050021410	-2.158755113

Chlorobenzene$^{\bullet+}$

C	-0.745475139	-0.031753542	-1.108588055
C	-1.977777437	-0.049417525	-0.377606734
C	0.435780155	0.008594476	-0.406596702
C	-2.006325689	-0.025891872	1.054832531
C	0.413219554	0.031865796	1.015697015
C	-0.813250965	0.014362994	1.736448640
H	1.385826539	0.022805499	-0.930218044
H	-2.961208852	-0.040270390	1.569223891
H	1.351256420	0.063577142	1.562547633
H	-0.800325507	0.032916606	2.821092126
Cl	-3.437021641	-0.099386337	-1.227889757
H	-0.768649334	-0.050620216	-2.192910942

Thiophenol

C	-0.741701868	-0.246304320	-1.109528458
C	-1.137489034	0.927681316	-0.453320994
C	-0.413277360	-1.384452975	-0.369491105
C	-1.200079915	0.946544916	0.948154623
C	-0.474934207	-1.366999404	1.026065117
C	-0.869999336	-0.195828226	1.678774821
H	-0.108106369	-2.287232503	-0.891003484
H	-1.505503095	1.850947805	1.466637809
H	-0.218701875	-2.253841850	1.597277259
H	-0.922880413	-0.167213244	2.763353037
H	-0.688427276	-0.277280831	-2.194095029
S	-1.572863461	2.426287775	-1.325395545
H	-1.374818152	1.952299424	-2.570336368

Thiophenol$^{\bullet+}$

C	-0.831592898	-0.295432586	-1.137626780
C	-1.284023069	0.877664849	-0.457830133
C	-0.397401085	-1.375229911	-0.399221661
C	-1.286279619	0.931706514	0.973900098
C	-0.402121245	-1.316388313	1.014760933
C	-0.847687233	-0.160402214	1.692692154
H	-0.051159550	-2.272635810	-0.900918458
H	-1.631432770	1.827933945	1.480468658
H	-0.057968624	-2.173443212	1.585587983
H	-0.844427931	-0.132668667	2.776993357
H	-0.830788076	-0.333456912	-2.222316564
S	-1.846633495	2.278902485	-1.281288321
H	-1.685014280	1.831823661	-2.547912784

Phenol

C	-0.869394973	-0.200657444	-1.171493521
C	-1.314649778	0.953345296	-0.517409912
C	-0.429210847	-1.295143227	-0.421719685
C	-1.319553418	1.013442994	0.880533042
C	-0.430662640	-1.245270529	0.974067946
C	-0.878147827	-0.085571820	1.617173219
H	-0.084943742	-2.187908954	-0.935873070
H	-1.668233526	1.918287642	1.367486289
H	-0.088569448	-2.097011478	1.553347226
H	-0.884143998	-0.034534248	2.702235041
H	-0.866448204	-0.244196786	-2.258748231
O	-1.759435215	2.060355928	-1.194896027
H	-1.708294630	1.907177280	-2.147414271

Phenol$^{\bullet+}$

C	-0.859638827	-0.226560213	-1.208526345
C	-1.313363210	0.949857634	-0.527059005
C	-0.430520745	-1.293129640	-0.459227593
C	-1.325514863	1.029437196	0.908793554
C	-0.441490656	-1.218110565	0.965121967
C	-0.891223361	-0.051667564	1.636143456
H	-0.081047207	-2.198247396	-0.944612183
H	-1.679051550	1.945619513	1.370169391
H	-0.099037362	-2.070726690	1.543751076
H	-0.889742607	-0.019495329	2.720302180
H	-0.861021283	-0.259018806	-2.294568994
O	-1.742325087	2.018240389	-1.159370910
H	-1.722573176	1.940536101	-2.131234062

Aniline

C	-1.541212812	-0.367946441	-1.060987320
C	-1.803947573	0.891177154	-0.492665906
C	-1.443349385	-1.501540446	-0.254027863

C	-1.967214149	0.980597704	0.901192264
C	-1.604091759	-1.409514094	1.131944558
C	-1.867806211	-0.159086930	1.699323198
H	-1.237757227	-2.463936128	-0.714701153
H	-2.178579087	1.945957037	1.355124939
H	-1.526320015	-2.293732441	1.756524661
H	-1.996807413	-0.066287064	2.774257319
H	-1.422175373	-0.455167799	-2.138449420
N	-1.959446180	2.021019738	-1.303020651
H	-1.516088397	1.976114861	-2.210272892
H	-1.812369832	2.911909573	-0.848812386

***Aniline*$^{\bullet+}$**

C	-1.536294268	-0.389537047	-1.089874231
C	-1.808115686	0.888874740	-0.492472348
C	-1.440790419	-1.501642764	-0.286850183
C	-1.975323981	1.000170177	0.930560752
C	-1.608384254	-1.384285197	1.114455245
C	-1.874818978	-0.127593671	1.710665693
H	-1.236698537	-2.472385290	-0.725649497
H	-2.178498550	1.971791681	1.370928702
H	-1.531535992	-2.268273795	1.739523971
H	-1.999529512	-0.057520979	2.785883769
H	-1.410015356	-0.461060276	-2.166080316
N	-1.905696938	1.977667756	-1.262509153
H	-1.792175812	1.929119943	-2.269551541
H	-2.096686411	2.892815511	-0.868304687

Ethynylbenzene

C	-1.915379650	-0.298635109	-0.822659491
C	-2.138125924	0.988635501	-0.295391736
C	-1.649909967	-1.370639001	0.028418607
C	-2.088656536	1.174699983	1.100152689
C	-1.602354364	-1.177377585	1.412541966
C	-1.822439402	0.097206361	1.944006857
H	-1.480004569	-2.358601666	-0.389446067
H	-2.259805410	2.165094169	1.509397178
H	-1.395215513	-2.014523427	2.072591755
H	-1.786747444	0.252618072	3.018294116
H	-1.952770305	-0.445232809	-1.897290081
C	-2.411191183	2.091582925	-1.165368521
C	-2.642051863	3.026125580	-1.902529202
H	-2.845841695	3.846515243	-2.552095457

***Ethynylbenzene*$^{\bullet+}$**

C	-1.912609576	-0.320501921	-0.848614745
C	-2.138455840	0.989982200	-0.296847954
C	-1.651271190	-1.373665118	-0.002986467

C	-2.090911510	1.194618389	1.127524397
C	-1.607440788	-1.156704232	1.396942989
C	-1.827800783	0.127454191	1.954774802
H	-1.478693864	-2.368364656	-0.399610801
H	-2.263881098	2.189704711	1.522712281
H	-1.400248404	-1.993745406	2.057624864
H	-1.787746929	0.261249025	3.030424795
H	-1.952800828	-0.453178028	-1.924309394
C	-2.403740289	2.061294750	-1.142007747
C	-2.637437872	3.007214832	-1.888263387
H	-2.842265196	3.832893144	-2.541473082

Benzaldehyde

C	-0.249730580	1.209088769	-0.000166695
C	-0.953878116	-0.003926485	-0.000291785
C	1.146157664	1.210940235	0.000001832
C	-0.251700516	-1.220937179	-0.000212510
C	1.839704933	-0.002709130	0.000179007
C	1.140497088	-1.217674220	0.000073150
H	1.690688268	2.150318324	0.000012468
H	-0.815435394	-2.148561729	-0.000571891
H	2.925963060	-0.004449879	0.000330678
H	1.686340839	-2.156482545	0.000268156
H	-0.798543869	2.148163569	-0.000192706
C	-2.434447944	0.016468890	-0.000538998
O	-3.146135458	-0.972768162	-0.000633351
H	-2.886093211	1.032096034	-0.000634706

***Benzaldehyde*$^{\bullet+}$**

C	-0.274071276	1.247415249	-0.010830563
C	-0.965958196	0.039910795	0.124950101
C	1.116846190	1.207851377	-0.082538907
C	-0.270102461	-1.223557230	0.114511302
C	1.812071486	-0.043946153	-0.079309295
C	1.119484547	-1.248108549	0.033738470
H	1.686859051	2.131600819	-0.108610416
H	-0.847375033	-2.138958420	0.195994028
H	2.895152204	-0.042109807	-0.158816117
H	1.651375426	-2.193166752	0.042205822
H	-0.801063677	2.196419511	-0.012400820
C	-2.446266471	0.025876382	0.163296255
O	-3.023803013	-0.974934226	-0.225342650
H	-3.001820336	0.932705717	0.454527081

1,2-dihydro-1,2-azaborine

B	-0.876539746	0.000000000	-1.208183571
N	-2.070419061	0.000000000	-0.402839450
C	0.418764093	0.000000000	-0.421323067
C	-2.062178953	0.000000000	0.965729126
C	0.362423474	0.000000000	0.957086514
C	-0.879270810	0.000000000	1.658104847
H	1.399551641	0.000000000	-0.891832175
H	-3.024737636	0.000000000	1.467623381
H	1.275244093	0.000000000	1.551940016
H	-0.901788429	0.000000000	2.742383061
H	-1.004707941	0.000000000	-2.395057780
H	-2.984338731	0.000000000	-0.837367560

1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.527944100	1.386684824	0.000000000
N	-1.378044396	0.187307194	0.000000000
C	0.997093490	1.085469561	0.000000000
C	-0.883582252	-1.044646271	0.000000000
C	1.447048373	-0.238475989	0.000000000
C	0.524989655	-1.287414612	0.000000000
H	1.735565057	1.883227715	0.000000000
H	-1.580456854	-1.878969059	0.000000000
H	2.507936073	-0.473181314	0.000000000
H	0.853263310	-2.321671710	0.000000000
H	-1.042308965	2.448643282	0.000000000
H	-2.392078442	0.273971926	0.000000000

1-phenyl-1,2-dihydro-1,2-azaborine

B	-1.450924272	-1.184645553	0.541914436
N	-0.712986474	-0.058044881	-0.001798373
C	-2.958974880	-1.069876893	0.510299351
C	-1.369226954	1.040426320	-0.510275994
C	-3.536527651	0.067983598	-0.010029648
C	-2.736445149	1.126290086	-0.526572456
H	-3.612954845	-1.849378499	0.894941982
H	-0.744606737	1.826043744	-0.921563291
H	-4.618881886	0.186156853	-0.043091782
H	-3.196557285	2.010999515	-0.953290471
H	-0.823142055	-2.094459667	0.985977667
C	0.725001750	-0.026564420	0.000983090
C	1.408300225	1.077309633	0.526375970
C	1.447288103	-1.108056531	-0.516022247
C	2.804940235	1.099865231	0.525796464
C	2.843021109	-1.082076968	-0.508033480
C	3.527434467	0.021274609	0.009658138
H	0.848143350	1.902304337	0.955674952
H	0.912897775	-1.958004081	-0.926555667

H	3.326040825	1.956768372	0.942574191
H	3.395161479	-1.924052760	-0.915021283
H	4.613062963	0.038917194	0.013026507

1-phenyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-1.448186357	-1.242414273	0.388339058
N	-0.687727094	-0.038454638	-0.071947372
C	-2.976426593	-1.107246873	0.432743612
C	-1.358101574	1.070101569	-0.441954544
C	-3.567239473	0.076236596	0.045396877
C	-2.757905848	1.149816703	-0.398198752
H	-3.608203792	-1.933490747	0.746843870
H	-0.776487400	1.908078169	-0.809333101
H	-4.645261150	0.210678219	0.059847356
H	-3.212107732	2.076123443	-0.734760755
H	-0.831231777	-2.201667969	0.690619673
C	0.735579554	-0.020187736	-0.015201486
C	1.413828172	1.144576608	0.404712543
C	1.460921128	-1.171935800	-0.391051167
C	2.801329626	1.157061518	0.428029431
C	2.848888266	-1.139084538	-0.378552042
C	3.524536080	0.019976461	0.030713203
H	0.858013673	2.005974456	0.759905086
H	0.940163485	-2.062351050	-0.722163270
H	3.325417637	2.041306906	0.774793136
H	3.408699428	-2.014640428	-0.689390979
H	4.609373717	0.034318376	0.055097249

1-methyl-1,2-dihydro-1,2-azaborine

B	-0.193338848	1.302924646	-0.000297991
N	-0.934963008	0.064317968	-0.000558896
C	1.315715562	1.177168763	-0.000033453
C	-0.295153312	-1.147259567	-0.000471974
C	1.882794751	-0.079376770	0.000436336
C	1.072629633	-1.249881712	0.000194556
H	1.978294585	2.040039497	-0.000263946
H	-0.928200694	-2.030707955	-0.001994856
H	2.964368712	-0.209406720	0.000461385
H	1.523041867	-2.236651719	0.000764799
H	-0.817499261	2.321459631	0.000007912
C	-2.403470425	0.031565628	0.000641466
H	-2.778803249	-0.481738115	0.892714848
H	-2.781914493	1.053288657	-0.002396914
H	-2.780268032	-0.487584798	-0.887404236

1-methyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.198867036	1.306726275	-0.000220321
N	-0.962418454	0.039299207	-0.000456866
C	1.345698042	1.168190114	-0.000050939
C	-0.321126484	-1.121108495	-0.000426279

C	1.928827195	-0.097503904	0.000343564
C	1.105451126	-1.226037960	0.000176959
H	1.992533688	2.041857283	-0.000204264
H	-0.919937567	-2.029664093	-0.001449631
H	3.007034269	-0.229862275	0.000468620
H	1.526746609	-2.226210099	0.000678609
H	-0.801089247	2.322523922	0.000040606
C	-2.448736508	0.032887554	0.000521514
H	-2.814388999	-0.474001595	0.896545776
H	-2.801830366	1.061783681	-0.002538040
H	-2.815847478	-0.479913193	-0.891512269

1-vinyl-1,2-dihydro-1,2-azaborine

B	-1.241545804	-0.252068403	-0.755027046
N	-1.529644579	1.091510791	-0.274056558
C	-0.893667261	-1.280342284	0.296504486
C	-1.456087418	1.377954296	1.072714451
C	-0.850563915	-0.905562141	1.621522685
C	-1.132257332	0.435082540	2.009783586
H	-0.665110838	-2.313698503	0.045582597
H	-1.677175818	2.401927180	1.357978565
H	-0.596871617	-1.620433902	2.403083211
H	-1.094205457	0.730803572	3.052539364
H	-1.282163436	-0.455606807	-1.926362864
C	-1.887730407	2.180417081	-1.120320739
H	-1.858861308	3.142109879	-0.614141754
C	-2.242515284	2.117661001	-2.406090003
H	-2.300910577	1.189450340	-2.960375302
H	-2.480093355	3.036356178	-2.929833764

1-vinyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.024219959	-1.190177941	-0.000568939
N	0.570161633	0.210396073	-0.000329099
C	-1.506824411	-1.325992354	-0.000909246
C	-0.285767276	1.245987563	-0.000161153
C	-2.296727588	-0.194440884	0.000850428
C	-1.683402607	1.079086277	0.000708085
H	-1.982998006	-2.302643166	-0.001652925
H	0.139766704	2.245210945	0.000082654
H	-3.381591560	-0.250039071	0.002199030
H	-2.287785071	1.980543331	0.000449610
H	0.782904965	-2.090923468	0.000522603
C	1.955201841	0.494979485	-0.001288917
H	2.184353900	1.556274450	-0.004234543
C	2.944440877	-0.418270877	0.001477731
H	2.784521538	-1.488588976	0.004828003
H	3.969833731	-0.065921718	0.000533126

1-chloro-1,2-dihydro-1,2-azaborine

B	-0.724892016	-0.032382289	-1.173923774
N	-1.940432856	-0.049217050	-0.394808482
C	0.529100219	0.012248037	-0.324963776
C	-1.994061319	-0.027131768	0.974907325
C	0.432060798	0.033088080	1.049476322
C	-0.832503075	0.013398165	1.701751939
H	1.520510311	0.028645276	-0.772411258
H	-2.975545794	-0.042780191	1.432335654
H	1.323904939	0.064751590	1.673031506
H	-0.903633189	0.029993762	2.783771109
Cl	-3.494316003	-0.100130411	-1.196902266
H	-0.802904525	-0.054459995	-2.358455971

1-chloro-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.270956514	-1.320629517	0.000073193
N	0.447888202	-0.018622158	-0.000181220
C	-1.814460366	-1.181247295	0.000037966
C	-0.178849937	1.152332885	0.000050736
C	-2.408935501	0.077159484	-0.000007653
C	-1.604467457	1.222577565	0.000010066
H	-2.450997946	-2.062718586	0.000020010
H	0.421890254	2.057485848	0.000344625
H	-3.488742360	0.195064605	-0.000307321
H	-2.042275838	2.215944374	0.000043763
Cl	2.174695356	-0.015515602	0.000015480
H	0.361651789	-2.313817562	-0.000004710

1-mercapto-1,2-dihydro-1,2-azaborine

B	-0.836178896	-0.319841071	-1.197173910
N	-1.279540366	0.860419289	-0.478596877
C	-0.361201632	-1.463565478	-0.322948353
C	-1.284122774	0.927422415	0.899147211
C	-0.387280639	-1.325321200	1.046628244
C	-0.851636915	-0.125156124	1.659818584
H	-0.000043969	-2.401409753	-0.739483200
H	-1.648776743	1.849451130	1.337591489
H	-0.055905741	-2.132055636	1.699005417
H	-0.872840271	-0.026686378	2.739869302
H	-0.871433164	-0.300300394	-2.386107088
S	-1.901405925	2.259604831	-1.335853666
H	-0.719196411	2.899678412	-1.486469001

1-mercapto -1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.263262607	1.307449560	-0.000405574
N	-0.495230342	0.010636155	-0.000424259
C	1.791379907	1.182342569	0.000172075
C	0.151847249	-1.164742316	-0.000382082
C	2.373230693	-0.067727594	0.000395404

C	1.557780520	-1.224920318	-0.000048426
H	2.428231644	2.062772067	0.000441603
H	-0.437037919	-2.077782999	-0.000351593
H	3.451828084	-0.196217503	0.000874958
H	2.006737271	-2.213168071	-0.000116097
H	-0.371965722	2.304877096	-0.000919947
S	-2.227456441	-0.014426280	0.000316982
H	-2.352827912	1.328810315	-0.001290472

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.864460711	-0.215644194	-1.253861337
N	-1.304433515	0.927363296	-0.507146382
C	-0.401762543	-1.363642167	-0.394401414
C	-1.320780444	1.016312033	0.846413654
C	-0.434039992	-1.236643758	0.983106354
C	-0.893333291	-0.047738472	1.606594128
H	-0.039774385	-2.298647482	-0.815557109
H	-1.681492207	1.951343933	1.258844762
H	-0.105842541	-2.052364188	1.624998623
H	-0.915845833	0.044532378	2.686502061
H	-0.909508109	-0.140657925	-2.446577419
O	-1.775147398	2.101921275	-1.130148132
H	-1.707292474	1.909242696	-2.078822943

1-hydroxy -1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.166965973	-1.323902830	0.000192495
N	0.911065640	-0.037393213	0.000066777
C	-1.364588719	-1.167986914	0.000063454
C	0.319758603	1.144427695	0.000562880
C	-1.929508012	0.098456200	-0.000248141
C	-1.101587869	1.235283902	-0.000120223
H	-2.017362612	-2.036818387	0.000012186
H	0.960109268	2.021852413	0.001539177
H	-3.006237644	0.239875496	-0.000857950
H	-1.527183799	2.233638919	-0.000407511
H	0.809238271	-2.317291628	0.000429223
O	2.282762036	0.009620018	-0.000622325
H	2.601139903	-0.912388186	0.003059400

1-amino-1,2-dihydro-1,2-azaborine

B	-1.552007784	-0.380574002	-1.144485101
N	-1.831461270	0.871862701	-0.485262202
C	-1.432471007	-1.576329867	-0.216149416
C	-1.977900029	0.975334885	0.876047469
C	-1.590778916	-1.403419577	1.141046783
C	-1.865495306	-0.118607958	1.693374503
H	-1.223953705	-2.578796066	-0.583940614
H	-2.186551452	1.968115762	1.264745358

H	-1.510139649	-2.244255839	1.828731609
H	-1.989189936	0.012793735	2.762942817
H	-1.440792674	-0.376721054	-2.327884561
N	-1.963230229	2.059733783	-1.269303315
H	-1.265938944	2.736408972	-0.964896155
H	-2.888808110	2.455888028	-1.117311029

1-amino-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.174758368	-1.316806645	0.002867478
N	0.941911489	-0.015833273	0.007815385
C	-1.337974942	-1.178419429	-0.000749266
C	0.316550793	1.184904321	0.002532813
C	-1.896914525	0.074526660	-0.002076126
C	-1.070252342	1.242279711	0.000148207
H	-1.987911535	-2.048423831	-0.004034968
H	0.932281742	2.078575765	-0.001286741
H	-2.973665086	0.218537390	-0.004394077
H	-1.525849675	2.227106443	0.000230061
H	0.840565210	-2.295608136	0.006843555
N	2.280463406	-0.079533382	-0.026090905
H	2.699580842	-0.991102516	0.111295576
H	2.824644954	0.764342672	0.115668172

1-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.155922098	-1.313460189	0.000250513
N	0.575301995	-0.048460063	0.000450208
C	-1.663347263	-1.188758162	-0.000239036
C	-0.078906157	1.176794714	0.000109975
C	-2.238274501	0.061691775	-0.000154329
C	-1.441599490	1.246680695	-0.000043554
H	-2.318470764	-2.056650113	-0.000790811
H	0.557577945	2.053898302	0.000111765
H	-3.320574892	0.181899506	-0.000131319
H	-1.909349576	2.225055654	-0.000245093
H	0.487883405	-2.312796608	0.000707345
C	1.938944744	-0.029385719	-0.000233184
C	3.147260852	-0.012584471	0.000166160
H	4.212518779	-0.006457392	-0.003952880

1-ethynyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.144471715	1.312406726	-0.000287979
N	-0.598949787	0.000489410	-0.000460082
C	1.680907929	1.192616452	0.000129536
C	0.063774493	-1.173938768	-0.000396685
C	2.274453745	-0.056582500	0.000605546
C	1.472021317	-1.219233070	0.000230070
H	2.313778279	2.075996455	-0.000009863
H	-0.531081633	-2.081701453	-0.000725719

H	3.354409183	-0.174145942	0.001091157
H	1.931316539	-2.202699397	0.000253041
H	-0.507491941	2.294356490	-0.000286375
C	-1.954492586	0.018958120	-0.001596213
C	-3.165560512	0.035899705	0.001802628
H	-4.235775501	0.060227691	-0.000010264

1-formyl-1,2-dihydro-1,2-azaborine

B	0.172748051	-1.348767446	-0.000298449
N	0.944169795	-0.104646009	-0.000583050
C	-1.333828792	-1.174820220	0.000026630
C	0.321439143	1.134072979	-0.000436768
C	-1.869877469	0.090324547	0.000377556
C	-1.034869121	1.253476849	0.000142258
H	-2.015259210	-2.022135101	-0.000030874
H	0.974187102	2.002064137	-0.001348329
H	-2.947968082	0.244319030	0.000579852
H	-1.472930857	2.245486178	0.000538466
H	0.769732336	-2.372152449	-0.000122612
C	2.363385922	-0.091101237	-0.000930607
O	3.068631068	-1.068513919	-0.001094268
H	2.773320408	0.936313809	-0.001029402

1-formyl -1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.201030544	1.331320917	-0.000190647
N	-0.963644067	0.072678944	-0.000418882
C	1.344517934	1.165139429	-0.000045387
C	-0.348136954	-1.116212442	-0.000369887
C	1.905527424	-0.115123853	0.000258575
C	1.070609575	-1.237106964	0.000165221
H	2.010150069	2.024701435	-0.000135532
H	-0.990241650	-1.995418533	-0.000931032
H	2.982343199	-0.260099370	0.000458843
H	1.484257042	-2.240623418	0.000544491
H	-0.797071245	2.351099411	-0.000036066
C	-2.442299523	0.070078216	-0.000739599
O	-3.062586702	-0.948461075	-0.000896749
H	-2.852438783	1.087898319	-0.000799745

2-phenyl-1,2-dihydro-1,2-azaborine

B	0.747147972	0.071573865	0.000000000
N	1.513780545	-1.155438522	0.000000000
C	1.613061560	1.325036187	0.000000000
C	2.880510473	-1.209899131	0.000000000
C	2.985227055	1.206888010	0.000000000
C	3.631485124	-0.064680287	0.000000000
H	1.202277883	2.332401018	0.000000000

H	3.333491880	-2.196486036	0.000000000
H	3.618051829	2.093627931	0.000000000
H	4.713239302	-0.138262498	0.000000000
H	1.050852001	-2.055514249	0.000000000
C	-0.827158087	0.018344350	0.000000000
C	-1.580568111	1.210324529	0.000000000
C	-1.557768561	-1.187940105	0.000000000
C	-2.976908615	1.203065288	0.000000000
C	-2.953702636	-1.210029910	0.000000000
C	-3.670554665	-0.010026581	0.000000000
H	-1.064777417	2.166290623	0.000000000
H	-1.038386637	-2.144699924	0.000000000
H	-3.523442142	2.142309293	0.000000000
H	-3.481454496	-2.159937394	0.000000000
H	-4.756907500	-0.021154659	0.000000000

2-phenyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.720112822	0.055101338	0.000000000
N	1.510076873	-1.192028365	0.000000000
C	1.595331347	1.325139236	0.000000000
C	2.842416212	-1.221429515	0.000000000
C	2.984116294	1.221802958	0.000000000
C	3.605426981	-0.035379051	0.000000000
H	1.174579370	2.326504260	0.000000000
H	3.329746599	-2.192034744	0.000000000
H	3.610920199	2.109559949	0.000000000
H	4.686162301	-0.124468488	0.000000000
H	1.053953962	-2.099125735	0.000000000
C	-0.813738649	0.010663390	0.000000000
C	-1.560769973	1.226483656	0.000000000
C	-1.553980229	-1.207830911	0.000000000
C	-2.947452158	1.225652672	0.000000000
C	-2.938656727	-1.213907620	0.000000000
C	-3.641207252	0.005696763	0.000000000
H	-1.039098558	2.177408728	0.000000000
H	-1.041666669	-2.166249698	0.000000000
H	-3.495864603	2.161825871	0.000000000
H	-3.483719582	-2.152073453	0.000000000
H	-4.727032552	0.001051517	0.000000000

2-methyl-1,2-dihydro-1,2-azaborine

B	-1.002418984	0.077749927	-0.000131043
N	-0.243786627	-1.152523845	-0.000055976
C	-0.130402888	1.328301822	-0.000237952
C	1.124820381	-1.216162403	-0.000039701
C	1.240605677	1.202929054	0.000187633
C	1.879536113	-0.074332311	0.000076815
H	-0.546968991	2.334468085	-0.000402908
H	1.573613120	-2.204708264	-0.000495676
H	1.880295338	2.085033309	0.000737941

H	2.961109225	-0.152997132	-0.000392773
H	-0.722740303	-2.044938686	0.001011307
C	-2.586922900	0.024256479	0.000114787
H	-2.996533059	-0.994225498	-0.000265746
H	-3.000127513	0.539417409	0.877176043
H	-3.000441580	0.540138507	-0.876368460

2-methyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-1.024590445	0.076723166	-0.000064473
N	-0.255464892	-1.192799508	-0.000021265
C	-0.100054484	1.337271002	-0.000143893
C	1.069089457	-1.248404180	-0.000041453
C	1.288955090	1.204175837	0.000138096
C	1.869415091	-0.067872998	0.000018434
H	-0.517582921	2.341707560	-0.000394724
H	1.542370298	-2.227011174	-0.000148314
H	1.938439366	2.075307017	0.000419523
H	2.947117832	-0.192601050	-0.000168387
H	-0.747491726	-2.083783572	0.000485721
C	-2.571624915	0.074487491	0.000059352
H	-3.038605683	-0.914407010	-0.000312283
H	-2.953229599	0.630123696	0.869941445
H	-2.953456277	0.630928031	-0.869186820

2-vinyl-1,2-dihydro-1,2-azaborine

B	0.556050552	0.309416184	0.000902489
N	0.026297838	-1.036870048	0.000924686
C	-0.514381510	1.389705976	0.000228640
C	-1.307756631	-1.331669778	0.000137924
C	-1.845090469	1.030308959	-0.000630288
C	-2.251038514	-0.336328143	-0.000720578
H	-0.274798010	2.451862645	0.000332233
H	-1.581146630	-2.382384026	0.000206682
H	-2.627259746	1.788662522	-0.001212029
H	-3.302040497	-0.603191055	-0.001391047
H	0.647013325	-1.836854190	0.001656948
C	2.101688081	0.566662268	0.000742083
H	2.422132839	1.611067068	0.001700595
C	3.082381040	-0.352402113	-0.001386637
H	2.882055802	-1.424297366	-0.002701324
H	4.136419502	-0.083540823	-0.001904102

2-vinyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.572680069	0.307893956	0.000794078
N	0.041394885	-1.073569104	0.000830688
C	-0.531847335	1.391088946	0.000225415
C	-1.257269944	-1.351186488	0.000139066
C	-1.877994422	1.026675847	-0.000577128
C	-2.238683829	-0.325949661	-0.000659929

H	-0.289053069	2.451150497	0.000343931
H	-1.556904705	-2.395542174	0.000205056
H	-2.664950106	1.775962587	-0.001075485
H	-3.280986038	-0.626373067	-0.001247628
H	0.665037169	-1.876164604	0.001495864
C	2.073305717	0.598271374	0.000690102
H	2.383522201	1.642933552	0.001671352
C	3.069246905	-0.328742769	-0.001272992
H	2.881695165	-1.401184945	-0.002553514
H	4.118427038	-0.045391703	-0.001725837

2-chloro-1,2-dihydro-1,2-azaborine

B	-0.826267997	0.000000000	-1.178699612
N	-2.043451037	0.000000000	-0.421424225
C	0.456583686	0.000000000	-0.383111838
C	-2.061559149	0.000000000	0.949195764
C	0.363266710	0.000000000	0.991502444
C	-0.895158446	0.000000000	1.665837758
H	1.441522133	0.000000000	-0.841795128
H	-3.035946647	0.000000000	1.426330480
H	1.263337974	0.000000000	1.604480023
H	-0.940448638	0.000000000	2.748949739
H	-2.942379037	0.000000000	-0.887888143
Cl	-0.952713556	0.000000000	-2.970660136

2-chloro-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.503381118	0.066667981	0.000000000
N	0.241497034	-1.203925805	0.000000000
C	0.370789814	1.341184101	0.000000000
C	1.568629092	-1.244207818	0.000000000
C	1.759986244	1.213891438	0.000000000
C	2.352360748	-0.054867278	0.000000000
H	-0.068036391	2.335412709	0.000000000
H	2.049750227	-2.218598270	0.000000000
H	2.402058612	2.090397610	0.000000000
H	3.431505116	-0.166293926	0.000000000
H	-0.253062721	-2.094481979	0.000000000
Cl	-2.232913037	0.031647210	0.000000000

2-mercapto-1,2-dihydro-1,2-azaborine

B	-0.862956091	-0.001297143	-1.064815556
N	-2.069322859	-0.002883315	-0.278251692
C	0.430259526	0.001271805	-0.268443452
C	-2.065289543	-0.001948506	1.095090305
C	0.358286657	0.002405435	1.104290347
C	-0.892714192	0.000879255	1.797453622
H	1.413649476	0.002127902	-0.732679454
H	-3.033604462	-0.003532070	1.585002080

H	1.267011639	0.004434224	1.704459513
H	-0.924418773	0.001745207	2.881060919
H	-2.984151750	-0.005299745	-0.710687894
S	-0.889893462	-0.001786114	-2.909627586
H	-2.226399746	-0.003272080	-3.095625778

2-mercapto -1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.521320640	0.018019784	0.000286274
N	-0.263941473	-1.222416888	0.000227077
C	-0.300592537	1.315495032	0.000346662
C	-1.598381442	-1.215099402	0.000017655
C	-1.691950163	1.238070373	-0.000117237
C	-2.334056947	-0.008705047	-0.000341379
H	0.162311775	2.298964661	0.000792695
H	-2.109026471	-2.173651903	0.000129930
H	-2.300968867	2.137847772	-0.000246612
H	-3.416422036	-0.077560651	-0.000653997
H	0.175710605	-2.138960206	0.000702295
S	2.314667665	0.068264522	-0.000157910
H	2.578481914	-1.257649223	-0.000874307

2-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.868727927	-0.002010034	-1.208749880
N	-2.077900122	-0.002474329	-0.407682361
C	0.430521448	-0.000431264	-0.409811822
C	-2.061577421	-0.000715254	0.968714567
C	0.365354527	0.001414340	0.960085362
C	-0.885628565	0.001372281	1.661861197
H	1.407059808	-0.000596386	-0.888352055
H	-3.025570929	-0.001173855	1.467439272
H	1.275986451	0.002823824	1.557878961
H	-0.910815704	0.002771838	2.745779863
H	-2.999064849	-0.003982348	-0.828030808
O	-0.902295671	-0.002693419	-2.593185206
H	-1.778088603	-0.003926082	-2.994304264

2-hydroxy -1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	0.999290159	0.057820015	0.000157875
N	0.236998590	-1.220138887	0.000317728
C	0.115709314	1.336883020	0.000378621
C	-1.091959577	-1.242566228	-0.000010176
C	-1.270911698	1.217389282	-0.000071503
C	-1.867949274	-0.051275258	-0.000336990
H	0.564804263	2.326747465	0.000817861
H	-1.583608263	-2.211674310	0.000039736
H	-1.911082321	2.095195124	-0.000124156
H	-2.947320950	-0.159462809	-0.000657913
H	0.700570154	-2.125969293	0.000577689
O	2.336216926	0.129381848	-0.000372113

H	2.888097292	-0.664537033	-0.000409886

2-amino-1,2-dihydro-1,2-azaborine

B	-0.858636940	0.000844500	-1.247862014
N	-2.069731889	-0.001403671	-0.441648367
C	0.438676283	0.001635669	-0.431068956
C	-2.058722453	-0.001058480	0.931311184
C	0.366705702	0.001262202	0.937440984
C	-0.888133217	-0.000408742	1.634567251
H	1.426084924	0.003819156	-0.890751258
H	-3.025244116	-0.001651025	1.426027677
H	1.274953546	0.002480462	1.539305002
H	-0.919682159	-0.000986984	2.718242339
H	-2.987146165	-0.001063561	-0.868333386
N	-0.941969444	0.001369429	-2.672609114
H	-1.800824118	0.010220448	-3.200722599
H	-0.118393287	0.008126740	-3.252841363

2-amino-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	1.004159261	0.074868027	-0.000187032
N	0.250149036	-1.203915269	0.000014058
C	0.120574603	1.343299432	0.000033958
C	-1.077796021	-1.242697038	0.000036708
C	-1.263221558	1.211455071	-0.000048912
C	-1.858096688	-0.061154688	0.000003619
H	0.541765899	2.345752576	0.000197716
H	-1.557692522	-2.217174525	0.000078788
H	-1.909072271	2.085108029	0.000031945
H	-2.937096592	-0.170234067	0.000121605
H	0.724228482	-2.103415987	0.000137243
N	2.399040712	0.065948501	0.000098472
H	2.981726004	-0.762729218	-0.000783041
H	2.940588595	0.921866828	0.000393212

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.798408932	-0.008417205	-1.226992623
N	-1.671381962	0.852486293	-0.464397394
C	0.086242633	-0.914324282	-0.391612977
C	-1.713046211	0.867253665	0.901080343
C	-0.004477781	-0.850514493	0.982540355
C	-0.904223705	0.040303693	1.637453814
H	0.792110206	-1.614795239	-0.830662175
H	-2.409533098	1.557604948	1.366113638
H	0.617889427	-1.488282758	1.608881350
H	-0.959152341	0.073998145	2.719837167
H	-2.297780659	1.491207745	-0.938818233
C	-0.844317907	0.073746599	-2.757157075
C	-0.880672862	0.139047957	-3.971907176

H	-0.908342985	0.197565282	-5.036981610

2-ethynyl-1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.617710382	0.077702636	-0.001814113
N	0.132008056	-1.193937171	-0.001301592
C	0.271625823	1.341944064	-0.001257655
C	1.458165809	-1.244730709	0.000473884
C	1.660832658	1.208498771	0.000636531
C	2.247473721	-0.061935054	0.001558323
H	-0.156027643	2.340765802	-0.002134595
H	1.933168441	-2.221917816	0.001114520
H	2.307993726	2.081342994	0.001332694
H	3.326104205	-0.177619692	0.003026725
H	-0.364250883	-2.082235521	-0.001925276
C	-2.112637369	0.051598009	-0.000752700
C	-3.334604553	0.030425888	0.001775957
H	-4.405880543	0.013745290	0.007502496

2-formyl-1,2-dihydro-1,2-azaborine

B	0.963010987	-0.143256926	-0.000101567
N	0.270422508	1.117027326	-0.000049870
C	0.083086125	-1.370129015	-0.000102523
C	-1.091883323	1.223787844	-0.000007394
C	-1.286509357	-1.197686134	0.000075634
C	-1.877925426	0.098316772	0.000042082
H	0.485135474	-2.379880755	-0.000134576
H	-1.513524735	2.223666084	-0.000140947
H	-1.956236317	-2.056481851	0.000292266
H	-2.956457177	0.211551665	-0.000068024
H	0.782918608	1.992523702	0.000361989
C	2.554133999	-0.096877868	-0.000115453
O	3.280544258	-1.082050610	-0.000116068
H	3.050325465	0.913383668	-0.000137000

2-formyl -1,2-dihydro-1,2-azaborine$^{\bullet+}$

B	-0.824874229	-0.037459525	-1.155512311
N	-1.700262324	0.850727561	-0.452249721
C	0.080591425	-0.945004636	-0.397276382
C	-1.711271984	0.872173247	0.904842169
C	0.004851251	-0.857942271	0.991860539
C	-0.877191409	0.036502617	1.631632474
H	0.774781109	-1.648612959	-0.845803906
H	-2.394006216	1.564386762	1.384993458
H	0.636298144	-1.489975186	1.612132654
H	-0.917277788	0.085098751	2.713955388
H	-2.342628344	1.495447274	-0.902542197
C	-0.878136878	0.004251944	-2.766571075
O	-0.224830068	-0.660705506	-3.532100370

H	-1.595077051	0.723564927	-3.240218033

Wheland intermediates in the chlorination of benzene (and derivatives) at the *orto-* position

Benzene

C	-1.924219913	-0.313823686	-0.853969049
C	-1.836092724	0.982132717	-0.293923885
C	-1.466848483	-1.473553330	-0.185498872
C	-1.304068568	1.135607659	0.960499170
C	-0.929929663	-1.355488838	1.070632666
C	-0.730972158	-0.022593489	1.681861988
H	-1.575269392	-2.445938155	-0.654086620
H	-0.590000526	-2.221891644	1.631094515
H	-2.376555957	-0.425260205	-1.836928178
H	-2.218777546	1.835760294	-0.843219315
H	-1.239000613	2.108724514	1.439180940
H	0.370691457	0.139748732	1.594717385
Cl	-1.069606321	0.004406556	3.449051133

Phenylbenzene

C	0.421896610	0.540679373	-0.143199317
C	1.024072223	1.772330652	0.156827574
C	1.339695498	-0.606499945	-0.512775085
C	2.398352615	1.950178678	0.072144564
C	2.799713007	-0.314443981	-0.605558449
C	3.298699444	0.912942512	-0.321444545
H	0.413292312	2.625918088	0.421932216
H	1.012884278	-1.060640373	-1.454878895
H	2.806545917	2.930419297	0.304140719
H	3.439718968	-1.141548889	-0.895902968
H	4.362059568	1.116171498	-0.382115217
Cl	1.174462351	-1.932142321	0.742520287
C	-1.005882423	0.344772093	-0.122703988
C	-1.609860949	-0.772606607	-0.765858423
C	-1.857647755	1.269712982	0.547221595
C	-2.985019421	-0.944511546	-0.749941302
C	-3.230133479	1.083841915	0.569845040
C	-3.799857128	-0.019415377	-0.082489806
H	-1.006310372	-1.494567987	-1.303008856
H	-1.438406616	2.109084365	1.088845191
H	-3.429028661	-1.793114578	-1.259160529

H	-3.861971924	1.788679197	1.099621524
H	-4.876549127	-0.157893222	-0.070191127

Toluene

C	0.220424164	1.044108728	-0.100585719
C	1.584808405	1.113559260	0.141271020
C	-0.359791413	-0.296880858	-0.427375312
C	2.364265303	-0.048952495	0.219021193
C	0.503281001	-1.489812249	-0.235092813
C	1.833157956	-1.352797338	0.034248367
H	2.049100613	2.078604450	0.317272885
H	-0.471728595	-0.246025079	-1.534931956
H	3.423165959	0.053028900	0.445217339
H	0.042601801	-2.462501179	-0.380214183
H	2.477947343	-2.219627785	0.129700114
Cl	-2.026681170	-0.558100947	0.199142720
C	-0.646958171	2.249052981	-0.104061258
H	-1.351218284	2.241212356	-0.942964779
H	-1.268110237	2.246345601	0.804041582
H	-0.059188798	3.167754623	-0.120980283

Styrene

C	-0.660837112	0.419239085	-0.155574861
C	-0.330464795	1.714996089	0.249857362
C	0.465524323	-0.504610797	-0.550429878
C	0.997866410	2.127021772	0.325166112
C	1.855271907	0.007356374	-0.404661902
C	2.099011906	1.282897116	-0.005713817
H	-1.108173223	2.417404099	0.525933878
H	0.319342687	-0.743322237	-1.618560370
H	1.205103726	3.140513661	0.659527836
H	2.658179626	-0.681669006	-0.647785569
H	3.112010748	1.659546934	0.083368473
Cl	0.334577444	-2.102541353	0.310336301
C	-2.008165587	-0.082080946	-0.275461705
H	-2.114546294	-1.104520557	-0.625680157
C	-3.128505908	0.617395771	0.023830432
H	-3.117852844	1.636672304	0.396909834
H	-4.105605804	0.161500493	-0.099583477

Chlorobenzene

C	0.217132433	0.744392273	0.078744555
C	-0.752286759	1.639393764	-0.332568298
C	-0.158391086	-0.632839999	0.548313186
C	-2.096620878	1.238827371	-0.345741916
C	-1.609498099	-0.963709446	0.474617705
C	-2.532729427	-0.051420435	0.060999216
H	-0.473895391	2.637217979	-0.653696550
H	0.145106799	-0.706467094	1.607418224
H	-2.839204612	1.955074926	-0.689983312

H	-1.891147114	-1.968136131	0.776822028
H	-3.587294046	-0.300949066	0.020474695
Cl	0.780105824	-1.916476869	-0.318855858
Cl	1.848028030	1.192257630	0.122060394

Thiophenol

C	0.050954281	0.800888439	0.089072072
C	-1.130073030	1.515437064	-0.158018433
C	-0.056377171	-0.659183810	0.461139497
C	-2.349484802	0.855351479	-0.221274327
C	-1.389955888	-1.296720928	0.255389672
C	-2.488293284	-0.554685602	-0.031563788
H	-1.091322380	2.581145427	-0.358816345
H	0.096564687	-0.681175639	1.557387470
H	-3.237385966	1.438742838	-0.451497877
H	-1.441944468	-2.369650488	0.412146439
H	-3.464630425	-1.015965185	-0.131116647
Cl	1.275235125	-1.668924041	-0.217031222
S	1.618718338	1.491506713	0.060911502
H	1.212220324	2.766380865	-0.130200014

Phenol

C	-0.228063346	1.025418442	0.146671355
C	-1.543923395	1.057303538	-0.317598315
C	0.409156753	-0.264064506	0.587974191
C	-2.264192334	-0.128294382	-0.374686139
C	-0.454942470	-1.475276622	0.470877550
C	-1.732638466	-1.396677459	0.023575077
H	-1.993388174	1.993413128	-0.635905828
H	0.709686387	-0.137214346	1.639735738
H	-3.285871658	-0.090136259	-0.744820367
H	-0.003935521	-2.418627302	0.762407241
H	-2.354788934	-2.281275707	-0.053363810
Cl	1.943739150	-0.541749686	-0.336844609
O	0.541635424	2.072609352	0.273193131
H	0.123055365	2.906311219	-0.007961240

Aniline

C	0.246228507	1.018819800	-0.105341196
C	1.651013343	1.073751016	0.096318991
C	-0.384608939	-0.310199422	-0.460972321
C	2.370786906	-0.090671056	0.189887360
C	0.456062510	-1.518209240	-0.187972979
C	1.774165925	-1.399592422	0.076011226
H	2.130391590	2.035579403	0.249536703
H	-0.502379625	-0.274139703	-1.558946069
H	3.436985476	-0.025536469	0.388964724
H	-0.031207857	-2.481939044	-0.292422549
H	2.395165545	-2.277771295	0.213717030
Cl	-2.061051287	-0.476897084	0.187393864

N	-0.509510538	2.096248179	-0.058996735
H	-1.521128319	2.030150444	-0.119220783
H	-0.109671352	3.013698333	0.104320430

Ethynylbenzene

C	0.237563194	0.826848016	0.090085685
C	-0.805315759	1.670719013	-0.289419961
C	-0.077370198	-0.581966321	0.526969175
C	-2.121742172	1.199075211	-0.313155611
C	-1.500106802	-1.001831466	0.425178966
C	-2.477223805	-0.129667256	0.048874557
H	-0.587133446	2.691027209	-0.584512400
H	0.190333431	-0.639001475	1.598123301
H	-2.907801519	1.880444117	-0.629389210
H	-1.724510065	-2.029461086	0.695280062
H	-3.517722565	-0.434820671	0.027388251
Cl	0.987163857	-1.793895029	-0.294449729
C	1.561415491	1.278044293	0.117823825
C	2.711159800	1.673206675	0.144719020
H	3.724030753	2.021810862	0.166803874

Benzaldehyde

C	0.433556675	-1.689008691	-0.168035874
C	0.618388449	-0.364757902	0.152391988
C	-0.873702107	-2.217602025	-0.265207300
C	-0.557072758	0.487797563	0.479703357
C	-2.033185161	-1.443862848	-0.027278060
C	-1.895760383	-0.116585457	0.288319554
H	-0.991511897	-3.261472302	-0.547768948
H	-0.491570410	0.654395346	1.579414113
H	-3.015601048	-1.891869005	-0.132159273
H	-2.758596850	0.525463657	0.443346657
H	1.301021534	-2.310763194	-0.369527260
C	2.024191283	0.188760765	0.255238778
O	2.967080177	-0.487080336	-0.085965139
H	2.135940166	1.212042263	0.648691071
Cl	-0.463411290	2.138068667	-0.252832826

Wheland intermediates in the chlorination of benzene (and derivatives) at the *meta*- position

Phenylbenzene

C	0.081749996	-0.426265252	-0.175002708
C	-0.905641103	0.543199405	-0.198367173
C	-0.358151065	-1.781073960	-0.220026193
C	-2.329256200	0.202481830	-0.395009528
C	-1.711739838	-2.176573560	-0.295859125
C	-2.697829763	-1.225617952	-0.335919008

H	-0.657166894	1.597367389	-0.117984496
H	0.399464860	-2.560527322	-0.196750262
H	-2.497669847	0.452039444	-1.471703923
H	-1.959679198	-3.232762020	-0.309358818
H	-3.750810540	-1.484233270	-0.391970923
Cl	-3.453774099	1.272607672	0.514005388
C	1.517821628	-0.086440810	-0.061152583
C	2.373909829	-0.866959225	0.736599469
C	2.039485712	1.024683972	-0.747115926
C	3.724157900	-0.538310682	0.846560817
C	3.391904247	1.345354823	-0.638982194
C	4.235219221	0.565909927	0.157963099
H	1.985241917	-1.708812460	1.303341323
H	1.400572941	1.620447761	-1.393306375
H	4.374083713	-1.138110457	1.475271970
H	3.788086703	2.196803982	-1.182598516
H	5.287327059	0.818411112	0.242597615

Toluene

C	-1.606685160	-0.467383437	-0.015574488
C	-0.324915249	-0.890093429	-0.290891072
C	-1.791743693	0.928508039	0.187096403
C	0.791573629	0.063300491	-0.470522414
C	-0.758052650	1.889027353	0.111837492
C	0.522598936	1.480756748	-0.155680186
H	-0.099919815	-1.942943113	-0.438897371
H	-2.793789662	1.278220103	0.429993419
H	0.946286554	0.076617139	-1.576564654
H	-0.981367906	2.934266917	0.297949949
H	1.353910706	2.178447170	-0.197949253
Cl	2.348902389	-0.531960949	0.209664753
C	-2.770257141	-1.416431894	0.111151973
H	-3.253819352	-1.308734146	1.087397733
H	-3.523855015	-1.207964763	-0.655746519
H	-2.451542831	-2.454558126	0.001304823

Styrene

C	1.290111115	-0.219488116	0.048957896
C	0.053140666	-0.788297082	0.299243610
C	1.306415173	1.187860992	-0.175473305
C	-1.166024357	0.026811689	0.464909848
C	0.167043589	2.016797232	-0.105866823
C	-1.061716770	1.465519437	0.153486911
H	-0.049293439	-1.861110149	0.439187775
H	2.251570459	1.656712809	-0.436122797
H	-1.328859452	0.022179703	1.570583906
H	0.267562932	3.079675565	-0.298973301
H	-1.967773311	2.063172904	0.187179209
Cl	-2.640233212	-0.745171913	-0.223731301
C	2.496101316	-1.059367763	-0.035794740

H	2.309018750	-2.130453364	-0.023664877
C	3.760407459	-0.620726486	-0.098121296
H	4.036851249	0.429799371	-0.089144079
H	4.582062268	-1.326619327	-0.150900232

Chlorobenzene

C	1.206021594	0.017833907	0.053526447
C	0.054381272	-0.682911116	0.321631950
C	1.128658438	1.416781420	-0.175367918
C	-1.233713369	0.028178852	0.473020600
C	-0.085582022	2.133248216	-0.124047770
C	-1.255810414	1.467486747	0.143020170
H	0.066394671	-1.757518745	0.478628489
H	2.047586488	1.949599666	-0.408852567
H	-1.402815992	0.021677649	1.578117396
H	-0.083869511	3.199633176	-0.323852690
H	-2.213306854	1.979320150	0.174697829
Cl	-2.624221722	-0.881163070	-0.216958205
Cl	2.733775103	-0.777522479	-0.063630600

Thiophenol

C	1.243749034	-0.024869374	0.053180334
C	0.063001317	-0.697124766	0.305949994
C	1.160376632	1.382461659	-0.166055142
C	-1.215083348	0.029056154	0.457703546
C	-0.040640475	2.115836466	-0.113632740
C	-1.225087786	1.467430870	0.135926257
H	0.033779845	-1.771498792	0.461715294
H	2.077424839	1.922372238	-0.395236753
H	-1.377609143	0.033237952	1.564496880
H	-0.020432686	3.183758600	-0.303762902
H	-2.176398453	1.990365301	0.161417601
Cl	-2.625390500	-0.865870755	-0.211979939
S	2.845392607	-0.761641976	-0.073041876
H	2.453497277	-2.028011313	0.169522498

Phenol

C	-1.561573846	-0.484695219	-0.016858761
C	-0.280756121	-0.911765408	-0.292514421
C	-1.789565297	0.906253873	0.188295432
C	0.810639726	0.068471732	-0.472523951
C	-0.771507712	1.873231140	0.106983561
C	0.517452384	1.481286107	-0.163610761
H	-0.040981944	-1.961552107	-0.437194510
H	-2.807129326	1.209015348	0.425919998
H	0.975217312	0.096641600	-1.577315989
H	-1.009862791	2.915962449	0.287859923
H	1.336501068	2.192269925	-0.216512620
Cl	2.379994722	-0.492084407	0.212551829
O	-2.643746952	-1.265850859	0.119383682

H	-2.457865550	-2.208485684	-0.010281390

Aniline

C	-1.606635638	-0.492167346	-0.005922966
C	-0.294920618	-0.906318105	-0.230444635
C	-1.813075736	0.911312953	0.171387057
C	0.790602597	0.068493025	-0.420220769
C	-0.790732923	1.871658255	0.093152684
C	0.508106079	1.485017646	-0.139760534
H	-0.045590193	-1.957062984	-0.343838404
H	-2.823465645	1.256542681	0.381138746
H	0.902333234	0.100734586	-1.535675485
H	-1.036288725	2.917237156	0.246592899
H	1.326205645	2.195628322	-0.196107296
Cl	2.385388958	-0.496582344	0.185094599
N	-2.650142735	-1.357698675	0.074195039
H	-2.511434086	-2.354061214	-0.001404535
H	-3.575310033	-1.046815580	0.328272456

Ethynylbenzene

C	1.360551895	-0.001206398	0.052877877
C	0.194145748	-0.701587295	0.310357838
C	1.253988392	1.405549309	-0.169865635
C	-1.097893371	-0.003277027	0.459438346
C	0.033572726	2.110298022	-0.128668571
C	-1.133432574	1.435038088	0.126107654
H	0.210198146	-1.776115378	0.465991282
H	2.167308478	1.951567375	-0.393142327
H	-1.257696634	-0.003622048	1.566331508
H	0.025645761	3.176809254	-0.327534253
H	-2.096267384	1.937127652	0.147162438
Cl	-2.487590160	-0.927487551	-0.212109553
C	2.624440414	-0.650560460	-0.033876373
C	3.702575228	-1.194451211	-0.106527588
H	4.654615033	-1.678457327	-0.169790629

Benzaldehyde

C	1.295008764	1.166056323	0.132916461
C	1.222189845	-0.232699583	-0.117324664
C	0.166104378	2.009854173	0.107710570
C	0.003505740	-0.801509175	-0.381102906
C	-1.068997617	1.467219873	-0.149835881
C	-1.212803086	0.034768077	-0.497375519
H	0.274510118	3.067427436	0.324424090
H	-0.102062609	-1.870286708	-0.556101772
H	-1.969814620	2.075100237	-0.151469015
H	-1.433649482	0.043468472	-1.590730427
H	2.278461595	1.573680069	0.364143309
C	2.489064451	-1.051254532	-0.036311519
O	3.547581221	-0.537482835	0.235123607

H	2.384106054	-2.132940982	-0.238462345
Cl	-2.657075225	-0.723222240	0.268746580

Wheland intermediates in the chlorination of benzene (and derivatives) at the *para-* position

Phenylbenzene

C	-0.201779711	0.045830616	0.225100611
C	0.530441780	1.277175232	0.053740655
C	0.541695623	-1.144579994	0.558518952
C	1.878852943	1.324666021	0.189096833
C	1.888395054	-1.120214195	0.714922802
C	2.675052606	0.132061350	0.576803427
H	0.002743397	2.172774417	-0.248195663
H	0.013775894	-2.076267140	0.715879106
H	2.421511980	2.249145684	0.016268508
H	2.433858235	-2.022951201	0.972776371
H	3.185449896	0.338625352	1.530989259
Cl	4.032254128	-0.121570359	-0.618994437
C	-1.632581947	0.005240817	0.054390164
C	-2.307498485	-1.224178070	-0.196087973
C	-2.412466738	1.195153946	0.131007823
C	-3.681017737	-1.254409828	-0.375763299
C	-3.788937575	1.151562702	-0.022109983
C	-4.426654531	-0.069996763	-0.282847648
H	-1.749171367	-2.147014437	-0.297338288
H	-1.943605300	2.145058843	0.357950914
H	-4.177881901	-2.194326323	-0.590986881
H	-4.371997413	2.062275393	0.063244815
H	-5.504168384	-0.099236697	-0.412826135

Toluene

C	-1.864154447	0.000716187	-0.083222295
C	-1.166998132	1.239556347	0.065014940
C	-1.167785807	-1.238729862	0.064775578
C	0.168273135	1.255864114	0.337310109
C	0.167450641	-1.256858739	0.336862222
C	0.923072489	-0.000745347	0.563282614
H	-1.710182053	2.168956630	-0.073520528
H	-1.711707330	-2.167695540	-0.074072632
H	0.715107634	2.190164860	0.427166681
H	0.713522812	-2.191619980	0.426286428
H	1.211010470	-0.001121835	1.633863104
Cl	2.490965849	0.000123201	-0.343208077
C	-3.318718654	0.000334756	-0.376237710
H	-3.629231776	-0.890223368	-0.928330228

H	-3.857983545	-0.020006962	0.586402021
H	-3.637248022	0.905634776	-0.898232645

Styrene

C	1.484035444	-0.227234661	0.024312677
C	0.662008077	-1.403194628	0.088868930
C	0.885219978	1.063112277	0.228176836
C	-0.671009998	-1.315909798	0.339984647
C	-0.444096900	1.178856799	0.480432719
C	-1.325635414	-0.010406951	0.607806281
H	1.122073915	-2.370568539	-0.085363159
H	1.491803101	1.957758185	0.156245358
H	-1.295987766	-2.203453419	0.371812986
H	-0.904126042	2.153373089	0.614141609
H	-1.722692900	-0.032168743	1.637829050
Cl	-2.795993537	0.180507239	-0.448960201
C	2.885168956	-0.405216214	-0.265538049
H	3.212604437	-1.426820175	-0.439259998
C	3.805505822	0.588003169	-0.325984183
H	3.570929927	1.633915878	-0.155679454
H	4.842987171	0.359156186	-0.548957521

Chlorobenzene

C	1.346745966	0.000004165	0.051066038
C	0.672726805	-1.251372683	0.168430132
C	0.672507555	1.251225942	0.168390385
C	-0.669446890	-1.258497731	0.401301592
C	-0.669613059	1.258045945	0.401613503
C	-1.434127071	-0.000241615	0.593879959
H	1.233702450	-2.171791705	0.049163066
H	1.233278276	2.171788631	0.049207053
H	-1.217531713	-2.193401106	0.476056091
H	-1.217529741	2.192876274	0.478693617
H	-1.803099885	-0.000935474	1.637448452
Cl	-2.930879002	0.000177714	-0.432139154
Cl	3.009792676	0.000151338	-0.257840679

Thiophenol

C	1.386848113	0.024357494	0.051254546
C	0.698318554	-1.230851716	0.194897786
C	0.676390361	1.267309996	0.182348285
C	-0.632468114	-1.249234840	0.454725572
C	-0.654625232	1.262144403	0.442994142
C	-1.417771069	0.000373847	0.637323078
H	1.250620469	-2.157963155	0.077303218
H	1.205614352	2.206137966	0.055869982
H	-1.166103577	-2.190240887	0.549090373
H	-1.205641512	2.194233177	0.527273832
H	-1.848600742	0.002502603	1.651679059
Cl	-2.859720531	-0.013448680	-0.478242003

S	3.058243828	-0.054978223	-0.292827638
H	3.294576303	1.273797291	-0.357450767

Phenol

C	1.797005373	0.007713490	-0.085325229
C	1.130350058	-1.249498557	0.083134914
C	1.119435736	1.261410244	0.083748067
C	-0.184525560	-1.259680886	0.408481014
C	-0.195999672	1.260476680	0.409209083
C	-0.950932015	-0.003017117	0.635639215
H	1.701103010	-2.158623799	-0.072833540
H	1.662509252	2.190168742	-0.068632800
H	-0.721797462	-2.195836582	0.527862515
H	-0.741435411	2.192339105	0.526265117
H	-1.320035534	-0.003522163	1.674439586
Cl	-2.448455248	-0.002130828	-0.397236753
O	3.059309635	-0.060683362	-0.412630140
H	3.490080062	0.805272813	-0.530940687

Aniline

C	1.825995305	0.000195655	-0.092806789
C	1.130010023	-1.254789877	0.086620470
C	1.129565566	1.254780034	0.087183058
C	-0.176231429	-1.258143135	0.424795863
C	-0.176730634	1.257404309	0.425244652
C	-0.944363181	-0.000476857	0.653115043
H	1.670954631	-2.183651425	-0.067142833
H	1.669900905	2.184018300	-0.066568108
H	-0.712979262	-2.193740129	0.548880988
H	-0.714112071	2.192657454	0.549219401
H	-1.339198321	-0.001674708	1.679374905
Cl	-2.423895036	0.000216302	-0.413925116
N	3.101840088	0.000429313	-0.431869472
H	3.615675664	-0.862403408	-0.571871547
H	3.615270574	0.863586303	-0.571477386

Ethynylbenzene

C	1.509327803	-0.000588686	0.051530676
C	0.813580781	-1.250010347	0.171992451
C	0.814080750	1.249057191	0.172633423
C	-0.527745396	-1.258607129	0.401587775
C	-0.527242187	1.257989682	0.402211894
C	-1.293476921	-0.000191052	0.589704349
H	1.369632579	-2.173628675	0.056401432
H	1.370492998	2.172473343	0.057362435
H	-1.077011137	-2.192532964	0.476715876
H	-1.076240094	2.192093295	0.477622525
H	-1.681038384	-0.000392069	1.625414143
Cl	-2.779086521	0.000581691	-0.458758550
C	2.886962919	-0.000548124	-0.203435131

C	4.083392111	0.001113902	-0.423678637
H	5.137426873	0.003052447	-0.618059533

Benzaldehyde

C	-0.899036896	-1.041212782	-0.171299321
C	-1.451055933	0.255320609	-0.025799485
C	0.453738310	-1.182121321	-0.338514358
C	-0.657985113	1.428174284	-0.060983314
C	1.325757752	0.006252154	-0.471980691
C	0.699478947	1.323568492	-0.228146043
H	0.917947620	-2.159856697	-0.433593151
H	-1.123937494	2.399838340	0.077114132
H	1.551036986	0.033346570	-1.567138912
H	1.343275158	2.198724376	-0.238786967
H	-1.562572917	-1.898518185	-0.113203816
C	-2.946971311	0.379210923	0.201285839
O	-3.649257814	-0.603049739	0.231722810
H	-3.341682488	1.401796295	0.334435200
Cl	2.925910175	-0.182315680	0.325867913

Intermediate in the chlorination of substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

N	1.042316278	1.330918075	0.052917269
B	-0.185909609	0.999969481	0.831187003
C	1.842010247	0.421644789	-0.463636214
C	-0.498277034	-0.528620473	0.891695264
C	1.602994536	-0.985996272	-0.334767469
C	0.512839345	-1.454995982	0.331094142
H	2.728617221	0.768472112	-0.990291489
H	-1.127723609	-0.940020991	1.675818306
H	2.339434062	-1.660545362	-0.756598482
H	0.382848468	-2.524964648	0.472705109
H	1.321453462	2.303238683	-0.058058859
Cl	-1.687291249	0.032348080	-0.479345172
H	-0.744038536	1.853911623	1.420343886

1-phenyl-1,2-dihydro-1,2-azaborine

B	1.048690953	-0.444026205	-0.890555652
N	0.134103655	0.425858135	-0.061983357
C	2.551363350	-0.024463079	-0.881381815
C	0.612411041	1.483636046	0.569282710
C	2.919671465	1.226345253	-0.199955550
C	1.980360144	1.915001899	0.499008186
H	3.227903690	-0.372151449	-1.656520375
H	-0.089489219	2.060365088	1.165311233

H	3.936289277	1.600892702	-0.276794017
H	2.231838414	2.830428251	1.023401143
H	0.574257490	-1.236845021	-1.620194087
C	-1.283064156	0.155711803	-0.043893518
C	-2.198395313	1.208822335	-0.181304212
C	-1.719644580	-1.166351214	0.109831796
C	-3.563810159	0.932321312	-0.138615315
C	-3.088011927	-1.426484342	0.158835293
C	-4.009933935	-0.381574801	0.036674588
H	-1.854856586	2.222026357	-0.366927296
H	-1.005159920	-1.975287967	0.216630257
H	-4.277366247	1.740320060	-0.261054951
H	-3.433201996	-2.446056194	0.293857687
H	-5.073966050	-0.592323086	0.064874450
Cl	2.458595998	-1.487376075	0.370589304

1-methyl-1,2-dihydro-1,2-azaborine

B	-0.080063889	0.699965333	0.859384365
N	-1.312736128	0.291833609	0.094225577
C	1.066156683	-0.354250319	0.873006048
C	-1.411824928	-0.902474052	-0.437169036
C	0.795504348	-1.675128776	0.273644132
C	-0.383068762	-1.908881313	-0.356377956
H	1.857933551	-0.313587017	1.615231257
H	-2.338913030	-1.145997627	-0.952620964
H	1.536625376	-2.464377351	0.363937498
H	-0.601686218	-2.872592873	-0.802778850
H	-0.133934264	1.671016971	1.526552287
C	-2.432490539	1.253028936	-0.000024538
H	-3.280525588	0.798100450	-0.512633265
H	-2.724765769	1.556850089	1.007427007
H	-2.095728523	2.134852673	-0.550537877
Cl	1.586965062	0.912254015	-0.478295889

1-vinyl-1,2-dihydro-1,2-azaborine

B	-0.129997888	-0.501884110	-0.817976420
N	-0.982880575	0.497920221	-0.052199270
C	1.386464688	-0.158358603	-0.880736349
C	-0.433207353	1.601015507	0.424359156
C	1.845839666	1.119222329	-0.321224291
C	0.956431072	1.937164985	0.300001674
H	2.033557327	-0.636112942	-1.610188684
H	-1.091900414	2.299061834	0.936109521
H	2.883489843	1.417716025	-0.438164688
H	1.266538263	2.890411282	0.713978501
H	-0.660147084	-1.291905137	-1.510255265
C	-2.387301113	0.309435884	0.116879381
H	-2.900797165	1.181669468	0.508604062
C	-3.037108403	-0.827802083	-0.148277980
H	-2.559739413	-1.723577482	-0.525479427

H	-4.106258943	-0.868854671	0.026420055
Cl	1.155215308	-1.501597389	0.507826889

1-chloro-1,2-dihydro-1,2-azaborine

N	0.896890870	0.207573525	-0.099890322
B	-0.135242643	-0.600191514	-0.859554380
C	0.655271493	1.382748879	0.435617835
C	-1.540415948	0.076597909	-0.869100955
C	-0.636885049	2.009422330	0.356018763
C	-1.685160880	1.416864091	-0.273316539
H	1.475576331	1.891599302	0.935933737
H	-2.289263995	-0.214381211	-1.600174608
H	-0.727315484	2.994323218	0.801035499
H	-2.632343202	1.940733802	-0.367086730
H	0.232227117	-1.487365928	-1.538919486
Cl	2.501492928	-0.424526193	-0.002784608
Cl	-1.603895619	-1.293905562	0.484764948

1-mercapto-1,2-dihydro-1,2-azaborine

N	0.937309897	0.159161841	-0.049895600
B	-0.107532502	-0.608079885	-0.832991779
C	0.677269112	1.337060862	0.484079941
C	-1.502308003	0.089854173	-0.888594134
C	-0.590562365	2.000512664	0.350875045
C	-1.632956830	1.437812818	-0.315034143
H	1.480359889	1.831992293	1.026104081
H	-2.239837248	-0.199577311	-1.631334803
H	-0.672077166	2.988798802	0.790121267
H	-2.559067142	1.988573138	-0.452207021
H	0.237621473	-1.519371516	-1.495250810
S	2.601697857	-0.406462506	-0.028944898
H	2.274380108	-1.700044904	0.171919599
Cl	-1.631455885	-1.267944274	0.481055528

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.039805169	-0.702609310	0.840568999
N	1.224991815	-0.320917319	0.100453069
C	-1.083686735	0.450670536	0.872705584
C	1.439061634	0.850792672	-0.433715329
C	-0.741008930	1.737819527	0.256653649
C	0.454969477	1.902639249	-0.365792267
H	-1.913065355	0.436975944	1.573325061
H	-1.437999777	2.566869384	0.332536554
H	0.023880174	-1.643610802	1.552874494
O	2.272608537	-1.205543183	0.005173746
H	1.996777727	-2.021956008	0.460561650
H	2.402718660	1.004710847	-0.912795646
H	0.726847712	2.849985248	-0.818123096
Cl	-1.593156499	-0.886772009	-0.483493520

1-amino-1,2-dihydro-1,2-azaborine (actually bound to B, rather than to C3)

B	0.461474746	0.298597825	-0.691667503
N	-0.238072530	-1.051956446	-0.166974283
C	-0.502301568	1.516585381	-0.535837611
C	-1.468829884	-1.053750896	0.321095036
C	-1.773630304	1.409212451	0.013124029
C	-2.218043308	0.148246107	0.416149620
H	-0.151500766	2.497931106	-0.851735044
H	-2.428511278	2.265236018	0.142807630
H	0.753871680	0.086602847	-1.842450295
N	0.454778625	-2.165295757	-0.273988189
H	0.116649461	-3.015501051	0.164983695
H	1.441366147	-2.060163312	-0.491154692
H	-1.896922663	-1.993978974	0.658271931
H	-3.210580874	0.045482735	0.848269106
Cl	1.969074883	0.563699993	0.360234129

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.033809958	0.244505430	-0.106562980
B	0.005134175	-0.592330342	-0.864193568
C	0.715693657	1.414679504	0.439286907
C	-1.425615993	0.021418603	-0.868800965
C	-0.595716536	1.980614123	0.363758740
C	-1.624233030	1.349383547	-0.266584218
H	1.514574533	1.956224416	0.938752104
H	-2.171197102	-0.304846478	-1.587768131
H	-0.731505785	2.959113896	0.811211297
H	-2.591468298	1.835875286	-0.355816950
H	0.406762498	-1.458355814	-1.552504407
C	2.315085943	-0.215546410	-0.041745124
C	3.436142904	-0.660148540	0.014846638
H	4.431588812	-1.049269490	0.061045667
Cl	-1.408533443	-1.359983262	0.486590385

1-formyl-1,2-dihydro-1,2-azaborine

B	0.126125251	-0.542608781	0.805884962
N	0.980314924	0.435689170	0.032216553
C	-1.376826908	-0.131088373	0.895483390
C	0.491027272	1.569982075	-0.439739233
C	-1.768659441	1.194857595	0.374010882
C	-0.868926657	1.979035767	-0.283450814
H	-2.023797423	-0.551395364	1.660179930
H	1.183970461	2.230831029	-0.960992759
H	-2.780781715	1.554030778	0.542892552
H	-1.148836786	2.949484980	-0.677812734
H	0.644773476	-1.406709168	1.409408872
C	2.413401161	0.164445260	-0.172063100
O	2.905733518	-0.862349677	0.172778968
H	2.935372817	0.998889325	-0.667589659

Cl	-1.346183712	-1.415006272	-0.511716911

2-phenyl-1,2-dihydro-1,2-azaborine

N	0.983221584	1.721418367	-0.289310447
B	0.361581384	0.437869857	0.132772083
C	2.265873428	2.003689991	-0.147551393
C	1.429844677	-0.643071698	0.610371709
C	3.214468711	1.090881517	0.401362900
C	2.834395026	-0.163056048	0.765184331
H	2.598848258	2.986719855	-0.474109838
H	1.121763624	-1.196731150	1.501611140
H	4.242247680	1.422777041	0.491846146
H	3.571616533	-0.865956719	1.145811065
H	0.409698055	2.458540404	-0.690166059
C	-1.150182179	0.262311973	0.097049335
C	-1.743031220	-0.929953331	0.588797496
C	-2.021249937	1.264481598	-0.406552206
C	-3.121097357	-1.110478397	0.577954120
C	-3.399291761	1.087821913	-0.420440710
C	-3.950753051	-0.101315251	0.073741154
H	-1.116750378	-1.726595268	0.978121257
H	-1.629621833	2.198458418	-0.803288417
H	-3.553013823	-2.030143340	0.958769853
H	-4.045839684	1.865972550	-0.812515196
H	-5.027538526	-0.240591950	0.065473338
Cl	1.527039652	-1.915193404	-0.728349027

2-methyl-1,2-dihydro-1,2-azaborine

N	1.453024211	0.968188257	-0.431380879
B	0.119338119	1.109494250	0.203143667
C	2.140282072	-0.164439819	-0.454346601
C	-0.468754457	-0.261986988	0.738302193
C	1.664528913	-1.385774172	0.103781713
C	0.427279118	-1.451443958	0.669768298
H	3.116608443	-0.143603068	-0.935011014
H	-0.939050487	-0.184288800	1.723979202
H	2.306818843	-2.256267519	0.036440413
H	0.054602142	-2.396644665	1.057837364
H	1.895865602	1.774370624	-0.867434749
C	-0.543248623	2.500081390	0.327603428
H	-0.199280119	2.959360470	1.270166565
H	-0.272318511	3.199112850	-0.471114999
H	-1.633607755	2.448191056	0.394194005
Cl	-1.849222721	-0.630621232	-0.430196188

2-vinyl-1,2-dihydro-1,2-azaborine

N	-0.711897083	1.473928312	-0.367090063
B	-0.782021340	0.113214692	0.219083465
C	0.398453719	2.191699785	-0.414145513

C	0.621795942	-0.447764690	0.701192862
C	1.655946622	1.733349211	0.077478248
C	1.782109413	0.482077148	0.598322392
H	0.332558440	3.179504987	-0.865962911
H	0.575822140	-0.882129990	1.706692701
H	2.504276869	2.402800132	-0.006413967
H	2.754336289	0.125518830	0.930514744
H	-1.539377270	1.907130197	-0.769188412
C	-2.103073558	-0.643144814	0.333580272
H	-2.075453756	-1.659744737	0.723639764
C	-3.314908969	-0.144390565	0.005699970
H	-3.461981536	0.860499699	-0.387831613
H	-4.226363287	-0.724303079	0.123698787
Cl	1.008633534	-1.864456180	-0.410755411

2-chloro-1,2-dihydro-1,2-azaborine

B	0.595574809	-0.492150522	-0.127955285
N	-0.043980954	-1.672855263	0.473913020
C	-0.389864767	0.598602275	-0.704898762
C	-1.356524829	-1.867888186	0.440635888
C	-1.832476776	0.215391381	-0.699954613
C	-2.271468302	-0.954009948	-0.153913310
H	-0.087730807	0.971083551	-1.689526099
H	-1.731707109	-2.779154432	0.902018094
H	-2.543852131	0.922153105	-1.120885203
H	-3.324346465	-1.210953012	-0.136046369
H	0.521795616	-2.389003063	0.926454206
Cl	2.316080453	-0.400659087	-0.159569197
Cl	-0.271834492	2.043812252	0.425999617

2-mercapto-1,2-dihydro-1,2-azaborine

B	0.641379045	-0.509779270	-0.100337996
N	-0.025834050	-1.676015379	0.517386255
C	-0.343134023	0.584140238	-0.696242989
C	-1.333834412	-1.875848285	0.444359847
C	-1.779634533	0.180984128	-0.751993635
C	-2.231190425	-0.981990038	-0.206431963
H	-0.018291604	0.978305175	-1.663746619
H	-1.722421494	-2.776363115	0.915206013
H	-2.479471704	0.874910897	-1.211375138
H	-3.281946624	-1.247116249	-0.225225733
H	0.506808158	-2.387957442	1.011266988
S	2.406451973	-0.336867115	-0.201386461
H	2.760494835	-1.463897868	0.453561654
Cl	-0.317915773	2.031345807	0.444625784

2-hydroxy-1,2-dihydro-1,2-azaborine

B	0.254104932	1.084195799	-0.196520449
N	1.576254914	0.823321266	0.439219511
C	-0.514341921	-0.201426912	-0.710860455

C	2.125371043	-0.382467893	0.448931452
C	0.263933574	-1.472401738	-0.660050458
C	1.508991626	-1.538791752	-0.109903868
H	-0.958806163	-0.052016198	-1.700370872
H	3.101498585	-0.476673924	0.920610397
H	-0.208968014	-2.372770258	-1.045165611
H	2.054670413	-2.473698258	-0.054920762
H	2.116203061	1.565229925	0.879558815
O	-0.263788632	2.301558488	-0.345295845
H	0.173851356	3.093350316	-0.005503621
Cl	-1.932739636	-0.469424893	0.427019215

2-amino-1,2-dihydro-1,2-azaborine

N	-1.720150633	-0.890818413	-0.180692368
B	-0.272074573	-1.057908139	0.150021810
C	-2.303738589	0.288460614	-0.258370355
C	0.478751402	0.290435004	0.543547616
C	-1.620839622	1.521727002	-0.023886014
C	-0.301893379	1.539655345	0.305643993
H	-3.354634198	0.306970262	-0.539379577
H	0.698678726	0.263663719	1.623416318
H	-2.185897916	2.438805206	-0.144606922
H	0.214339756	2.488659363	0.431472409
H	-2.297911561	-1.693826949	-0.418824492
N	0.299315680	-2.312978107	0.130694412
H	1.290817767	-2.447053945	0.288838059
H	-0.183948122	-3.176295362	-0.081903602
Cl	2.108394546	0.419224595	-0.255164699

2-ethynyl-1,2-dihydro-1,2-azaborine

B	0.638617842	0.579397021	0.145401315
N	-0.113915941	1.699604676	-0.456667271
C	-0.262840781	-0.588892185	0.718035623
C	-1.436247430	1.778788465	-0.431632936
C	-1.732891084	-0.340862152	0.702709671
C	-2.271120573	0.785449105	0.156491689
H	0.063403148	-0.945295595	1.700362797
H	-1.889578481	2.653724183	-0.893189757
H	-2.382433777	-1.109065017	1.115916849
H	-3.342587738	0.947048367	0.130210944
H	0.386427315	2.464454269	-0.904656808
C	2.129286122	0.631515029	0.171692859
C	3.345774197	0.678502206	0.204525362
H	4.415680783	0.719849063	0.234818560
Cl	0.002044850	-2.009793956	-0.425011969

2-formyl-1,2-dihydro-1,2-azaborine

B	0.461903370	-0.698729715	0.092998993
N	-0.582669882	-1.555366657	0.663360253
C	-0.053462098	0.540964506	-0.713990479

C	-1.874596528	-1.377595688	0.393712882
C	-1.520168663	0.605467298	-0.952989537
C	-2.369568500	-0.321659972	-0.419340266
H	0.541522248	0.805178492	-1.591789437
H	-2.574148381	-2.084940044	0.835047247
H	-1.914475859	1.431932462	-1.540135259
H	-3.440620597	-0.267149678	-0.577286051
H	-0.351219753	-2.348617462	1.258744629
C	2.008436805	-1.058668513	0.218374357
O	2.734186074	-0.744497404	-0.711669644
H	2.426267851	-1.612680046	1.085756300
Cl	0.297619840	1.853841083	0.551769955

Intermediate in the chlorination of substituted 1,2-dihydro-1,2-azaborines on C4

1,2-dihydro-1,2-azaborine

B	1.763485057	-1.238464592	-0.000044302
N	2.340593591	0.094066135	-0.002407568
C	0.199472121	-1.306964471	0.001608162
C	1.589024104	1.204353805	0.000301417
C	-0.503160274	0.003080299	0.001194090
C	0.184488930	1.200398230	0.002039093
H	-0.150032213	-1.912872754	-0.852659540
H	2.114349998	2.156773585	0.000534649
H	-0.146229960	-1.909287571	0.860250931
H	-0.336450615	2.150340122	0.004505155
H	2.480160483	-2.178123043	0.001684668
Cl	-2.207537440	0.016628033	-0.001067125
H	3.347901364	0.230166044	-0.004587903

1-methyl-1,2-dihydro-1,2-azaborine

B	-1.282654352	1.301758912	-0.000704110
N	-1.938944906	0.000411745	-0.002073366
C	0.280904683	1.325692444	0.001167157
C	-1.198649785	-1.115965261	-0.000191611
C	0.943957942	-0.001754077	0.000888037
C	0.209265986	-1.165355194	0.001429122
H	0.643784368	1.923296504	-0.853379626
H	-1.744309355	-2.058298783	0.000491245
H	0.639425035	1.919899917	0.860081229
H	0.687986284	-2.137390487	0.000862148
H	-1.950417851	2.278046293	0.000071005

C	-3.419235684	-0.140421248	0.000522955
H	-3.744320461	-0.627906361	0.922551361
H	-3.862017084	0.851919163	-0.055939910
H	-3.738831508	-0.727380329	-0.863260588
Cl	2.649454188	-0.074263454	-0.000588219

1-vinyl-1,2-dihydro-1,2-azaborine

B	0.985201201	-1.158407495	-0.060995701
N	1.567702592	0.189187222	-0.029919730
C	-0.569895961	-1.284089618	-0.026288061
C	0.740263370	1.249469901	-0.003298630
C	-1.324464339	-0.007393572	0.002417000
C	-0.666540768	1.199196759	0.014194422
H	-0.911555240	-1.906782527	-0.870852881
H	1.215409902	2.227993501	0.007050251
H	-0.856217640	-1.905358745	0.841445278
H	-1.207149584	2.138069175	0.035850532
H	1.693109523	-2.100356503	-0.114361165
C	2.984258015	0.450008650	-0.055521415
H	3.222870733	1.496976711	-0.211453368
C	3.938352270	-0.466533214	0.102152301
H	3.749778123	-1.519420943	0.271611804
H	4.973574727	-0.147827929	0.062296137
Cl	-3.031140165	-0.053010066	0.019013086

1-mercapto-1,2-dihydro-1,2-azaborine

B	-0.786650608	1.345520986	-0.019195250
N	-1.452777492	0.044317897	-0.053946584
C	0.778318191	1.335912182	-0.033034942
C	-0.736195130	-1.095217915	-0.072200677
C	1.419261930	-0.002822344	-0.014350276
C	0.669114273	-1.158087045	-0.047250302
H	1.115992836	1.885578119	-0.931530146
H	1.178340960	1.963573654	0.780136700
H	-1.440224526	2.329017090	-0.005417294
H	-1.304748723	-2.022087074	-0.101279667
H	1.135509231	-2.136316376	-0.052371659
Cl	3.120605763	-0.099839796	0.042061235
S	-3.217455156	-0.102259786	0.093188401
H	-3.480453527	0.331314468	-1.159515864

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-1.254805405	1.321413853	-0.000041066
N	-1.874475684	0.010508939	0.003144071
C	0.305726860	1.327490984	0.001546414
C	-1.173588087	-1.125797250	0.002829574
C	0.966575631	-0.005161500	0.000558282
C	0.233829512	-1.170050419	0.002358322

H	0.671659601	1.924556174	-0.852163327
H	0.665763167	1.918488723	0.862457962
H	-1.950742204	2.279011806	0.000025539
O	-3.248659608	-0.196247258	-0.007239730
H	-3.664542850	0.683374242	0.028750103
H	-1.761860035	-2.040516151	0.003545005
H	0.711115709	-2.142716864	0.003500538
Cl	2.671084406	-0.071965573	-0.001766243

1-amino-1,2-dihydro-1,2-azaborine

B	-1.260663818	1.335116510	0.022447202
N	-1.872684415	0.017241373	-0.057570616
C	0.227217514	1.307533219	0.182833846
C	-1.171615505	-1.183026135	0.047875256
C	0.936332026	0.045333899	0.404130064
C	0.169735159	-1.205742410	0.223951353
H	0.837350395	2.207238720	0.196088858
H	1.052119341	0.092948660	1.521733354
H	-1.964882571	2.277694071	-0.105581620
N	-3.204709811	-0.090415046	-0.197108234
H	-3.579091162	-0.964953484	-0.547222782
H	-3.689747197	0.769095321	-0.425409947
H	-1.758002589	-2.091956362	-0.033728398
H	0.687762675	-2.154641194	0.302044937
Cl	2.617142106	-0.039455795	-0.225954173

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.595090140	0.020619711	0.001511717
B	0.928185288	1.334499624	0.001804397
C	0.863509792	-1.121089055	0.003670230
C	-0.632560011	1.330865694	0.002195823
C	-0.537596059	-1.165319125	0.002314229
C	-1.282208456	-0.003974196	0.000331752
H	1.430545907	-2.048236099	0.005783491
H	-1.000168851	1.926520385	-0.852026314
H	-1.013655099	-2.138914747	0.003900616
H	-0.997216340	1.921482316	0.861400153
H	1.600771957	2.303759760	0.003606681
C	2.962365908	-0.064238411	0.001616144
C	4.167251582	-0.110025124	-0.006727072
H	5.235746263	-0.151952774	-0.010894121
Cl	-2.983831146	-0.091571201	-0.002679806

2-methyl-1,2-dihydro-1,2-azaborine

N	1.823870385	-0.979044971	0.003281542
B	1.699541486	0.484911312	0.002956022
C	0.776957999	-1.807359385	-0.000832039
C	0.207734531	1.005399942	0.002567547
C	-0.564484014	-1.381512437	-0.003123161

C	-0.854925382	-0.035591450	-0.000012827
H	0.989578830	-2.874217546	-0.001511427
H	0.046662599	1.681136015	-0.854152508
H	-1.346840204	-2.130685799	-0.004162419
H	0.045364248	1.676990222	0.862362117
H	2.741677221	-1.416617921	0.004434855
C	2.960879757	1.391090678	-0.002949362
H	2.940930258	2.096899852	0.838017087
H	3.910647360	0.849216532	0.037701827
H	2.976312839	2.019471784	-0.904487679
Cl	-2.486931455	0.468694004	-0.000123784

2-vinyl-1,2-dihydro-1,2-azaborine

N	-1.353729068	1.184177895	0.007857420
B	-1.351745471	-0.288530149	0.009523701
C	-0.240358115	1.914322062	0.002406214
C	0.088085385	-0.938889008	0.000983999
C	1.061431732	1.372448287	-0.002576681
C	1.235341502	0.008592954	-0.001442676
H	-0.357515632	2.995741736	0.004310091
H	0.185614652	-1.615842217	-0.864635446
H	1.904720627	2.052270275	-0.006684669
H	0.195861019	-1.628234287	0.855000767
H	-2.224660023	1.707144350	0.015627705
C	-2.654556027	-1.097563153	0.018274301
H	-2.579634015	-2.184305192	0.054216381
C	-3.897561950	-0.575600718	-0.023138536
H	-4.094526753	0.494778407	-0.066516072
H	-4.785796542	-1.201699976	-0.020199093
Cl	2.819008471	-0.635709686	-0.003427350

2-chloro-1,2-dihydro-1,2-azaborine

B	-1.280735131	0.048723250	0.001176006
N	-1.181567716	-1.407955986	0.000269420
C	0.076111601	0.840806979	0.009304544
C	-0.004120339	-2.040328519	-0.000321010
C	1.300450046	-0.009580710	0.002125991
C	1.241795008	-1.386262352	0.000184866
H	0.114890843	1.542836427	-0.839533103
H	-0.030537001	-3.127543129	-0.001806204
H	0.111115576	1.515408904	0.881127345
H	2.141726032	-1.989282344	-0.002527348
H	-2.017895240	-1.987640386	-0.000981039
Cl	-2.847310313	0.788200563	-0.002577139
Cl	2.817367979	0.767514146	-0.002822408

2-hydroxy-1,2-dihydro-1,2-azaborine

B	-1.662815467	0.499760899	-0.000621819
N	-1.838379533	-0.970358924	-0.002027225
C	-0.172407144	1.016978750	0.000303086

C	-0.795883448	-1.801294620	0.000567850
C	0.866646832	-0.048843569	0.000390671
C	0.551640229	-1.388693732	0.001579230
H	-0.006229938	1.683771560	-0.860858656
H	-1.015930368	-2.866436203	0.000649142
H	-0.007400827	1.681731660	0.863357627
H	1.321447598	-2.150728212	0.002380748
H	-2.755951816	-1.408123806	-0.002046614
O	-2.681110027	1.367173348	0.000942037
H	-3.599595536	1.067688928	-0.000796617
Cl	2.506364185	0.425752889	-0.000475604

2-amino-1,2-dihydro-1,2-azaborine

N	1.843048338	-0.959719535	0.000099600
B	1.675324993	0.518548402	0.000116188
C	0.812863859	-1.792204855	-0.000280844
C	0.174285490	1.033902955	-0.000107568
C	-0.541097330	-1.380372163	0.000370555
C	-0.856665304	-0.046166506	0.000208419
H	1.034928223	-2.856912705	-0.001457120
H	-0.013049138	1.687507921	-0.865882118
H	-1.309893521	-2.143276152	0.000793926
H	-0.013088487	1.686621473	0.866421446
H	2.764150456	-1.389082088	-0.001466735
N	2.795276546	1.334364683	0.000094985
H	2.735374838	2.344067183	-0.001161492
H	3.752136946	1.005425439	0.000028504
Cl	-2.501889489	0.426839233	-0.000101398

2-formyl-1,2-dihydro-1,2-azaborine

B	-1.405169074	-0.198769921	-0.004104391
N	-1.160451836	-1.626320060	-0.000752717
C	-0.141067015	0.722691096	-0.005317376
C	0.082412147	-2.140647192	0.003272912
C	1.163798617	0.016937079	-0.000275595
C	1.249133266	-1.364744306	0.003052743
H	-0.186240012	1.419190794	-0.861270186
H	0.167135007	-3.224960456	0.005703139
H	-0.190236935	1.427968875	0.843000932
H	2.207616639	-1.869893851	0.005038374
H	-1.922666753	-2.300660401	-0.000051789
C	-2.890860460	0.387530767	-0.005570545
O	-3.053100977	1.596759238	0.008522028
H	-3.777110581	-0.285011229	-0.018589566
Cl	2.594405415	0.938885638	0.000109983

Intermediate in the chlorination of substituted 1,2-dihydro-1,2-azaborines on C5

1,2-dihydro-1,2-azaborine

B	2.241389100	0.049396164	-0.417929947
N	1.407709625	1.264631141	-0.082606588
C	1.575533086	-1.292464104	-0.144564110
C	0.208231110	1.200529448	0.407336262
C	0.313907732	-1.336588529	0.341024761
C	-0.462878621	-0.101061954	0.668772878
H	2.085803796	-2.229388785	-0.348600819
H	-0.336782674	2.118960463	0.619789500
H	-0.210275927	-2.270509613	0.530265400
H	-0.789904642	-0.113645760	1.718767087
H	3.312472018	0.269936686	-0.862347841
Cl	-1.998923973	0.003740497	-0.312524394
H	1.787072853	2.196551558	-0.253217421

1-phenyl-1,2-dihydro-1,2-azaborine

B	-0.457073468	-1.884952390	0.017298294
N	0.019570323	-0.448724679	0.157031988
C	-1.941064838	-2.147203786	0.230223858
C	-0.832147760	0.507000490	0.402716426
C	-2.781723512	-1.120673196	0.483541111
C	-2.291377353	0.284221801	0.597320382
H	-2.347722779	-3.152806836	0.170089692
H	-0.464941258	1.529667914	0.453577823
H	-3.851835748	-1.253471189	0.624157060
H	-2.572380333	0.711280878	1.570914259
H	0.374077892	-2.680581656	-0.241304640
C	1.435728802	-0.136027871	0.059921461
C	2.027627064	0.666768447	1.041777703
C	2.173393394	-0.643057592	-1.014451485
C	3.382361596	0.981184088	0.930686954
C	3.523555134	-0.310201739	-1.116995840
C	4.127700476	0.498717978	-0.148579556
H	1.456907678	1.004584426	1.902059977
H	1.703320119	-1.263978198	-1.769565171
H	3.855136735	1.588585343	1.695186578
H	4.102483019	-0.683486118	-1.955052578
H	5.181867044	0.742674292	-0.229583679
Cl	-3.106356753	1.359821417	-0.635455811

1-methyl-1,2-dihydro-1,2-azaborine

B	1.758511736	-1.000634929	-0.350726391
N	1.492943117	0.442621652	0.037220597

C	0.612213234	-1.984876204	-0.181150880
C	0.334858618	0.807521769	0.490050948
C	-0.586021692	-1.551456419	0.269798583
C	-0.812876513	-0.128071246	0.659456700
H	0.726292262	-3.035018444	-0.434413814
H	0.173883440	1.852188391	0.752693451
H	-1.445936771	-2.207031123	0.385524699
H	-1.148420498	-0.065315575	1.704773658
H	2.844638138	-1.219595278	-0.761526618
C	2.584466410	1.434247742	-0.129519646
H	2.251868206	2.421324195	0.192584894
H	3.441784120	1.112013115	0.464451765
H	2.871644415	1.459930689	-1.182706317
Cl	-2.163332440	0.616802162	-0.317246122

1-vinyl-1,2-dihydro-1,2-azaborine

B	-1.245076926	1.311124871	-0.286044349
N	-1.208162136	-0.151672223	0.140531938
C	0.046556730	2.103799321	-0.176558157
C	-0.084381636	-0.669363237	0.559289169
C	1.183788469	1.505290699	0.238935723
C	1.200656845	0.072889907	0.652185401
H	0.078871766	3.153588004	-0.453987589
H	-0.072835734	-1.718406013	0.849302478
H	2.137133517	2.024231281	0.303742922
H	1.578500607	-0.027661953	1.679673878
H	-2.273276400	1.725571264	-0.681563624
C	-2.365950294	-1.006694725	0.082840509
H	-2.153974665	-2.030426901	0.373776823
C	-3.589665912	-0.619684601	-0.279020535
H	-3.853596894	0.387455980	-0.573858107
H	-4.381552017	-1.360564212	-0.280307830
Cl	2.371941240	-0.889826019	-0.371104375

1-chloro-1,2-dihydro-1,2-azaborine

N	1.107102278	-0.091362301	-0.080436045
B	1.034017560	-1.552840811	0.348410683
C	0.091591053	0.577715491	-0.533523747
C	-0.335670805	-2.195131678	0.195397744
C	-1.257760371	-0.045167838	-0.663959118
C	-1.387652008	-1.474778446	-0.253727128
H	0.216898957	1.622007939	-0.812811302
H	-0.490757931	-3.236479660	0.464133578
H	-1.586637393	0.090328620	-1.704966375
H	-2.386644821	-1.893170687	-0.351588608
H	2.036829394	-2.019205197	0.753170790
Cl	2.629741112	0.726146197	0.072243174
Cl	-2.343347293	1.032632486	0.328837406

1-mercapto-1,2-dihydro-1,2-azaborine

N	1.156465099	-0.097540747	-0.129730605
B	1.059948418	-1.553141699	0.307249180
C	0.119211628	0.544385733	-0.586091250
C	-0.314456359	-2.194291352	0.227410379
C	-1.240021709	-0.063298232	-0.661864669
C	-1.375981994	-1.476983880	-0.203530186
H	0.231708711	1.579489259	-0.904675972
H	-0.467436074	-3.227135798	0.527727467
H	-1.601588042	0.042160549	-1.694670821
H	-2.381786766	-1.887104547	-0.255081558
H	2.070645522	-2.051062186	0.660913715
S	2.657101506	0.807790932	0.111380089
H	3.451556515	-0.249802813	-0.152471521
Cl	-2.299037950	1.051197915	0.325843388

1-hydroxy-1,2-dihydro-1,2-azaborine

B	1.756980402	-1.010610417	-0.351326623
N	1.456959898	0.421437524	0.029297117
C	0.613970976	-1.986732313	-0.167081017
C	0.311189955	0.827285920	0.475760662
C	-0.584198845	-1.544609937	0.282241269
C	-0.825767898	-0.117410640	0.654418505
H	0.728228159	-3.039604844	-0.408255909
H	-1.440748243	-2.202825956	0.407037469
H	2.853149068	-1.200402187	-0.755458702
O	2.413063441	1.402489255	-0.101395978
H	3.216097276	0.971132765	-0.448165894
H	0.192481577	1.883452341	0.708655968
H	-1.152435510	-0.052000409	1.702915479
Cl	-2.200681271	0.581041460	-0.316876604

1-amino-1,2-dihydro-1,2-azaborine

B	1.758288797	-0.993848193	-0.351193109
N	1.481181714	0.461038712	0.009070321
C	0.619399993	-1.971353214	-0.160195336
C	0.322935683	0.839380683	0.465430578
C	-0.578225474	-1.531506253	0.289292930
C	-0.814418134	-0.103149538	0.653523017
H	0.737710082	-3.024944867	-0.396041465
H	-1.434326643	-2.189232056	0.419672439
H	2.845798460	-1.200291530	-0.765880407
N	2.545843609	1.332940644	-0.065779442
H	2.278269242	2.310502253	-0.136565065
H	3.221794727	1.042835518	-0.764005280
H	0.171080503	1.885965052	0.720841961
H	-1.144578985	-0.034025974	1.699827919
Cl	-2.204034558	0.578759603	-0.317426951

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-1.257702796	-0.044267928	0.086514913
B	-1.158830041	-1.511119734	-0.357484936
C	-0.215422065	0.601818910	0.554806365
C	0.205131246	-2.161673914	-0.209726748
C	1.127079968	-0.021185643	0.669581864
C	1.257728407	-1.447180006	0.246860113
H	-0.339968459	1.640584391	0.852424080
H	0.360493621	-3.199992434	-0.488866853
H	1.480308761	0.111363707	1.702175149
H	2.256843166	-1.866446835	0.339446382
H	-2.161673089	-1.971071965	-0.771832972
C	-2.467503353	0.587094916	-0.026099900
C	-3.553410830	1.099521974	-0.138022617
H	-4.517310556	1.554511640	-0.235848277
Cl	2.203977104	1.061395059	-0.338959781

1-formyl-1,2-dihydro-1,2-azaborine

B	-1.204465024	1.338766581	-0.300721697
N	-1.139848408	-0.114080504	0.163235079
C	0.099660721	2.120294833	-0.198374506
C	-0.038792511	-0.641095700	0.614803063
C	1.231036844	1.521252293	0.234516958
C	1.250612450	0.095305373	0.678131780
H	0.146172232	3.164711630	-0.493802784
H	-0.045812268	-1.682513720	0.941001865
H	2.187084085	2.036378992	0.291310336
H	1.667016783	-0.004213846	1.689896454
H	-2.249789348	1.706475226	-0.696428150
C	-2.352526589	-0.991595010	0.102247713
O	-3.387872779	-0.577026517	-0.298111973
H	-2.145159730	-2.011860428	0.462421833
Cl	2.332775317	-0.926423414	-0.388753148

2-phenyl-1,2-dihydro-1,2-azaborine

N	-0.638862814	-1.098078684	0.455164321
B	0.182959984	0.173107158	0.274702778
C	-1.921402665	-1.129731541	0.621788701
C	-0.675535083	1.450418864	0.328545448
C	-2.753141359	0.104590637	0.623781712
C	-2.014832775	1.394426810	0.475348194
H	-2.421407989	-2.089235267	0.741127848
H	-0.228014391	2.436262931	0.241116844
H	-3.389875231	0.103457899	1.517177354
H	-2.637404962	2.285322764	0.497642403
H	-0.169016058	-2.002247217	0.439605290
C	1.685527683	0.038794676	0.067867563
C	2.471882375	1.209732698	-0.099580912
C	2.361725635	-1.209933762	0.029052540
C	3.846442122	1.137667976	-0.293992961

C	3.735103527	-1.286687346	-0.164858218
C	4.479541578	-0.110544275	-0.326861881
H	1.997889199	2.185493852	-0.076645506
H	1.821536542	-2.146866993	0.149817203
H	4.427195738	2.045555279	-0.420034625
H	4.230279648	-2.251797915	-0.190650634
H	5.553133315	-0.168901328	-0.478305101
Cl	-3.915145566	-0.174849484	-0.771282509

2-methyl-1,2-dihydro-1,2-azaborine

N	-1.024620640	1.182512880	0.198072589
B	-1.869790529	-0.053687607	-0.096983257
C	0.221315086	1.152797202	0.549594084
C	-1.097838432	-1.371338003	0.067207335
C	0.972951901	-0.124762655	0.682449609
C	0.208145032	-1.379473847	0.406269734
H	0.749352984	2.086287318	0.738131602
H	-1.586985347	-2.327109750	-0.103018336
H	1.435231276	-0.153736361	1.678674704
H	0.782287865	-2.297368186	0.507346581
H	-1.452151987	2.105099859	0.108083699
C	-3.342139621	0.149630645	-0.523656754
H	-4.008458013	-0.427390895	0.133139963
H	-3.697247915	1.184207273	-0.543922580
H	-3.499822711	-0.280611812	-1.523987115
Cl	2.366385314	0.086405500	-0.483015705

2-vinyl-1,2-dihydro-1,2-azaborine

N	-0.787407750	0.938107155	0.383849499
B	-1.480586593	-0.364994057	0.011387847
C	0.467888444	1.033165881	0.684546494
C	-0.548644995	-1.583983495	0.029351358
C	1.381451954	-0.142661978	0.666854883
C	0.763519986	-1.457998439	0.318024847
H	0.885109275	2.005898239	0.939305944
H	-0.927547923	-2.575973885	-0.203140753
H	1.910959154	-0.190670664	1.627386257
H	1.447762239	-2.302920860	0.319586003
H	-1.319079675	1.807980682	0.399839211
C	-2.966769767	-0.345370996	-0.338195642
H	-3.428566706	-1.297894915	-0.595518687
C	-3.765905458	0.744636722	-0.361912592
H	-3.419850877	1.750219942	-0.124584406
H	-4.818585218	0.680888369	-0.624246838
Cl	2.662179242	0.344075703	-0.550109809

2-chloro-1,2-dihydro-1,2-azaborine

B	-1.355230302	0.122025249	0.058136669
N	-0.559035999	-1.135277448	0.335076083
C	-0.577909328	1.430785457	0.144527864

C	0.703258915	-1.124388967	0.629166224
C	0.742965098	1.407197444	0.422637583
C	1.490492008	0.138021754	0.684722341
H	-1.063807428	2.387244740	-0.024829765
H	1.215006737	-2.066229229	0.819772644
H	1.342476129	2.312697026	0.476040748
H	2.021051432	0.179824727	1.645383588
H	-1.023789187	-2.043950916	0.286266448
Cl	-3.023973574	-0.100251461	-0.321493171
Cl	2.793261416	-0.141135970	-0.568798642

2-mercapto-1,2-dihydro-1,2-azaborine

B	-1.383385217	0.068759316	0.067741013
N	-0.555869025	-1.166353671	0.350724301
C	-0.620883762	1.394450973	0.172923494
C	0.706036337	-1.124276997	0.647997808
C	0.697562858	1.403360854	0.453256042
C	1.473890889	0.149557045	0.695187427
H	-1.120794166	2.346535218	0.016352716
H	1.235178719	-2.055231248	0.843207180
H	1.273360630	2.322980052	0.517649091
H	2.036451785	0.193004878	1.635888999
H	-0.976224478	-2.094693599	0.308953251
S	-3.106752504	-0.043604263	-0.355116805
H	-3.260256313	-1.385308707	-0.318414858
Cl	2.747664341	-0.120949562	-0.599467712

2-hydroxy-1,2-dihydro-1,2-azaborine

B	-1.824200905	0.034512337	-0.111918358
N	-0.986414476	-1.209173399	0.197727714
C	-1.086049946	1.368926159	0.061492441
C	0.251398019	-1.146360856	0.576330285
C	0.210031752	1.390944161	0.423382145
C	0.986555329	0.143168643	0.701921865
H	-1.602018716	2.308158679	-0.117153278
H	0.790540035	-2.068388925	0.787676607
H	0.769823953	2.315634676	0.537983298
H	1.467374571	0.177887094	1.687783972
H	-1.383255261	-2.145901671	0.112342095
O	-3.094577450	-0.079901295	-0.500733610
H	-3.539184397	-0.929928761	-0.613373376
Cl	2.361369385	-0.083065965	-0.488977623

2-amino-1,2-dihydro-1,2-azaborine

N	1.005661269	-1.190428874	0.216269906
B	1.834852790	0.045037323	-0.113551799
C	-0.228664148	-1.136506579	0.599217579
C	1.087126064	1.380693573	0.061665147
C	-0.979189599	0.146801707	0.707487468
C	-0.206414435	1.397187440	0.430367279

H	-0.756161015	-2.061321930	0.825438634
H	1.583495245	2.332230017	-0.111724214
H	-1.481283032	0.184419441	1.681310831
H	-0.768300623	2.319801027	0.549686719
H	1.412772787	-2.122783284	0.140702190
N	3.140374370	-0.153127706	-0.526326297
H	3.743892345	0.625488611	-0.760276995
H	3.602179737	-1.046466789	-0.639908909
Cl	-2.337108293	-0.096463116	-0.505918740

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-1.508372501	0.142301541	0.060354056
N	-0.709068361	-1.117635408	0.348407723
C	-0.701456724	1.440338986	0.129209341
C	0.555472978	-1.120185659	0.626016701
C	0.622403125	1.407001003	0.393157520
C	1.357939261	0.133480240	0.663542839
H	-1.173608501	2.402665981	-0.044787454
H	1.059634292	-2.065486302	0.819346742
H	1.233223891	2.305785207	0.429981648
H	1.890925907	0.179007294	1.622762339
H	-1.181438553	-2.021985791	0.314755023
C	-2.956081751	-0.044791112	-0.253196127
C	-4.137339895	-0.197660259	-0.510023539
H	-5.177768825	-0.321377730	-0.732764000
Cl	2.660060837	-0.166344249	-0.587833518

2-formyl-1,2-dihydro-1,2-azaborine

B	1.422719341	0.175001132	0.059535180
N	0.488226992	1.351892973	0.203441581
C	0.800782714	-1.194240180	0.275348367
C	-0.772096314	1.228421299	0.491538193
C	-0.521599004	-1.300263458	0.540700260
C	-1.407462783	-0.103317777	0.679826191
H	1.403736403	-2.094640986	0.197363685
H	-1.393180087	2.118437734	0.580639604
H	-1.019767166	-2.257902191	0.673517991
H	-1.924137157	-0.107485398	1.650439324
H	0.834325987	2.303447633	0.065519032
C	2.947263849	0.458267152	-0.307004608
O	3.717029033	-0.483558298	-0.396461392
H	3.324700414	1.491679619	-0.480167863
Cl	-2.738188723	-0.104496916	-0.572970643

Intermediate in the chlorination of substituted 1,2-dihydro-1,2-azaborines on C6

1-methyl-1,2-dihydro-1,2-azaborine

B	1.417160674	1.172570501	-0.448361227
N	0.142282666	1.137125269	0.145608173
C	2.211916973	-0.186928211	-0.471993014
C	-0.397095226	-0.056331640	0.687910919
C	1.706273022	-1.340621710	0.112057627
C	0.459286382	-1.265711735	0.722160200
H	3.193337863	-0.246759527	-0.941173861
H	-0.909980827	0.116660694	1.638485763
H	2.251281623	-2.279964612	0.118319742
H	0.035450896	-2.124125107	1.236359874
H	1.857967466	2.182335270	-0.877517989
C	-0.740010682	2.315194984	0.235661432
H	-0.992583492	2.521207539	1.280226102
H	-0.222305079	3.174066912	-0.187249927
H	-1.660881127	2.134946467	-0.328675546
Cl	-1.717496713	-0.799022359	-0.414263687

1-vinyl-1,2-dihydro-1,2-azaborine

B	-0.205356570	1.744985398	-0.298914777
N	-0.642298432	0.513808277	0.252785169
C	1.332991899	1.921046086	-0.462296387
C	0.298354846	-0.495030337	0.665740056
C	2.245594591	0.976820179	0.013801937
C	1.746528831	-0.177888941	0.583648869
H	1.736663452	2.818370920	-0.929497529
H	0.049194276	-0.859379092	1.669155911
H	3.319442988	1.122546344	-0.057591446
H	2.408562005	-0.944801107	0.976213525
H	-0.979079612	2.597704354	-0.562341859
C	-2.002456177	0.164553838	0.475652673
H	-2.151603878	-0.588689670	1.243467292
C	-3.041375456	0.679502694	-0.195772928
H	-2.931048022	1.396409439	-1.001184805
H	-4.045594693	0.366232755	0.065376606
Cl	0.197692488	-1.978579445	-0.418452264

1-mercapto-1,2-dihydro-1,2-azaborine

N	-0.475347056	-0.689090486	0.071947590
B	0.263561121	-1.742038459	-0.516660888
C	0.148489512	0.477231906	0.641221924
C	1.811206959	-1.582997530	-0.463948037
C	1.631131036	0.462858671	0.752431651

C	2.429447759	-0.511893327	0.183952216
H	-0.312917578	0.744001276	1.598489863
H	2.455078895	-2.340629814	-0.908804093
H	2.061106678	1.304302758	1.288682528
H	3.509894289	-0.428386030	0.255105384
H	-0.288758210	-2.682268071	-0.975293831
S	-2.216681300	-0.644718987	0.192924873
H	-2.435188397	-1.384779022	-0.913318601
Cl	-0.075638112	1.948129572	-0.434645910

1-hydroxy-1,2-dihydro-1,2-azaborine

B	1.443067513	1.173215950	-0.443630896
N	0.172318592	1.054728315	0.133671117
C	2.244308966	-0.159590185	-0.459630064
C	-0.403205496	-0.146428521	0.653026364
C	1.749973406	-1.343288807	0.097729334
C	0.488587659	-1.334406443	0.661663330
H	3.240023951	-0.192772987	-0.900499693
H	2.330349634	-2.260985687	0.096797812
H	1.827293409	2.219690587	-0.840947969
O	-0.722209501	2.089777019	0.312580695
H	-0.366832772	2.858406956	-0.170206024
H	-0.845227742	0.048476564	1.636591140
H	0.062591746	-2.226263603	1.112725484
Cl	-1.773051036	-0.736570018	-0.410727733

1-amino-1,2-dihydro-1,2-azaborine

B	-1.491964181	-1.201737522	-0.344456651
N	-0.158406862	-1.042319142	0.104716718
C	-2.325365329	0.089552040	-0.385448391
C	0.371284772	0.220642289	0.577590422
C	-1.827580620	1.331888854	0.051519396
C	-0.532142422	1.400986724	0.496596301
H	-3.339310355	0.073541682	-0.782839893
H	-2.433794651	2.232126484	0.015883624
H	-1.871725950	-2.276729710	-0.662675723
N	0.693736666	-2.104281816	0.312216360
H	1.643016225	-1.921489703	-0.013205881
H	0.304412896	-2.964424002	-0.061589434
H	0.680240700	0.090462278	1.623569066
H	-0.084256966	2.340158811	0.808185317
Cl	1.882710336	0.664044597	-0.339267353

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-0.459042503	-0.780248237	0.089921115
B	0.393323595	-1.772780363	-0.475973455
C	0.045797603	0.464223946	0.643079333
C	1.917576032	-1.442342720	-0.439960207
C	1.520806997	0.615920807	0.706392808
C	2.417315937	-0.286270023	0.160664579

H	-0.414253727	0.653518733	1.618353616
H	2.637626620	-2.131889781	-0.878628202
H	1.866270854	1.525922000	1.189905246
H	3.481822887	-0.075823873	0.206968443
H	-0.066776511	-2.770709947	-0.905291797
C	-1.806377612	-0.930030487	0.140907986
C	-3.008519293	-1.054401875	0.195618949
H	-4.071507588	-1.164188176	0.234052338
Cl	-0.411836828	1.888307632	-0.411117318

2-formyl-1,2-dihydro-1,2-azaborine

B	1.240426550	-0.073967432	-0.409669616
N	0.047177433	-0.653250338	-0.857250494
C	1.129124128	1.351215685	0.225372546
C	-1.226527166	-0.024568357	-0.735017852
C	-0.084595220	2.036571343	0.215347194
C	-1.215804254	1.373313985	-0.238529646
H	1.997906582	1.831978197	0.671689337
H	-1.786907702	-0.091149788	-1.674954702
H	-0.179095456	3.047868790	0.600477879
H	-2.188663943	1.857385615	-0.205419017
H	0.016648987	-1.571373938	-1.291016234
C	2.642526531	-0.827201225	-0.322572623
O	3.175100836	-0.652737682	0.761631556
H	3.097819130	-1.499050495	-1.075424823
Cl	-2.316467693	-0.861146249	0.503156925

Intermediate in the bromination of substituted 1,2-dihydro-1,2-azaborines on C3

1-phenyl-1,2-dihydro-1,2-azaborine

B	1.043786691	-0.379167377	-0.936377880
N	0.126810344	0.475644958	-0.094208668
C	2.539588784	0.048788292	-0.923409547
C	0.596840134	1.541962276	0.530550888
C	2.905476727	1.285160697	-0.228425213
C	1.958962676	1.982706179	0.456170542
H	3.223546447	-0.297809248	-1.692177598
H	-0.106771030	2.112042969	1.130389475
H	3.923291046	1.658939167	-0.292794163
H	2.206498955	2.900613938	0.977844296
H	0.565359693	-1.146537727	-1.690961103
C	-1.284739452	0.184318173	-0.059457791
C	-2.220959428	1.225388472	-0.135654555
C	-1.697219699	-1.150213597	0.046265631
C	-3.580118731	0.923731630	-0.074722579

C	-3.059560252	-1.435843868	0.115734616
C	-4.001233865	-0.403533680	0.057215755
H	-1.900409867	2.251240115	-0.289281463
H	-0.968655115	-1.951249986	0.101590207
H	-4.309207419	1.723589278	-0.150476257
H	-3.384685115	-2.466092428	0.215076100
H	-5.060784030	-0.633498748	0.099925889
Br	2.467864711	-1.551842532	0.406843294

2-formyl-1,2-dihydro-1,2-azaborine

N	1.000308819	1.616782536	-0.285822643
B	0.348400847	0.374304707	0.204934839
C	2.273903718	1.910868860	-0.083300131
C	1.385359273	-0.678985946	0.755378308
C	3.184919360	1.024610927	0.557493453
C	2.771031729	-0.203950744	0.981031630
H	2.621831718	2.883620749	-0.423855497
H	1.044148168	-1.367087479	1.527043689
H	4.207899247	1.355871974	0.691478343
H	3.475300792	-0.875255436	1.466585567
H	0.438499817	2.347388070	-0.715055380
C	-1.167557811	0.220688972	0.152312552
C	-1.820861216	-0.709767148	0.998587298
C	-1.973892459	1.003618756	-0.712023454
C	-3.205077328	-0.846114025	0.986050138
C	-3.356644728	0.861273763	-0.735636988
C	-3.973939874	-0.060704564	0.119149023
H	-1.241946834	-1.326879905	1.679278901
H	-1.521451518	1.713535853	-1.401336306
H	-3.688159998	-1.558982256	1.646377347
H	-3.955528937	1.458905999	-1.415112052
H	-5.054338122	-0.167564669	0.107890477
Br	1.565734566	-1.846078777	-0.882949654

Intermediate in the bromination of substituted 1,2-dihydro-1,2-azaborines on C5

1-phenyl-1,2-dihydro-1,2-azaborine

B	1.000272258	-0.416715226	-1.084365489
N	0.112247930	0.402635902	-0.171263121
C	2.456527592	0.011946168	-1.200896424
C	0.604277983	1.405031836	0.507400057
C	2.917973675	1.033705679	-0.445713044
C	2.032230015	1.790971201	0.474015586
H	3.145776225	-0.502281473	-1.864391580
H	-0.064491200	1.968654842	1.153317458
H	3.956055803	1.357107392	-0.469518615
H	2.134261722	2.875065503	0.363849217

H	0.482721273	-1.320784698	-1.637818435
C	-1.313089109	0.128822959	-0.102922464
C	-2.219116973	1.185999683	-0.243178551
C	-1.747749840	-1.184182589	0.102403747
C	-3.586162807	0.920961387	-0.159954066
C	-3.117245298	-1.431010598	0.194314822
C	-4.035051558	-0.383613788	0.063200756
H	-1.870792585	2.191367895	-0.461812020
H	-1.036114000	-1.995586544	0.211562752
H	-4.296944823	1.730939042	-0.285126697
H	-3.465705391	-2.443512921	0.368512078
H	-5.099225701	-0.586636531	0.123330750
Br	2.601708311	1.452985162	2.359862217

2-formyl-1,2-dihydro-1,2-azaborine

N	1.023379287	1.768087809	0.006183734
B	0.387880228	0.442754268	0.386284487
C	2.291426237	2.030164967	0.100789777
C	1.401514554	-0.568729840	0.955443190
C	3.272168837	1.000761044	0.505636241
C	2.721976089	-0.291992211	0.987229613
H	2.649707044	3.026505220	-0.149467679
H	1.086053244	-1.539479676	1.326744974
H	4.040210396	1.422447107	1.157630193
H	3.458045089	-1.003174498	1.353637462
H	0.432757774	2.531179105	-0.319601241
C	-1.111654536	0.269149823	0.177267367
C	-1.763657573	-0.877132306	0.703141272
C	-1.909870411	1.206096560	-0.530573030
C	-3.131136312	-1.069675168	0.541134301
C	-3.275704313	1.015093663	-0.698970549
C	-3.888459525	-0.124304925	-0.160645004
H	-1.191988889	-1.619601609	1.250496670
H	-1.468002648	2.094612907	-0.976964356
H	-3.610003940	-1.950856723	0.955485732
H	-3.865419795	1.741250897	-1.248835397
H	-4.955933173	-0.274565665	-0.290431480
Br	4.231841348	0.749545514	-1.243434889

Products of the bromination of 1-phenyl-1,2-dihydro-1,2-azaborine on C3

Product brominated on B

B	-0.639453425	-0.146427538	-0.989731449
N	0.369481880	-0.655571430	-0.092901359
C	-2.006398879	-0.780940221	-0.925651668

C	0.070260502	-1.682141283	0.777782293
C	-2.214873847	-1.800869573	-0.025465947
C	-1.171291976	-2.255437163	0.831637106
H	-2.828929838	-0.463486034	-1.560557209
H	0.883272104	-2.006396980	1.418493914
H	-3.187245221	-2.284785306	0.052293157
H	-1.343775236	-3.059779803	1.537976433
C	1.722731636	-0.144192960	-0.038813188
C	2.711966898	-0.717583283	-0.839881000
C	2.034845287	0.897311792	0.836848180
C	4.026139183	-0.251971063	-0.754217970
C	3.350596095	1.359042555	0.919918003
C	4.346771989	0.787421720	0.123444197
H	2.450126560	-1.521069834	-1.521238347
H	1.251790947	1.336821706	1.446794349
H	4.796021666	-0.698137133	-1.376585491
H	3.593825402	2.169017506	1.601014549
H	5.368561603	1.149393360	0.187437016
Br	-0.183193010	1.304951496	-2.204383006

Product brominated on C3

B	-0.553603308	-0.069677148	-0.957375703
N	0.433327054	-0.692788406	-0.102526355
C	-1.921589719	-0.714259382	-0.929183852
C	0.125296957	-1.786155493	0.674360656
C	-2.164249760	-1.811156443	-0.138350674
C	-1.125220294	-2.344547322	0.672851561
H	0.920579406	-2.169424248	1.303632569
H	-3.142763674	-2.284541483	-0.114133633
H	-1.318777363	-3.197720099	1.313225392
H	-0.232117749	0.861827154	-1.618904439
C	1.790071932	-0.210356472	-0.058640585
C	2.857285131	-1.091582251	-0.268315607
C	2.040196662	1.143235220	0.189269924
C	4.170601116	-0.619298645	-0.214286630
C	3.355203672	1.610087350	0.232535854
C	4.424206976	0.732150346	0.032956279
H	2.658847408	-2.135724326	-0.490007692
H	1.208025824	1.818955643	0.355731796
H	4.993680373	-1.307614829	-0.381843498
H	3.542352704	2.661502458	0.429182587
H	5.445700029	1.098210695	0.069098530
Br	-3.333366551	-0.015761140	-2.009400187

Wheland intermediates in the nitration of benzene (and derivatives) at the *orto*- position

Benzene

C	-1.590384855	1.238965949	-0.157089995
C	-2.102293216	-0.001727701	-0.603971113
C	-0.529524358	1.253833157	0.718942995
C	-1.592073753	-1.238699138	-0.145170929
C	0.093300057	0.005076448	1.101771019
C	-0.531373964	-1.246359117	0.731153820
H	-0.119961508	2.186105094	1.096345708
H	-2.048702329	-2.165609745	-0.475333564
H	0.769306251	0.008408688	1.951057994
H	-0.123035650	-2.175527013	1.117425241
H	-2.045630009	2.163214537	-0.496507111
N	1.542352394	-0.002675817	-0.273770598
O	1.158562356	-0.010946010	-1.394498621
O	2.591428436	0.004205613	0.280716816
H	-2.931351831	-0.004479831	-1.306907826

Phenylbenzene

C	-0.331181971	0.721021902	0.198075613
C	-1.309197258	-0.371535642	0.553928285
C	-0.862915949	1.988700347	-0.084901071
C	-2.764637324	-0.032297868	0.561814581
C	-2.229151928	2.228314610	-0.048999937
C	-3.191529548	1.220805901	0.279707741
H	-1.057815936	-0.807437772	1.527951766
H	-0.200884630	2.816817853	-0.304927788
H	-3.449020471	-0.838555089	0.808357609
H	-2.584642545	3.230378656	-0.273801632
H	-4.246910201	1.469892042	0.296045415
N	-1.171398007	-1.603484909	-0.426353372
O	-1.547573681	-2.666083850	0.033340796
O	-0.746914829	-1.377655948	-1.544394183
C	1.079884562	0.440276386	0.177228610
C	1.979936613	1.304662456	-0.511028211
C	1.618168524	-0.709620069	0.822812328
C	3.336785143	1.028836047	-0.550701776
C	2.977705088	-0.971485797	0.788954275
C	3.841635273	-0.105591817	0.101290911
H	1.605534446	2.162883954	-1.056153810
H	0.978974350	-1.382521923	1.384162836
H	4.006100223	1.686142408	-1.095305405
H	3.373481642	-1.842451674	1.300153473
H	4.906407094	-0.315575528	0.073942586

Toluene

C	-0.600912799	1.035563133	0.237000269
C	0.186367291	-0.203997664	0.517961685
C	-1.927349105	0.880852998	-0.129929589
C	-0.441286103	-1.519745032	0.237064610
C	-2.480521038	-0.393476442	-0.331235261

C	-1.747925212	-1.596143782	-0.142133446
H	0.411510976	-0.186504410	1.600651307
H	-2.544892136	1.759444316	-0.287403299
H	0.178189166	-2.401788276	0.372840271
H	-3.515419467	-0.462139337	-0.658546558
H	-2.222722863	-2.554378692	-0.322872391
N	1.644339337	-0.225446305	-0.107191943
O	2.367469995	-1.086650843	0.350536554
O	1.885923612	0.579799218	-0.983836861
C	0.019875649	2.373226798	0.412206356
H	-0.735784331	3.144162640	0.575093724
H	0.750528412	2.390476938	1.226821129
H	0.576731306	2.625589420	-0.502880950

Styrene

C	-0.909846917	0.193720343	0.239319707
C	0.500317001	-0.195590619	0.580403129
C	-1.770473513	-0.812538636	-0.204430801
C	0.914528696	-1.605145669	0.344754119
C	-1.319943788	-2.120088697	-0.374962552
C	0.019227003	-2.526863442	-0.095056217
H	0.675939448	0.041451230	1.642047701
H	-2.808694891	-0.587825055	-0.419214161
H	1.952175356	-1.852024229	0.548418724
H	-2.021142820	-2.864871450	-0.742712301
H	0.311901797	-3.559210475	-0.252498660
N	1.581273026	0.724515542	-0.138656635
O	2.705559754	0.614599866	0.306845384
O	1.196952325	1.418040055	-1.059924895
C	-1.293499496	1.565718798	0.453811136
H	-0.558047044	2.213604053	0.922727397
C	-2.481888429	2.106242738	0.090216144
H	-3.261960033	1.547232523	-0.416991013
H	-2.688507869	3.153780188	0.284368810

Chlorobenzene

C	-0.599799395	0.724347924	0.140108213
C	0.175555229	-0.455586950	0.611444176
C	-1.874462903	0.571585002	-0.369109935
C	-0.499669416	-1.773339077	0.514962843
C	-2.437017543	-0.712908517	-0.434842362
C	-1.764641850	-1.880866602	0.019157173
H	0.540608352	-0.283667583	1.633129257
H	-2.435883361	1.435529505	-0.708044717
H	0.069796441	-2.639393312	0.840577440
H	-3.433881665	-0.815519931	-0.857030272
H	-2.255728706	-2.845294943	-0.050774888
N	1.595509719	-0.628822619	-0.185548381
O	2.338492392	-1.425912872	0.337854460
O	1.738347731	0.022097521	-1.193104903

Cl	0.115062403	2.252553289	0.275464878

Thiophenol

C	-0.616948525	0.714037392	0.119315367
C	0.208673911	-0.482952231	0.518221677
C	-1.950176311	0.505953774	-0.268408137
C	-0.422638632	-1.823701260	0.331858136
C	-2.475683009	-0.773629454	-0.358172593
C	-1.714696761	-1.946654596	-0.054552281
H	0.447528001	-0.381777484	1.589727334
H	-2.570615739	1.359647009	-0.523640512
H	0.205974247	-2.682374686	0.543176617
H	-3.503640753	-0.888552572	-0.691491701
H	-2.170742109	-2.924924235	-0.159563906
N	1.669823446	-0.537852254	-0.114131511
O	2.302506793	-1.527597369	0.185692250
O	2.026868872	0.399912052	-0.802314577
S	-0.079684182	2.336015286	0.210336390
H	1.216055628	2.109572941	0.508851790

Phenol

C	-0.513652026	1.026656595	0.068079500
C	0.180183263	-0.260458485	0.468137400
C	-1.898431417	1.009613535	-0.162133806
C	-0.586359019	-1.520902506	0.241927791
C	-2.564819429	-0.198350268	-0.205663550
C	-1.911873045	-1.468542148	-0.018657227
H	0.313386004	-0.172204744	1.564586774
H	-2.398837111	1.950818877	-0.363264988
H	-0.050543088	-2.455566647	0.366468835
H	-3.629110722	-0.194172372	-0.426423382
H	-2.490911267	-2.380234691	-0.116654657
N	1.646116398	-0.343688567	-0.030203776
O	2.082613401	-1.431192282	-0.315653700
O	2.270052229	0.723908887	-0.040301930
O	0.129327561	2.147286665	0.019086561
H	1.111580607	1.985040216	0.077517202

Aniline

C	-0.490128506	1.066396811	0.072250612
C	0.192974228	-0.206359880	0.550773619
C	-1.868100982	1.009951533	-0.274812311
C	-0.597239577	-1.468272159	0.411312909
C	-2.532989886	-0.187324487	-0.277434786
C	-1.898321428	-1.440335279	0.063588909
H	0.407160829	-0.060859362	1.622399870
H	-2.370765359	1.925492550	-0.570806138
H	-0.083226227	-2.392423801	0.649402083
H	-3.579351539	-0.200810633	-0.569539251
H	-2.477873571	-2.355469621	0.014968839

N	1.625090844	-0.364338149	-0.052252489
O	1.913399654	-1.440603146	-0.526979188
O	2.357554402	0.616787294	0.048078983
N	0.178722735	2.198831370	0.050377686
H	1.182504279	2.206360597	0.228037178
H	-0.268962384	3.060276630	-0.245227587

Ethynylbenzene

C	-0.223034656	0.997974163	0.151077844
C	-0.019347901	-0.425886514	0.576849073
C	-1.480510125	1.396860080	-0.296513706
C	-1.176469519	-1.344971218	0.439807655
C	-2.527401537	0.471441186	-0.375667732
C	-2.385012052	-0.893339412	0.002077805
H	0.323456305	-0.435558359	1.623016914
H	-1.642091505	2.428875268	-0.587446310
H	-1.009692542	-2.385144166	0.704543749
H	-3.489483876	0.810421762	-0.751598569
H	-3.231237543	-1.566267701	-0.083820888
N	1.223968748	-1.127130335	-0.157892338
O	1.536032282	-2.195411738	0.324357991
O	1.704843419	-0.546518294	-1.106314105
C	0.840183940	1.899560509	0.256929701
C	1.766637801	2.681585696	0.358721670
H	2.582265121	3.371784728	0.443661632

Benzaldehyde

C	-1.127608087	-1.172755951	0.528104200
C	-0.957510007	-0.091953970	-0.315323990
C	-0.138622261	-2.181913217	0.583660712
C	0.278479335	0.031363857	-1.048306663
C	1.015415955	-2.143942591	-0.228100151
C	1.217748145	-1.065392486	-1.064971503
H	-0.285983904	-3.024981443	1.253496593
H	0.346804124	0.783150425	-1.830422052
H	1.728246670	-2.961006330	-0.194526251
H	2.091851999	-1.004196809	-1.706734395
H	-2.034044654	-1.248970576	1.121247021
C	-2.024813363	0.961155014	-0.440208699
O	-3.053023929	0.898994565	0.193497594
H	-1.821074438	1.786316337	-1.149515357
N	1.360673430	1.120103477	0.320794089
O	1.369370866	0.654135753	1.406227304
O	1.793895410	2.072425465	-0.233307800

Wheland intermediates in the nitration of benzene (and derivatives) at the *meta*- position

Phenylbenzene

C	-0.321076371	-0.520015992	0.177825860
C	0.703927444	0.408657127	0.239599575
C	0.064965406	-1.892924782	0.175952082
C	2.099515746	-0.008489095	0.452878994
C	1.402656721	-2.343549625	0.245118680
C	2.427443930	-1.437800629	0.325784525
H	0.510203648	1.474149966	0.165818065
H	-0.719911726	-2.641391478	0.101209100
H	2.300546599	0.222733179	1.525399447
H	1.609131237	-3.408132360	0.211448261
H	3.471533432	-1.732063707	0.355161438
N	3.149564874	0.942817636	-0.238296185
O	2.765003163	2.070775398	-0.472047016
O	4.250066554	0.463877385	-0.424438130
C	-1.739210767	-0.116945258	0.061644412
C	-2.628133342	-0.848925713	-0.746635846
C	-2.211633478	1.011351945	0.756323341
C	-3.960407247	-0.455126833	-0.859411692
C	-3.546783346	1.396201442	0.646465587
C	-4.422009034	0.665369690	-0.162126818
H	-2.279084282	-1.702445625	-1.321445855
H	-1.549110582	1.570278625	1.411519650
H	-4.634641716	-1.016707872	-1.497678231
H	-3.904621740	2.259671295	1.197585807
H	-5.460710586	0.967744372	-0.248833622

Toluene

C	1.829093275	-0.466744550	0.004466739
C	0.534744748	-0.854879975	0.271906232
C	2.059133073	0.925425663	-0.183651113
C	-0.531895196	0.140224736	0.481548355
C	1.054331941	1.916202608	-0.096053119
C	-0.239182516	1.547419127	0.166146185
H	0.265262049	-1.901241012	0.382874260
H	3.067948283	1.244634077	-0.439778627
H	-0.722564601	0.130890001	1.579721299
H	1.306504840	2.954892688	-0.281823608
H	-1.056172267	2.261870332	0.193101280
N	-1.946738688	-0.338371016	-0.044362685
O	-2.091301924	-1.539543239	-0.137366609
O	-2.751871651	0.544269470	-0.257362122
C	2.959917722	-1.451623630	-0.141758600
H	3.441745707	-1.346284463	-1.119091836
H	3.723397502	-1.276507275	0.623752423
H	2.607745475	-2.479774580	-0.042162878

Styrene

C	1.521548315	-0.197385574	0.046913767
C	0.267287221	-0.727051977	0.296959538

C	1.585059317	1.209401411	-0.180255330
C	-0.906377748	0.139190833	0.479141738
C	0.471921596	2.074481108	-0.112928016
C	-0.774813441	1.566315897	0.148133147
H	0.119236615	-1.796793252	0.413233445
H	2.541169865	1.643821559	-0.459603092
H	-1.109726345	0.126033850	1.575473883
H	0.603920581	3.131216183	-0.320052515
H	-1.668296958	2.182733248	0.158210444
N	-2.254572590	-0.500828064	-0.053456932
O	-2.244351520	-1.705550304	-0.196500734
O	-3.169862484	0.278383602	-0.220171937
C	2.697657024	-1.076593148	-0.047281791
H	2.475081779	-2.140894053	-0.049204287
C	3.975650104	-0.677974621	-0.103298299
H	4.286023905	0.362817578	-0.078341990
H	4.774136807	-1.409437428	-0.163550881

Chlorobenzene

C	1.432696638	0.035762816	0.052371590
C	0.251493738	-0.613296262	0.322244393
C	1.419999855	1.437984190	-0.177811112
C	-0.983780375	0.168231915	0.493545553
C	0.238808725	2.207826395	-0.120881385
C	-0.960914222	1.597102764	0.148112130
H	0.204212100	-1.690193610	0.453343429
H	2.358173867	1.924422924	-0.434532443
H	-1.204543449	0.139218250	1.585738914
H	0.284464998	3.271308823	-0.330602947
H	-1.900946375	2.140654351	0.154002189
N	-2.281240808	-0.586418017	-0.051549955
O	-2.173806680	-1.787381559	-0.165738929
O	-3.244308849	0.122168922	-0.247252936
Cl	2.919388410	-0.828950469	-0.077854192

Thiophenol

C	1.470260617	-0.006331667	0.052464611
C	0.263075830	-0.629721484	0.306039705
C	1.447729698	1.404370729	-0.168507713
C	-0.965363179	0.162519512	0.475440753
C	0.277284947	2.186793607	-0.117396561
C	-0.934001913	1.590889894	0.133550924
H	0.177606798	-1.704034045	0.435862064
H	2.383620655	1.901608826	-0.417070210
H	-1.172394910	0.151133280	1.571678372
H	0.338915708	3.250501236	-0.321542933
H	-1.869552815	2.141492892	0.132056914
N	-2.268098151	-0.575508202	-0.049264816
O	-2.173465276	-1.777892428	-0.179211751
O	-3.234800695	0.136667654	-0.221025585

S	3.036651414	-0.810149210	-0.083132399
H	2.591834123	-2.059483394	0.157255634

Phenol

C	1.787043477	-0.475836135	0.019689026
C	0.497236044	-0.872230011	0.298439749
C	2.048234768	0.907741289	-0.206753489
C	-0.550427707	0.143526285	0.484793901
C	1.052384462	1.898209040	-0.131737647
C	-0.245698906	1.540734553	0.144526004
H	0.221536395	-1.914703341	0.428022747
H	3.067026264	1.180196102	-0.473797234
H	-0.761066124	0.172251812	1.579124396
H	1.309750413	2.931993644	-0.336229884
H	-1.057858412	2.260931986	0.162632236
N	-1.976681472	-0.319990962	-0.045473716
O	-2.103627078	-1.510530254	-0.237760485
O	-2.798955264	0.564121250	-0.157065843
O	2.848872546	-1.282684565	-0.109537976
H	2.641440182	-2.220265021	0.025947397

Aniline

C	1.830309146	-0.481240235	0.012878084
C	0.513190246	-0.866039471	0.254414568
C	2.063083697	0.915138241	-0.198682075
C	-0.533388445	0.141586909	0.449440305
C	1.060410803	1.897918097	-0.127493492
C	-0.242793224	1.544291503	0.128242172
H	0.231098924	-1.908899362	0.358945867
H	3.072929362	1.232752866	-0.450538269
H	-0.709657527	0.170776778	1.552072914
H	1.321982142	2.933454760	-0.317749904
H	-1.055443520	2.262379764	0.153977409
N	-1.962476550	-0.325187634	-0.040173546
O	-2.094333838	-1.516165999	-0.234467160
O	-2.794555014	0.554599765	-0.127156621
N	2.854425803	-1.367459147	-0.064001664
H	2.697634406	-2.359439158	0.033697290
H	3.785898649	-1.078272226	-0.320986164

Ethynylbenzene

C	1.589481578	0.017056215	0.051582842
C	0.393960493	-0.630084382	0.314396480
C	1.547881809	1.428528611	-0.171370513
C	-0.847872100	0.139251394	0.481289866
C	0.360151617	2.187897092	-0.125156745
C	-0.836826493	1.568415824	0.131669821
H	0.350534671	-1.706631661	0.446054322
H	2.481070667	1.928246392	-0.419391569
H	-1.057302778	0.117687309	1.576320275

H	0.397700140	3.251797783	-0.334181326
H	-1.782056807	2.102571860	0.128688111
N	-2.136061243	-0.623687497	-0.050938084
O	-2.024892517	-1.826199211	-0.157601168
O	-3.106634860	0.075601656	-0.250644137
C	2.820384626	-0.689403881	-0.049842074
C	3.869749807	-1.286119607	-0.129149421
H	4.796269614	-1.816317158	-0.204729750

Benzaldehyde

C	1.581032700	1.186852471	0.118430322
C	1.455586887	-0.212539456	-0.107680304
C	0.480326175	2.067913863	0.084273697
C	0.217103043	-0.743812900	-0.359696362
C	-0.775331092	1.567458669	-0.159735391
C	-0.948645113	0.145471733	-0.508020173
H	0.623229924	3.122544024	0.295243945
H	0.063871219	-1.812047506	-0.496082158
H	-1.661328277	2.195856110	-0.140583144
H	-1.198292887	0.134619423	-1.593386423
H	2.575655796	1.561313981	0.357354677
C	2.690715670	-1.077868232	-0.004948039
O	3.767163333	-0.596975336	0.254794862
H	2.544368710	-2.159058963	-0.181789055
N	-2.292285316	-0.481093862	0.076592475
O	-3.169467760	0.315567188	0.328992837
O	-2.303300432	-1.689966687	0.163262047

Wheland intermediates in the nitration of benzene (and derivatives) at the *para-* position

Phenylbenzene

C	-0.488401327	0.026418332	0.200779256
C	0.250319226	1.260465731	0.075568994
C	0.258336220	-1.182047035	0.457592971
C	1.599554104	1.300958682	0.203096922
C	1.605947185	-1.173672307	0.605577988
C	2.371866724	0.095284819	0.587069486
H	-0.272254452	2.168563175	-0.196235325
H	-0.266921139	-2.123682753	0.550845102
H	2.152560030	2.220980734	0.045201030
H	2.156412812	-2.090543532	0.787252525
H	2.775902932	0.262425479	1.603921567
N	3.706797463	-0.029734230	-0.236422375
O	4.193364566	1.016553206	-0.622850407
O	4.152252126	-1.154604721	-0.368006375
C	-1.919370302	-0.000171218	0.040598927

C	-2.606979974	-1.216049995	-0.243998947
C	-2.690355549	1.192581749	0.165292568
C	-3.982005146	-1.229908880	-0.410650692
C	-4.068111553	1.164247824	0.024583621
C	-4.717593059	-0.043439737	-0.271048387
H	-2.058228135	-2.139667371	-0.382510906
H	-2.212862043	2.131062974	0.419999976
H	-4.488279255	-2.158444638	-0.651768574
H	-4.643280370	2.075899371	0.145734928
H	-5.796448354	-0.060356754	-0.391795992

Toluene

C	2.136175535	-0.003579047	0.079591624
C	1.433340077	1.236068631	-0.044157566
C	1.433238956	-1.240536891	-0.054779561
C	0.092313930	1.258044437	-0.285359449
C	0.090781052	-1.259714358	-0.293861294
C	-0.641545230	0.000185347	-0.537202919
H	1.976309525	2.165146538	0.098422645
H	1.975403542	-2.170969721	0.079342256
H	-0.466093057	2.187765783	-0.335573631
H	-0.467893720	-2.188909662	-0.350761532
H	-0.895923295	0.003176909	-1.618701091
N	-2.089667620	0.000324806	0.092947188
O	-2.585011543	1.094839034	0.269727585
O	-2.577301741	-1.093840008	0.292305379
C	3.593345594	0.002603437	0.357266449
H	3.955670247	-0.953842821	0.737571445
H	4.121106751	0.206341777	-0.590018894
H	3.872016954	0.813418755	1.037908397

Styrene

C	1.768168334	-0.230213117	0.014535546
C	0.949998365	-1.409274777	0.082421971
C	1.151753697	1.059232081	0.170856160
C	-0.388911733	-1.330457558	0.304237052
C	-0.182516239	1.173504790	0.396228282
C	-1.030805268	-0.026198558	0.583937070
H	1.415162916	-2.376701875	-0.077523067
H	1.748268579	1.958248015	0.073323030
H	-1.016463213	-2.215805803	0.316307997
H	-0.661393326	2.143924084	0.476762544
H	-1.356415238	-0.040186463	1.643277886
N	-2.429619721	0.114603082	-0.137249406
O	-3.002236545	-0.927390554	-0.388746294
O	-2.816298822	1.251415395	-0.324897347
C	3.174315906	-0.403192096	-0.247175158
H	3.512479484	-1.425574800	-0.393796006
C	4.089032658	0.596080973	-0.308693921
H	3.843438037	1.643440080	-0.164382780

H	5.132843432	0.370877172	-0.504272671

Chlorobenzene

C	1.622647262	0.000136684	0.044088144
C	0.942583866	-1.249797916	0.144906928
C	0.942539377	1.250116108	0.144132883
C	-0.404016924	-1.259952080	0.353375327
C	-0.404388177	1.260134027	0.350438135
C	-1.144489282	0.000237789	0.575234677
H	1.500799931	-2.171554892	0.022325720
H	1.500805355	2.171835567	0.021427955
H	-0.962336799	-2.190326451	0.394253511
H	-0.962789951	2.190479256	0.391077221
H	-1.464439926	0.002289613	1.638188516
N	-2.564574660	-0.000251876	-0.136982270
O	-3.041369763	-1.095008900	-0.351452311
O	-3.043013327	1.094417018	-0.348353414
Cl	3.287599168	-0.000007024	-0.249398838

Thiophenol

C	1.666012539	0.031022798	0.039044611
C	0.976197341	-1.222112693	0.201555869
C	0.943861639	1.272460130	0.109191002
C	-0.359581817	-1.243338865	0.433936077
C	-0.392244174	1.271900870	0.343477405
C	-1.126240087	0.012494884	0.616615048
H	1.530992257	-2.150736010	0.109866056
H	1.465908908	2.209713519	-0.053779090
H	-0.897992958	-2.181413656	0.520644889
H	-0.959248366	2.197302264	0.365036380
H	-1.479516659	0.049250991	1.664914290
N	-2.510062103	-0.019330202	-0.147853537
O	-2.923496919	-1.118876134	-0.458823204
O	-3.044819229	1.060471894	-0.307041575
S	3.342098824	-0.052375063	-0.276950509
H	3.575906877	1.275199653	-0.374963192

Phenol

C	2.080530684	0.008615374	-0.080912740
C	1.403035713	-1.247402717	0.056368204
C	1.392199261	1.261551914	0.049429803
C	0.076116570	-1.260762722	0.329577626
C	0.064612049	1.264329864	0.322671351
C	-0.666264921	-0.000479757	0.584493436
H	1.973589032	-2.157681439	-0.094354680
H	1.933703172	2.190999442	-0.104385978
H	-0.475738287	-2.192361771	0.403686093
H	-0.496325757	2.191358654	0.387858312
H	-0.954463615	0.002705114	1.653781233
N	-2.089037532	-0.003130782	-0.098872252

O	-2.570887836	-1.097745633	-0.311171390
O	-2.580580333	1.090545198	-0.297961599
O	3.352953335	-0.062191130	-0.362948163
H	3.791338177	0.801959546	-0.467175430

Aniline

C	2.104111169	0.008225179	-0.091517988
C	1.407703998	-1.245510145	0.102568164
C	1.388783272	1.261627839	0.011944958
C	0.091227032	-1.252455413	0.397359038
C	0.072793301	1.268735311	0.309314772
C	-0.662994318	0.011620579	0.617498473
H	1.954475108	-2.175809841	-0.018735988
H	1.920145202	2.189423645	-0.177775558
H	-0.450605128	-2.185214067	0.511706074
H	-0.486904151	2.196950133	0.359301881
H	-0.973626328	0.048718880	1.677033260
N	-2.057304581	-0.012327510	-0.104690390
O	-2.485382163	-1.108490564	-0.416008387
O	-2.598735842	1.068855752	-0.243347934
N	3.388948630	0.006646640	-0.391496238
H	3.912845009	-0.856605691	-0.486260226
H	3.900577611	0.868449350	-0.547111935

Ethynylbenzene

C	1.793741176	-0.000470864	0.043000036
C	1.092226454	-1.248751407	0.145064523
C	1.092687043	1.247968435	0.147076499
C	-0.253515972	-1.260695562	0.348702182
C	-0.253118540	1.259853489	0.350126170
C	-0.995826551	-0.000355539	0.570714852
H	1.645853022	-2.173360388	0.025268053
H	1.646523201	2.172538785	0.028396252
H	-0.812754023	-2.190155926	0.388255468
H	-0.812307205	2.189329814	0.390064588
H	-1.323476396	-0.000955626	1.630847886
N	-2.407561992	0.000385112	-0.150640209
O	-2.888113993	-1.093504927	-0.366731452
O	-2.885831318	1.094870665	-0.369016872
C	3.172944644	-0.000707711	-0.198343143
C	4.371715502	0.000906156	-0.407059113
H	5.427748354	0.002403348	-0.591208179

Benzaldehyde

C	-0.951131541	0.201463376	1.128794324
C	-1.435240542	-0.297887277	-0.107009935
C	0.305277751	-0.157187717	1.558317789
C	-0.676649533	-1.193102224	-0.896381172
C	1.137928870	-0.972010196	0.710031959
C	0.586546421	-1.560914887	-0.484781390

H	0.698037479	0.194703411	2.507544292
H	-1.098680120	-1.592150507	-1.814465339
H	2.052602303	-1.388187569	1.120282013
H	1.188184683	-2.256578152	-1.062165886
H	-1.596663972	0.849172035	1.713678991
C	-2.810701204	0.118509744	-0.568572265
O	-3.481012129	0.893669716	0.074483242
H	-3.163177952	-0.322903886	-1.518348641
N	2.105061517	0.581440237	-0.267432667
O	3.265573158	0.455575504	-0.077038432
O	1.377373161	1.323035136	-0.828574548

Intermediate in the nitration of substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

N	-1.943650487	-1.140664283	-0.213523082
B	-0.516130034	-1.354157978	0.002764762
C	-2.522354546	0.061110947	-0.175563111
C	0.254481705	-0.055374460	0.447682543
C	-1.810188672	1.259575523	0.085404052
C	-0.461074865	1.232696651	0.305333867
H	-3.587823748	0.104460914	-0.392285421
H	0.354964244	-0.239656256	1.541448341
H	-2.357647002	2.194607127	0.051497185
H	0.105290372	2.155119553	0.406670483
H	-2.541729704	-1.924069639	-0.469042577
N	1.722031510	0.009331107	-0.018684042
O	2.099034554	1.070480970	-0.490398124
O	2.364992738	-1.013083433	0.129133345
H	-0.056299405	-2.433035812	-0.101119920

1-phenyl-1,2-dihydro-1,2-azaborine

B	0.701171348	0.472825862	0.364772698
N	-0.360919989	-0.473164615	-0.009229558
C	2.142767121	-0.140052668	0.498820473
C	-0.054116913	-1.727697887	-0.350905604
C	2.344884173	-1.506261073	-0.039781689
C	1.265460686	-2.265637815	-0.371075069
H	2.247987389	-0.207353928	1.603831871
H	-0.884423410	-2.353493443	-0.669486108
H	3.355506285	-1.893534339	-0.131356673

H	1.379655207	-3.289536448	-0.708907122
H	0.432581759	1.592599157	0.606557841
C	-1.757804892	-0.061199195	-0.016201292
C	-2.704384784	-0.852383896	0.643592127
C	-2.120797796	1.115376393	-0.677351055
C	-4.043793032	-0.460301375	0.624392677
C	-3.463859553	1.491716437	-0.690623589
C	-4.423932343	0.707005311	-0.043108732
H	-2.401782481	-1.737050154	1.196808061
H	-1.378435831	1.717334897	-1.191354778
H	-4.783771891	-1.059807437	1.144031491
H	-3.758825112	2.396453485	-1.211582298
H	-5.465634275	1.010338968	-0.052006103
N	3.261602532	0.839003133	0.109958566
O	4.088392160	0.432905176	-0.693435114
O	3.213573533	1.937777296	0.634001465

1-methyl-1,2-dihydro-1,2-azaborine

B	0.500306919	-0.987609283	0.158623377
N	1.851701597	-0.459007827	-0.037332716
C	-0.604922364	0.083890074	0.484170586
C	2.066300710	0.856421038	-0.060545682
C	-0.247756777	1.502510298	0.264894338
C	1.057715524	1.849900105	0.081902116
H	-0.707692844	-0.054683926	1.583708623
H	3.091923155	1.177008135	-0.238845195
H	-1.032338871	2.253935651	0.285454822
H	1.359494097	2.887415188	-0.006922825
H	0.312392751	-2.150144561	0.125118764
C	3.006883284	-1.369046907	-0.285573188
H	3.752992397	-1.233958482	0.500453605
H	2.648846953	-2.396273464	-0.269805121
H	3.445956355	-1.151427013	-1.261337098
N	-2.003862641	-0.281235892	-0.039526216
O	-2.591127050	0.581803983	-0.674431625
O	-2.390973557	-1.405325801	0.223557345

1-vinyl-1,2-dihydro-1,2-azaborine

B	-0.423585054	0.682757006	0.108290349
N	-1.637587555	-0.142633778	-0.035502366
C	0.889315935	-0.099298351	0.467879032
C	-1.528896961	-1.477364371	-0.048929249
C	0.876066346	-1.565476093	0.268584339
C	-0.314438126	-2.202666356	0.090380493
H	0.930262024	0.078182030	1.566260674
H	-2.450398980	-2.032545154	-0.211406479
H	1.813482433	-2.113202281	0.299114415
H	-0.369851955	-3.282794238	0.014378956

H	-0.476509707	1.851695736	-0.001446849
C	-2.936788590	0.433445706	-0.280569291
H	-3.650363939	-0.272398765	-0.692494924
C	-3.262117123	1.699217304	-0.018974082
H	-2.581570743	2.427220188	0.406647079
H	-4.269940734	2.032864435	-0.239075935
N	2.169599429	0.579264188	-0.039319082
O	2.945301128	-0.121148341	-0.671958375
O	2.286193017	1.761425945	0.232078447

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.465991718	0.994462814	0.178159815
N	-1.803834615	0.439058835	-0.005422428
C	0.624810338	-0.093882600	0.477008997
C	-2.057090656	-0.863707916	-0.079161047
C	0.259807261	-1.509144826	0.241003863
C	-1.043906967	-1.854291566	0.042568640
H	0.742369959	0.022981364	1.578474001
H	1.043844002	-2.260666967	0.263013255
H	-0.314127765	2.163575179	0.158522602
O	-2.909195792	1.232054120	-0.271951579
H	-2.673268642	2.145123712	-0.026019256
H	-3.093694488	-1.131275935	-0.273380731
H	-1.346345247	-2.889753961	-0.065089665
N	2.035674957	0.277714441	-0.039211812
O	2.682767284	-0.617957989	-0.553129056
O	2.362464020	1.438570787	0.127248398

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.622351101	-0.012783312	-0.045924942
B	0.371039495	-0.785071310	-0.227886003
C	1.608100381	1.334273291	0.033692757
C	-0.906020917	0.091884889	-0.482534114
C	0.429422720	2.115315828	-0.038606710
C	-0.798353638	1.541747091	-0.210081164
H	2.570933253	1.811460908	0.198547388
H	-1.015076014	-0.021195927	-1.585022434
H	0.536045400	3.187237587	0.085476388
H	-1.705549736	2.138951699	-0.179978388
H	0.416753038	-1.959957081	-0.229808926
C	2.805627192	-0.684715848	0.114720481
C	3.831782150	-1.300537548	0.262946272
H	4.742534669	-1.847867889	0.389977810
N	-2.209371634	-0.535696573	0.051327408
O	-2.940675785	0.196868536	0.698561827
O	-2.379799860	-1.709014344	-0.223241256

1-formyl-1,2-dihydro-1,2-azaborine

B	0.405800387	0.688990971	-0.200181085

N	1.593462492	-0.164694728	-0.005042655
C	-0.919028754	-0.109033985	-0.489293567
C	1.496881414	-1.498995054	0.063777148
C	-0.901363344	-1.565941400	-0.234253608
C	0.285154621	-2.220838672	-0.045631865
H	-1.010795854	0.022875114	-1.591038170
H	2.422602047	-2.044855524	0.247959241
H	-1.844216228	-2.107046057	-0.225671485
H	0.323018784	-3.298075443	0.071425680
H	0.510468436	1.858596122	-0.181436566
C	2.932562983	0.444121898	0.195928220
O	3.094765835	1.618043111	0.120452502
H	3.707704427	-0.309243778	0.408218505
N	-2.197027772	0.577247642	0.039578715
O	-2.975148540	-0.131247352	0.659673366
O	-2.300763126	1.762342061	-0.210293739

2-phenyl-1,2-dihydro-1,2-azaborine

N	0.868570040	1.925424295	-0.157436067
B	0.288748273	0.604185121	0.197358337
C	2.145531432	2.233915253	-0.046143252
C	1.394249345	-0.467332480	0.655271706
C	3.137377428	1.313050823	0.415953124
C	2.803803317	0.037742237	0.728403819
H	2.442342940	3.243144027	-0.324008437
H	1.128314147	-0.933644742	1.610041757
H	4.160274624	1.665362250	0.483654927
H	3.576071647	-0.660544083	1.044276102
H	0.259580383	2.669688724	-0.487845251
C	-1.210687580	0.377349442	0.124467371
C	-1.793511127	-0.795747032	0.676095918
C	-2.085523126	1.317603716	-0.487254808
C	-3.165354000	-1.012510907	0.622645291
C	-3.454704161	1.098019190	-0.550271954
C	-3.996566588	-0.067679324	0.008798606
H	-1.167839521	-1.542133191	1.154408692
H	-1.698908017	2.224914187	-0.945899054
H	-3.590292699	-1.912628636	1.054341244
H	-4.102973306	1.823274095	-1.030840502
H	-5.068037969	-0.238008794	-0.034929624
N	1.383799482	-1.643769235	-0.358308792
O	0.865658486	-2.687878479	-0.006801365
O	1.890147088	-1.400775828	-1.447992786

2-methyl-1,2-dihydro-1,2-azaborine

N	-2.020354093	-0.710902247	-0.121505969
B	-0.616280253	-1.063795858	0.188741007
C	-2.477011566	0.527271773	-0.264826016

C	0.269143367	0.231371482	0.471601161
C	-1.660289425	1.680812500	-0.117410161
C	-0.335331161	1.555071571	0.176829173
H	-3.525759096	0.642846930	-0.531314819
H	0.428098698	0.215027409	1.569897143
H	-2.112528000	2.651685144	-0.283888102
H	0.312001013	2.427961811	0.225961333
H	-2.692171650	-1.458544287	-0.285392821
C	-0.201898345	-2.547188580	0.281446279
H	0.604510318	-2.726692644	0.998651698
H	-1.032774548	-3.226615631	0.499866853
H	0.217286494	-2.845288635	-0.693085585
N	1.729540348	0.195620870	-0.057301429
O	2.400848493	1.189550913	0.158330408
O	2.074583589	-0.819899847	-0.637118948

2-vinyl-1,2-dihydro-1,2-azaborine

N	-1.692190228	0.948514311	-0.237191717
B	-0.901216011	-0.234647716	0.174126077
C	-1.203732896	2.174850743	-0.337309635
C	0.609158076	0.132701051	0.541806511
C	0.153607985	2.504061846	-0.055466095
C	1.039309127	1.538622638	0.311316981
H	-1.882936851	2.954650329	-0.675653914
H	0.741417263	-0.062360958	1.621931694
H	0.462917939	3.534771317	-0.185360203
H	2.091347477	1.774484964	0.456137667
H	-2.668452969	0.839073266	-0.500946624
N	1.669042622	-0.815062500	-0.090508933
O	2.827538091	-0.617966980	0.229392611
O	1.246027976	-1.666111988	-0.857516047
C	-1.548491560	-1.607570786	0.320276929
C	-2.866125109	-1.859915327	0.155921030
H	-3.597368542	-1.096023049	-0.105099929
H	-3.278312540	-2.857655997	0.280730075
H	-0.912965806	-2.452345627	0.576806218

2-chloro-1,2-dihydro-1,2-azaborine

N	-1.605616124	1.015904632	-0.386489799
B	-0.893158024	-0.152981268	0.153436990
C	-1.078194440	2.231732439	-0.402837457
C	0.580801699	0.127917921	0.676321199
C	0.225729027	2.530838791	0.094857798
C	1.027023594	1.551595567	0.594426024
H	-1.686697835	3.029626438	-0.823873731
H	0.734775747	-0.242727845	1.698470858
H	0.559832105	3.560782871	0.040960888
H	2.033771822	1.784459062	0.935887681

H	-2.546245090	0.911302885	-0.764573942
Cl	-1.717699151	-1.658374627	0.265795460
N	1.595582288	-0.703352027	-0.180087573
O	2.689900029	-0.904446659	0.300070654
O	1.179258655	-1.041187873	-1.281542987

2-mercapto-1,2-dihydro-1,2-azaborine

N	1.706385344	1.144000314	-0.204658134
B	0.273308873	0.903967024	0.081322420
C	2.627164739	0.192250967	-0.207239071
C	-0.037379931	-0.598032187	0.531273427
C	2.339047040	-1.176925542	0.061550404
C	1.069890600	-1.577333060	0.340311013
H	3.642769661	0.487837280	-0.461873848
H	-0.234634458	-0.547348905	1.618463297
H	3.153676033	-1.888559131	-0.007710830
H	0.839499961	-2.632004764	0.462698779
H	2.029111778	2.072272984	-0.468336514
S	-0.949290975	2.185521833	-0.012108480
H	-0.109735912	3.189330467	-0.356462214
N	-1.366091394	-1.144675386	-0.022862953
O	-1.341062974	-2.244092584	-0.553066230
O	-2.335206254	-0.418294399	0.126314136

2-hydroxy-1,2-dihydro-1,2-azaborine

N	-1.907231989	-0.629510123	-0.310181929
B	-0.602341106	-1.021664659	0.293379119
C	-2.276587297	0.634762090	-0.422745194
C	0.345665511	0.186389981	0.712533986
C	-1.475895243	1.738970807	0.006711108
C	-0.235505056	1.550650455	0.530024650
H	-3.247813553	0.829456087	-0.873508327
H	-1.888176471	2.733258178	-0.122764724
H	-2.565849192	-1.323326307	-0.658743270
O	-0.244296622	-2.276184999	0.544812974
H	-0.774621083	-3.036131614	0.269772561
H	0.727466816	0.078921423	1.735268889
H	0.374832228	2.406074160	0.812667994
N	1.625862742	0.128969145	-0.179479604
O	2.630542790	0.655064180	0.250152917
O	1.471926358	-0.427894099	-1.261565751

2-amino-1,2-dihydro-1,2-azaborine

N	-1.948588110	-0.877159376	-0.211491240
B	-0.495918849	-1.090285840	0.068323645
C	-2.521083741	0.308819706	-0.203258349
C	0.267018316	0.235731219	0.546962034

C	-1.812394718	1.522028072	0.069440587
C	-0.485138555	1.511270059	0.353157410
H	-3.579693405	0.354082077	-0.450342284
H	0.439074450	0.120925335	1.631663332
H	-2.365770417	2.451556594	0.001318021
H	0.055307850	2.444815972	0.481753804
H	-2.542493188	-1.660896606	-0.473881208
N	0.062748542	-2.340935277	-0.047765961
H	-0.426818729	-3.181762597	-0.327191169
H	1.056257666	-2.478127014	0.107532251
N	1.686159528	0.333652066	-0.019802559
O	1.999563962	1.364833055	-0.592071744
O	2.395384333	-0.650554705	0.153271359

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.305677966	-0.946087966	0.175748769
N	0.788962283	-1.801912369	-0.323989525
C	0.156501197	0.496271101	0.670476319
C	2.054565725	-1.417153414	-0.358890589
C	1.617813128	0.785833444	0.559081559
C	2.499778677	-0.136405635	0.089258407
H	-0.166281897	0.693910866	1.701966162
H	2.778699592	-2.124217732	-0.758598680
H	1.962958555	1.772693519	0.861457899
H	3.559931436	0.079784697	0.021369999
H	0.579671415	-2.735354280	-0.672973106
C	-1.688429555	-1.492734600	0.257127370
C	-2.823001017	-1.929608605	0.332254502
H	-3.821059938	-2.314058488	0.396139028
N	-0.580612859	1.584673606	-0.166986897
O	-0.689599225	2.689491794	0.323470668
O	-0.954122435	1.214675681	-1.274577698

Cylic intermediate in the nitration of substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

N	1.497976025	-1.158791064	0.030933100
B	0.147235845	-1.103217667	-0.708898622
C	2.128915002	-0.114291714	0.477769324
C	-0.363460751	0.440452820	-0.925062394
C	1.628327125	1.241933527	0.330538036
C	0.488050242	1.529858211	-0.333522282
H	3.093220886	-0.262782056	0.960665811
H	-0.868637078	0.752503524	-1.842798695
H	2.243315813	2.035128580	0.742237723
H	0.180766261	2.564632616	-0.462293284

H	0.020800275	-1.945464167	-1.533829584
N	-1.450803176	0.023158423	0.072254980
O	-1.045933696	-1.181677661	0.372127390
O	-2.427281576	0.542450784	0.489229856
H	1.968845561	-2.055584592	0.137189808

1-phenyl-1,2-dihydro-1,2-azaborine

N	0.099208618	0.533418870	-0.265523300
B	-0.904277989	-0.523521925	-0.806502012
C	-0.313135120	1.716840395	0.102912144
C	-2.449815608	0.003259767	-0.866302002
C	-1.697691687	2.159769498	0.067966993
C	-2.716838718	1.394578499	-0.372175638
H	0.440125902	2.424081591	0.441967291
H	-3.111073065	-0.291782432	-1.685319901
H	-1.879402685	3.176996056	0.399519170
H	-3.731150767	1.783022686	-0.393211178
H	-0.464473032	-1.221365291	-1.655966485
N	-2.649527083	-1.015763946	0.264097975
O	-1.417210672	-1.412893678	0.438955527
O	-3.588802839	-1.420869000	0.858997200
C	1.491506380	0.181355960	-0.108327225
C	2.172724784	-0.450144895	-1.157106278
C	2.140795347	0.481373284	1.097871445
C	3.523858963	-0.754484263	-0.998246310
C	3.489042020	0.159127347	1.245641550
C	4.182880830	-0.453749851	0.198189365
H	1.669432165	-0.673413203	-2.090117381
H	1.590385997	0.916362815	1.926745737
H	4.061975864	-1.227162089	-1.813171218
H	3.990264800	0.372232453	2.184002840
H	5.231472893	-0.706002459	0.317346334

1-methyl-1,2-dihydro-1,2-azaborine

N	-1.554353225	0.303695759	-0.027323896
B	-0.264622322	0.748748381	-0.762419497
C	-1.686591887	-0.898612071	0.442751704
C	0.846674431	-0.442373246	-0.911605009
C	-0.671407702	-1.939407248	0.342307161
C	0.507750808	-1.765058340	-0.286891325
H	-2.627240048	-1.152950055	0.929200124
H	1.455943226	-0.541188461	-1.813807610
H	-0.925130832	-2.898943522	0.780781228
H	1.216923613	-2.584825536	-0.362826629
H	-0.470878905	1.531648795	-1.630387409
N	1.637760125	0.424399404	0.076153065
O	0.759798301	1.361242512	0.321260335
O	2.729447838	0.375874440	0.527278547
C	-2.653670191	1.281749554	0.076939675

H	-2.961068885	1.570613109	-0.931188804
H	-3.497503533	0.853919833	0.619612801
H	-2.289907968	2.170567492	0.598405992

1-vinyl-1,2-dihydro-1,2-azaborine

N	-1.256140446	0.117591100	0.004061635
B	-0.018731453	0.713815491	-0.723163914
C	-1.231495060	-1.090483867	0.502542511
C	1.199905058	-0.362028483	-0.931402629
C	-0.123176849	-2.014358438	0.351389943
C	1.007638511	-1.721029934	-0.325234156
H	-2.109741596	-1.426116549	1.049307427
H	1.797646826	-0.380955428	-1.846198619
H	-0.257461644	-2.996307330	0.793360633
H	1.787844755	-2.468155024	-0.441909136
H	-0.301373129	1.508356848	-1.556664786
N	1.923018273	0.550995796	0.065338665
O	0.957388465	1.375288305	0.374429729
O	3.029415856	0.607501866	0.478389448
C	-2.435362334	0.929008541	0.071935921
H	-2.221305378	1.986342426	0.179755800
C	-3.676351208	0.452769645	-0.050732912
H	-3.895539415	-0.591605048	-0.252031047
H	-4.518613037	1.131801763	0.017443565

1-chloro-1,2-dihydro-1,2-azaborine

N	-1.153631523	-0.170986760	-0.061042324
B	-0.008834640	0.582316015	-0.805849510
C	-1.048866824	-1.373796359	0.422940111
C	1.337743754	-0.345383221	-0.899571396
C	0.179216570	-2.149462096	0.340833748
C	1.298356930	-1.706443937	-0.268702686
H	-1.922839138	-1.816778024	0.895677145
H	1.971492001	-0.308096757	-1.790025634
H	0.141953081	-3.140115380	0.782178141
H	2.177049458	-2.343088168	-0.326503216
H	-0.400055432	1.251063597	-1.700085145
Cl	-2.674564160	0.636260415	0.059435920
N	1.887975703	0.698098996	0.086555098
O	0.818365195	1.432417638	0.262901278
O	2.942845193	0.897473786	0.577721228

1-mercapto-1,2-dihydro-1,2-azaborine

N	-1.206852163	-0.160482019	-0.065170184
B	-0.035185169	0.575036917	-0.788128467
C	-1.064364670	-1.361754831	0.426813537
C	1.316132569	-0.337398545	-0.908619427
C	0.165166281	-2.131048587	0.341288341
C	1.282052044	-1.697908005	-0.279086166
H	-1.922706720	-1.825848124	0.910032596

H	1.945160436	-0.292797647	-1.801715064
H	0.132941509	-3.121026078	0.784803127
H	2.159096168	-2.335336812	-0.343478196
H	-0.407437095	1.275111447	-1.672154305
S	-2.760369989	0.628685202	0.076071043
H	-2.385980933	1.705280308	-0.642765559
N	1.868990454	0.697005298	0.085194285
O	0.789892056	1.409663558	0.297184371
O	2.927851756	0.905059650	0.564737533

1-hydroxy-1,2-dihydro-1,2-azaborine

N	-1.501742434	0.304909394	-0.034355809
B	-0.213920790	0.773445574	-0.756575762
C	-1.693305826	-0.885870228	0.438655866
C	0.858247382	-0.450657379	-0.917139343
C	-0.685642782	-1.930984481	0.334960091
C	0.494316607	-1.770061091	-0.297800747
H	-2.656617699	-1.086378674	0.902018902
H	1.463689865	-0.553013084	-1.821661065
H	-0.952275382	-2.888940216	0.768905847
H	1.189927603	-2.600097127	-0.379902815
H	-0.449789842	1.565788392	-1.611829561
O	-2.552679544	1.176762512	0.118088634
H	-2.350325385	1.956743781	-0.431181751
N	1.670313111	0.397486366	0.078553388
O	0.806078716	1.356885537	0.316032475
O	2.752921308	0.325648573	0.541198799

1-amino-1,2-dihydro-1,2-azaborine

B	0.243174526	-0.774682205	0.734824837
N	1.542338220	-0.315478441	-0.002472811
C	-0.842853188	0.430738556	0.929964112
C	1.682153246	0.893635535	-0.470930796
C	-0.500571831	1.757065325	0.320653354
C	0.665302517	1.921598611	-0.337251245
H	-1.440616217	0.512562371	1.841301290
H	2.626440423	1.150873111	-0.946089656
H	-1.196621462	2.583824137	0.424215384
H	0.912955956	2.884258069	-0.772694926
H	0.472487395	-1.584058742	1.571410599
N	2.585724626	-1.202427128	0.012757923
H	3.312946906	-1.015678094	-0.671187291
H	2.278233716	-2.167829839	0.041382402
N	-1.655753963	-0.406814786	-0.073725548
O	-0.776535244	-1.338780172	-0.356879442
O	-2.747448407	-0.345392784	-0.519071888

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.313311222	-0.179152920	0.055814168
B	0.154970738	0.587150533	0.786659609

C	1.147522385	-1.388857141	-0.438565664
C	-1.211324109	-0.304767966	0.905400459
C	-0.092516479	-2.125348211	-0.352711733
C	-1.200289308	-1.663879268	0.270146907
H	2.007346023	-1.852953647	-0.915696897
H	-1.840639203	-0.257927532	1.798052785
H	-0.087780677	-3.115677236	-0.796262309
H	-2.090230853	-2.284264672	0.331975737
H	0.549018587	1.278415087	1.662973653
N	-1.748365887	0.740364649	-0.083875009
O	-0.658077761	1.428545937	-0.305694822
O	-2.810209388	0.972200933	-0.546916076
C	2.522222739	0.439601439	-0.021503488
C	3.567721944	1.041694426	-0.079294209
H	4.499395521	1.565071081	-0.128198250

1-formyl-1,2-dihydro-1,2-azaborine

N	-1.207148806	-0.093748340	0.181353668
B	0.063171536	-0.684844375	0.827643023
C	-1.242933469	1.110181732	-0.333520627
C	1.298179565	0.390465311	0.892122278
C	-0.123704732	2.024508482	-0.329970988
C	1.060509233	1.730644302	0.255617261
H	-2.197176599	1.428300628	-0.755033456
H	1.970564248	0.444610564	1.752242470
H	-0.289852615	2.997969463	-0.779475437
H	1.852340441	2.475118492	0.285217865
H	-0.163295301	-1.444891991	1.710496041
N	1.935285199	-0.563712516	-0.126559860
O	0.949789976	-1.400662032	-0.312181892
O	3.001381228	-0.634967187	-0.630299600
C	-2.464408224	-0.872667558	0.174768114
O	-3.453053841	-0.462330007	-0.353133898
H	-2.354006273	-1.829785047	0.699755678

2-phenyl-1,2-dihydro-1,2-azaborine

N	0.800115540	1.410063031	-0.964530599
B	0.310501411	0.148666925	-0.207473758
C	1.892276334	2.060925112	-0.693171280
C	1.400394841	-0.301662586	0.937069324
C	2.841514073	1.627816937	0.315484579
C	2.628791166	0.547609574	1.098864974
H	2.086753845	2.988325072	-1.228574171
H	1.066078862	-0.741032652	1.880808737
H	3.725007168	2.242466735	0.451058398
H	3.345970925	0.290906760	1.874290581
N	1.685377616	-1.459913743	-0.018439752
O	0.934511448	-1.148338191	-1.030034479
O	2.364950677	-2.428312841	0.063430964

H	0.167650687	1.838354237	-1.639022843
C	-1.238838891	0.068515631	-0.026327346
C	-1.835112162	0.272679994	1.235042588
C	-2.086457826	-0.171969885	-1.130095204
C	-3.221916438	0.240014359	1.390541991
C	-3.471564877	-0.212155740	-0.976981889
C	-4.040760887	-0.004035908	0.284674908
H	-1.215538469	0.465047388	2.108243414
H	-1.662723777	-0.354887175	-2.115920562
H	-3.662382193	0.400218570	2.369630720
H	-4.106892622	-0.410556982	-1.834490423
H	-5.119306752	-0.034443106	0.404459655

2-methyl-1,2-dihydro-1,2-azaborine

N	1.485955993	-0.757782180	0.577422953
B	0.154582726	-1.032159684	-0.174092301
C	2.110900744	0.380601153	0.593225432
C	-0.363523650	0.335117216	-0.935129500
C	1.618840261	1.569113091	-0.081904918
C	0.484077008	1.570777759	-0.813661932
H	3.062381317	0.438878486	1.119082079
H	-0.877812353	0.274234940	-1.898216248
H	2.230548915	2.461761081	-0.006154487
H	0.176582857	2.472935971	-1.336501137
N	-1.440104699	0.334474467	0.151307056
O	-1.057738695	-0.670285694	0.882046344
O	-2.399573026	1.001410624	0.346447726
H	1.952717594	-1.536425279	1.040227932
C	0.017227942	-2.481710555	-0.766783259
H	-0.958699753	-2.641557707	-1.238100982
H	0.776665080	-2.668913241	-1.536383270
H	0.132011814	-3.258160271	-0.000201942

2-vinyl-1,2-dihydro-1,2-azaborine

N	-0.121245123	-1.524774368	0.875109222
B	-0.743900843	-0.250836161	0.250463347
C	1.016969871	-2.041422101	0.519237229
C	0.253107085	0.393482840	-0.883748393
C	1.880347216	-1.445014101	-0.483760836
C	1.541308989	-0.328374253	-1.163932198
H	1.322320361	-2.980439245	0.977180349
H	-0.154449284	0.883200938	-1.772063211
H	2.806544196	-1.965530884	-0.702698149
H	2.198988301	0.054377391	-1.940162013
N	0.483370373	1.484287488	0.163162674
O	-0.194448522	1.022415049	1.168530054
O	1.081851611	2.507282421	0.146202510
H	-0.673907139	-2.062207785	1.541277845

C	-2.298520584	-0.276864080	0.145035690
H	-2.878530667	-0.406287898	1.062306720
C	-2.985016755	-0.165200827	-1.004461004
H	-2.492735286	-0.039681220	-1.967119018
H	-4.070693342	-0.198892234	-1.034604318

2-chloro-1,2-dihydro-1,2-azaborine

N	-0.386007596	-1.431423709	0.786316640
B	-0.673139908	-0.102186870	0.064020696
C	0.693370697	-2.135311527	0.610055811
C	0.563864285	0.333782974	-0.916441584
C	1.783013664	-1.724281847	-0.257976066
C	1.745419381	-0.589381287	-0.990555485
H	0.770505601	-3.090251736	1.126542279
H	0.353232054	0.842843790	-1.861078194
H	2.628949038	-2.399744802	-0.328714459
H	2.563838157	-0.346625536	-1.663335337
N	0.785962789	1.418737798	0.145212259
O	-0.148628866	1.107422087	1.004058219
O	1.547001597	2.315060478	0.256532873
H	-1.115140955	-1.835211336	1.374059758
Cl	-2.380025128	0.080788322	-0.397210996

2-mercapto-1,2-dihydro-1,2-azaborine

N	-0.337166873	-1.460756709	0.805887558
B	-0.691774164	-0.137638159	0.098504964
C	0.756579712	-2.132837603	0.587482025
C	0.503739919	0.352951190	-0.904505599
C	1.809536436	-1.671644177	-0.296736123
C	1.713532365	-0.529573053	-1.012663059
H	0.869991655	-3.098972859	1.075051890
H	0.265142399	0.864761005	-1.841127276
H	2.678186859	-2.313683999	-0.396662237
H	2.509042693	-0.246803550	-1.697032569
N	0.722198821	1.436523739	0.157788370
O	-0.147943364	1.075631656	1.057754575
O	1.433549970	2.379562287	0.226495795
H	-1.034996140	-1.911604767	1.395247956
S	-2.440352018	0.036476060	-0.465537794
H	-3.021488660	-0.044719516	0.751023122

2-hydroxy-1,2-dihydro-1,2-azaborine

N	1.551077925	-0.574206337	0.583173821
B	0.312021838	-0.996152903	-0.226016258
C	2.019022730	0.635762570	0.627319580
C	-0.420098415	0.289246646	-0.933978094
C	1.387303450	1.755738189	-0.050222075

C	0.273111719	1.618367791	-0.801387086
H	2.940333040	0.811491321	1.179500499
H	-0.917001403	0.175440932	-1.901596882
H	1.877792001	2.718980937	0.040295449
H	-0.137627656	2.477694590	-1.325036946
N	-1.490981632	0.155850437	0.148072618
O	-1.050107134	-0.813605818	0.871214964
O	-2.492775715	0.767617731	0.335906539
H	2.094638276	-1.311277489	1.032369663
O	0.471123764	-2.267899668	-0.679168120
H	-0.158971665	-2.643503757	-1.304465871

2-ethynyl-1,2-dihydro-1,2-azaborine

N	-0.400958592	-1.472326552	0.760527674
B	-0.772797020	-0.145140038	0.058062609
C	0.713277096	-2.114868593	0.575278094
C	0.440947078	0.359866110	-0.931112094
C	1.772428890	-1.639849044	-0.297439375
C	1.663298227	-0.507377724	-1.025896182
H	0.844759159	-3.069723749	1.080961469
H	0.205924643	0.869662510	-1.868980730
H	2.653375049	-2.267415300	-0.380070686
H	2.459958437	-0.220664521	-1.707569270
N	0.636562713	1.439323285	0.136049587
O	-0.249767010	1.080575782	1.019324225
O	1.354409983	2.375846448	0.224743251
H	-1.105666943	-1.925803529	1.340357416
C	-2.250013948	-0.025201703	-0.295036176
C	-3.428122435	0.038564041	-0.584051206
H	-4.464658836	0.106147283	-0.839840172

2-formyl-1,2-dihydro-1,2-azaborine

N	-1.091042717	-1.005347447	0.587528678
B	-0.618390013	0.295071135	-0.060177061
C	-0.421354751	-2.115251633	0.571767012
C	0.758543125	0.100921664	-0.942860829
C	0.870716136	-2.242368287	-0.083906856
C	1.411433052	-1.251935841	-0.826473168
H	-0.867620471	-2.997276986	1.028145007
H	1.358337938	-3.209519335	-0.021907852
H	2.335106303	-1.426717430	-1.372486716
N	1.342884522	1.033157934	0.119165446
O	0.325055457	1.115893685	0.941512179
O	2.370574499	1.602935622	0.240566608
H	-2.054604351	-1.014783436	0.934152644
C	-1.908736491	1.158023696	-0.501022657
O	-3.015488917	0.691597719	-0.274620072
H	-1.822902332	2.151332041	-0.987967384
H	0.923080584	0.563285882	-1.919768368

Intermediate in the nitration of substituted 1,2-dihydro-1,2-azaborines on C4

1-phenyl-1,2-dihydro-1,2-azaborine

B	-0.165612702	-1.322301071	0.450744331
N	0.520114107	-0.085787812	0.115780121
C	-1.676871194	-1.235292210	0.505151057
C	-0.169401585	1.102702345	-0.137414851
C	-2.318860024	0.065727449	0.418464644
C	-1.516147152	1.212289777	-0.040548902
H	-2.329018689	-2.084319541	0.695424457
H	0.427719386	1.938084393	-0.479749027
H	-2.534275223	0.279264487	1.497882208
H	-2.011352321	2.147535948	-0.270889609
H	0.455861976	-2.298566255	0.678495615
C	1.938492679	-0.036548669	0.017975415
C	2.640360325	1.113492129	0.442828933
C	2.642951965	-1.146935691	-0.494346929
C	4.026662899	1.140554183	0.361288742
C	4.027425343	-1.094791976	-0.590900880
C	4.724372980	0.043078159	-0.161513213
H	2.114761550	1.947825175	0.894402524
H	2.104453890	-2.015268502	-0.854027760
H	4.567100353	2.011029178	0.717650389
H	4.566196260	-1.937517790	-1.010739357
H	5.806825149	0.073906923	-0.232174877
N	-3.796990417	0.039677473	-0.144185580
O	-4.183928115	1.069415361	-0.659337113
O	-4.405650630	-0.996295610	0.030042728

1-methyl-1,2-dihydro-1,2-azaborine

B	1.537778400	-1.299967700	0.002739835
N	2.191485465	0.027570077	-0.000096639
C	-0.016818740	-1.336118949	0.003434617
C	1.458099314	1.130246241	-0.003156466
C	-0.659643687	-0.011939404	0.000352523
C	0.028217670	1.155501130	-0.003192296
H	-0.386050600	-1.942970636	-0.843786230
H	1.990248336	2.079877125	-0.005534407
H	-0.384502951	-1.938797427	0.854443742
H	-0.482391821	2.111614525	-0.005518303
H	2.234624068	-2.254392216	0.004223875
C	3.673969779	0.122530439	0.000006525
H	4.060953193	-0.377030158	0.890256835
H	4.061477387	-0.380266461	-0.888157054
H	3.984650245	1.167468508	-0.001278765
N	-2.157858528	0.049057019	0.000057915
O	-2.669112012	1.161207406	0.006477360

O	-2.732834769	-1.032253663	-0.006705330

1-vinyl-1,2-dihydro-1,2-azaborine

B	1.240044179	-1.181180879	0.007341407
N	1.796227059	0.160152663	-0.016782443
C	-0.270071860	-1.253041952	0.150522871
C	0.999175592	1.301465323	0.076726043
C	-1.019398509	-0.038034213	0.402874131
C	-0.346346005	1.257872721	0.238074420
H	-0.841501563	-2.177616269	0.109910107
H	1.516046595	2.251086472	-0.001542110
H	-1.166669332	-0.136653644	1.513245220
H	-0.925947185	2.170143372	0.308444361
H	1.932789235	-2.121319563	-0.151550689
C	3.177929933	0.415802279	-0.199206573
H	3.412325622	1.453831208	-0.409686050
C	4.158144197	-0.499686711	-0.104569998
H	3.990375003	-1.542158735	0.136427210
H	5.181796052	-0.181456386	-0.267851576
N	-2.528746434	-0.063110688	-0.072487140
O	-3.031320730	-1.164770539	-0.151855645
O	-3.032447472	1.022158826	-0.276462204

1-mercapto-1,2-dihydro-1,2-azaborine

B	-1.065352388	1.335352052	0.060603196
N	-1.682832140	0.021613896	0.030564007
C	0.442716185	1.308608675	0.186580727
C	-0.980570140	-1.178673933	0.132781547
C	1.118551240	0.048603193	0.443555884
C	0.364361686	-1.207015827	0.294453950
H	1.072374897	2.194208594	0.134774933
H	-1.552149256	-2.096814499	0.059345692
H	1.327917329	0.128100390	1.542593299
H	0.889012422	-2.152402706	0.365533957
H	-1.746726939	2.293063477	-0.060675373
S	-3.391679777	0.010110741	-0.188691261
H	-3.538214773	-1.333088229	-0.212188887
N	2.611834584	-0.026210384	-0.097156866
O	3.034673858	-1.142760568	-0.312751347
O	3.179413735	1.039979925	-0.202037953

1-hydroxy-1,2-dihydro-1,2-azaborine

B	1.510229485	-1.346336102	-0.001637489
N	2.085070885	-0.023241746	-0.043974939
C	-0.000386933	-1.305337434	0.142561152
C	1.414337656	1.180285266	0.067070567
C	-0.670375588	-0.044618786	0.403270821
C	0.068874513	1.216132700	0.245291802
H	-0.634695745	-2.188783058	0.102246022
H	2.008205922	2.085915791	-0.013118677

H	-0.818474379	-0.139359631	1.514120461
H	-0.456364916	2.159810030	0.330718312
H	2.205090539	-2.286942265	-0.136174908
O	3.432077533	0.015162282	-0.235500347
H	3.727602757	0.939710548	-0.340787651
N	-2.186428438	0.022797376	-0.064454441
O	-2.622079250	1.137766646	-0.259086672
O	-2.750316986	-1.046889025	-0.145014259

1-amino-1,2-dihydro-1,2-azaborine

B	1.521765513	-1.301586566	0.023643914
N	2.174009433	0.034986979	0.023579751
C	-0.025855307	-1.332512273	0.009608062
C	1.444049736	1.144071692	-0.006226753
C	-0.675291499	-0.009360947	0.001335340
C	0.016299222	1.155222531	-0.008010657
H	-0.368974949	-1.934508019	-0.853210457
H	1.980911052	2.089967557	-0.035175642
H	-0.404489597	-1.949047700	0.844999386
H	-0.494817821	2.111193888	-0.017620778
H	2.233643145	-2.245161671	0.038398875
N	3.553953369	0.108769274	-0.074226992
H	3.994464840	-0.737625847	0.270800680
H	3.946646129	0.951989698	0.335400772
N	-2.165228635	0.046476142	-0.001413938
O	-2.683668248	1.156003287	0.022323224
O	-2.738419567	-1.037010543	-0.027319700

2-methyl-1,2-dihydro-1,2-azaborine

N	2.083738148	-0.985925525	0.002123923
B	1.924611871	0.494791823	0.006463180
C	1.072965898	-1.838016458	-0.003126806
C	0.425218733	0.972594086	0.004841416
C	-0.294417447	-1.430044448	-0.004853039
C	-0.581638502	-0.103959413	-0.000140240
H	1.308813027	-2.900585910	-0.003818890
H	0.236816170	1.649347030	-0.847487557
H	-1.077350901	-2.179188363	-0.008019457
H	0.229992371	1.649787062	0.854818541
H	3.016597323	-1.395053978	0.004903902
C	3.173286879	1.410798337	-0.001021600
H	3.116487957	2.162863206	0.796624406
H	4.130167564	0.888593285	0.092027890
H	3.203850138	1.991329333	-0.935001864
N	-2.032773016	0.294595882	-0.000150079
O	-2.856774398	-0.610114197	0.005112128
O	-2.252571104	1.498850296	-0.005167095

2-mercapto-1,2-dihydro-1,2-azaborine

B	1.553907236	0.031734523	0.001013074
N	1.477678898	-1.453792717	0.006570103
C	0.163936896	0.778743011	0.000023353
C	0.336085442	-2.117477086	0.007046995
C	-1.004026833	-0.127018404	0.000181073
C	-0.942585272	-1.480662555	0.003861797
H	0.078121966	1.469372139	0.855433018
H	0.388279994	-3.204325219	0.009456105
H	0.079939169	1.468585296	-0.856211602
H	-1.840929904	-2.086639261	0.003300312
H	2.321014988	-2.023889981	0.008118354
S	3.101225667	0.910893710	-0.006036353
H	3.942265337	-0.145748955	-0.005279334
N	-2.368466479	0.506675935	-0.001309940
O	-2.385226966	1.730468621	0.019271765
O	-3.331265598	-0.248433022	-0.021779336

2-amino-1,2-dihydro-1,2-azaborine

N	2.098493252	-0.965177397	0.005796542
B	1.900447914	0.524969018	-0.005374999
C	1.101000396	-1.819735218	0.013138485
C	0.393249676	1.008151890	-0.005034888
C	-0.275888349	-1.420411760	0.010209330
C	-0.584894089	-0.103253651	0.000560930
H	1.343034704	-2.880463791	0.021629384
H	0.178963278	1.660799841	-0.866100037
H	-1.048789868	-2.179742197	0.014900761
H	0.182432082	1.663852567	0.854622525
H	3.032881493	-1.369636600	0.007617510
N	3.014541684	1.343049095	-0.013128692
H	2.945028664	2.352959402	-0.020697178
H	3.975374579	1.024711264	-0.010266718
N	-2.042836410	0.264974305	-0.001327611
O	-2.851165854	-0.653724431	-0.033531308
O	-2.288492730	1.464420333	0.030544883

Intermediate in the nitration of substituted 1,2-dihydro-1,2-azaborines on C5

1,2-dihydro-1,2-azaborine

B	2.340253835	0.053555923	-0.499635152
N	1.534557269	1.289532615	-0.177370758
C	1.773784035	-1.251862178	0.052954692
C	0.397199153	1.263036068	0.449963488
C	0.572123396	-1.255729684	0.672683735
C	-0.231355799	-0.015946188	0.839312307
H	2.312618035	-2.189805302	-0.046731402

H	-0.122752445	2.198497716	0.655443687
H	0.119547796	-2.163526589	1.065858045
H	-0.724589771	0.071181742	1.809936052
H	3.322153010	0.228484641	-1.130391884
N	-1.552116162	-0.073200646	-0.179060507
O	-2.601439502	0.215960070	0.343463665
O	-1.306516156	-0.394097837	-1.318785303
H	1.887544330	2.205750358	-0.455985957

1-phenyl-1,2-dihydro-1,2-azaborine

B	-0.140458614	-1.994622627	-0.081172410
N	0.260419591	-0.542308907	0.131349325
C	-1.612598842	-2.341231560	0.099272635
C	-0.638742293	0.360941846	0.402393744
C	-2.507775191	-1.377823674	0.403504837
C	-2.075491272	0.036162998	0.627517344
H	-1.969556578	-3.358934258	-0.032125831
H	-0.325500406	1.398087007	0.482872830
H	-3.572829192	-1.562468874	0.520516151
H	-2.329617176	0.339698464	1.657164110
H	0.730225814	-2.732506473	-0.376022038
C	1.658597702	-0.155225539	0.063158903
C	2.192206383	0.656899979	1.071427395
C	2.438004169	-0.596685668	-1.011593493
C	3.528483019	1.047133470	0.987688965
C	3.768098534	-0.186479545	-1.087061757
C	4.313633861	0.631233207	-0.091365663
H	1.592478939	0.943462539	1.930565503
H	2.013350936	-1.221222115	-1.790036593
H	3.956773766	1.661523916	1.772476998
H	4.377507983	-0.506007362	-1.925700729
H	5.354043602	0.933466800	-0.150737221
N	-2.942787606	1.004595735	-0.241026531
O	-4.143533037	0.897251518	-0.108164576
O	-2.331591008	1.773841914	-0.970626395

1-methyl-1,2-dihydro-1,2-azaborine

B	1.997128486	-1.015718700	-0.391392090
N	1.722256293	0.402490312	0.083222340
C	0.847640970	-2.008925401	-0.304997073
C	0.553552325	0.749620820	0.518144919
C	-0.357347799	-1.610050596	0.156211950
C	-0.578682134	-0.215150429	0.650741464
H	0.964037723	-3.037741730	-0.633782637
H	0.385452585	1.780712559	0.821202161
H	-1.224828408	-2.263506852	0.212230725
H	-0.873055646	-0.239592994	1.713064930
H	3.088082337	-1.206401829	-0.801785992
C	2.820231464	1.398536961	0.002029747
H	2.477215855	2.369807655	0.358760479

H	3.655933615	1.044474270	0.608958470
H	3.143230604	1.471817939	-1.038455130
N	-1.822279882	0.411096255	-0.053880747
O	-2.858240567	-0.208037246	0.046557262
O	-1.625565319	1.464833094	-0.647835114

1-vinyl-1,2-dihydro-1,2-azaborine

B	-1.522404019	1.315023626	-0.347939771
N	-1.435366264	-0.128119745	0.141300942
C	-0.252331643	2.149319530	-0.291337237
C	-0.292437163	-0.602140486	0.556554403
C	0.905245824	1.611372571	0.146941262
C	0.954425266	0.205615594	0.651168366
H	-0.251091553	3.181118153	-0.631511236
H	-0.244319443	-1.643170283	0.866015707
H	1.847780690	2.152582297	0.177208687
H	1.283640100	0.199429955	1.703383878
H	-2.563336735	1.677224654	-0.759936074
C	-2.566450567	-1.019354966	0.120725693
H	-2.308298322	-2.041597619	0.377266134
C	-3.818506263	-0.660261024	-0.166818998
H	-4.126508557	0.345267321	-0.422298687
H	-4.588458469	-1.423685017	-0.143633226
N	2.096320114	-0.581446366	-0.076256478
O	3.201239432	-0.089062854	-0.009387076
O	1.761725033	-1.612874327	-0.644737909

1-chloro-1,2-dihydro-1,2-azaborine

N	1.359595585	-0.081628218	-0.064351119
B	1.429198234	-1.576961791	0.227095623
C	0.269206986	0.542311933	-0.393529259
C	0.100223233	-2.307533228	0.108260225
C	-0.999575044	-0.201567082	-0.601914437
C	-1.027535556	-1.646409004	-0.237813804
H	0.276035134	1.621587496	-0.532567037
H	0.034284100	-3.370963957	0.321877549
H	-1.248412398	-0.084396101	-1.673433619
H	-1.997675792	-2.129967409	-0.309787419
H	2.487859286	-1.994122715	0.529722373
Cl	2.809776468	0.849680036	0.122185763
N	-2.175103171	0.634017918	0.064165850
O	-3.110042608	-0.012779153	0.478371575
O	-2.030714626	1.843150652	0.047227526

1-mercapto-1,2-dihydro-1,2-azaborine

N	1.378310029	-0.070684371	-0.034277261
B	1.346167865	-1.524724371	0.425863401
C	0.308280750	0.530834728	-0.467356489
C	0.023466220	-2.255604429	0.274795482
C	-0.988581967	-0.183202350	-0.646312582

C	-1.063102351	-1.607396890	-0.199232270
H	0.359347740	1.584378954	-0.733550820
H	-0.078237142	-3.295157803	0.574066141
H	-1.264574654	-0.114099353	-1.712097301
H	-2.041893686	-2.071693346	-0.293322204
H	2.351158534	-1.939324134	0.886860054
S	2.901352146	0.822764713	-0.055146020
H	3.448887008	0.100848023	0.943440858
N	-2.108663541	0.657809407	0.058080912
O	-1.735169136	1.660483693	0.650923225
O	-3.235948141	0.229084364	-0.054743699

1-hydroxy-1,2-dihydro-1,2-azaborine

B	2.082996676	-0.989437536	-0.277688037
N	1.690110016	0.444147616	0.000567724
C	0.975846290	-2.009040559	-0.101278257
C	0.502064552	0.817797080	0.358758532
C	-0.263772638	-1.609777400	0.269844464
C	-0.561049224	-0.187748816	0.606645739
H	1.147336372	-3.063736736	-0.296550986
H	-1.096646015	-2.299387152	0.374891250
H	3.203408796	-1.143964840	-0.625237941
O	2.592811192	1.467350079	-0.164184443
H	3.436069958	1.061754879	-0.440184727
H	0.302443693	1.879439147	0.486229742
H	-0.823325039	-0.115057339	1.677954623
N	-1.905060888	0.329631549	-0.059834338
O	-2.031218725	1.539339557	-0.111369693
O	-2.685831629	-0.528855590	-0.406343435

1-amino-1,2-dihydro-1,2-azaborine

B	-1.990039292	1.000770330	-0.406013028
N	-1.701933968	-0.424109808	0.060689292
C	-0.852307112	1.994587170	-0.299093605
C	-0.538026044	-0.768623290	0.528347630
C	0.351042990	1.597952355	0.171808700
C	0.581388791	0.203802451	0.660752692
H	-0.973634221	3.024333723	-0.622836548
H	-0.380616636	-1.795109964	0.848367311
H	1.213108885	2.257678249	0.235821148
H	0.897295380	0.232410577	1.715527725
H	-3.079349497	1.169905795	-0.831500823
N	-2.760358862	-1.299865022	0.057224219
H	-2.495138230	-2.280726668	0.050852571
H	-3.458346684	-1.053553934	-0.635898068
N	1.839843501	-0.396025927	-0.061491446
O	1.667634251	-1.446228364	-0.664730564
O	2.863029788	0.243908301	0.050270916

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.399049797	0.026987985	0.140373623
B	1.292517103	1.392721636	-0.555812392
C	0.390976166	-0.474519360	0.817396694
C	0.033132003	2.192616224	-0.254651858
C	-0.919779194	0.198034169	0.864942157
C	-0.987745166	1.616240320	0.416814899
H	0.525635175	-1.438945680	1.302947007
H	-0.073171378	3.218837334	-0.595201739
H	-1.428219849	0.003092177	1.810165665
H	-1.923276658	2.131447057	0.623411325
H	2.212477597	1.677551168	-1.234750188
C	2.584045312	-0.647833029	0.056893702
C	3.634088261	-1.232238226	-0.051774928
H	4.566083472	-1.750878047	-0.144762214
N	-1.854003297	-0.677268294	-0.201460849
O	-2.885741701	-1.099195125	0.259505599
O	-1.402214279	-0.771759159	-1.322126418

1-formyl-1,2-dihydro-1,2-azaborine

B	-1.596463087	1.353370623	-0.165228120
N	-1.404483837	-0.137486581	0.099232707
C	-0.332365310	2.199983387	-0.070016839
C	-0.244040332	-0.643217881	0.401068351
C	0.856201005	1.640665191	0.249724217
C	0.958668877	0.194543156	0.601575719
H	-0.361181547	3.265955266	-0.278083288
H	-0.139683784	-1.722770750	0.523144481
H	1.781444549	2.206749007	0.310789847
H	1.233213516	0.085562561	1.667985406
H	-2.687477534	1.691208476	-0.447137780
C	-2.557564808	-1.092681405	-0.036497808
O	-3.645933528	-0.699000684	-0.286693477
H	-2.250026562	-2.138186746	0.123448729
N	2.188735310	-0.540707792	-0.086854293
O	3.031563062	0.180014648	-0.568847727
O	2.168984557	-1.757326603	-0.020959379

2-phenyl-1,2-dihydro-1,2-azaborine

N	-0.338934148	-1.128487054	0.281012501
B	0.487066519	0.152510140	0.219495604
C	-1.622185334	-1.180400849	0.433379113
C	-0.380794026	1.420055893	0.332621861
C	-2.431262253	0.049302451	0.642925506
C	-1.716751346	1.354481786	0.501801567
H	-2.133742011	-2.140327569	0.415246716
H	0.058954289	2.411724498	0.277691786
H	-2.891632515	-0.036087546	1.642812699
H	-2.342581658	2.238082899	0.581664835
H	0.126524237	-2.027397451	0.159218660

C	1.992750344	0.033749189	0.041349638
C	2.773395931	1.214147428	-0.086040939
C	2.679428818	-1.209651685	-0.004428309
C	4.151993762	1.155550571	-0.252352921
C	4.057228671	-1.272332551	-0.167476432
C	4.795301239	-0.087498234	-0.293189047
H	2.291520243	2.185871834	-0.056136640
H	2.144819646	-2.152221048	0.095118753
H	4.728396717	2.069661763	-0.349895524
H	4.561003402	-2.232840090	-0.196985702
H	5.872353082	-0.134964662	-0.422120408
N	-3.708204756	-0.054247866	-0.280555518
O	-4.154793803	0.992157989	-0.697508428
O	-4.147343203	-1.181523380	-0.450943623

2-methyl-1,2-dihydro-1,2-azaborine

N	1.321529275	1.198359173	-0.040503409
B	2.178900933	-0.060086589	0.085153494
C	0.055662392	1.207505030	-0.313190253
C	1.379283396	-1.355247392	-0.123615001
C	-0.673421167	-0.047834401	-0.620520222
C	0.060975291	-1.332151078	-0.411252265
H	-0.495355858	2.146300729	-0.331459713
H	1.859558859	-2.325579586	-0.025544646
H	-0.995765791	0.033958917	-1.674788548
H	-0.529310927	-2.233700590	-0.547386818
H	1.752277452	2.107323422	0.135936287
C	3.674785175	0.102567726	0.436753437
H	4.296507728	-0.488248028	-0.249545025
H	4.055856449	1.127900017	0.450375554
H	3.864210998	-0.337559801	1.428371933
N	-2.068994074	0.005281292	0.120228873
O	-2.581904583	1.109984781	0.190416105
O	-2.507517072	-1.055083650	0.506581880

2-vinyl-1,2-dihydro-1,2-azaborine

N	1.061757754	-0.886702299	0.456093955
B	1.728395886	0.399306179	-0.020817774
C	-0.192070517	-0.998406059	0.747435076
C	0.768200829	1.595394297	-0.101105234
C	-1.114704317	0.177592238	0.704748169
C	-0.535864185	1.473673753	0.217264783
H	-0.587153215	-1.964857563	1.051012808
H	1.121551011	2.569173641	-0.430895135
H	-1.555826196	0.306944235	1.705692318
H	-1.244370204	2.296223624	0.158513222
H	1.613172410	-1.741640687	0.529918148
C	3.210932442	0.379647813	-0.377761854
H	3.651026067	1.314489321	-0.722839915
C	4.033164674	-0.691992054	-0.308128241

H	3.709882969	-1.679242362	0.020440883
H	5.082889817	-0.630092591	-0.582482667
N	-2.322448036	-0.236309254	-0.183163819
O	-3.243470987	0.546699731	-0.244964590
O	-2.214156316	-1.320450828	-0.750664317

2-chloro-1,2-dihydro-1,2-azaborine

N	-0.852193014	1.166239690	0.142975051
B	-1.658548263	-0.112150797	0.037356327
C	0.421365633	1.191131536	0.382100650
C	-0.863208909	-1.403254888	0.200924889
C	1.181116252	-0.056191650	0.645353260
C	0.462638866	-1.352480981	0.451416885
H	0.953386776	2.140744225	0.397566169
H	-1.340905102	-2.374196862	0.106479411
H	1.556834339	0.019044574	1.682047292
H	1.071346570	-2.245117364	0.563096278
H	-1.315112764	2.064240814	-0.012883415
Cl	-3.343125636	0.069563213	-0.280695818
N	2.543521652	0.027969242	-0.163874963
O	2.981051489	-1.022335053	-0.575008731
O	3.028685558	1.142841863	-0.251395419

2-mercapto-1,2-dihydro-1,2-azaborine

N	-0.856072227	1.201955150	0.138038560
B	-1.690881305	-0.057897121	0.033364673
C	0.415710361	1.202067464	0.390299494
C	-0.903428362	-1.361249728	0.211527761
C	1.160320483	-0.053565753	0.662401146
C	0.418270362	-1.337237361	0.475125826
H	0.962366921	2.142945411	0.405446749
H	-1.389514954	-2.329233348	0.123229183
H	1.553858734	0.025639207	1.691147857
H	1.006704687	-2.240904812	0.601227169
H	-1.276099140	2.117756560	-0.023593094
S	-3.435421851	0.003944997	-0.297616500
H	-3.603942864	1.342586011	-0.367888096
N	2.509271130	0.008640708	-0.170129597
O	2.928228233	-1.048516545	-0.584208998
O	3.009958931	1.116786364	-0.273774279

2-hydroxy-1,2-dihydro-1,2-azaborine

N	-1.289246975	1.226778903	0.014208471
B	-2.137983484	-0.044467738	-0.100868447
C	-0.027377119	1.212688208	0.306731277
C	-1.362161793	-1.351264298	0.114792946
C	0.687050170	-0.048365154	0.632139832
C	-0.052103214	-1.332038377	0.422475687
H	0.537454685	2.143347969	0.323581571
H	1.012485924	0.043609682	1.683910535

H	-1.690865846	2.145850543	-0.178822008
O	-3.436900534	0.025154990	-0.388135866
H	-3.909579548	0.856519013	-0.524024099
H	-1.864959068	-2.309067271	0.013476248
H	0.529511969	-2.235733621	0.577098956
N	2.083863986	-0.003312231	-0.112080192
O	2.507852886	-1.063109025	-0.514218627
O	2.610447903	1.096438602	-0.169407189

2-amino-1,2-dihydro-1,2-azaborine

N	-1.301720747	1.124762518	0.347638647
B	-2.070954362	-0.106332309	-0.122892574
C	-0.061438786	1.102495714	0.705198098
C	-1.252669610	-1.412846489	-0.115323600
C	0.733363963	-0.169383228	0.735758906
C	0.032925871	-1.417088216	0.274750448
H	0.419307636	2.027320123	1.014032078
H	-1.694722292	-2.357333415	-0.422875429
H	1.147203238	-0.301424760	1.746227340
H	0.645299491	-2.314787683	0.292275680
H	-1.756934571	2.037994640	0.372448999
N	-3.387968793	0.071132924	-0.501940938
H	-3.952195193	-0.703990838	-0.828564788
H	-3.897861299	0.945618369	-0.503347944
N	1.974637266	0.098120904	-0.154272565
O	1.941528600	1.148507814	-0.795457113
O	2.844600228	-0.743120710	-0.155715086

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-1.820251977	0.125145705	0.045699556
N	-1.004879206	-1.155159168	0.143666387
C	-1.003340220	1.408617142	0.213071764
C	0.269730771	-1.189253525	0.367173358
C	0.325108895	1.352748773	0.449136717
C	1.038671035	0.053009969	0.633708109
H	-1.472999168	2.384231811	0.129349491
H	0.799548454	-2.140096682	0.370788390
H	0.939293972	2.241800768	0.558607719
H	1.416128210	-0.031376569	1.668935417
H	-1.471276990	-2.050575845	-0.010347552
C	-3.278281375	-0.031214726	-0.226948688
C	-4.470129912	-0.143067841	-0.455297592
H	-5.518726562	-0.239641607	-0.652499833
N	2.394028217	-0.036310018	-0.179673841
O	2.818992871	1.006050033	-0.625521167
O	2.892563153	-1.147923091	-0.240380589

2-formyl-1,2-dihydro-1,2-azaborine

B	-1.737460388	0.184763802	-0.022055755
N	-0.809718040	1.374701513	-0.072361174

C	-1.079721155	-1.167783084	-0.242757662
C	0.466352955	1.281460403	-0.298373671
C	0.251082610	-1.247722869	-0.475863617
C	1.092341303	-0.022185117	-0.616837253
H	-1.665378420	-2.081548139	-0.191211738
H	1.095213662	2.169782928	-0.266281648
H	0.771536375	-2.191393736	-0.614490065
H	1.453316428	0.060167481	-1.660000400
H	-1.167738812	2.313391427	0.116395012
C	-3.281268863	0.431351812	0.282207457
O	-4.035441040	-0.527035179	0.301593078
H	-3.685762521	1.451242255	0.471462083
N	2.477308322	-0.110560059	0.157857811
O	2.819529917	-1.218674595	0.499717776
O	3.067453794	0.947171298	0.288161031

Intermediate in the nitration of substituted 1,2-dihydro-1,2-azaborines on C6

1-amino-1,2-dihydro-1,2-azaborine

B	1.878123530	0.988339227	-0.261055576
N	0.541552185	1.018783430	0.207524726
C	2.483330447	-0.422448015	-0.436861045
C	-0.164323876	-0.162019497	0.591087568
C	1.787250334	-1.588336167	-0.079781900
C	0.493237630	-1.467977877	0.371573812
H	3.468105840	-0.546530844	-0.885328913
H	2.221371151	-2.575606224	-0.207455683
H	2.441080650	2.004346239	-0.485727204
N	-0.116469246	2.196450299	0.553619663
H	-0.973511979	2.312281118	0.010558441
H	0.507668356	2.988130473	0.424942959
H	-0.484985817	-0.080494331	1.638199814
H	-0.129590544	-2.337270446	0.565997221
N	-1.611278948	-0.278251149	-0.153260693
O	-2.304162809	-1.181533177	0.253875190
O	-1.845013261	0.550270301	-1.007859289

Cyclic product of the nitration of substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

N	1.427250208	-1.228002894	0.208016505

B	0.106127375	-1.098004220	-0.562671453
C	2.253051796	-0.177407723	0.300517901
C	-0.253441915	0.431702761	-0.490464818
C	1.909473602	1.163846507	0.039051588
C	0.565550098	1.507812187	-0.190844630
H	3.260826302	-0.385798393	0.654643449
H	2.665884692	1.921269180	0.207105658
H	0.204190260	2.519006331	-0.014300742
H	0.054308059	-1.780257301	-1.550259654
N	-1.496585961	0.129414212	0.014971860
O	-1.370888732	-1.225765807	0.142199892
O	-2.502922448	0.738352878	0.319749958
H	1.820329781	-2.118871213	0.488623305

1-phenyl-1,2-dihydro-1,2-azaborine

N	-0.084378553	0.568898538	0.348854856
B	0.996966344	-0.434203246	0.845261775
C	0.290178897	1.859019817	0.282717741
C	2.365411808	0.154554214	0.352691475
C	1.613121909	2.348388163	0.207523596
C	2.691044264	1.466090380	0.043175190
H	-0.516111218	2.586451245	0.232754996
H	1.738739911	3.420422129	0.106048388
H	3.633972297	1.789704874	-0.391263419
H	0.799127534	-0.821302490	1.965269723
N	2.641371591	-1.021449500	-0.291613183
O	1.461440155	-1.692354225	-0.039021815
O	3.560573262	-1.505428059	-0.922297643
C	-1.443360157	0.204355604	0.125535271
C	-1.965736457	-0.925727292	0.773656207
C	-2.258354058	0.929959729	-0.759002329
C	-3.294483161	-1.295565749	0.568226371
C	-3.587965948	0.554941002	-0.953082638
C	-4.114581693	-0.555518441	-0.288048865
H	-1.335990030	-1.500927422	1.442204249
H	-1.847718439	1.760793488	-1.323486384
H	-3.688377795	-2.167784070	1.081160396
H	-4.205609067	1.120925866	-1.644103433
H	-5.146952901	-0.850400899	-0.448361814

1-methyl-1,2-dihydro-1,2-azaborine

N	-1.494488603	0.468071003	0.012349112
B	-0.159496092	0.718524110	-0.738650081
C	-1.887098430	-0.788881503	0.188937140
C	0.714403581	-0.557841479	-0.471732642
C	-1.078579554	-1.952181206	0.067405512
C	0.302596377	-1.836618256	-0.099816546
H	-2.917701119	-0.927619136	0.515288528
H	-1.544538564	-2.905075377	0.290511567
H	0.974356150	-2.654180948	0.152628382

H	-0.351191635	1.230380859	-1.811449518
N	1.708274512	0.226920298	0.037175390
O	1.083718158	1.462273957	-0.048886500
O	2.830273185	0.081504008	0.484816549
C	-2.390979748	1.577572896	0.324208236
H	-2.565991544	2.171474254	-0.579365359
H	-3.346071621	1.216201725	0.715308576
H	-1.923272499	2.226359321	1.072149742

1-vinyl-1,2-dihydro-1,2-azaborine

N	-1.257410537	0.091368998	-0.275128780
B	0.089881434	0.539997915	-0.886945014
C	-1.424361810	-1.226144073	-0.041643591
C	1.150991865	-0.512947751	-0.403697941
C	-0.403624734	-2.188785284	0.061586887
C	0.947767338	-1.798065759	0.068240806
H	-2.451582602	-1.549563303	0.108517219
H	-0.698732713	-3.205336060	0.295319210
H	1.718569861	-2.421359104	0.516058018
H	-0.026724502	0.948495419	-2.011064197
N	1.928849233	0.496750493	0.113067975
O	1.099967189	1.562528275	-0.123707686
O	3.015943782	0.601226414	0.643651765
C	-2.328076666	0.998369334	-0.129862660
H	-2.239819534	1.860153248	-0.786033091
C	-3.349342070	0.884873116	0.729250155
H	-3.426457969	0.077703299	1.450690228
H	-4.132770729	1.633553116	0.735156242

1-chloro-1,2-dihydro-1,2-azaborine

N	-1.137489196	-0.113559255	-0.098585841
B	0.074605405	0.534767765	-0.819036708
C	-1.206539447	-1.431496306	0.112487639
C	1.239229489	-0.463450241	-0.443790918
C	-0.096611571	-2.306702635	0.082838734
C	1.198630675	-1.789612058	-0.031298771
H	-2.183819142	-1.830113362	0.369972683
H	-0.280110104	-3.349785926	0.312125728
H	2.067179745	-2.359789156	0.289968773
H	-0.206760411	0.935575552	-1.912208508
N	1.960357945	0.588839942	0.057428723
O	1.029117394	1.594253118	-0.110987252
O	3.058429669	0.772175379	0.538525048
Cl	-2.594659747	0.805210960	0.201882080

1-mercapto-1,2-dihydro-1,2-azaborine

N	-1.201856243	-0.102486820	-0.117258557
B	0.040959387	0.510145785	-0.809247761
C	-1.249602074	-1.428311207	0.094773568
C	1.214717290	-0.470572030	-0.444356347

C	-0.139200619	-2.300102263	0.086668923
C	1.162390065	-1.787276266	-0.010178633
H	-2.226359167	-1.834100755	0.348657378
H	-0.322183022	-3.340725960	0.328418711
H	2.021238710	-2.351670470	0.346021413
H	-0.219699084	0.922906698	-1.908819739
S	-2.618330668	0.846265542	0.258135952
H	-2.798022262	1.315409436	-0.998730774
N	1.936727877	0.585962380	0.053817737
O	1.002517303	1.585222341	-0.099025466
O	3.041592139	0.773112023	0.519208744

1-hydroxy-1,2-dihydro-1,2-azaborine

N	1.432115549	-0.434097317	0.012250107
B	0.112154986	-0.762990611	-0.737076361
C	1.858171486	0.801247233	0.193873326
C	-0.736182873	0.544846569	-0.500175774
C	1.038894171	1.962706957	0.072590674
C	-0.326452528	1.839683937	-0.146426354
H	2.895817482	0.895436588	0.503562955
H	1.499939574	2.918432165	0.292228150
H	-1.006400467	2.667522126	0.039362979
H	0.359818901	-1.312128554	-1.781577604
O	2.366180985	-1.422797603	0.351877517
H	2.160337945	-2.165707974	-0.240860743
N	-1.725011808	-0.218396433	0.037970692
O	-1.106684953	-1.472826042	-0.048034622
O	-2.828884083	-0.059813909	0.519524607

1-amino-1,2-dihydro-1,2-azaborine

N	-1.462642712	0.456118363	0.007200414
B	-0.141908216	0.734668524	-0.743110685
C	-1.876275388	-0.795534341	0.186546313
C	0.724504027	-0.553274713	-0.487818501
C	-1.064830708	-1.954756067	0.072700641
C	0.313817991	-1.832364505	-0.109318579
H	-2.913905213	-0.892469331	0.496866086
H	-1.525567713	-2.909151294	0.299349319
H	0.991638075	-2.647129436	0.135457227
H	-0.341819859	1.269743665	-1.803837598
N	1.718944876	0.223673008	0.034893274
O	1.099035473	1.462925260	-0.042381380
O	2.834821464	0.069744120	0.491737113
N	-2.412965476	1.470348385	0.331747894
H	-2.421572489	2.126056222	-0.450325235
H	-2.050187105	1.980835137	1.137421407

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.318082306	-0.095141951	0.090461274
B	0.069171849	0.521096322	0.796386336

C	1.336179539	-1.440077092	-0.118662922
C	-1.117208468	-0.441925315	0.430566299
C	0.219897981	-2.283132711	-0.102157700
C	-1.082944116	-1.747128870	-0.014562341
H	2.307326165	-1.856728210	-0.371998569
H	0.382575639	-3.326888702	-0.344495617
H	-1.943942750	-2.290466277	-0.397463854
H	0.321458536	0.932607398	1.892003786
N	-1.837828282	0.629972515	-0.054266822
O	-0.891512668	1.609130156	0.077319234
O	-2.949465532	0.827988320	-0.494390511
C	2.442584108	0.626870537	-0.124354234
C	3.415564519	1.322003664	-0.313009554
H	4.274504680	1.930562181	-0.477710421

2-phenyl-1,2-dihydro-1,2-azaborine

N	-0.866147198	-1.335786527	-1.172832760
B	-0.401206030	-0.040327241	-0.460383201
C	-1.621104740	-2.227678362	-0.525727389
C	-1.553721939	0.217471959	0.598114771
C	-2.356368192	-1.982384854	0.655757677
C	-2.472492533	-0.672537516	1.141174817
H	-1.712267419	-3.209989267	-0.986114090
H	-2.965563379	-2.788350484	1.047594673
H	-3.294532568	-0.382218697	1.792625148
N	-1.779930952	1.455624132	0.062910216
O	-0.888454037	1.421962985	-0.985164665
O	-2.516959643	2.398383554	0.273777760
H	-0.451901578	-1.659988223	-2.040368542
C	1.169881440	-0.001197265	-0.170522523
C	1.885599805	1.210745028	-0.098600018
C	1.895980356	-1.186863895	0.056181813
C	3.253895836	1.236640592	0.182964070
C	3.264001510	-1.170941849	0.342771018
C	3.949248716	0.044825479	0.406003673
H	1.361371064	2.145121639	-0.273889959
H	1.385624573	-2.146708930	0.016051049
H	3.777970768	2.187783284	0.226721581
H	3.792551610	-2.104710304	0.516319280
H	5.013165525	0.063672263	0.625803809

2-methyl-1,2-dihydro-1,2-azaborine

N	-1.418521697	0.767920053	0.761446680
B	-0.127085222	0.974718423	-0.060199401
C	-2.225826580	-0.264520968	0.488827589
C	0.269467424	-0.486214164	-0.511118275
C	-1.868182780	-1.414368562	-0.243995503
C	-0.522801996	-1.620228801	-0.596489045
H	-3.224317953	-0.225602820	0.920487084

H	-2.606196794	-2.201616664	-0.342780195
H	-0.136980953	-2.620141590	-0.786283356
N	1.506261532	-0.359622373	0.077965235
O	1.371155481	0.860650288	0.665379105
O	2.512996070	-1.035694613	0.169102720
H	-1.812754026	1.484441164	1.360933200
C	-0.128811340	2.286948874	-0.969422916
H	0.761667567	2.346576476	-1.604768733
H	-1.009114512	2.314966824	-1.623918493
H	-0.150605796	3.199765114	-0.357300172

2-vinyl-1,2-dihydro-1,2-azaborine

N	1.413020150	0.011397777	-1.122763011
B	0.214640158	0.666337306	-0.408752798
C	2.086101499	-0.976424846	-0.518829939
C	-0.350433869	-0.467709883	0.528308208
C	1.617125837	-1.745628773	0.564736576
C	0.282557100	-1.613062288	0.985715022
H	3.055775068	-1.229613292	-0.942974930
H	2.244302396	-2.554855567	0.919642342
H	-0.223574655	-2.417846713	1.515503455
N	-1.592060961	-0.365026186	-0.058479587
O	-1.324970913	0.541848093	-1.037406342
O	-2.684213508	-0.873424033	0.097879793
H	1.874215679	0.426191869	-1.924734468
C	0.445983173	2.180264312	-0.005210915
H	0.540347031	2.919261088	-0.807566748
C	0.546880577	2.631839450	1.253395322
H	0.461913127	1.961049088	2.106629440
H	0.711276704	3.682171342	1.486469299

2-chloro-1,2-dihydro-1,2-azaborine

N	-0.961085360	-0.946296040	1.033996649
B	-0.518237641	0.289116507	0.242927741
C	-0.668044015	-2.162750312	0.567828794
C	0.767301088	-0.164780240	-0.533175123
C	0.317902480	-2.457685142	-0.403101304
C	1.182475921	-1.454655322	-0.854829358
H	-1.204759590	-2.994861891	1.018567348
H	0.482087382	-3.499382359	-0.652029863
H	2.132296716	-1.696276660	-1.326865745
N	1.460608219	0.860250985	0.049015194
O	0.449459587	1.394001154	0.838761344
O	2.595489291	1.280040936	0.061568162
H	-1.667531183	-0.904263816	1.760960853
Cl	-1.971148576	1.123721904	-0.525273794

2-mercapto-1,2-dihydro-1,2-azaborine

N	-1.038980274	-0.908160503	1.000752895
B	-0.527050382	0.317283589	0.227158235

C	-0.786287740	-2.137017009	0.537984502
C	0.766382270	-0.203369840	-0.507073762
C	0.213297855	-2.472976412	-0.402696181
C	1.135634007	-1.505844713	-0.822799285
H	-1.372147476	-2.945649085	0.970336011
H	0.339592994	-3.520258063	-0.650458368
H	2.090444751	-1.787027916	-1.262136466
N	1.492756480	0.806860809	0.056358608
O	0.496735776	1.393394684	0.826107007
O	2.639476789	1.202209093	0.048773069
H	-1.758722463	-0.838751582	1.712731966
S	-2.018796653	1.219691056	-0.529930837
H	-1.401165105	2.387578686	-0.789610745

2-ethynyl-1,2-dihydro-1,2-azaborine

N	-0.932361872	-1.050052546	1.012716127
B	-0.654358795	0.259338671	0.243088375
C	-0.501973467	-2.216025478	0.521863698
C	0.677114303	-0.040643218	-0.552685271
C	0.494165886	-2.376425795	-0.465742309
C	1.235478997	-1.265893104	-0.893751825
H	-0.927311539	-3.113300119	0.967112116
H	0.782395873	-3.386113495	-0.733047510
H	2.217842447	-1.383501937	-1.346795059
N	1.278240150	1.041689537	0.034690306
O	0.265811362	1.447928543	0.870080668
O	2.361794164	1.585563117	-0.005317635
H	-1.623799226	-1.110119453	1.752102232
C	-1.946957392	0.891941577	-0.347192820
C	-2.976178103	1.343349413	-0.811326580
H	-3.869796322	1.755569327	-1.223725712

2-formyl-1,2-dihydro-1,2-azaborine

N	-1.195291032	0.639308985	-0.929075131
B	-0.452576180	-0.450597734	-0.154149658
C	-1.095834681	1.909629302	-0.538637177
C	0.774076726	0.268861709	0.515822477
C	-0.098504498	2.434676898	0.319027462
C	0.965539160	1.629956657	0.739617172
H	-1.823565308	2.602258507	-0.956597411
H	-0.106070731	3.502200139	0.504461662
H	1.892571531	2.064999262	1.107144599
N	1.622868393	-0.653793912	-0.032466226
O	0.705107564	-1.388127633	-0.768901917
O	2.811175364	-0.896250529	-0.025249057
H	-1.979443395	0.424068222	-1.535950446
C	-1.473625919	-1.441570587	0.617710788
O	-2.689498411	-1.397360033	0.474558231
H	-1.048506014	-2.209454566	1.308576150

Substituted 1,2-dihydro-1,2-azaborines nitrated on C3

1,2-dihydro-1,2-azaborine

B	0.550686755	-1.322044914	0.000000000
N	1.976566280	-1.107359980	0.000000000
C	-0.236564489	-0.025964137	0.000000000
C	2.570122158	0.119203233	0.000000000
C	0.403488769	1.196320768	0.000000000
C	1.817443358	1.269399050	0.000000000
H	3.655112499	0.145313858	0.000000000
H	-0.185138313	2.108796131	0.000000000
H	2.315553044	2.231512970	0.000000000
H	0.140417247	-2.432506559	0.000000000
H	2.604000038	-1.902089755	0.000000000
N	-1.704444310	-0.015585950	0.000000000
O	-2.293716342	1.071386291	0.000000000
O	-2.277975095	-1.107661745	0.000000000

1-phenyl-1,2-dihydro-1,2-azaborine

B	-0.703509034	0.527117140	-0.083328465
N	0.350539903	-0.454427889	0.114254926
C	-2.103413186	-0.042639812	-0.004342603
C	0.069740397	-1.774072706	0.346445899
C	-2.318588084	-1.386158803	0.221610342
C	-1.217959214	-2.253496677	0.401059039
H	0.921338148	-2.426636516	0.505989807
H	-3.332060009	-1.772561469	0.267309425
H	-1.376492291	-3.307298490	0.597508309
H	-0.398878602	1.647475631	-0.303433458
C	1.740799076	-0.073390874	0.037012993
C	2.611581422	-0.763753807	-0.813366191
C	2.211329369	0.993176936	0.809098091
C	3.955839063	-0.390542165	-0.881572746
C	3.554905361	1.363918761	0.731015545
C	4.431137047	0.673081044	-0.110690434
H	2.235034622	-1.569989697	-1.435621833
H	1.529802712	1.521547030	1.467237697
H	4.625906714	-0.924401235	-1.548633741
H	3.916334334	2.190954210	1.334497048
H	5.475356496	0.964352548	-0.168283785
N	-3.286799732	0.808232260	-0.176025155
O	-3.099876509	2.016206652	-0.342434054
O	-4.406598210	0.284170212	-0.143661467

1-methyl-1,2-dihydro-1,2-azaborine

B	0.511947664	0.971783905	0.000203686
N	1.855424237	0.437422570	0.000504023

C	-0.576701643	-0.081919725	-0.000120442
C	2.096204586	-0.904710087	0.000372932
C	-0.268112671	-1.426170389	-0.000497602
C	1.083960069	-1.836769077	-0.000237702
H	3.138636620	-1.211294812	0.001441191
H	-1.063454341	-2.165095270	-0.000649985
H	1.337932267	-2.890183950	-0.000643976
H	0.369356098	2.147445112	0.000037937
C	3.032867363	1.322910552	-0.000366899
H	3.641573511	1.149880213	-0.893375591
H	2.695803063	2.358313799	0.002791571
H	3.645956910	1.145845342	0.888833565
N	-1.998226284	0.281898144	0.000011035
O	-2.844322639	-0.620249134	0.000360314
O	-2.277847943	1.483613794	-0.000215314

1-vinyl-1,2-dihydro-1,2-azaborine

B	0.419253695	-0.674249894	0.059220276
N	1.627937087	0.139404319	0.041275706
C	-0.868903756	0.114773920	0.003664702
C	1.553706428	1.507816453	-0.000496060
C	-0.867331113	1.493224766	-0.039057787
C	0.362063714	2.189316872	-0.041142742
H	2.499433768	2.040690881	-0.003969023
H	-1.805644475	2.038176363	-0.068395640
H	0.380150814	3.272190612	-0.074356987
H	0.511715057	-1.848304337	0.130973265
C	2.945382295	-0.415945136	0.078967784
H	3.714831308	0.326065643	0.273135619
C	3.276167926	-1.695089209	-0.103736941
H	2.553345663	-2.474184194	-0.310612917
H	4.320383015	-1.978314656	-0.040775441
N	-2.174485885	-0.556672259	0.002916396
O	-2.181011126	-1.790091643	-0.004430439
O	-3.198502554	0.136427838	0.007278203

1-chloro-1,2-dihydro-1,2-azaborine

B	0.212055083	-0.772487989	0.000084468
N	1.427364694	0.012527727	-0.000188998
C	-1.021620334	0.108363235	0.000052831
C	1.485403179	1.376733628	0.000042934
C	-0.936472725	1.484144752	0.000050065
C	0.327657030	2.117209084	0.000084838
H	2.469182096	1.830090781	0.000349893
H	-1.843491552	2.080287901	-0.000222317
H	0.403530631	3.198047895	0.000175646
Cl	2.970699230	-0.802116240	-0.000017941
H	0.278563320	-1.949787735	-0.000046078
N	-2.367894409	-0.483919260	0.000000939
O	-2.444971375	-1.713864256	0.000132867

O	-3.345860596	0.270790008	-0.000176402

1-mercapto-1,2-dihydro-1,2-azaborine

B	-0.245194011	0.766965824	-0.005124089
N	-1.481287210	0.004731835	0.008589315
C	0.995900715	-0.105240444	0.000465177
C	-1.512709835	-1.367437703	0.006141300
C	0.908966726	-1.479893994	0.001773581
C	-0.358101700	-2.110490115	0.003106626
H	-2.493644442	-1.829250072	0.004461879
H	1.814772451	-2.078384906	0.000017703
H	-0.432894975	-3.191578671	0.001397062
H	-0.297009590	1.946636244	-0.014594162
S	-3.034726603	0.830413378	-0.046217447
H	-3.153203596	1.022583008	1.286784070
N	2.342107179	0.483974062	-0.000475600
O	3.320663972	-0.271112348	-0.006585254
O	2.422462607	1.714188716	0.006244869

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.469144066	-0.974749417	-0.000116535
N	-1.791869338	-0.411195741	0.000048646
C	0.600188375	0.088140686	-0.000108207
C	-2.083166332	0.908800499	-0.000503021
C	0.281160525	1.434914829	0.000173003
C	-1.067671363	1.842927002	0.000025123
H	-3.136413036	1.164751918	-0.001545793
H	1.074982406	2.174890451	0.000718085
H	-1.327087556	2.894507840	0.000129498
H	-0.364013644	-2.156398699	-0.000221941
O	-2.942147121	-1.218679318	0.000603565
H	-2.601485766	-2.128049639	-0.003475527
N	2.022365666	-0.272091740	-0.000011617
O	2.301728753	-1.473984073	-0.000131465
O	2.864557144	0.631825690	0.000162586

1-amino-1,2-dihydro-1,2-azaborine

B	-0.492861950	0.972310571	0.001843260
N	-1.829071264	0.422050690	0.000940751
C	0.589663925	-0.083292485	0.001324991
C	-2.089901041	-0.914015321	-0.000859375
C	0.276227856	-1.428874860	-0.001229980
C	-1.073354065	-1.843191634	-0.002155818
H	-3.140082965	-1.182494998	-0.001982231
H	1.072630693	-2.166675236	-0.004184754
H	-1.325479250	-2.896798124	-0.003782506
H	-0.369408297	2.150708681	0.002907294
N	-3.007643483	1.242629531	0.001050804
H	-2.959190517	1.847079398	0.818868587
H	-2.960267575	1.845812167	-0.817794663

N	2.011070664	0.278939050	0.000175926
O	2.856256123	-0.623360187	0.004124638
O	2.290361130	1.480939444	-0.004724031

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-1.610810668	-0.025153218	0.000807757
B	-0.363849625	-0.788891704	0.001942547
C	-1.635683470	1.356749745	0.000336323
C	0.874177471	0.082185186	0.001277359
C	-0.480230894	2.090620858	-0.000812395
C	0.787517710	1.456197569	-0.000802330
H	-2.618233523	1.814080993	0.000888948
H	-0.549399060	3.171897684	0.000122796
H	1.693588631	2.054260176	-0.001554384
H	-0.431711631	-1.967000726	0.004745942
C	-2.812751356	-0.675431042	0.000144650
C	-3.872652408	-1.253345573	-0.001845674
H	-4.807714083	-1.764849679	0.001995811
N	2.220206283	-0.508268674	-0.000054000
O	3.198547898	0.246357924	0.000035605
O	2.297813244	-1.738288800	-0.001146197

1-formyl-1,2-dihydro-1,2-azaborine

N	-1.496483436	-0.229106173	-0.001160436
B	-0.195455368	-0.879710080	-0.000368466
C	-1.645329070	1.142715604	-0.000256420
C	0.972083819	0.085738871	0.000350904
C	-0.557922889	1.970195795	0.001695279
C	0.764330892	1.444578353	0.001451582
H	-2.667050061	1.504085421	-0.001240850
H	-0.713307775	3.042661335	0.003566223
H	1.614813859	2.119848137	0.002100847
H	-0.160605932	-2.062163644	-0.001011618
N	2.363000680	-0.389454818	-0.000283755
O	2.540718023	-1.609246359	0.002816527
O	3.274031208	0.443960664	-0.003330551
C	-2.683021206	-1.021291807	-0.000591841
O	-3.799426071	-0.562963439	-0.000139061
H	-2.458226347	-2.097347796	-0.000505722

2-phenyl-1,2-dihydro-1,2-azaborine

B	0.313450392	-0.600820380	0.038285806
N	0.654392500	-2.008776210	0.163255585
C	1.575109194	0.265190258	-0.028699552
C	1.910630580	-2.522259294	0.220969374
C	2.832569635	-0.302994877	0.041502121
C	3.009785540	-1.699868843	0.164664354
H	2.002608653	-3.599503957	0.318268678
H	3.702817563	0.343952492	-0.011038193
H	4.004509670	-2.126127896	0.211348775

H	-0.101346038	-2.679656175	0.243659280
C	-1.220182171	-0.271367631	0.022578934
C	-1.788125872	0.757658390	0.799014031
C	-2.102248418	-1.075764722	-0.728469006
C	-3.167621826	0.963343045	0.835145435
C	-3.483464235	-0.862451908	-0.714014422
C	-4.020602155	0.156222359	0.075630327
H	-1.144081944	1.412106719	1.377201462
H	-1.705807668	-1.865534115	-1.364625163
H	-3.577342363	1.761055979	1.448301012
H	-4.135152868	-1.486251572	-1.319581096
H	-5.093581760	0.325189697	0.094710519
N	1.551757779	1.724019174	-0.207348721
O	0.474747681	2.245147487	-0.507321315
O	2.601277436	2.361712515	-0.059732626

2-methyl-1,2-dihydro-1,2-azaborine

B	-0.560779552	-1.049136816	0.000010911
N	-1.988676872	-0.783409075	0.000043345
C	0.239981087	0.256095038	0.000064243
C	-2.565401158	0.448806292	0.000097564
C	-0.386965964	1.485620414	-0.000107339
C	-1.797928862	1.588276476	0.000029364
H	-3.650240653	0.488706787	0.000375412
H	0.217771618	2.387393937	-0.000409037
H	-2.278674043	2.559017961	0.000309958
H	-2.630003565	-1.567955381	-0.000568868
C	-0.072973028	-2.544541603	-0.000225861
H	-0.902130477	-3.263874591	0.000130941
H	0.559500244	-2.752940227	-0.870497289
H	0.560328329	-2.752981194	0.869418511
N	1.706007721	0.276185369	0.000044467
O	2.288200883	-0.814138285	0.000328739
O	2.295663701	1.363242837	-0.000228415

2-vinyl-1,2-dihydro-1,2-azaborine

B	0.819454994	0.356026307	-0.111955731
N	1.867875002	-0.649324002	-0.124234758
C	-0.566270800	-0.285457330	-0.019764266
C	1.673818170	-1.990675721	-0.041103851
C	-0.713574933	-1.656009081	0.067657870
C	0.407518474	-2.517139267	0.059508280
H	2.556523525	-2.622182307	-0.064276340
H	-1.712014706	-2.075440911	0.144276234
H	0.276480371	-3.590481726	0.124135979
H	2.830160690	-0.346417161	-0.221147709
C	1.240736434	1.856478125	-0.183379117
H	0.546584476	2.566120293	-0.626339915
C	2.394479432	2.340522274	0.309348378
H	3.121569492	1.712389938	0.824941306

H	2.652671298	3.395330533	0.250824320
N	-1.805932654	0.498603646	0.000623495
O	-1.707207640	1.724798863	-0.115380408
O	-2.886869586	-0.087620887	0.129165260

2-chloro-1,2-dihydro-1,2-azaborine

B	0.655351856	-0.589105711	0.000000000
N	2.029271938	-0.148142989	0.000000000
C	-0.345133378	0.558084331	0.000000000
C	2.420672164	1.154924626	0.000000000
C	0.112792839	1.861228944	0.000000000
C	1.493494908	2.168032595	0.000000000
H	3.488288147	1.348429115	0.000000000
H	-0.615759181	2.666172964	0.000000000
H	1.825403292	3.198957084	0.000000000
H	2.766399968	-0.844035932	0.000000000
Cl	0.400124319	-2.343545710	0.000000000
N	-1.802718831	0.381101897	0.000000000
O	-2.235468915	-0.771841008	0.000000000
O	-2.521291645	1.387536576	0.000000000

2-mercapto-1,2-dihydro-1,2-azaborine

B	-0.459681539	0.785684454	-0.000081435
N	-1.910140467	0.778566166	-0.000355458
C	0.126799949	-0.624627896	0.000037329
C	-2.673487376	-0.349588472	-0.000342115
C	-0.694128545	-1.731134004	0.000247284
C	-2.103925006	-1.599024569	0.000111274
H	-3.749899735	-0.211107192	-0.000714965
H	-0.243284680	-2.719006120	0.000465647
H	-2.738527248	-2.476614731	0.000232027
H	-2.424167300	1.650987998	-0.000975581
S	0.479016186	2.349967317	0.000499545
H	-0.601291001	3.166800346	0.001164362
N	1.565691467	-0.865630098	-0.000171388
O	2.297278937	0.131911518	-0.001348312
O	1.987796288	-2.027386611	0.000815919

2-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.581897182	1.026717627	0.000167089
N	-2.013638267	0.743097338	-0.000391977
C	0.265576112	-0.255826824	0.000040616
C	-2.551766911	-0.511440286	-0.000367947
C	-0.342952502	-1.489542875	0.000174972
C	-1.755757639	-1.626783738	0.000028685
H	-3.634937199	-0.579979455	-0.000742803
H	0.282026263	-2.377405782	0.000277341
H	-2.210903236	-2.609534194	0.000083907
H	-2.686408291	1.500665232	-0.000731127
O	-0.114799196	2.312187286	0.000990268

H	-0.784730244	3.005048146	0.000857539
N	1.729336841	-0.246103008	-0.000147872
O	2.287751380	0.852814222	-0.001306588
O	2.335472167	-1.326308097	0.000782796

2-amino-1,2-dihydro-1,2-azaborine

B	-0.563625343	1.046634875	-0.000460192
N	-2.006745896	0.790044773	-0.000539841
C	0.251928284	-0.264084958	-0.000501028
C	-2.563887411	-0.449150920	0.000534856
C	-0.380658353	-1.486932682	0.000258308
C	-1.794695108	-1.588185632	0.000610671
H	-3.648566643	-0.498541405	0.001173184
H	0.222263955	-2.390054547	0.000780878
H	-2.276079328	-2.558229398	0.001028754
H	-2.660383528	1.563226922	0.000076866
N	-0.073719262	2.365596157	-0.001446346
H	-0.645772659	3.195636432	0.006374793
H	0.923249979	2.524183682	0.002845198
N	1.703374845	-0.272553423	0.000041222
O	2.280088813	0.829929649	0.001905423
O	2.313988605	-1.347915920	-0.001336964

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.351776790	-0.902232952	-0.000372428
N	-1.795016504	-1.049189834	0.000274244
C	0.078115227	0.560465980	-0.000048281
C	-2.681658754	-0.020427430	0.000376412
C	-0.863929317	1.569770539	-0.000026212
C	-2.248859134	1.284695838	0.000135184
H	-3.736456976	-0.275809459	0.000620272
H	-0.527093712	2.601850144	-0.000031374
H	-2.974190641	2.089213286	0.000157635
H	-2.189259176	-1.982641971	0.000388339
C	0.471966341	-2.182013529	-0.002896912
C	1.129292758	-3.204534214	0.002065689
H	1.710697363	-4.099496853	-0.003118915
N	1.485189403	0.979331839	0.000094374
O	2.340690011	0.092850106	0.000690475
O	1.746166874	2.188852678	-0.000336150

2-formyl-1,2-dihydro-1,2-azaborine

B	0.762651640	-0.306031737	-0.001728550
N	1.786758946	0.702264548	-0.001278118
C	-0.636210035	0.268328246	0.000383264
C	1.558459337	2.035269190	0.001585045
C	-0.829024936	1.639712708	0.003191489
C	0.268471132	2.526557369	0.004575759
H	2.422386478	2.692371550	0.001596166
H	-1.841141033	2.033379547	0.004796596

H	0.106059648	3.597642047	0.008150688
H	2.750860504	0.372714521	-0.003124085
C	1.355145999	-1.795557790	-0.004756036
O	2.575333447	-1.949808586	-0.003702875
H	0.698502256	-2.683710802	-0.008124630
N	-1.835242413	-0.574215069	0.000496036
O	-2.946827978	-0.039495569	-0.016577289
O	-1.659682023	-1.797841137	0.018211188

Substituted 1,2-dihydro-1,2-azaborines O-nitrated on B

1,2-dihydro-1,2-azaborine

N	-0.897572587	-1.243927194	-0.000021876
B	0.050203076	-0.164163739	0.001254748
C	-2.252183165	-1.039813369	-0.001215199
C	-0.525636052	1.236089310	0.001545457
C	-2.769093017	0.227331990	-0.000627817
C	-1.896692444	1.359496431	0.000167231
H	-2.881862057	-1.923351089	-0.002519360
H	0.077690398	2.138541540	0.003551730
H	-3.844871578	0.360371851	-0.001396175
H	-2.356722693	2.346568165	0.000698288
N	2.368767355	0.453758902	-0.004549842
O	1.401903380	-0.593052522	0.002505057
O	3.463924116	0.014891631	0.000755590
H	-0.578399263	-2.205249585	-0.000717133

1-phenyl-1,2-dihydro-1,2-azaborine

N	0.226530846	0.862029797	0.089789484
B	1.353419388	-0.047244495	0.000092420
C	0.442155584	2.222040052	0.168239035
C	2.739906060	0.561156549	-0.001139680
C	1.696708327	2.766088751	0.168893209
C	2.848582578	1.928602284	0.083242985
H	-0.448816864	2.835646338	0.245666244
H	3.647040775	-0.031420772	-0.066992141
H	1.798360492	3.842819245	0.244952724
H	3.826743458	2.406934879	0.088005880
N	2.114426880	-2.308289668	-0.229370513
O	1.009165604	-1.419829051	-0.082721973
O	1.748819295	-3.429740030	-0.263682912
C	-1.146357050	0.417493543	0.056691233
C	-1.636262569	-0.427951630	1.056351333
C	-1.988712891	0.846998953	-0.974299212
C	-2.968811798	-0.842390322	1.021083082
C	-3.323459203	0.435373435	-0.999452780
C	-3.816404246	-0.410788105	-0.003185702
H	-0.975753098	-0.758274657	1.850616233

H	-1.594342195	1.486826553	-1.758046344
H	-3.344587846	-1.500979118	1.798345928
H	-3.972439382	0.769026662	-1.803706422
H	-4.852575985	-0.734506033	-0.026145098

1-methyl-1,2-dihydro-1,2-azaborine

N	-0.912814284	-0.949300276	-0.002930978
B	0.093826120	0.084593427	-0.001056594
C	-2.243498898	-0.614164994	-0.001405506
C	-0.378752706	1.523127697	0.000198527
C	-2.675614738	0.684719314	0.000666803
C	-1.733765598	1.756134305	0.001149418
H	-2.943651273	-1.444783297	-0.002559341
H	0.296824362	2.372927769	0.001366665
H	-3.741487705	0.883152869	0.000948665
H	-2.120846243	2.773863246	0.003077210
N	2.438251008	0.615411556	0.001413432
O	1.433519237	-0.392220117	-0.001472458
O	3.516005484	0.133260321	-0.000223272
C	-0.589718893	-2.384966857	0.002971545
H	-0.974850701	-2.857990099	0.912288260
H	-1.032877082	-2.877187391	-0.868616339
H	0.490593887	-2.513320581	-0.029601115

1-vinyl-1,2-dihydro-1,2-azaborine

N	-0.939823562	-0.484204150	-0.075094106
B	0.281449198	0.306198953	-0.019066499
C	-2.162860853	0.155499044	-0.085577207
C	0.146033743	1.812382159	0.057916298
C	-2.278153851	1.514043348	-0.017181375
C	-1.118695088	2.345548319	0.062968629
H	-3.035565520	-0.477891976	-0.178991465
H	0.997698208	2.482912701	0.113666483
H	-3.269426585	1.952613684	-0.043214983
H	-1.267519188	3.422586946	0.117858935
N	2.686990626	0.308552618	0.029263225
O	1.475767748	-0.453976822	-0.033903676
O	3.626703895	-0.401336737	0.008314556
C	-0.881614951	-1.906521646	-0.100919051
H	0.104081359	-2.275654255	-0.355513960
C	-1.876476472	-2.758139664	0.168896964
H	-2.872035845	-2.457095781	0.475043447
H	-1.687549409	-3.822728733	0.097110026

1-chloro-1,2-dihydro-1,2-azaborine

N	-0.921924634	-0.477614550	-0.000175577
B	0.226534574	0.405741966	0.000284369
C	-2.221807312	-0.033995517	0.000064877
C	-0.114699755	1.883140122	0.000561387
C	-2.493908700	1.306413486	-0.000136155

C	-1.435240067	2.262795066	-0.000132145
H	-2.993587194	-0.793649695	-0.000112829
H	0.650560968	2.653557906	0.001094571
H	-3.530982483	1.622088453	-0.000042961
H	-1.705021670	3.317166033	0.000477157
Cl	-0.711232492	-2.207211292	-0.000078466
N	2.605794456	0.686078122	-0.001944988
O	1.484446829	-0.219520304	0.000689637
O	3.618667368	0.089789501	0.000784893

1-mercapto-1,2-dihydro-1,2-azaborine

N	-0.924723327	-0.529524364	0.022880131
B	0.201703612	0.386512951	0.001250623
C	-2.224576649	-0.063018272	0.036677592
C	-0.129655085	1.865443984	-0.022361131
C	-2.504595373	1.274268068	0.015051962
C	-1.451522598	2.238281378	-0.017954948
H	-2.999992114	-0.819908856	0.062235396
H	0.631619110	2.639243979	-0.045043318
H	-3.542574843	1.587437633	0.026857120
H	-1.728226096	3.291091483	-0.036294504
S	-0.716478509	-2.269686686	-0.063150839
H	-0.266611317	-2.444003762	1.199280217
N	2.581021996	0.685956036	-0.035063576
O	1.473718512	-0.223248652	0.035034038
O	3.601975051	0.101582963	0.016385978

1-hydroxy-1,2-dihydro-1,2-azaborine

N	-0.877240491	-0.889317401	-0.000059905
B	0.103945535	0.162922794	-0.000224698
C	-2.216946307	-0.679638479	0.000899061
C	-0.450860819	1.561644210	-0.000782927
C	-2.710177816	0.603339583	0.000626085
C	-1.823772744	1.715153155	-0.000020449
H	-2.834386699	-1.570335647	0.001011928
H	0.172686997	2.450612478	-0.001804996
H	-3.784186211	0.747151816	0.000324904
H	-2.262213509	2.711261630	-0.000673036
O	-0.513250692	-2.247209231	-0.000611460
H	0.460482231	-2.233899465	0.000125140
N	2.475608308	0.654619211	-0.000125717
O	1.430789863	-0.337423529	-0.000469707
O	3.534303446	0.144205474	0.000920854

1-amino-1,2-dihydro-1,2-azaborine

N	-0.898380960	-0.925638967	0.001182577
B	0.100163961	0.117144095	0.011752440
C	-2.237361551	-0.643262929	-0.010473713
C	-0.406202911	1.539873614	0.016047654
C	-2.691358367	0.649715775	-0.011002319

C	-1.769529335	1.737035349	0.001284474
H	-2.887768331	-1.510223199	-0.019291692
H	-3.760319824	0.828951923	-0.020205818
H	-2.177648092	2.746507015	0.001027945
N	2.447980481	0.635984462	-0.022298345
O	1.432705424	-0.370610160	0.016944858
O	3.520650744	0.147659597	-0.004350190
N	-0.581054931	-2.322855829	-0.000947881
H	-0.028877430	-2.514011459	0.833578695
H	0.035467122	-2.495792169	-0.793075271
H	0.245838755	2.407988539	0.025598753

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-0.929417153	-0.668895325	0.000393341
B	0.141161110	0.327460537	0.000639759
C	-2.265574863	-0.277856687	0.000384308
C	-0.285964442	1.780979506	-0.000407886
C	-2.621133826	1.036445531	0.000055922
C	-1.627767632	2.067200137	-0.000676373
H	-2.986669900	-1.086423333	0.001097413
H	0.423130642	2.602711707	-0.000671564
H	-3.675541296	1.288231774	0.000961416
H	-1.972483793	3.099696512	-0.001801132
N	2.496315302	0.766288587	-0.001239731
O	1.438389345	-0.211665399	0.002856149
O	3.547070125	0.239073331	-0.000541876
C	-0.664695338	-2.006349153	-0.001481958
C	-0.430511851	-3.191295433	-0.000193366
H	-0.212190774	-4.234078949	-0.003927749

1-formyl-1,2-dihydro-1,2-azaborine

N	-0.926601769	-0.445705336	-0.001818752
B	0.328371949	0.306235399	-0.008511855
C	-2.148557436	0.216992080	0.007071736
C	0.225558787	1.820332285	-0.010610331
C	-2.216948739	1.574446772	0.010041584
C	-1.026086079	2.377163072	0.002736118
H	-3.018922204	-0.427468988	0.009637665
H	1.090486890	2.475682574	-0.014624128
H	-3.192447660	2.047661959	0.017667191
H	-1.148660256	3.458844682	0.008283077
N	2.737979777	0.259607532	-0.018190082
O	1.492344978	-0.485595463	-0.002669088
O	3.653959800	-0.471569517	0.022688082
C	-0.954308831	-1.863349584	-0.005037376
O	-1.974491647	-2.516600646	-0.000284043
H	0.049455808	-2.305740315	-0.013209260

Substituted 1,2-dihydro-1,2-azaborines halogenated on B

1,2-dihydro-1,2-azaborine

N	0.250374548	-1.158726958	-0.000331999
B	-0.468698161	0.081445812	-0.000095003
C	1.619805698	-1.219605544	0.000389988
C	0.366606497	1.338836613	-0.000016279
C	2.372496012	-0.076115384	0.000019469
C	1.737638742	1.202676577	0.000120778
H	2.066029070	-2.208547861	-0.000878884
H	-0.061092362	2.337630544	-0.000993425
H	3.453689449	-0.154822364	-0.000878480
H	2.378567447	2.083081383	-0.000103443
H	-0.243855103	-2.042675046	0.000299007
Cl	-2.263651471	0.010431682	0.000060130

1-phenyl-1,2-dihydro-1,2-azaborine

B	-1.441340567	0.645572952	-0.054980646
N	-0.549426372	-0.487683521	0.055867073
C	-2.924025263	0.361397036	-0.032341439
C	-1.064110687	-1.763678010	0.165634845
C	-3.344769707	-0.942936337	0.083179607
C	-2.409126966	-2.013531543	0.181942366
H	-3.667514126	1.150360727	-0.108292785
H	-0.331406211	-2.559106776	0.248462461
H	-4.405700064	-1.187351861	0.101431887
H	-2.746842169	-3.039452779	0.277461592
C	0.892871859	-0.380092114	0.042193228
C	1.606113538	-0.787724467	-1.088179081
C	1.565832433	0.111286530	1.163285835
C	3.000955107	-0.705270052	-1.093838108
C	2.959699429	0.194628204	1.150534672
C	3.679698519	-0.213893391	0.024203632
H	1.068375109	-1.154561995	-1.957187625
H	0.998283857	0.428030680	2.032200362
H	3.553743521	-1.019154490	-1.974247837
H	3.481605207	0.578827528	2.021816661
H	4.763475089	-0.147179676	0.017234018
Cl	-0.764425925	2.299289014	-0.228787413

1-methyl-1,2-dihydro-1,2-azaborine

B	0.372320299	0.374783492	-0.001085265
N	-0.223780698	-0.938632397	-0.002068272
C	-0.551224480	1.565768231	-0.000190588
C	-1.590644227	-1.065123469	-0.000151116
C	-1.909482598	1.338775908	0.000863983
C	-2.433583567	0.015594959	0.000553973

H	-0.187145191	2.589630395	-0.000941866
H	-1.976499830	-2.079751645	-0.001699287
H	-2.613970376	2.168984046	0.001728455
H	-3.503753868	-0.158560984	-0.000014969
C	0.581916870	-2.169898879	0.001229465
H	-0.076185250	-3.040513889	-0.023805026
H	1.240487485	-2.195691095	-0.870073410
H	1.202207362	-2.217136678	0.899727023
Cl	2.168558207	0.508105568	0.000236843

1-vinyl-1,2-dihydro-1,2-azaborine

B	-0.057482803	0.626094379	-0.005318244
N	0.115257388	-0.813905679	-0.094156254
C	1.191368800	1.468047414	0.121419073
C	1.397743244	-1.335951149	-0.098796512
C	2.418074161	0.850594320	0.128310623
C	2.520324156	-0.566566390	0.011774839
H	1.144642353	2.551042881	0.197981649
H	1.462004837	-2.415844694	-0.182126502
H	3.336922526	1.428021180	0.214226226
H	3.487678800	-1.056314788	0.008764595
C	-0.920072283	-1.794298535	-0.236848373
H	-0.661051491	-2.590279840	-0.930825133
C	-2.089845199	-1.805706067	0.401125081
H	-2.383695074	-1.042623745	1.110492618
H	-2.793468877	-2.605520886	0.197645664
Cl	-1.681878997	1.386583917	-0.090588353

1-chloro-1,2-dihydro-1,2-azaborine

N	-0.122771652	0.656661822	0.000106986
B	0.040984633	-0.781209707	0.000193236
C	-1.350628115	1.276849989	-0.000589031
C	-1.256342638	-1.558502209	0.000885766
C	-2.502710825	0.539508552	-0.000830734
C	-2.454504323	-0.884395931	0.000709037
H	-1.345172838	2.359534582	-0.002816749
H	-1.262482997	-2.645411687	0.000975392
H	-3.450101089	1.066631931	-0.003195336
H	-3.397565596	-1.427462341	0.001241954
Cl	1.245769966	1.736586643	0.000446114
Cl	1.658743873	-1.519949791	-0.000500492

1-mercapto-1,2-dihydro-1,2-azaborine

N	-0.094387669	0.693480741	0.018306681
B	0.046213832	-0.750358225	-0.009516044
C	-1.346480101	1.282144935	0.035264305
C	-1.236130754	-1.551021559	-0.026633952
C	-2.493306374	0.539161138	0.017071967
C	-2.438223349	-0.885671989	-0.015468908
H	-1.358781145	2.365381349	0.060713110

H	-1.234311058	-2.637551829	-0.050911618
H	-3.445398905	1.057994771	0.031424543
H	-3.378720933	-1.433728652	-0.030372414
S	1.266835726	1.800314617	-0.058962599
H	1.674166503	1.644925961	1.220526375
Cl	1.666708971	-1.505050684	0.010573845

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-0.378489399	-0.431796717	-0.000268443
N	0.230543925	0.868351036	-0.000813050
C	0.573579909	-1.591311279	-0.000805645
C	1.575020983	1.067202499	0.000790137
C	1.930836187	-1.332289529	-0.000372581
C	2.434705554	-0.004524087	0.000769757
H	0.234506731	-2.623672709	-0.000798915
H	2.648604281	-2.150252331	-0.001206979
O	-0.499343147	2.066731994	-0.000599303
H	-1.431434714	1.782136920	-0.001125767
H	1.895156494	2.102397158	0.001214218
H	3.501338436	0.187370262	0.003368152
Cl	-2.177536198	-0.498283641	0.000511435

1-ethynyl-1,2-dihydro-1,2-azaborine

N	0.029531317	-0.766396642	-0.001118660
B	-0.049759724	0.691535458	-0.000145768
C	1.267026119	-1.408178003	-0.001620963
C	1.263329677	1.437461050	0.001705835
C	2.434890435	-0.707456813	-0.000461112
C	2.435449467	0.722171360	0.001747878
H	1.227314919	-2.490696808	-0.005112590
H	1.307941735	2.522994278	0.002281361
H	3.368176673	-1.259175906	-0.002999684
H	3.398281298	1.229823542	0.003006671
C	-1.076709431	-1.564315521	-0.000638513
C	-2.048629849	-2.281118822	0.001946184
H	-2.908149955	-2.910644360	0.012181099
Cl	-1.647568628	1.477494129	-0.000695256

1-formyl-1,2-dihydro-1,2-azaborine

B	-0.060307979	-0.636423513	0.000325779
N	0.149275177	0.817853566	0.002131088
C	1.190616290	-1.494842605	-0.001597320
C	1.448576329	1.323421920	0.002906791
C	2.422676559	-0.897621344	-0.002443682
C	2.550457482	0.529431149	-0.000143471
H	1.129607313	-2.579729862	-0.003041503
H	1.529710542	2.405671757	0.005829248
H	3.334626603	-1.491714391	-0.005317296
H	3.529059287	0.996161306	-0.000506055

C	-0.868560746	1.814531988	0.000266589
O	-2.055247190	1.617321034	-0.004157255
H	-0.437513248	2.832819477	0.003737969
Cl	-1.676767840	-1.366758416	0.001272326

Substituted 1,2-dihydro-1,2-azaborines halogenated on C3

1,2-dihydro-1,2-azaborine

N	1.729479781	-1.116357560	-0.000375729
B	0.307355033	-1.308718591	0.000319410
C	2.341516073	0.109136220	0.000049597
C	-0.479768727	-0.010986618	-0.000633564
C	1.594896707	1.257585410	0.000192997
C	0.171442391	1.200368040	-0.000283147
H	3.426148041	0.123349076	0.000561235
H	2.097374787	2.218126312	0.001748644
H	-0.388854991	2.132398380	0.000779845
H	2.347660446	-1.917961581	0.001543573
Cl	-2.246269421	-0.022164413	0.000114102
H	-0.129238371	-2.414668289	0.001165603

1-phenyl-1,2-dihydro-1,2-azaborine

B	-0.912616084	0.608100668	-0.117145429
N	0.108818659	-0.389175626	0.114880569
C	-2.336270835	0.095848242	-0.034579806
C	-0.212622028	-1.701257639	0.384334660
C	-2.593103230	-1.227710065	0.230244817
C	-1.512704397	-2.127472733	0.444231155
H	0.617424223	-2.373265535	0.570012106
H	-3.612508580	-1.601995447	0.283796269
H	-1.710570178	-3.168968884	0.671412215
H	-0.586076775	1.721247226	-0.368246484
C	1.507694610	-0.052563801	0.035207723
C	2.364670757	-0.792882785	-0.787580240
C	2.008409908	1.021647999	0.778163649
C	3.719657063	-0.461514733	-0.858863714
C	3.362532404	1.351601053	0.696839072
C	4.222937696	0.611082613	-0.118416979
H	1.967639426	-1.607683415	-1.385218229
H	1.339571641	1.586458165	1.418809727
H	4.377429849	-1.035789845	-1.504506502
H	3.745077722	2.185005880	1.278456592
H	5.275803129	0.869374063	-0.178132800
Cl	-3.699122181	1.189800928	-0.295877351

1-methyl-1,2-dihydro-1,2-azaborine

B	0.287988551	-0.992054491	0.000336285
N	1.622443343	-0.455528964	0.000776073
C	-0.819305146	0.044477136	0.000082265
C	1.857643458	0.895603226	-0.000224897
C	-0.522736013	1.386253490	0.000154154
C	0.835346927	1.808742946	-0.000002813
H	2.897450995	1.208840671	-0.000624056
H	-1.310182901	2.135960403	0.000127553
H	1.074959443	2.866163518	-0.000853163
H	0.140583266	-2.172609622	0.000093476
C	2.805652902	-1.328970583	-0.000574088
H	3.415752486	-1.150809328	0.891163103
H	2.480794241	-2.368762319	-0.002186321
H	3.417583416	-1.146473032	-0.890059073
Cl	-2.515974202	-0.450115855	-0.000155233

1-vinyl-1,2-dihydro-1,2-azaborine

B	0.216588543	0.721955849	-0.070238001
N	1.396248601	-0.119981187	-0.053579588
C	-1.104121099	-0.015363010	-0.001410724
C	1.283045174	-1.494195624	-0.004116264
C	-1.144560705	-1.387444647	0.051191452
C	0.071244245	-2.126008184	0.048408073
H	2.212276691	-2.054085893	-0.001540339
H	-2.089771181	-1.923034068	0.090487915
H	0.048373073	-3.209098414	0.089132697
H	0.334492250	1.898642975	-0.150650315
C	2.727602206	0.393100711	-0.097819703
H	3.468348855	-0.363527810	-0.342463545
C	3.107213024	1.651447524	0.132977751
H	2.414933331	2.442094244	0.394467761
H	4.157809675	1.905364213	0.052743140
Cl	-2.626632566	0.880419967	-0.004587739

1-chloro-1,2-dihydro-1,2-azaborine

N	-1.195712445	0.008909078	0.000779728
B	-0.002787185	0.813793393	0.000371783
C	-1.226549431	-1.363344277	-0.000256896
C	1.261244134	-0.027085679	0.000042418
C	-0.050215157	-2.065019808	-0.000085064
C	1.206804160	-1.400626200	0.000027507
H	-2.199370228	-1.837826865	-0.000605087
H	-0.094683530	-3.148164140	0.000492312
H	2.116278929	-1.995582547	0.000387868
H	-0.083139367	1.994691199	0.001066203
Cl	-2.759759856	0.788057643	-0.000221398
Cl	2.838169109	0.762315277	-0.000153194

1-mercapto-1,2-dihydro-1,2-azaborine

N	-1.251046028	0.026229431	0.006501035
B	-0.034890826	0.807451825	-0.004122459
C	-1.254631352	-1.354147620	0.000576900
C	1.235117743	-0.025817722	0.001172040
C	-0.082133806	-2.058964700	0.000453305
C	1.179110324	-1.397626206	0.002367566
H	-2.224476787	-1.837054366	-0.007525017
H	-0.126153230	-3.142334812	-0.005338633
H	2.087136740	-1.995441234	0.002002104
H	-0.099212242	1.991267922	-0.008463896
S	-2.817616471	0.819582600	-0.043509082
H	-2.980703408	0.935966960	1.294182274
Cl	2.814723855	0.762318768	0.000164606

1-hydroxy-1,2-dihydro-1,2-azaborine

B	0.249822464	0.995603808	-0.000106286
N	1.561808450	0.425897056	-0.000467928
C	-0.841827929	-0.046813488	-0.000284401
C	1.845300436	-0.902568832	-0.000495523
C	-0.535459735	-1.391797587	0.000149427
C	0.817642007	-1.815441862	0.000403558
H	-1.322594234	-2.141106738	0.000086556
H	0.144257575	2.181979290	0.001012007
O	2.723262790	1.223062262	0.000522947
H	2.390516166	2.134750638	-0.000885846
H	2.895389854	-1.167995697	-0.000510702
H	1.059338361	-2.871794908	0.000686212
Cl	-2.539804007	0.436693449	0.000048331

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-1.377094773	-0.047577265	0.001269766
B	-0.150795447	-0.830962544	0.000866509
C	-1.372191286	1.342307615	0.000348625
C	1.118224381	-0.001987483	0.000490822
C	-0.197980620	2.036452425	-0.000556735
C	1.062759142	1.369643778	-0.000237997
H	-2.343512448	1.821399999	0.000625132
H	-0.234545515	3.119867365	-0.002192062
H	1.971250424	1.966640450	-0.001461529
H	-0.233823338	-2.012800781	0.000933895
C	-2.592199645	-0.669796630	0.000178123
C	-3.667639535	-1.219713341	-0.000765412
H	-4.615308495	-1.706718234	-0.007209440
Cl	2.694703177	-0.791609169	-0.000326936

1-formyl-1,2-dihydro-1,2-azaborine

B	-0.189327857	0.729657133	0.000277290
N	-1.364871089	-0.132221748	-0.000668374

C	1.132470929	-0.019863818	-0.000154186
C	-1.263817548	-1.515441564	-0.000332169
C	1.164593659	-1.390688580	-0.000463375
C	-0.053468686	-2.138886368	-0.000160139
H	-2.197049907	-2.069414559	-0.000258547
H	2.109316365	-1.928747683	-0.000241281
H	-0.020233568	-3.222426087	0.001310492
H	-0.333813359	1.902219211	0.001366188
C	-2.684249780	0.402343337	0.001975546
O	-2.954606458	1.575491492	-0.001331666
H	-3.456545294	-0.388575923	0.007716058
Cl	2.654874442	0.867077127	0.000207269

Wheland intermediates of acylation of benzene derivatives at the *orto*- position

Benzene

C	2.146517222	-0.315270471	0.324761104
C	-0.476714275	0.282133467	-0.530897766
C	1.759007000	1.038704331	0.211887694
C	0.486397838	1.340862095	-0.206440650
H	3.152135211	-0.545443410	0.668175033
H	-0.802074637	0.426964808	-1.585552933
H	2.465471439	1.825152421	0.454914645
H	0.171261160	2.377415874	-0.303731670
C	-1.931714246	0.524645643	0.138208580
O	-2.665529759	-0.378717251	0.381961653
H	-2.171256257	1.590596345	0.290604601
C	1.270591770	-1.379405519	0.018852283
H	1.608760208	-2.404731509	0.124009709
C	-0.012143061	-1.101943501	-0.386592223
H	-0.721668564	-1.899839862	-0.587858774

Phenylbenzene

C	-0.557988007	0.424591769	-0.180576009
C	-3.435743850	0.632125135	-0.298999627
C	-1.220916052	1.610984313	0.173754531
C	-2.604024488	1.712337784	0.118039135
H	-4.509615576	0.770173174	-0.361654226
H	-0.646823624	2.491394805	0.436255065
H	-3.068664789	2.659338792	0.378819272
C	-1.395760412	-0.767976771	-0.506616501
H	-1.034365211	-1.267563321	-1.421093854
C	-2.860166620	-0.556054349	-0.622677321
H	-3.468640035	-1.400196160	-0.936725192
C	0.884592352	0.322944516	-0.178514292
C	1.666367686	1.180835138	0.641836670
C	1.560114682	-0.633834499	-0.980967462
C	3.048992659	1.072343612	0.665983007

C	2.944201847	-0.723839640	-0.967207776
C	3.692848634	0.124945200	-0.140816737
H	1.183774751	1.891943088	1.302353952
H	1.006040068	-1.277924979	-1.655457338
H	3.629609893	1.717018336	1.317252128
H	3.445790932	-1.445129057	-1.603601509
H	4.775652426	0.049102225	-0.127493827
C	-1.181579016	-1.952692453	0.558124124
O	-0.371906052	-1.922376332	1.434098729
H	-1.851214553	-2.811212127	0.374695818

Toluene

C	2.148723429	-0.375615989	0.495190807
C	-0.289853204	0.466863000	-0.648213791
C	2.025441343	0.975619274	0.080008194
C	0.854302606	1.388440701	-0.487345774
H	3.080112073	-0.698452124	0.953704055
H	-0.634813819	0.499652652	-1.699177892
H	2.855627454	1.660814940	0.212264072
H	0.728948424	2.419767217	-0.808426099
C	-1.572637759	1.162370309	0.051537802
O	-2.321885487	0.591322417	0.780036526
H	-1.683376362	2.219936991	-0.242291131
C	1.121621036	-1.311229173	0.328215490
H	1.278220575	-2.337669318	0.644247206
C	-0.088914848	-0.947234213	-0.247514506
C	-1.196922891	-1.919932936	-0.420497343
H	-1.944217134	-1.732378317	0.367820210
H	-1.720409778	-1.788775888	-1.372906643
H	-0.851533057	-2.951224006	-0.330613497

Styrene

C	-1.673433025	-1.496446922	-0.505046670
C	-0.348507511	0.709687470	0.660415134
C	-2.449989284	-0.388449173	-0.063313332
C	-1.821012556	0.672079193	0.515899599
H	-2.180732340	-2.334201104	-0.976063255
H	-0.092330274	0.965015284	1.705857354
H	-3.527272949	-0.401053150	-0.187393479
H	-2.387440149	1.535867846	0.854761191
C	0.173482359	2.042889780	-0.079092908
O	1.100437644	2.062919951	-0.828707214
H	-0.410572885	2.935848466	0.203671364
C	-0.292374506	-1.557959254	-0.344241203
H	0.230435852	-2.449466152	-0.670568507
C	0.409659615	-0.505667526	0.253134690
C	1.835936712	-0.512075954	0.487122000
H	2.239347876	0.321946398	1.054567942
C	2.697631592	-1.452940301	0.038428816
H	2.392181020	-2.308323714	-0.555798824

H	3.758092171	-1.370961392	0.253226316

Chlorobenzene

C	2.014455857	1.139034122	-0.560701514
C	0.229255236	-0.667547733	0.696086058
C	2.537000672	-0.036377137	0.037693165
C	1.686380028	-0.902116123	0.666225041
H	2.694509463	1.816271041	-1.071012700
H	-0.173611419	-0.811824794	1.712679003
H	3.602511006	-0.234083814	-0.003093965
H	2.062488615	-1.812301338	1.126871417
C	-0.468658419	-1.954324223	-0.046799809
O	-1.251090776	-1.848406453	-0.931857397
H	-0.132938919	-2.906890248	0.395110194
C	0.655592145	1.471959749	-0.510986650
H	0.297049388	2.394147827	-0.954946433
C	-0.224556459	0.619360675	0.134658758
Cl	-1.874751137	1.003523696	0.248673697

Thiophenol

C	-0.818383365	-2.213894838	0.359558228
C	-0.386635623	0.451836879	-0.505219685
C	0.478032312	-1.710633947	0.397400014
C	0.739256037	-0.417520298	-0.066153611
H	-0.160243655	0.894909623	-1.491173953
H	1.284775641	-2.339618210	0.759626388
C	-0.467484595	1.825026162	0.362599543
O	-1.435608188	2.514002876	0.347066587
H	0.467842564	2.058633116	0.906490488
C	-1.922543839	-1.460446021	-0.130455432
H	-2.911105392	-1.905719076	-0.149253574
C	-1.723658296	-0.180997028	-0.549990173
H	-2.548117876	0.440494682	-0.885893745
H	-0.991070660	-3.225389992	0.717761676
S	2.316681345	0.284769743	-0.134312510
H	2.982925265	-0.722138120	0.469963411

Phenol

C	2.093232375	-0.750171081	0.350768888
C	-0.499559318	-0.000920456	-0.520354412
C	1.778049339	0.603909323	0.337502857
C	0.516726594	0.992725771	-0.112703230
H	-0.842918944	0.256150742	-1.540014536
H	2.505332952	1.345030107	0.656193809
C	-1.892823724	0.225701565	0.267786360
O	-2.694515871	-0.647025324	0.371779879
H	-2.024301083	1.257948937	0.636663803
C	1.179025558	-1.763616816	-0.063076566
H	1.484034226	-2.803455288	-0.026574128
C	-0.068955021	-1.414665985	-0.479376706

H	-0.803295673	-2.162069679	-0.763519362
H	3.079697367	-1.047257866	0.697175387
O	0.102037757	2.244114732	-0.191671786
H	0.766960523	2.894829146	0.094616732

Aniline

C	2.046177206	-0.827284330	0.359424642
C	-0.520724457	0.044560733	-0.514611369
C	1.799568361	0.526874034	0.347439198
C	0.557431812	1.006273788	-0.128886185
H	-0.889802977	0.302213892	-1.522075813
H	2.561088173	1.230275953	0.669654356
C	-1.835942309	0.252829284	0.368663650
O	-2.746284864	-0.517083292	0.318766655
H	-1.841510363	1.168475200	0.992391828
C	1.084509411	-1.800784986	-0.078211260
H	1.345256599	-2.852971772	-0.054081958
C	-0.136042278	-1.397120508	-0.499806529
H	-0.901536512	-2.104038160	-0.802463711
H	3.012854594	-1.175282031	0.713088268
N	0.301511234	2.310039175	-0.200198791
H	0.995039709	2.994714697	0.078915908
H	-0.545856405	2.677957954	-0.614601898

Ethynylbenzene

C	-1.349672925	-1.938345551	0.332387729
C	-0.191065591	0.510853205	-0.496924778
C	0.044318694	-1.820160717	0.353687392
C	0.649501319	-0.639467752	-0.075028052
H	0.132784614	0.837676114	-1.503994989
H	0.658291133	-2.650548387	0.684222601
C	0.196388153	1.874528972	0.297415076
O	-0.546690944	2.801411580	0.339525805
H	1.211766309	1.852061117	0.730839143
C	-2.196872657	-0.888864447	-0.103766585
H	-3.272381737	-1.028766547	-0.098658218
C	-1.646617226	0.299140981	-0.500665115
H	-2.270685961	1.136636721	-0.798942741
H	-1.797209249	-2.870645771	0.666845988
C	2.049504066	-0.502177466	-0.099472089
C	3.258267691	-0.377439035	-0.121556554
H	4.324614372	-0.278069661	-0.140321195

Benzaldehyde

C	2.176138736	1.010968572	0.403346512
C	-0.051785231	-0.402167115	-0.611890611
C	0.893367772	1.587753544	0.503325040
C	-0.201670413	0.929911826	-0.025207410
H	-0.665726739	-0.538270912	-1.518011282
H	0.774049516	2.560023627	0.973024545

C	-1.031854211	-1.513993063	0.293839316
O	-0.649311012	-2.581249943	0.598980003
H	-2.022678827	-1.048279946	0.432095970
C	2.377816618	-0.231071453	-0.227208640
H	3.379428385	-0.639007052	-0.311900504
C	1.296271821	-0.917896864	-0.740286107
H	1.435187342	-1.891292996	-1.202758418
H	3.029343991	1.543961788	0.814156470
C	-1.560376267	1.540068703	0.045130514
O	-2.546079482	0.917240112	-0.306595008
H	-1.628184786	2.565687337	0.447005160

Wheland intermediates of acylation of benzene derivatives at the *meta*- position

Phenylbenzene

C	0.179491408	0.361219952	0.177112036
C	2.976613486	1.018708891	0.389485753
C	0.798507915	1.416844682	-0.551253071
C	2.154572781	1.773005253	-0.414238490
H	4.029488741	1.258332610	0.506463991
H	0.182940068	1.992309422	-1.237427325
H	2.536589090	2.637843306	-0.946354841
C	1.006144762	-0.393949702	0.994872775
H	0.596235415	-1.198417202	1.598608137
C	2.450711635	-0.197131699	1.000165735
H	2.945589952	-0.495881199	1.926337978
C	-1.275846759	0.115555075	0.079881807
C	-2.176020587	1.192515717	-0.016912174
C	-1.779296690	-1.198100235	0.087375406
C	-3.547679695	0.958696733	-0.100700317
C	-3.151244675	-1.427780704	-0.002839116
C	-4.037474848	-0.350688301	-0.095414772
H	-1.813039669	2.216315132	0.009369126
H	-1.099328233	-2.044509168	0.124722975
H	-4.233611498	1.797367801	-0.161735952
H	-3.527207461	-2.445739567	-0.010685873
H	-5.105571557	-0.530777009	-0.163807148
C	3.015212827	-1.399176409	-0.097476340
O	2.650661401	-1.473865065	-1.217109563
H	3.740201738	-2.057969544	0.405308563

Toluene

C	-1.770464704	-0.756558263	0.294645926
C	0.881071043	-0.326878809	-0.529270929
C	-0.892876771	-1.859561826	0.229468694
C	0.405064051	-1.666909659	-0.173441647
H	-2.790788882	-0.932415591	0.630165088

H	1.238446429	-0.366286179	-1.583423523
H	-1.250966031	-2.847451795	0.499242297
H	1.096528350	-2.503855899	-0.236466424
C	2.304336470	0.027075837	0.138879295
O	2.620925672	1.146944996	0.390194556
H	2.950795323	-0.854435609	0.289726664
C	-1.394684015	0.571536925	-0.039994429
C	-0.086357879	0.771876000	-0.428335860
H	0.275414937	1.772275562	-0.651213360
C	-2.396514801	1.693232906	0.055729584
H	-2.798342286	1.770608520	1.071264153
H	-1.946706335	2.652548518	-0.206500434
H	-3.240137898	1.516350729	-0.619774247

Styrene

C	1.024174058	1.594153389	0.280510240
C	-1.233286666	0.132261723	-0.525216522
C	-0.228415589	2.240443289	0.253361949
C	-1.344328793	1.540333355	-0.132230739
H	1.890439031	2.167954658	0.602772402
H	-1.606305646	0.045172618	-1.571040251
H	-0.298283122	3.283901220	0.541710797
H	-2.320731845	2.017828765	-0.158261082
C	-2.368694236	-0.793700869	0.151981344
O	-2.192547814	-1.950072728	0.372763197
H	-3.314988231	-0.257479276	0.337643067
C	1.220069541	0.229519169	-0.071414838
C	0.098190622	-0.475187439	-0.475678816
H	0.173488863	-1.520513731	-0.759863696
C	2.573256317	-0.351105096	0.004206274
H	3.387953455	0.369327804	0.023410361
C	2.855024076	-1.658326635	0.079690015
H	2.091966791	-2.431568768	0.108501655
H	3.883775461	-1.997201958	0.136089043

Chlorobenzene

C	1.037968733	1.410490232	0.298451112
C	-1.366802083	0.196676572	-0.539218005
C	-0.134310945	2.188917593	0.237793416
C	-1.313342314	1.612856176	-0.173489820
H	1.964403105	1.865894758	0.638782356
H	-1.753948285	0.121962354	-1.580007582
H	-0.093184633	3.236363688	0.517188659
H	-2.224947654	2.202920538	-0.229599528
C	-2.616474509	-0.581429146	0.158549343
O	-2.573108643	-1.744304205	0.394590313
H	-3.489435671	0.070050273	0.330221895
C	1.050433304	0.040254585	-0.060828693
C	-0.118917781	-0.566351604	-0.458884158
H	-0.144299041	-1.626120415	-0.695935389

Cl	2.530261276	-0.847439834	0.033384316

Thiophenol

C	-0.960742221	-1.410590467	-0.215892782
C	1.205811658	0.204296992	0.566579836
C	-1.218068268	-0.034480229	0.036959330
C	-0.145388526	0.750973231	0.426794588
H	1.536877345	0.385968769	1.614398228
H	-0.292252406	1.807580672	0.641720098
C	2.337017922	1.131585734	-0.135110456
O	3.382305562	0.683478880	-0.481267935
H	2.050958926	2.194244072	-0.206737330
C	0.314245005	-1.991075278	-0.086486589
H	0.439166258	-3.047145705	-0.301548729
C	1.390070825	-1.217183469	0.280329069
H	2.392465627	-1.630273812	0.340749735
H	-1.780312428	-2.048828928	-0.536903047
S	-2.816428719	0.708164997	-0.121639875
H	-3.481647606	-0.415993707	-0.451448306

Phenol

C	-1.580373978	-1.055666809	-0.242517427
C	0.811425967	0.197241063	0.559321771
C	-1.590355840	0.345744662	-0.030944977
C	-0.418506486	0.963169095	0.369852771
H	1.159072419	0.353775619	1.605473587
H	-0.421243249	2.035961977	0.545905810
C	2.102197216	0.895860654	-0.144675411
O	3.064531987	0.266212758	-0.442593779
H	1.997217217	1.987193270	-0.260991555
C	-0.424024325	-1.837648711	-0.062846938
H	-0.473098852	-2.905690261	-0.246508611
C	0.757081332	-1.243291418	0.315968158
H	1.672481342	-1.818055855	0.417868239
H	-2.497206408	-1.545692260	-0.565283673
O	-2.679705054	1.115452701	-0.195681820
H	-3.465946493	0.617963721	-0.465267503

Aniline

C	-1.595608084	-1.042674929	-0.223676728
C	0.806443645	0.203495148	0.530166925
C	-1.622712597	0.372558471	-0.025948987
C	-0.423666138	0.975906965	0.347238255
H	1.134029880	0.334950730	1.587881040
H	-0.384389401	2.048992182	0.519239174
C	2.096746654	0.889469982	-0.149852621
O	3.075791619	0.264448962	-0.411813657
H	1.992011345	1.977421368	-0.299979401
C	-0.443840482	-1.825028544	-0.059199204
H	-0.503044686	-2.894193485	-0.233416218

C	0.750382736	-1.236801086	0.293072181
H	1.667022177	-1.811446107	0.380155345
H	-2.516262059	-1.536512385	-0.527200954
N	-2.777738275	1.066593609	-0.205901307
H	-3.639163738	0.603714059	-0.450801693
H	-2.823599607	2.062394121	-0.054512046

Ethynylbenzene

C	-1.069028421	-1.384584169	-0.228995959
C	1.096368837	0.230421210	0.579463050
C	-1.323575434	-0.007841279	0.043506922
C	-0.254792793	0.778722389	0.443654610
H	1.432090978	0.405761500	1.626447962
H	-0.416695150	1.830815121	0.664596591
C	2.221794986	1.163043239	-0.123389282
O	3.249560045	0.713076560	-0.516630030
H	1.948695841	2.231321656	-0.149335571
C	0.206065826	-1.966072125	-0.102489908
H	0.337514519	-3.019010651	-0.328279628
C	1.275776051	-1.191262999	0.277830619
H	2.278251273	-1.605161047	0.338306020
H	-1.902133693	-2.000929246	-0.556411252
C	-2.638043464	0.523445736	-0.095891215
C	-3.756325034	0.970041237	-0.212856863
H	-4.744681916	1.366833032	-0.311899789

Benzaldehyde

C	-0.902833479	-1.597731817	-0.265370716
C	1.064293851	0.227623929	0.610237501
C	-1.278620011	-0.257969020	-0.024032013
C	-0.324006706	0.636197953	0.415315272
H	1.367166609	0.479161171	1.650271474
H	-0.624151444	1.665769153	0.607186368
C	2.111120925	1.262837320	-0.105556321
O	3.153622251	0.892705887	-0.534063087
H	1.756792067	2.306606370	-0.093248511
C	0.418014748	-2.057956615	-0.076788984
H	0.662581517	-3.095380237	-0.278605219
C	1.386508826	-1.177578204	0.341267255
H	2.419117183	-1.495977267	0.454320116
H	-1.658171845	-2.298193718	-0.618430050
C	-2.698568088	0.211856636	-0.231353465
O	-3.017097047	1.360992085	-0.036474203
H	-3.421887045	-0.553634233	-0.569438754

Wheland intermediates of acylation of benzene derivatives at the *para*- position

Phenylbenzene

C	-0.093299390	-0.136036936	-0.196388908
C	2.782770854	-0.371482618	-0.474910557
C	0.579840284	-1.375020133	0.088950529
C	1.928809978	-1.494718766	-0.032397819
H	3.299255611	-0.688265257	-1.406856881
H	0.008505297	-2.221102517	0.449888385
H	2.409498658	-2.438502968	0.214458575
C	4.033849350	-0.163665685	0.468100512
O	4.464207579	0.918578415	0.744515769
H	4.493675332	-1.107317968	0.816076913
C	0.705457258	0.979830097	-0.626019622
H	0.220894863	1.915328203	-0.875814550
C	2.054902052	0.882673655	-0.756073241
H	2.638409511	1.743372001	-1.068820405
C	-1.527215927	-0.014541321	-0.044319775
C	-2.362987735	-1.164670982	-0.056126842
C	-2.138887520	1.258131106	0.120998530
C	-3.738238738	-1.042891949	0.075826312
C	-3.512435676	1.369204633	0.279620195
C	-4.316672833	0.221791675	0.251061420
H	-1.940245745	-2.149259954	-0.218026771
H	-1.533964280	2.155636304	0.174635262
H	-4.365050405	-1.927553922	0.040032524
H	-3.961581296	2.345248706	0.429229597
H	-5.392436673	0.312722098	0.365335745

Toluene

C	-1.773220758	0.099298304	0.071604378
C	0.992567388	-0.309261659	-0.548636220
C	-1.229461920	-1.218882205	0.063342866
C	0.088301012	-1.426958370	-0.231778802
H	1.389931519	-0.478322327	-1.574032747
H	-1.878176590	-2.058044359	0.293834478
H	0.493018257	-2.436631096	-0.238239546
C	2.379980973	-0.389024547	0.244359962
O	2.988802162	0.588211941	0.555815651
H	2.727671367	-1.420895088	0.427796564
C	-0.935608032	1.211293934	-0.232396919
H	-1.361194936	2.209796916	-0.219126077
C	0.389037373	1.032226689	-0.515422591
H	1.036758711	1.883401579	-0.705841471
C	-3.199490829	0.315913015	0.435370442
H	-3.822717580	-0.546495601	0.186656630
H	-3.264044852	0.452759782	1.527023077
H	-3.607291649	1.219961417	-0.023066530

Styrene

C	1.386603138	-0.231777575	-0.054588534
C	-1.396311810	0.298061811	-0.567154435

C	0.901873101	1.116379881	-0.098290128
C	-0.412730797	1.375995753	-0.339676731
H	-1.828334133	0.445126103	-1.581498160
H	1.584921566	1.941465189	0.064598365
H	-0.763611938	2.404944827	-0.368953641
C	-2.720299000	0.488567592	0.292507438
O	-3.343801550	-0.435587891	0.722392304
H	-3.024889813	1.543857479	0.414105387
C	0.466005736	-1.307508825	-0.268880158
H	0.836662621	-2.326771250	-0.225863025
C	-0.856272248	-1.072110622	-0.498966466
H	-1.552808830	-1.896868070	-0.618421176
C	2.768681928	-0.565416319	0.209002763
H	3.008844925	-1.625435675	0.212550356
C	3.761269103	0.322311922	0.447334828
H	3.613092607	1.397375039	0.465461387
H	4.772093320	-0.025091511	0.635800099

Chlorobenzene

C	1.256619800	0.000346366	-0.048145825
C	-1.514534982	0.319348550	-0.547701916
C	0.695524594	1.306191072	0.000872649
C	-0.639348084	1.463513960	-0.243729668
H	-1.974781256	0.496742648	-1.544442873
H	1.333329871	2.152931355	0.229406564
H	-1.077919589	2.458461251	-0.214785024
C	-2.868683353	0.325535224	0.318560306
O	-3.426742280	-0.682795156	0.620824859
H	-3.238226757	1.338504511	0.555016143
C	0.473502090	-1.149152781	-0.340809912
H	0.945452659	-2.125381561	-0.358987542
C	-0.864725981	-1.001011135	-0.571562221
H	-1.488707248	-1.870806731	-0.757290630
Cl	2.913852810	-0.192332155	0.267884342

Thiophenol

C	1.301078284	-0.026391627	-0.047237050
C	-1.496860034	0.320010558	-0.566156551
C	0.722351563	1.285981817	-0.001408918
C	-0.603764868	1.455140115	-0.248860027
H	-1.933121746	0.504345082	-1.571644533
H	1.352530898	2.138569797	0.231889437
H	-1.033257183	2.453617036	-0.215102035
C	-2.827505089	0.333967209	0.299799969
O	-3.358576819	-0.670289561	0.672321449
H	-3.230865695	1.345781173	0.486412750
C	0.484029803	-1.164095583	-0.351337203
H	0.927359586	-2.154312153	-0.375688836
C	-0.845586294	-1.006199967	-0.586539297
H	-1.472537193	-1.872188939	-0.778314423

S	2.978395476	-0.143917143	0.292635728
H	3.097573628	-1.481522898	0.149645182

Phenol

C	-1.721053628	0.110059477	0.087009902
C	1.011753247	-0.316911754	-0.571631846
C	-1.208896598	-1.224368894	0.077882607
C	0.096342281	-1.430806583	-0.236245468
H	1.382389476	-0.490299493	-1.604811907
H	-1.883265896	-2.036617331	0.326992338
H	0.493558827	-2.443060251	-0.246890112
C	2.386727754	-0.398017798	0.218834604
O	2.973106642	0.579284870	0.579373067
H	2.761177872	-1.427343938	0.363649707
C	-0.895364082	1.235153212	-0.226694061
H	-1.317926816	2.235949676	-0.199198861
C	0.413862137	1.034680178	-0.528583124
H	1.066438516	1.879589090	-0.728986089
O	-2.985116748	0.234652678	0.411167174
H	-3.304448484	1.154292982	0.411896804

Aniline

C	-1.742331396	0.102760952	0.096363519
C	1.012537357	-0.318307865	-0.602764030
C	-1.195968114	-1.233111620	0.093524152
C	0.100155054	-1.432920518	-0.236828254
H	1.367757680	-0.506756315	-1.637241014
H	-1.839282959	-2.066537123	0.359398787
H	0.503302618	-2.442775738	-0.237736636
C	2.364787121	-0.382813419	0.197589918
O	2.897041596	0.592629654	0.647441510
H	2.795275029	-1.398299314	0.280463406
C	-0.904324971	1.226100304	-0.246024350
H	-1.329870082	2.225010149	-0.225457801
C	0.394524604	1.031227988	-0.564809255
H	1.034068355	1.879731106	-0.788209968
N	-3.010052357	0.297994485	0.424147779
H	-3.417532837	1.225563382	0.439754979
H	-3.618965842	-0.470894094	0.678117522

Ethynylbenzene

C	1.420210932	-0.002907660	-0.045490956
C	-1.375641541	0.310831136	-0.537976724
C	0.832258633	1.300985914	0.012088949
C	-0.502313510	1.456508135	-0.225300631
H	-1.832814980	0.495213010	-1.535038415
H	1.462939785	2.151683394	0.244977217
H	-0.946717518	2.448271179	-0.183676515
C	-2.720694814	0.310735537	0.329131563
O	-3.268014642	-0.698868375	0.651751046

H	-3.103185352	1.321790961	0.555457603
C	0.618793570	-1.149583240	-0.346603192
H	1.089671303	-2.125821333	-0.378165704
C	-0.719333145	-1.007704542	-0.571106056
H	-1.341276721	-1.877228512	-0.763336898
C	2.792657271	-0.159598933	0.208256335
C	3.980173272	-0.295475452	0.428988434
H	5.026873832	-0.416690887	0.622477603

Benzaldehyde

C	1.325064239	-0.259565991	-0.058060728
C	-1.402789761	0.294360036	-0.558086865
C	0.898761243	1.088555442	-0.115771949
C	-0.421715534	1.367567774	-0.363155982
H	-1.899061053	0.441719417	-1.542719666
H	1.632749861	1.873368265	0.037578112
H	-0.762360182	2.399296593	-0.416240545
C	-2.751963103	0.507903697	0.332200389
O	-3.429706540	-0.408248726	0.665613712
H	-2.972771723	1.569088651	0.535113901
C	0.428771054	-1.334899197	-0.252757109
H	0.792282964	-2.357105418	-0.196423557
C	-0.901154831	-1.080155994	-0.486964569
H	-1.615482076	-1.891715966	-0.595298840
C	2.783666842	-0.546052712	0.228987771
O	3.570760343	0.353208257	0.410739373
H	3.078481226	-1.610162492	0.260135573

Wheland intermediates of acylation of substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

B	0.160780231	1.318584611	-0.664977429
N	1.308023631	1.137610287	0.207813683
C	-0.601650503	-0.002120491	-1.029569635
C	1.727734112	-0.064833862	0.617574345
C	0.113863224	-1.250208792	-0.725458716
C	1.170122150	-1.274749559	0.147284919
H	-1.077772484	-0.008093076	-2.013815451
H	2.568730905	-0.086313083	1.306840728
H	-0.246258340	-2.182842608	-1.154377856
H	1.633734461	-2.204480376	0.456239285
H	-0.186265300	2.412658827	-0.946986032
H	1.830441854	1.940120301	0.549972489
C	-1.858209883	0.148160487	-0.000836106
O	-1.780489805	-0.094981204	1.164407801
H	-2.766314998	0.523362914	-0.501470076

1-phenyl-1,2-dihydro-1,2-azaborine

N	-0.038808707	0.281467124	0.287283837
B	0.921017345	-0.829533513	0.313995917
C	0.396724239	1.543346047	0.379396717
C	2.433357545	-0.463661172	0.469217137
C	1.764140407	1.920155168	0.454958995
C	2.753665518	0.982315038	0.457441711
H	-0.369372737	2.314906878	0.380089404
H	2.625658454	-0.841045201	1.502336511
H	1.987720164	2.980700063	0.487372070
H	3.797751781	1.285554736	0.442009387
H	0.513763571	-1.936339176	0.242274237
C	-1.456991612	0.041006137	0.076237809
C	-2.121523912	-0.883869771	0.886695008
C	-2.126424223	0.735079623	-0.937601676
C	-3.484946002	-1.099520075	0.686385636
C	-3.490167873	0.507037884	-1.128335181
C	-4.169276717	-0.405995907	-0.317269434
H	-1.592750988	-1.410678642	1.674483361
H	-1.588711378	1.413107019	-1.594222688
H	-4.012366921	-1.806173792	1.318475149
H	-4.014436424	1.031702017	-1.920147829
H	-5.228544966	-0.583425231	-0.471445417
C	3.407086547	-1.325237237	-0.376206898
O	4.263993157	-0.840819146	-1.067413053
H	3.251281024	-2.416412745	-0.292659464

1-methyl-1,2-dihydro-1,2-azaborine

B	0.409633222	-1.051386567	0.381940825
N	1.610423399	-0.321166450	-0.036604634
C	-0.888155460	-0.218204376	0.627816479
C	1.563444962	0.997266104	-0.213754479
C	-0.782740312	1.231808693	0.342208724
C	0.399954734	1.794986155	-0.033523967
H	-1.060986747	-0.341077868	1.721692715
H	2.485575518	1.480199307	-0.531600616
H	-1.676488437	1.846229781	0.422236993
H	0.487495915	2.857746189	-0.229311177
H	0.491044432	-2.223541748	0.523971546
C	2.878980667	-1.054873251	-0.280751589
H	3.654863848	-0.363118419	-0.609697973
H	3.192815199	-1.545066418	0.642646170
H	2.712709746	-1.811359584	-1.049708912
C	-2.178590620	-0.872190450	0.042812033
O	-2.937867322	-0.277198504	-0.672437717
H	-2.333719088	-1.923569335	0.345667039

1-vinyl-1,2-dihydro-1,2-azaborine

B	0.141831369	-0.548882782	0.707052490
N	1.165857937	0.285454909	0.052344347

C	-1.323024044	0.003622826	0.757188147
C	0.821071177	1.492827560	-0.414192479
C	-1.512554905	1.377491487	0.236366663
C	-0.477061505	2.058453717	-0.335420036
H	-1.709477617	-0.045372935	1.792069845
H	1.614593505	2.072627103	-0.881031702
H	-2.495790009	1.841297801	0.288525917
H	-0.610226005	3.054691467	-0.741869172
H	0.457316625	-1.582728082	1.176272797
C	2.541506982	-0.119598134	-0.080868273
H	3.213382190	0.702848786	-0.303716180
C	2.976168246	-1.374642764	0.029620544
H	2.333075800	-2.223680258	0.227435728
H	4.035422918	-1.570361508	-0.092198323
C	-2.295518578	-0.972862024	-0.015691659
O	-1.884899814	-1.811904478	-0.769374942
H	-3.370732491	-0.817215924	0.186490823

1-chloro-1,2-dihydro-1,2-azaborine

B	0.020193912	0.657985684	-0.975508526
N	0.924658065	-0.109367448	-0.122651604
C	-1.447446043	0.114368012	-1.004709893
C	0.554661205	-1.224914664	0.518684345
C	-1.648980793	-1.240024944	-0.473552590
C	-0.712715782	-1.825702895	0.334578238
H	-1.979713502	0.297812434	-1.942119667
H	1.294827774	-1.688581581	1.165788827
H	-2.586496118	-1.754168548	-0.671770100
H	-0.889278167	-2.776423394	0.824903293
Cl	2.566666485	0.417939120	0.077271158
H	0.396886454	1.657471015	-1.475614235
C	-2.122252764	1.188312710	0.033920463
O	-1.995120596	1.114490107	1.216496359
H	-2.676990951	1.983765736	-0.490631010

1-mercapto-1,2-dihydro-1,2-azaborine

B	-0.077209105	-0.687169421	-0.637731165
N	1.063223617	-0.018901523	-0.004301893
C	-1.410735527	0.135124619	-0.678089284
C	0.972103131	1.246971944	0.436014728
C	-1.282351693	1.569245252	-0.388312918
C	-0.166742055	2.064821098	0.234561211
H	-2.035685433	-0.082955723	-1.548621958
H	1.852410348	1.655274268	0.927424369
H	-2.108385643	2.237429168	-0.622363802
H	-0.097884213	3.101603761	0.545223837
H	0.026918380	-1.810564880	-0.985042658
S	2.671402413	-0.767741723	0.009431123
H	2.296164202	-1.841614127	0.736940755
C	-2.247613973	-0.585172570	0.521637522

O	-2.980680895	-1.494772326	0.292809548
H	-2.065690173	-0.170245956	1.528375621

1-hydroxy-1,2-dihydro-1,2-azaborine

B	0.295898495	-0.860202940	0.884894740
N	1.324532350	-0.270070848	0.042576253
C	-1.011509932	-0.012912784	0.997087132
C	1.218129588	0.934958184	-0.512587730
C	-0.923420100	1.377897297	0.515701050
C	0.115795054	1.791955462	-0.267536913
H	-1.514284623	-0.096379391	1.965750835
H	2.055974997	1.242053988	-1.133981632
H	-1.733473650	2.066148306	0.743836097
H	0.149153917	2.785308866	-0.699947970
H	0.465912496	-1.950838495	1.311030052
O	2.559603362	-0.871486961	-0.170593409
H	2.419284308	-1.833555445	-0.116235699
C	-1.978643290	-0.864145837	-0.001168454
O	-1.936664594	-0.763352070	-1.189240852
H	-2.649476226	-1.549788284	0.543302532

1-amino-1,2-dihydro-1,2-azaborine

B	0.103308022	-0.845483850	0.613581923
N	1.400230748	-0.455971055	0.060843442
C	-0.993416328	0.271682411	0.671455115
C	1.641558317	0.795343930	-0.337292950
C	-0.582116526	1.606611725	0.178326433
C	0.673675893	1.832107483	-0.309747934
H	-1.306998456	0.380087870	1.730527193
H	2.650776547	0.984632094	-0.696135528
H	-1.303152844	2.422377729	0.189263592
H	0.975361072	2.807346663	-0.674474130
H	-0.030669244	-1.955125100	0.996565455
N	2.498955286	-1.352112084	-0.068260325
H	2.480533722	-1.767485704	-0.999803831
H	2.390045140	-2.094552136	0.618520838
C	-2.346936959	-0.161823136	-0.011438406
O	-2.447136942	-1.177291791	-0.641268465
H	-3.186149334	0.542903982	0.135513908

1-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.034170474	-0.698404221	-0.622941818
N	-1.212338051	-0.010007814	-0.051893121
C	1.296959799	0.117396933	-0.633261241
C	-1.131864262	1.273879181	0.366403810
C	1.172288290	1.550335142	-0.330201435
C	0.028146328	2.064595317	0.225297538
H	1.914376089	-0.080402964	-1.515465427
H	-2.038920054	1.694930446	0.791904465
H	2.020637209	2.208440318	-0.506670447

H	-0.040584705	3.104841600	0.523805537
H	-0.150781306	-1.825156897	-0.949813874
C	-2.411287002	-0.666560273	0.033882056
C	2.169663983	-0.627640063	0.529198484
O	2.878621125	-1.545454857	0.262302161
H	2.032394033	-0.223009201	1.546429329
C	-3.460087161	-1.259285558	0.088681404
H	-4.388501801	-1.787983648	0.138898544

1-formyl-1,2-dihydro-1,2-azaborine

B	0.119976876	-0.634347124	0.603752087
N	1.174500733	0.177491558	-0.024072246
C	-1.286345348	0.050084502	0.693974012
C	0.942018566	1.444657325	-0.414745113
C	-1.310321627	1.493372585	0.450148719
C	-0.266600060	2.128155185	-0.185919570
H	-1.888160884	-0.259765814	1.551567930
H	1.770181174	1.965978103	-0.894083515
H	-2.191486141	2.068005701	0.729618071
H	-0.319196231	3.175702056	-0.460800803
H	0.351286064	-1.747849436	0.908084030
C	2.535743939	-0.357556375	-0.215472722
O	2.825896555	-1.463180965	0.114026086
H	3.213940629	0.374369283	-0.683354501
C	-2.072957656	-0.704684115	-0.541646057
O	-2.783642540	-1.630334443	-0.323521316
H	-1.871033954	-0.287378138	-1.542986559

2-phenyl-1,2-dihydro-1,2-azaborine

B	-0.378238124	-0.279972059	-0.282992066
N	-1.083610062	-1.524783420	0.082180912
C	-1.381609969	0.900435882	-0.640085049
C	-2.394686575	-1.697631941	-0.034741207
C	-2.754881108	0.485066345	-0.987132631
C	-3.256811893	-0.722974793	-0.600353757
H	-0.985215386	1.640255079	-1.339903043
H	-2.796728095	-2.660819396	0.271179052
H	-3.401400485	1.193007213	-1.501005963
H	-4.295544561	-0.989540337	-0.756482398
H	-0.558440245	-2.332359678	0.405767066
C	1.141811565	-0.168693903	-0.166279507
C	1.833519589	0.900445767	-0.790060374
C	1.914852880	-1.112394061	0.557558856
C	3.217536008	1.018213039	-0.700917594
C	3.296665995	-0.993466880	0.656321875
C	3.949913001	0.071978102	0.024106105
H	1.286528668	1.635230562	-1.373950424
H	1.437001130	-1.939544537	1.077730379
H	3.727234904	1.838607877	-1.195637216
H	3.867041587	-1.721475313	1.223943772

H	5.029428991	0.162701169	0.096214910
C	-1.396906425	1.651119374	0.773997603
O	-2.085525976	1.322218142	1.697013034
H	-0.667610689	2.479396937	0.822126469

2-methyl-1,2-dihydro-1,2-azaborine

B	-1.005089584	-0.564106233	0.208160272
N	-0.158818656	-1.466798081	-0.585454779
C	-0.174967100	0.568403024	0.941499710
C	1.172856126	-1.423600432	-0.588891461
C	1.273679888	0.324266792	1.064959669
C	1.920404330	-0.564527233	0.252409615
H	-0.624304969	0.925474686	1.872222580
H	1.689082851	-2.126119933	-1.239445558
H	1.847980132	0.920927016	1.770410972
H	2.999168164	-0.668101952	0.259954597
H	-0.586017299	-2.181018402	-1.170345959
C	-2.549332510	-0.716694551	0.219191725
H	-2.954461495	-1.313852801	-0.603596306
H	-2.839274425	-1.221025411	1.155038129
H	-3.076160553	0.244533252	0.238788841
C	-0.401254016	1.778281041	-0.100912950
O	0.197967240	1.883227591	-1.130205626
H	-1.192764559	2.476705518	0.222293432

2-vinyl-1,2-dihydro-1,2-azaborine

B	-0.780203749	-0.137682303	0.358084016
N	-0.403947546	-1.310572087	-0.449324504
C	0.471357350	0.639055306	0.943579675
C	0.843493110	-1.756344851	-0.561543807
C	1.739086071	-0.116080437	0.959986405
C	1.933440166	-1.203066979	0.156998573
H	0.275556015	1.150649516	1.890361950
H	1.003179570	-2.623228603	-1.198767530
H	2.559865210	0.249584825	1.573127513
H	2.895254658	-1.696956401	0.083020305
H	-1.111711970	-1.850074564	-0.940193316
C	-2.234606121	0.325731736	0.495234232
H	-2.453354415	1.122151406	1.206610718
C	-3.279955174	-0.169082995	-0.200853488
H	-3.180011031	-0.957120851	-0.945849131
H	-4.291903334	0.201792113	-0.061570375
C	0.587697096	1.821364362	-0.138983595
O	1.110040687	1.689897841	-1.207664902
H	0.100867783	2.755240110	0.192322235

2-chloro-1,2-dihydro-1,2-azaborine

B	0.444723672	-0.495360337	-0.163029239
N	-0.365159421	-1.519233514	0.503661448
C	-0.343834783	0.723400700	-0.772178633

C	-1.694129622	-1.469296303	0.541335914
C	-1.821238783	0.584300119	-0.732382682
C	-2.447762307	-0.438280932	-0.074590929
H	-0.025203797	0.933076017	-1.806532718
H	-2.204954536	-2.276326297	1.061787727
H	-2.428850986	1.350722323	-1.211277178
H	-3.528562610	-0.497269107	-0.019413320
H	0.082287654	-2.315821072	0.953491922
Cl	2.159330564	-0.705716780	-0.226358004
C	0.015954285	2.081025594	-0.017697344
O	0.539997424	2.090619262	1.058147158
H	-0.266337907	2.996678979	-0.566916078

2-mercapto-1,2-dihydro-1,2-azaborine

B	0.496413130	-0.508673335	-0.143542767
N	-0.328851231	-1.518653987	0.546541337
C	-0.307115367	0.700284129	-0.781189136
C	-1.655406416	-1.487681846	0.548226801
C	-1.783621056	0.520563797	-0.793277142
C	-2.410478178	-0.494043610	-0.129013522
H	0.029540724	0.928385573	-1.804670871
H	-2.168296805	-2.281430359	1.086666354
H	-2.390561428	1.260519118	-1.312793927
H	-3.491003119	-0.574938303	-0.107567703
H	0.097477529	-2.298726369	1.040192140
S	2.268536440	-0.634097581	-0.267388194
H	2.447815459	-1.766961988	0.444771175
C	-0.039661867	2.058738078	-0.003484147
O	0.425931372	2.084543223	1.100511875
H	-0.326956264	2.969914614	-0.558849662

2-hydroxy-1,2-dihydro-1,2-azaborine

N	1.366172361	-1.211177867	0.065171907
B	-0.071334009	-0.886338739	-0.138344229
C	2.296329792	-0.284241614	0.180125934
C	-0.386079052	0.644202477	-0.406182103
C	2.015448400	1.115771098	0.103936727
C	0.753550974	1.565961372	-0.136984865
H	3.315917970	-0.616336494	0.364377160
H	-0.559074866	0.708596215	-1.503836399
H	2.840988525	1.801715070	0.255242638
H	0.573743317	2.640169632	-0.162722648
C	-1.757701759	1.084393040	0.145841185
O	-2.671787916	0.298044501	0.230917828
H	-1.874573495	2.145499642	0.433399676
H	1.646039783	-2.184225795	0.181809719
O	-0.924159847	-1.903295173	-0.074375808
H	-1.861964079	-1.636797049	-0.098372414

2-amino-1,2-dihydro-1,2-azaborine

N	1.404520835	1.198020541	-0.085968594
B	-0.050613952	0.927505855	0.136720322
C	2.307872368	0.244704080	-0.191848248
C	-0.401165777	-0.601700833	0.414616482
C	1.991204196	-1.144460732	-0.094457496
C	0.718007529	-1.551088830	0.158305607
H	3.335165339	0.547536910	-0.382696608
H	-0.585734793	-0.666298178	1.509397377
H	2.796015956	-1.855930335	-0.238547557
H	0.508645786	-2.619697870	0.197761782
C	-1.764046029	-1.072035868	-0.142466033
O	-2.701703386	-0.321517057	-0.254650824
H	-1.846280859	-2.145021644	-0.402684436
H	1.740122983	2.150006925	-0.213917112
N	-0.957336175	1.965608960	0.103815956
H	-1.951730937	1.773581770	0.163589697
H	-0.735417474	2.940742679	-0.049271052

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.387830421	-0.686229327	0.152831715
N	0.642069555	-1.561835641	-0.428009312
C	0.142155844	0.727101018	0.618396546
C	1.935775325	-1.249639720	-0.454986041
C	1.609913666	0.839033163	0.714961849
C	2.452854398	-0.060438864	0.117174625
H	-0.367800328	1.115124470	1.504125877
H	2.611747430	-1.973802117	-0.904100281
H	2.033298458	1.697519954	1.233161474
H	3.528265287	0.075470245	0.122315144
H	0.382458347	-2.473592081	-0.798189872
C	-1.811102656	-1.141109664	0.182749517
C	-2.971917541	-1.506533214	0.219139280
H	-3.992922364	-1.827788057	0.255104936
C	-0.367993940	1.735166819	-0.539442800
O	-1.315484423	2.438221553	-0.370075729
H	0.214085924	1.703557489	-1.477622158

2-formyl-1,2-dihydro-1,2-azaborine

B	0.501250666	-0.768882947	-0.212287016
N	-0.495570684	-1.497853896	0.542302088
C	-0.030131334	0.500173116	-0.958994461
C	-1.793395856	-1.148336145	0.548635351
C	-1.481192969	0.580617835	-1.102671526
C	-2.317844051	-0.142037383	-0.283863896
H	0.528336666	0.811198312	-1.843275242
H	-2.453896881	-1.722145246	1.194090293
H	-1.907303918	1.273798623	-1.824647587
H	-3.392027688	0.002081775	-0.297435782
H	-0.246078527	-2.296144793	1.121655401

C	2.062467905	-1.049589003	-0.079656043
O	2.800994005	-0.077971832	-0.175959710
H	2.493593088	-2.049738612	0.131266219
C	0.433286344	1.623173497	0.186331722
O	-0.136581708	1.759774557	1.219956621
H	1.331676525	2.166267274	-0.141436418

Wheland intermediates of acylation of substituted 1,2-dihydro-1,2-azaborines on C4

1-phenyl-1,2-dihydro-1,2-azaborine

B	0.624094644	-1.065422990	-0.691405249
N	-0.128653628	0.044579866	-0.142439261
C	2.125479017	-0.857356083	-0.766542493
C	0.488119184	1.219802317	0.277288649
C	2.725064478	0.395790873	-0.359454239
C	1.825906727	1.424926219	0.181375116
H	2.808619307	-1.621460631	-1.131603405
H	-0.159896027	1.967022885	0.717390584
H	3.283223653	0.815265143	-1.227665547
H	2.234864790	2.369122124	0.526850123
H	0.056674583	-2.024101369	-1.082593604
C	-1.551934543	-0.020500249	-0.026227406
C	-2.340103059	1.111971884	-0.310106248
C	-2.160530127	-1.228750406	0.361426959
C	-3.724825014	1.026274655	-0.211023072
C	-3.545376974	-1.293855903	0.474574443
C	-4.331331893	-0.171670479	0.187000538
H	-1.883070339	2.030779739	-0.662118152
H	-1.551924634	-2.090790717	0.608116584
H	-4.333059027	1.890083715	-0.457842164
H	-4.012213805	-2.218841555	0.796158685
H	-5.411676779	-0.230213964	0.270458917
C	4.064189557	0.161006344	0.548208558
O	4.803468692	-0.747269053	0.354051945
H	4.209454188	0.944948878	1.310650431

Wheland intermediates of acylation of substituted 1,2-dihydro-1,2-azaborines on C5

1,2-dihydro-1,2-azaborine

B	2.145701199	0.339399596	0.438928721
N	1.609134886	-1.050466696	0.251473571
C	1.213865316	1.454244581	-0.010046454
C	0.434597521	-1.314782408	-0.251971032
C	-0.013062652	1.150955450	-0.497679673

C	-0.495247708	-0.253222657	-0.649140515
H	0.141536770	-2.359115302	-0.359872453
H	-0.723085793	1.919846738	-0.792722836
H	-0.763413612	-0.454110564	-1.706865680
H	3.223295111	0.418247508	0.915999939
H	2.183416036	-1.848682764	0.520744713
H	1.496258243	2.500157586	0.067806163
C	-1.922109730	-0.505792596	0.038302797
O	-2.502926772	0.372488078	0.597242688
H	-2.321276778	-1.527310292	-0.093881949

1-phenyl-1,2-dihydro-1,2-azaborine

B	-0.590642869	1.912634598	0.074539731
N	-0.122646229	0.487023382	-0.118314533
C	-2.080674766	2.173677372	-0.081288334
C	-0.978739108	-0.469680952	-0.361998674
C	-2.917809626	1.151310555	-0.371523538
C	-2.430255700	-0.250401769	-0.529257908
H	-2.492800636	3.173361593	0.023576259
H	-0.603708199	-1.489132258	-0.418533755
H	-3.987868471	1.303303171	-0.505513991
H	-2.680042741	-0.597494257	-1.554243728
H	0.246678091	2.705340633	0.324272506
C	1.295637389	0.167900299	-0.055586658
C	1.869198316	-0.593859225	-1.079047227
C	2.052281139	0.628381225	1.025791921
C	3.225485680	-0.913963444	-1.004803953
C	3.403986439	0.291614001	1.090757551
C	3.990537308	-0.476430101	0.079397743
H	1.281591431	-0.899193797	-1.940046367
H	1.595355990	1.216492395	1.814590155
H	3.682901954	-1.492477424	-1.800440174
H	3.997827198	0.630124625	1.933192559
H	5.045338606	-0.725162059	0.132466225
C	-3.244327052	-1.282057839	0.342639617
O	-2.737002945	-2.237156859	0.861168465
H	-4.324779352	-1.058182828	0.403953545

1-methyl-1,2-dihydro-1,2-azaborine

B	-1.812062414	0.803994314	-0.363437177
N	-1.316246387	-0.560439591	0.056254274
C	-0.823031498	1.952786705	-0.266156139
C	-0.096774218	-0.735994236	0.468496397
C	0.433852718	1.717927101	0.178835676
C	0.892264637	0.355928329	0.583668250
H	-1.098152648	2.965321078	-0.547262493
H	0.227175454	-1.744179682	0.722185712
H	1.171770566	2.514248759	0.264902850
H	1.192634554	0.386634044	1.652120224

H	-2.932117621	0.845091845	-0.739013627
C	2.249146347	-0.064986980	-0.103841135
O	2.465681904	-1.183672531	-0.477598420
H	2.981467998	0.758329174	-0.183867120
C	-2.247895567	-1.712624076	-0.038305515
H	-3.109836948	-1.517821113	0.602673303
H	-2.587094313	-1.803063770	-1.071854783
H	-1.747726838	-2.630050211	0.272738503

1-vinyl-1,2-dihydro-1,2-azaborine

B	1.219468963	-1.295031860	-0.325585758
N	1.077290748	0.151428871	0.109551461
C	-0.023942908	-2.163532051	-0.258208213
C	-0.090535713	0.604273175	0.489910054
C	-1.198695083	-1.638802864	0.160068897
C	-1.317689002	-0.209832723	0.568239410
H	0.007947663	-3.209350240	-0.550371194
H	-0.171078668	1.659333129	0.745117716
H	-2.109093999	-2.233508092	0.217758375
H	-1.647145573	-0.170629516	1.628204686
H	2.280169036	-1.641138954	-0.702338359
C	2.179425950	1.082105716	0.075581293
H	1.875838577	2.107561063	0.259164341
C	3.452691594	0.753269387	-0.140056215
H	3.803265171	-0.254954814	-0.318729072
H	4.194887662	1.543830259	-0.134852132
C	-2.515166948	0.535422499	-0.143917909
O	-2.450650584	1.681055693	-0.491165366
H	-3.418486204	-0.089470748	-0.263686664

1-chloro-1,2-dihydro-1,2-azaborine

B	0.499438783	1.392059436	0.702437132
N	0.888571633	0.161483097	-0.090761889
C	-0.881132573	1.939567219	0.372731763
C	0.074802293	-0.473684163	-0.886048919
C	-1.720398673	1.232097873	-0.419787905
C	-1.348772645	-0.116497625	-0.947793701
H	-1.215097793	2.891948690	0.775419889
H	0.450563865	-1.327927831	-1.445582673
H	-2.727608801	1.573366559	-0.650091142
H	-1.736187430	-0.307714180	-1.954412209
Cl	2.528074350	-0.395046414	0.017449012
H	1.304748111	1.804866813	1.456711395
C	-2.128439400	-1.181330751	0.021878599
O	-1.703072574	-1.481302587	1.092726935
H	-3.078898891	-1.539839342	-0.407036667

1-mercapto-1,2-dihydro-1,2-azaborine

B	-0.930047133	1.526374051	-0.290705859
N	-1.144987223	0.078345081	0.098044147

C	0.481892319	2.057181612	-0.132495414
C	-0.171954599	-0.659456482	0.568474642
C	1.468672136	1.240198660	0.305490435
C	1.213046973	-0.174513435	0.694298706
H	0.728930383	3.082805233	-0.392287262
H	-0.402389522	-1.684501014	0.859479929
H	2.500733177	1.571627852	0.389255409
H	1.491556658	-0.323499386	1.758313919
H	-1.885002629	2.105227880	-0.676047025
S	-2.707911666	-0.704637927	-0.193373915
H	-3.430610106	0.368476786	0.187888869
C	2.211241379	-1.205611291	-0.002502466
O	3.085662140	-0.834351464	-0.725735203
H	2.048937004	-2.263367403	0.273609116

1-hydroxy-1,2-dihydro-1,2-azaborine

B	-1.572251033	1.156859214	-0.322562351
N	-1.497148328	-0.314769712	-0.030308477
C	-0.298879938	1.928795885	-0.057810432
C	-0.435514598	-0.918465840	0.417520934
C	0.806321516	1.276486564	0.381486184
C	0.820690268	-0.187635964	0.653983407
H	-0.239105913	2.998783700	-0.234764063
H	-0.514707100	-1.989966915	0.595791629
H	1.750341249	1.790379726	0.544530273
H	1.082445157	-0.359993172	1.718795198
H	-2.616616051	1.537173907	-0.731307698
O	-2.588062514	-1.136408539	-0.224715709
H	-3.312127994	-0.568510392	-0.546981182
C	2.038462266	-0.941527145	-0.052697353
O	2.896221827	-0.339048547	-0.623396213
H	2.036099842	-2.039095583	0.074104639

1-amino-1,2-dihydro-1,2-azaborine

B	-1.574358730	1.136238599	-0.319463737
N	-1.520399498	-0.355654159	-0.050101593
C	-0.308478001	1.915197245	-0.051479848
C	-0.439664315	-0.930769508	0.403901260
C	0.800475755	1.270619500	0.385384762
C	0.816628668	-0.193215300	0.655360195
H	-0.257465992	2.986079781	-0.225789221
H	-0.477770235	-2.000777832	0.605307176
H	1.742824824	1.787449806	0.549052642
H	1.059719945	-0.355557477	1.726479079
H	-2.610327775	1.527451934	-0.734994420
N	-2.701247934	-1.064081334	-0.186517791
H	-2.565553661	-2.052474499	-0.378490114
H	-3.324126247	-0.613499966	-0.848313919
C	2.033268490	-0.933847753	-0.038438221
O	2.877998173	-0.338108455	-0.640223480

H	2.055489686	-2.029142692	0.114480548

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-1.153162912	0.036140130	-0.076077411
B	-1.195034763	1.514477743	0.299149365
C	-0.033819267	-0.558351313	-0.435439114
C	0.131212818	2.249321277	0.235619394
C	1.249544339	0.150951123	-0.520739725
C	1.253013087	1.594012464	-0.145579573
H	-0.065637289	-1.624550322	-0.649431166
H	0.202145127	3.302622515	0.491752967
H	1.581677149	0.057307393	-1.577030635
H	2.217109554	2.097185707	-0.204809275
H	-2.255962073	1.924338094	0.609659144
C	-2.316481984	-0.686087472	-0.006158947
C	-3.354871636	-1.292326294	0.081024176
H	-4.274805217	-1.834316087	0.151516026
C	2.391999754	-0.701136013	0.190176294
O	2.298809468	-1.882052685	0.356144420
H	3.278044889	-0.105227837	0.472427944

1-formyl-1,2-dihydro-1,2-azaborine

B	-1.074482870	1.321247184	-0.267464351
N	-1.141727799	-0.144840619	0.118498838
C	0.279595469	1.984210136	-0.063985882
C	-0.098582203	-0.791092135	0.578355631
C	1.335672589	1.263381099	0.378957948
C	1.224979551	-0.184932466	0.716452565
H	0.428318043	3.035846162	-0.292121083
H	-0.232910442	-1.841485095	0.848058298
H	2.325987630	1.697085118	0.495039890
H	1.553469587	-0.371745297	1.758839648
H	-2.067304788	1.793371677	-0.687997443
C	-2.419403273	-0.903401894	0.000189998
O	-3.411667992	-0.388396027	-0.396081480
H	-2.312383902	-1.952801263	0.320436963
C	2.303316781	-1.093888720	-0.063669283
O	3.054994602	-0.612714183	-0.852061067
H	2.304199853	-2.158302763	0.230396648

2-phenyl-1,2-dihydro-1,2-azaborine

B	-0.103044832	-0.240466738	-0.188354642
N	0.773034870	0.983790954	-0.400445767
C	0.708693046	-1.546817062	-0.145004149
C	2.061626523	0.965531071	-0.536807305
C	2.049461409	-1.543280325	-0.299780135
C	2.840914297	-0.289253313	-0.522877166
H	0.228555434	-2.508849111	0.009420906
H	2.594699915	1.909143697	-0.639540179
H	2.628737545	-2.464830663	-0.276461154

H	3.344412990	-0.349642070	-1.510465953
H	0.340169451	1.906234322	-0.413118752
C	-1.608321048	-0.042278558	-0.037733334
C	-2.440592009	-1.169474585	0.186166094
C	-2.239131211	1.226965912	-0.110559547
C	-3.817771578	-1.037211913	0.328727495
C	-3.615086514	1.364387048	0.030072030
C	-4.406573798	0.230009001	0.250733286
H	-2.002129247	-2.160134004	0.249928993
H	-1.661814839	2.133677783	-0.280854123
H	-4.434005745	-1.913816661	0.500062333
H	-4.074835163	2.345419087	-0.030326753
H	-5.481504896	0.335503445	0.361661040
C	4.068883697	-0.146053544	0.447693030
O	4.442977669	0.913233547	0.872297681
H	4.567950863	-1.104155634	0.681481654

2-methyl-1,2-dihydro-1,2-azaborine

N	-0.862547303	-1.147340876	-0.237346132
B	-1.843257248	-0.030414555	0.079820272
C	0.399675065	-0.978212148	-0.492537066
C	-1.191822498	1.358315490	0.083906023
C	1.017881323	0.358211534	-0.528063749
C	0.121472968	1.509518799	-0.197236197
H	1.029588799	-1.849919433	-0.664183110
H	-1.774143631	2.248385378	0.307953898
H	1.398949071	0.486052439	-1.563589335
H	0.593996726	2.490712105	-0.208052595
H	-1.196419259	-2.111701555	-0.230480504
C	-3.305938346	-0.426435664	0.400971586
H	-4.010632589	0.386641784	0.204381900
H	-3.657429652	-1.327834438	-0.114181400
H	-3.384585259	-0.638225359	1.480802643
C	2.378846894	0.345718494	0.278436885
O	2.979976777	-0.665580706	0.507134436
H	2.730842731	1.349444796	0.576507274

2-vinyl-1,2-dihydro-1,2-azaborine

B	-1.445766033	0.337434079	-0.038584754
N	-0.640807127	-0.896680844	0.319484850
C	-0.601188133	1.615660823	-0.107151410
C	0.634769455	-0.901603092	0.556060505
C	0.723800130	1.586903441	0.155627051
C	1.447775488	0.329210643	0.527521321
H	-1.051533115	2.570286659	-0.367159005
H	1.131613201	-1.848896681	0.759284200
H	1.335198385	2.487122058	0.116630671
H	1.863982789	0.442439191	1.550947193
H	-1.102962209	-1.804689146	0.354627087
C	-2.947710468	0.206637260	-0.296444485

H	-3.483785084	1.112638504	-0.577044106
C	-3.675855589	-0.927054237	-0.203406537
H	-3.252563583	-1.892390839	0.072932021
H	-4.744767143	-0.943000157	-0.398614373
C	2.765578418	0.084124237	-0.304306604
O	3.175496844	-1.014723283	-0.556384914
H	3.284263256	1.012825519	-0.603160908

2-chloro-1,2-dihydro-1,2-azaborine

N	-0.832761854	1.154442898	0.171364265
B	-1.630167138	-0.117441890	0.056956474
C	0.429069182	1.182638338	0.495416928
C	-0.863044584	-1.399378456	0.347118569
C	1.201955302	-0.041413448	0.738329290
C	0.452532074	-1.331986797	0.650595626
H	0.917775048	2.154314397	0.566586310
H	-1.343899697	-2.372070192	0.300596038
H	1.658821417	0.072589525	1.742300346
H	1.043518175	-2.226093777	0.832498825
H	-1.293564639	2.048857085	-0.001669226
Cl	-3.292960427	0.054890677	-0.390765919
C	2.521679206	-0.023970613	-0.168923579
O	2.821901429	-0.962805526	-0.840462499
H	3.130603269	0.893638734	-0.079958789

2-mercapto-1,2-dihydro-1,2-azaborine

N	0.594232897	-1.270419239	0.038073197
B	1.304802632	0.059935131	0.065825048
C	-0.670741208	-1.417113472	0.313739490
C	0.419625881	1.245763088	0.455904891
C	-1.547053965	-0.285113070	0.644382924
C	-0.892743081	1.059590586	0.706051392
H	-1.085330463	-2.424480419	0.276714145
H	0.819768188	2.253797600	0.523738791
H	-2.018404478	-0.535836679	1.616410990
H	-1.552314759	1.886794487	0.954314012
H	1.102582230	-2.122159811	-0.196428190
S	3.035940795	0.203348135	-0.334005419
H	3.310383716	-1.090701227	-0.607018919
C	-2.825403133	-0.314195371	-0.308270588
O	-3.172107321	0.656097758	-0.911710935
H	-3.372820652	-1.274477613	-0.323242245

2-hydroxy-1,2-dihydro-1,2-azaborine

N	1.080410049	-1.213219199	-0.053052948
B	1.747816503	0.156539742	-0.106943239
C	-0.157746293	-1.388122579	0.311495697
C	0.841696886	1.322504554	0.300051934
C	-1.045748912	-0.272878227	0.666104654
C	-0.441999268	1.097259443	0.640534237

H	-0.544778993	-2.407150751	0.332967362
H	-1.439529625	-0.507055971	1.675994240
H	1.599079862	-2.057209594	-0.296537310
O	3.022136547	0.283243532	-0.490655727
H	3.569684096	-0.469630292	-0.746431121
H	1.219416976	2.341109044	0.302429061
H	-1.118020807	1.906125380	0.904736490
C	-2.385169947	-0.382248474	-0.193348039
O	-2.802763433	0.549433358	-0.812187148
H	-2.901413761	-1.357592771	-0.128093216

2-amino-1,2-dihydro-1,2-azaborine

N	-0.833692448	1.159777741	0.279952846
B	-1.791135855	0.043687591	-0.112009724
C	0.410426500	0.969164771	0.583189114
C	-1.155957608	-1.358549482	-0.119834913
C	1.033824537	-0.373653629	0.596666593
C	0.138382741	-1.519784162	0.212075533
H	1.031329505	1.833007305	0.813599428
H	-1.731719061	-2.241634189	-0.385517304
H	1.402072637	-0.530079106	1.631404465
H	0.607133141	-2.501905935	0.222142960
H	-1.153001300	2.128605260	0.293360863
N	-3.094897235	0.394180062	-0.421257559
H	-3.777377724	-0.300652745	-0.696667260
H	-3.480578140	1.329471572	-0.408889528
C	2.364983948	-0.339697886	-0.230872846
O	2.847286842	0.678870670	-0.649004657
H	2.825076990	-1.333541992	-0.380019412

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-1.468846806	0.122051036	0.020202244
N	-0.564374277	-1.047198952	0.341883566
C	-0.754024893	1.471348650	-0.055394307
C	0.713539473	-0.946363375	0.547758117
C	0.576697205	1.545364670	0.173479554
C	1.413168213	0.350620103	0.509836364
H	1.293969784	-1.849472033	0.729622779
H	1.108486323	2.494742024	0.132464579
H	1.849049548	0.490170456	1.521845094
H	-0.966006324	-1.984713726	0.377104579
C	-2.916835504	-0.183902645	-0.194207900
C	-4.097349543	-0.422370576	-0.375812630
H	-5.136849719	-0.624157677	-0.535383578
H	-1.294987161	2.383195179	-0.290366654
C	2.732523615	0.224908052	-0.355601819
O	3.255610848	-0.829992170	-0.578644106
H	3.134566695	1.194464228	-0.700112467

2-formyl-1,2-dihydro-1,2-azaborine

N	-0.672293047	0.808476840	0.308823427
B	-1.398421925	-0.445249445	-0.044801906
C	0.601890510	0.873631762	0.545454142
C	-0.555052640	-1.703998056	-0.118800841
C	1.450624438	-0.330922695	0.505774659
C	0.774557314	-1.612746861	0.142313727
H	1.060852724	1.839209436	0.753251513
H	1.885429701	-0.436419110	1.522405722
H	1.420100866	-2.489542773	0.106457624
H	-1.240543066	1.664401123	0.333197049
C	-2.951240923	-0.154893191	-0.291104665
O	-3.327748184	1.005540355	-0.168991191
H	-3.676954972	-0.944076199	-0.560059257
H	-0.968340396	-2.676388116	-0.372544606
C	2.777891623	-0.038810885	-0.323577570
O	3.193340341	1.071129929	-0.484196629
H	3.281293310	-0.948496143	-0.695486582

Wheland intermediates of acylation of substituted 1,2-dihydro-1,2-azaborines on C6

1,2-dihydro-1,2-azaborine

B	-1.199143783	1.460704292	0.018891843
N	0.037361611	1.063072500	-0.519091653
C	-2.126739788	0.273166775	0.448686613
C	0.468088219	-0.279268663	-0.663845401
C	-1.727309542	-1.048128809	0.281359740
C	-0.475685718	-1.313289765	-0.272743247
H	-3.101574976	0.449764931	0.900660356
H	0.799867499	-0.493332063	-1.701402310
H	-2.363867083	-1.880394628	0.568884468
H	-0.157869460	-2.344912295	-0.413913545
H	-1.474850716	2.604709002	0.129715247
H	0.734626969	1.759445354	-0.768109885
C	1.896991113	-0.548076338	0.085961009
O	2.474443650	0.345027936	0.613446933
H	2.265410122	-1.582794683	-0.009870941

1-phenyl-1,2-dihydro-1,2-azaborine

B	1.139306840	1.529458538	-0.563183716
N	0.479369894	0.466180743	0.115636518
C	2.678048125	1.570381003	-0.416749552
C	1.223138731	-0.584092071	0.735769889
C	3.361604503	0.652958461	0.380272820
C	2.648403322	-0.384295687	0.964765205
H	3.262757785	2.356231605	-0.891429992
H	0.712485159	-0.984740309	1.621790093
H	4.432900964	0.723070542	0.546433251

H	3.160646604	-1.139657363	1.556507423
H	0.511920526	2.359897132	-1.123668195
C	-0.945868076	0.317105797	0.110672996
C	-1.629663147	0.019843855	1.303613370
C	-1.655283624	0.482897798	-1.090107144
C	-3.015910730	-0.115673214	1.287398704
C	-3.040462528	0.339455240	-1.093774208
C	-3.723608425	0.039347400	0.090281447
H	-1.097459535	-0.042279627	2.248385749
H	-1.120926887	0.691518469	-2.009917056
H	-3.545224007	-0.321021115	2.212034240
H	-3.586964691	0.454344621	-2.024034206
H	-4.803627540	-0.065293252	0.082050271
C	1.231499282	-1.922567455	-0.239647365
O	0.987128230	-1.846830755	-1.397810641
H	1.450934368	-2.851991411	0.310957441

1-vinyl-1,2-dihydro-1,2-azaborine

B	-0.030675660	-1.544268577	-0.452469261
N	0.515730413	-0.491201962	0.337775152
C	-1.563909791	-1.515517962	-0.651847540
C	-0.309935553	0.568020092	0.824932561
C	-2.368597505	-0.573645063	-0.012583784
C	-1.757462988	0.422125454	0.736304622
H	-2.059154541	-2.266752206	-1.264419461
H	0.003606902	0.900550722	1.824556701
H	-3.451990438	-0.596607722	-0.088277958
H	-2.355217690	1.187673218	1.226168566
H	0.661472836	-2.410357517	-0.860036075
C	1.898654778	-0.355982779	0.635906289
H	2.106837656	0.208902400	1.541013795
C	2.895592304	-0.856813151	-0.104571607
H	2.732543911	-1.391480001	-1.032952026
H	3.919014227	-0.722694648	0.226426724
C	-0.060264550	1.948997313	-0.064451625
O	0.445191842	1.905540130	-1.135600421
H	-0.380137691	2.862717470	0.462639725

1-chloro-1,2-dihydro-1,2-azaborine

B	-0.267523694	-1.492342055	-0.708723112
N	0.416075255	-0.576924243	0.128308584
C	-1.816219679	-1.347881816	-0.637313325
C	-0.199686767	0.483275919	0.839462777
C	-2.436268801	-0.429508880	0.203385788
C	-1.646036755	0.437712197	0.953456529
H	-2.455023392	-1.990229331	-1.241598832
H	0.307998862	0.706119977	1.785450220
H	-3.517557532	-0.369021253	0.287074326
H	-2.106737890	1.180923178	1.601449341

Cl	2.143550115	-0.558886379	0.194249574
H	0.316877842	-2.292884582	-1.347861966
C	0.006394408	1.942462413	-0.006090549
O	0.173983692	1.935934280	-1.174184741
H	-0.006778300	2.818839680	0.661145909

1-mercapto-1,2-dihydro-1,2-azaborine

B	-0.123100226	1.424562164	0.755089560
N	0.538248657	0.541809522	-0.140962829
C	-1.679451407	1.391309422	0.671297803
C	-0.171023414	-0.447876552	-0.881294004
C	-2.343865752	0.607574960	-0.265291883
C	-1.599847677	-0.267131677	-1.054631321
H	-2.283526449	2.028993076	1.314769369
H	0.349413989	-0.752093480	-1.796185198
H	-3.422567971	0.647665198	-0.387342579
H	-2.096579594	-0.920569629	-1.769303934
H	0.491228696	2.162341410	1.442904503
S	2.285654769	0.400030447	-0.121902717
H	2.470880107	0.791432965	-1.404281130
C	-0.167368792	-1.895631561	0.010520761
O	-0.192941855	-1.869175291	1.190814882
H	-0.107094726	-2.788805849	-0.631095694

1-hydroxy-1,2-dihydro-1,2-azaborine

B	0.864526578	-1.402042732	0.544347958
N	-0.195425184	-0.932562546	-0.254443742
C	2.035935132	-0.402552275	0.644446655
C	-0.293100074	0.360656657	-0.817175602
C	2.025920757	0.822554009	-0.027070135
C	0.909384201	1.180079513	-0.769282359
H	2.917987311	-0.641836420	1.235976858
H	-0.760590428	0.325357483	-1.810964532
H	2.873705510	1.499926041	0.016534085
H	0.872668284	2.133904418	-1.290337217
H	0.805874490	-2.477775058	1.036081866
O	-1.362787984	-1.630794673	-0.501532211
H	-1.340823661	-2.423992376	0.063982654
C	-1.410640522	1.267351022	0.037666953
O	-1.738076428	0.956604113	1.129991634
H	-1.790060622	2.121028804	-0.546220674

1-amino-1,2-dihydro-1,2-azaborine

B	-1.117195378	-1.398795856	-0.327565909
N	0.104377502	-0.899885414	0.196558315
C	-2.235764492	-0.360844060	-0.474149879
C	0.286257205	0.465038357	0.616382514
C	-2.071893291	0.975026047	-0.076097554
C	-0.861640419	1.372510766	0.447227323
H	-3.189298906	-0.633853593	-0.922840176

H	0.560393569	0.466523804	1.687535328
H	-2.872521657	1.701306919	-0.181760819
H	-0.698089953	2.407519023	0.738428124
H	-1.190220361	-2.542550776	-0.626138760
N	1.188251861	-1.715973711	0.469306461
H	2.040275560	-1.371007991	0.023091577
H	0.979763300	-2.672059870	0.195522175
C	1.563511614	1.159372454	-0.043759769
O	2.294833568	0.571467427	-0.784805523
H	1.717915645	2.203592449	0.276632766

1-ethynyl-1,2-dihydro-1,2-azaborine

B	-0.419997048	-1.553952912	-0.610135171
N	0.404379989	-0.668502209	0.157067508
C	-1.930710827	-1.209446984	-0.603895163
C	-0.109424577	0.518163094	0.787112461
C	-2.437483294	-0.143083927	0.135699514
C	-1.555902342	0.673564595	0.834492075
H	-2.639839488	-1.814182425	-1.166288064
H	0.352156058	0.673240840	1.772795484
H	-3.502228886	0.067891698	0.179536448
H	-1.932270773	1.523431137	1.400302230
H	0.067415759	-2.478048498	-1.158862236
C	1.746405746	-0.849960166	0.241203488
C	2.941891683	-1.018620303	0.315657375
H	3.998898011	-1.165866576	0.378620594
C	0.400112355	1.872191528	-0.020035440
O	0.856139335	1.798098993	-1.110632648
H	0.290979469	2.791585997	0.577769184

1-formyl-1,2-dihydro-1,2-azaborine

B	0.349542528	1.315153057	0.659917049
N	0.684555010	0.256024201	-0.242905579
C	-1.165096093	1.701084597	0.681278430
C	-0.315100616	-0.495473890	-0.912944555
C	-2.071938137	1.121020185	-0.193327415
C	-1.642853563	0.064757747	-1.003673913
H	-1.534276636	2.471827280	1.355641474
H	0.035972000	-0.967676818	-1.836407713
H	-3.107690423	1.444065741	-0.249622899
H	-2.351823022	-0.445986600	-1.652879195
H	1.185913241	1.862953633	1.282380586
C	2.052467553	-0.170952744	-0.442884146
O	2.985875207	0.373919135	0.066338725
H	2.136975759	-1.037243106	-1.123536698
C	-0.709851359	-1.875296439	0.055147124
O	-0.645944845	-1.797964002	1.229623325
H	-0.961704988	-2.760635775	-0.549618878

2-chloro-1,2-dihydro-1,2-azaborine

B	0.995322208	0.150268757	-0.083097625
N	0.014373798	-0.485635829	-0.883126517
C	0.519879199	1.459291845	0.620147925
C	-1.324175033	-0.062501167	-0.950839086
C	-0.755452351	1.956031621	0.402139871
C	-1.644676247	1.232740677	-0.403118074
H	1.183511238	2.018254258	1.277342646
H	-1.809300976	-0.277375725	-1.910240817
H	-1.086548699	2.891239950	0.844833100
H	-2.655786429	1.602943575	-0.560348709
H	0.231840777	-1.347896829	-1.374043363
Cl	2.624914517	-0.465427834	0.047726659
C	-2.312026149	-1.025582870	0.099907018
O	-1.825552822	-1.571378513	1.023754189
H	-3.357447454	-1.081137482	-0.243483776

2-mercapto-1,2-dihydro-1,2-azaborine

B	1.080601020	0.021011860	-0.094104797
N	-0.129375978	-0.551469010	-0.563967330
C	0.966290003	1.513426688	0.353371228
C	-1.371090299	0.135577348	-0.619396582
C	-0.245100683	2.193479027	0.287796088
C	-1.369264081	1.527485888	-0.192151753
H	1.826048050	2.055434283	0.745605387
H	-1.803909515	0.126670595	-1.645312785
H	-0.335363093	3.230449273	0.598452498
H	-2.318186446	2.057398460	-0.257080637
H	-0.197711258	-1.538059558	-0.792505787
S	2.697970918	-0.762164665	0.061008423
H	2.380437035	-1.996132337	-0.384162725
C	-2.550562833	-0.676289660	0.133979490
O	-2.344396474	-1.766960452	0.564348248
H	-3.529763855	-0.168105626	0.140338535

2-hydroxy-1,2-dihydro-1,2-azaborine

B	-1.366867916	0.588513594	-0.054304793
N	-0.040728919	0.742688914	-0.553063905
C	-1.731222823	-0.876729891	0.385360463
C	0.903762568	-0.311494459	-0.633260447
C	-0.813057838	-1.911093873	0.280558673
C	0.458612192	-1.634281657	-0.220880035
H	-2.714659582	-1.097322357	0.798576288
H	1.308460584	-0.428291126	-1.663496454
H	-1.055119592	-2.927240973	0.578908077
H	1.185239141	-2.439984718	-0.312163050
H	0.343891635	1.656105681	-0.775280817
O	-2.313820706	1.540987886	0.087759727
H	-2.121244776	2.452734848	-0.165342200
C	2.293765511	0.052985004	0.116885137

O	2.456031648	1.137647410	0.578700598
H	3.055055869	-0.744595541	0.088657963

2-amino-1,2-dihydro-1,2-azaborine

B	-1.396143019	0.575722577	-0.051865663
N	-0.064128324	0.742226081	-0.559612598
C	-1.726739781	-0.891824183	0.392510316
C	0.894036349	-0.292510800	-0.641258020
C	-0.792128006	-1.912171818	0.283168756
C	0.472084417	-1.621193004	-0.227369929
H	-2.696562758	-1.151788040	0.816442675
H	1.307826691	-0.405323394	-1.669423703
H	-1.018146008	-2.930524014	0.586185544
H	1.208018430	-2.417914760	-0.320905903
H	0.303967006	1.661668436	-0.779591651
N	-2.344273382	1.599283326	0.064694422
H	-2.181991525	2.563106755	-0.194061801
H	-3.272958316	1.447164374	0.431083006
C	2.281662293	0.079492377	0.111153880
O	2.429924720	1.155600782	0.597805323
H	3.057785377	-0.703104389	0.059725495

2-ethynyl-1,2-dihydro-1,2-azaborine

B	-1.188333646	0.112963125	0.073605149
N	-0.037277970	-0.528603351	0.593192038
C	-0.932117670	1.582448106	-0.413954292
C	1.252876406	0.048338515	0.659625807
C	0.324005124	2.169055847	-0.313831239
C	1.377545166	1.428377557	0.218429247
H	-1.734658700	2.174037295	-0.851399096
H	1.683790242	-0.019150662	1.681141796
H	0.506539686	3.189380039	-0.639498887
H	2.364690101	1.880205376	0.298919450
H	-0.085529911	-1.502697068	0.878331524
C	-2.534675846	-0.559075925	-0.005541265
C	-3.622217041	-1.100185535	-0.066618213
H	-4.580034201	-1.573790891	-0.123146730
C	2.374215850	-0.852418555	-0.115706027
O	2.073559501	-1.886659980	-0.616226801
H	3.395827191	-0.440098165	-0.062801182

2-formyl-1,2-dihydro-1,2-azaborine

B	1.052713105	-0.242635659	0.050271045
N	-0.192685399	-0.670771959	-0.427554469
C	1.161086594	1.271867548	0.402366372
C	-1.313379648	0.187837832	-0.617687246
C	0.049325607	2.103363042	0.288506788
C	-1.130309997	1.585314263	-0.237206479
H	2.096115027	1.696061913	0.764027876
H	-1.658456328	0.188831188	-1.675322341

H	0.090698536	3.155187767	0.557555459
H	-1.981779740	2.245125631	-0.395542385
H	-0.396168441	-1.655305313	-0.585595544
C	2.351816738	-1.162525761	0.136715647
O	3.401096794	-0.599687677	-0.134405020
H	2.345689477	-2.248747313	0.362384867
C	-2.640251596	-0.433261677	0.063889102
O	-2.624232166	-1.538089556	0.507026302
H	-3.529154828	0.217218217	0.014559469

Cyclic intermediates of acylation of substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

N	0.719343011	1.384170728	0.203597861
B	-0.609334718	0.813368052	0.700349016
C	1.689131111	0.656743782	-0.280139800
C	-0.630970125	-0.839957151	0.696539390
C	1.645108888	-0.783800423	-0.349541557
C	0.610698016	-1.496731556	0.161085433
H	2.596543760	1.166290979	-0.599456245
H	-1.053675812	-1.411462295	1.530271861
H	2.524543182	-1.283924521	-0.739940014
H	0.682662621	-2.581778755	0.196452622
H	-1.164434617	1.466809612	1.518374736
C	-1.616515107	-0.606783038	-0.403003970
O	-1.624223101	0.629292732	-0.605380508
H	-2.256818794	-1.282469588	-0.982675023
H	0.898960468	2.382218236	0.289859505

1-phenyl-1,2-dihydro-1,2-azaborine

N	0.268432908	0.308489109	0.244374634
B	1.183080937	-0.922887993	0.430546485
C	0.781366925	1.508646040	0.138257496
C	2.785427481	-0.577954392	0.558398452
C	2.193761828	1.815633526	0.208092500
C	3.141176880	0.879951114	0.440470858
H	0.083219146	2.335148002	0.026296019
H	3.411072653	-1.084593816	1.301628071
H	2.461246262	2.863919003	0.128041577
H	4.179945438	1.181360409	0.552478907
H	0.696435030	-1.831006106	1.013009407
C	2.821181232	-1.229491679	-0.783685072
O	1.625670129	-1.455517000	-1.087744740
H	3.637787450	-1.496758387	-1.465322459
C	-1.163231880	0.133985083	0.125825905
C	-1.846411556	-0.648576717	1.064206250
C	-1.844409084	0.754417065	-0.929637293
C	-3.229918079	-0.782578288	0.953916017

C	-3.227155649	0.602173224	-1.033144323
C	-3.921494418	-0.161329171	-0.091052654
H	-1.314776910	-1.124193384	1.880101234
H	-1.299256797	1.313001453	-1.684692467
H	-3.767464952	-1.373464814	1.688154551
H	-3.756102512	1.067699957	-1.858241227
H	-4.996665796	-0.280483312	-0.175865577

1-methyl-1,2-dihydro-1,2-azaborine

N	-1.241108260	-0.040522417	0.095186660
B	-0.053195843	-0.849219149	0.645999558
C	-1.084681122	1.173632160	-0.349227891
C	1.361336746	-0.010273930	0.732874623
C	0.165689419	1.904873084	-0.326084804
C	1.296760625	1.401286013	0.217380835
H	-1.967410891	1.687624662	-0.727067261
H	2.018167247	-0.089175952	1.606214668
H	0.136855688	2.921927500	-0.701939776
H	2.181232622	2.029558387	0.292545434
H	-0.350950661	-1.677347545	1.441706534
C	1.737458104	-0.948189379	-0.365835380
O	0.699116219	-1.597191445	-0.637009674
H	2.674895935	-1.127890046	-0.905699873
C	-2.575101916	-0.669960594	0.118783154
H	-2.826594596	-0.918625271	1.152821614
H	-3.325062275	0.005022644	-0.295889054
H	-2.544673283	-1.593498311	-0.464323417

1-vinyl-1,2-dihydro-1,2-azaborine

N	0.909674964	-0.095160041	0.017635774
B	-0.271426047	-0.880385572	-0.585223312
C	0.739452141	1.115989605	0.493430156
C	-1.640327370	0.013112142	-0.819597998
C	-0.476813593	1.879131965	0.361569573
C	-1.565961134	1.422054423	-0.302021954
H	1.593051334	1.582955085	0.979496647
H	-2.225429050	-0.048391238	-1.743211238
H	-0.456901733	2.889019271	0.757286195
H	-2.412337095	2.085298903	-0.464562380
H	0.040500699	-1.755496759	-1.320972216
C	-2.144480907	-0.883231997	0.262400473
O	-1.153300351	-1.541898206	0.657767498
H	-3.136337215	-1.028828686	0.706501297
C	2.202571994	-0.713263971	0.010154325
H	2.167194201	-1.784152114	0.174207505
C	3.339451301	-0.056932534	-0.231476908
H	3.373330501	0.998524796	-0.484732070
H	4.281890442	-0.592115241	-0.209921565

1-chloro-1,2-dihydro-1,2-azaborine

N	0.783432004	0.213373644	-0.063644557
B	-0.216854732	-0.820812204	-0.628509294
C	0.448227707	1.402609866	0.358703213
C	-1.747211582	-0.207629367	-0.733626532
C	-0.908310262	1.899497691	0.313771036
C	-1.929112756	1.197104189	-0.231189928
H	1.238585898	2.053166845	0.726551041
H	-2.366732776	-0.397203395	-1.617701165
H	-1.058060260	2.909834556	0.679183453
H	-2.907513440	1.663343201	-0.321264451
H	0.238640169	-1.565836045	-1.425871494
C	-1.974860232	-1.201147810	0.359807506
O	-0.843519292	-1.669765330	0.633170811
H	-2.872566467	-1.540646860	0.889595113
Cl	2.460255460	-0.213786607	-0.058581979

1-mercapto-1,2-dihydro-1,2-azaborine

N	0.824310746	0.247937144	-0.122900320
B	-0.190881374	-0.792708262	-0.656289483
C	0.446335415	1.426172055	0.303222081
C	-1.739100795	-0.241403333	-0.711694810
C	-0.925918948	1.885473864	0.305522131
C	-1.950244391	1.155812822	-0.190330048
H	1.217788605	2.111689288	0.650124552
H	-2.377063001	-0.445474343	-1.578972556
H	-1.090549403	2.892251935	0.674639700
H	-2.948864172	1.584304896	-0.224913225
H	0.255784604	-1.526364860	-1.476036517
S	2.521671998	-0.182448858	-0.001127239
H	2.477089813	-1.030827609	-1.048603238
C	-1.901764471	-1.238407938	0.387339447
O	-0.746678125	-1.673535786	0.619876309
H	-2.766359481	-1.596303289	0.958510311

1-hydroxy-1,2-dihydro-1,2-azaborine

N	1.186562510	0.084060821	0.093823000
B	-0.013383171	0.880051371	0.633964332
C	1.127162878	-1.139747618	-0.338115042
C	-1.375587543	-0.037931392	0.735285773
C	-0.098233504	-1.911188624	-0.318448932
C	-1.250977411	-1.448126165	0.214951422
H	2.058214041	-1.583615344	-0.683107021
H	-2.028151189	0.012881823	1.613671790
H	-0.028761558	-2.926394566	-0.693750804
H	-2.114122042	-2.105652770	0.278978340
H	0.297759272	1.713323768	1.422878639
C	-1.797311032	0.868661416	-0.373980502
O	-0.788369296	1.572906150	-0.632852880
H	-2.727949521	0.983294321	-0.941446197

O	2.443222172	0.650710412	0.078622401
H	2.362035265	1.512467321	0.526089430

1-amino-1,2-dihydro-1,2-azaborine

B	0.027855400	0.880562599	-0.609237746
N	1.234561407	0.076367299	-0.059768572
C	-1.351987768	0.000302461	-0.767558028
C	1.106104778	-1.149514222	0.374249041
C	-1.267045291	-1.411284468	-0.246169482
C	-0.136171595	-1.887940228	0.320690122
H	-1.982031214	0.069912379	-1.660134618
H	1.999153133	-1.653835642	0.738013570
H	-2.139086135	-2.053990795	-0.331691712
H	-0.099834861	-2.902613664	0.702813071
H	0.343445845	1.741031924	-1.361813563
N	2.471827736	0.660179531	-0.206671659
H	3.204165442	0.226895655	0.348565622
H	2.430933396	1.668406519	-0.106228786
C	-1.780971703	0.887875880	0.350596327
O	-0.755226531	1.538523469	0.678707016
H	-2.731623219	1.028748037	0.877397265

1-ethynyl-1,2-dihydro-1,2-azaborine

N	-0.927039548	0.257760158	0.072361302
B	0.057816310	-0.812675108	0.629743226
C	-0.503568776	1.429808667	-0.369879406
C	1.612932234	-0.277251859	0.745947120
C	0.865476783	1.859494147	-0.313032607
C	1.853690482	1.119181425	0.249483772
H	-1.258615095	2.111904102	-0.753266835
H	2.227486319	-0.502530472	1.624546161
H	1.068282218	2.861073681	-0.676849781
H	2.847213574	1.549008798	0.353736271
H	-0.428641506	-1.554599422	1.412475904
C	1.795901460	-1.262741236	-0.362573934
O	0.644041974	-1.668430481	-0.649679945
H	2.678866506	-1.637369310	-0.893481756
C	-2.256225149	-0.036500974	0.074720470
C	-3.422716660	-0.349011845	0.081844876
H	-4.457932774	-0.616573627	0.090908131

1-formyl-1,2-dihydro-1,2-azaborine

N	0.853249485	0.076188061	0.173452032
B	-0.360913118	0.876512945	0.651068430
C	0.746014979	-1.149287635	-0.298643136
C	-1.756376028	-0.008261241	0.709926744
C	-0.476134828	-1.897898222	-0.322950583
C	-1.630230311	-1.417905375	0.213160010
H	1.673553105	-1.616745328	-0.630097316
H	-2.451211491	0.055790093	1.554517186

H	-0.420423914	-2.915817680	-0.693377037
H	-2.489530906	-2.080064394	0.298371875
H	-0.119091480	1.735385180	1.432400466
C	-2.123489962	0.909363956	-0.413762769
O	-1.092863026	1.573352702	-0.668476163
H	-3.055876831	1.066563293	-0.968800289
C	2.204728380	0.650355487	0.263889423
O	3.165517830	0.076117728	-0.154952248
H	2.198297852	1.635270657	0.747914266

2-phenyl-1,2-dihydro-1,2-azaborine

N	1.161286622	-1.400121722	-0.216855857
B	0.499640458	-0.061885606	0.138573643
C	2.364149170	-1.526382868	-0.709910999
C	1.535257897	1.198528486	-0.088027081
C	3.248034288	-0.411713078	-0.941303979
C	2.856972561	0.867861249	-0.717749282
H	2.690951312	-2.522557752	-1.002042262
H	1.149192412	2.158198658	-0.450319822
H	4.214723626	-0.631062001	-1.380699234
H	3.520918041	1.681424354	-1.002045701
C	1.653296682	1.174960514	1.406884605
O	0.984172350	0.215156547	1.830774822
H	2.214508138	1.827882362	2.087518334
H	0.589817181	-2.242727400	-0.191345697
C	-1.046944156	-0.008286454	-0.007708314
C	-1.664762630	0.902458126	-0.889123497
C	-1.874845229	-0.899925537	0.710751696
C	-3.051051011	0.921000332	-1.052106373
C	-3.259777217	-0.878350991	0.557569108
C	-3.849237023	0.031729329	-0.327791660
H	-1.060286469	1.598969584	-1.464899941
H	-1.438003137	-1.599878928	1.421061054
H	-3.507287883	1.626334698	-1.739615633
H	-3.880454459	-1.563185660	1.126924564
H	-4.927827368	0.046987003	-0.450542315

2-methyl-1,2-dihydro-1,2-azaborine

N	-0.183494701	1.400651985	0.362372914
B	0.824295613	0.385919643	-0.211806422
C	-1.474295103	1.220050866	0.419490487
C	0.047042171	-0.975849653	-0.747325088
C	-2.136290862	0.034445913	-0.067739324
C	-1.452242920	-0.968561722	-0.671686245
H	-2.083260235	2.029731313	0.817849541
H	0.397412885	-1.481488132	-1.654759029
H	-3.218677445	0.013745627	-0.005919901
H	-2.004840112	-1.793648450	-1.116276753
C	0.628000057	-1.575186999	0.494796324
O	1.212701764	-0.657325665	1.106093654

H	0.595167348	-2.596333286	0.895170969
H	0.157630683	2.312318320	0.661819368
C	2.126689535	0.990296371	-0.841125846
H	2.840443937	0.218318522	-1.147762938
H	1.883501282	1.569274053	-1.741849051
H	2.653739505	1.662337230	-0.152603174

2-vinyl-1,2-dihydro-1,2-azaborine

N	-0.361901717	1.272844468	0.722138871
B	0.605356747	0.200312899	0.201790495
C	-1.621777573	1.357251840	0.389502253
C	-0.161370217	-0.879809152	-0.776766779
C	-2.273511911	0.429195511	-0.500763260
C	-1.595977405	-0.580543315	-1.101900883
H	-2.192541992	2.200331875	0.774275215
H	0.366801919	-1.294968340	-1.642888447
H	-3.315127278	0.619177862	-0.734578660
H	-2.106360558	-1.194253016	-1.841105865
C	-0.074738823	-1.783288932	0.416746012
O	0.432884372	-1.132707478	1.349596417
H	-0.387722125	-2.826631113	0.549671020
H	0.008210744	2.035462473	1.286329316
C	2.094839814	0.622624068	0.092197346
H	2.588779359	1.033535065	0.976231194
C	2.819774608	0.541347914	-1.036559655
H	2.405955344	0.153053864	-1.965188857
H	3.854802694	0.868994755	-1.083809499

2-chloro-1,2-dihydro-1,2-azaborine

N	-0.241980029	1.252172129	0.644134411
B	0.524441919	0.069747434	0.048976128
C	-1.522647255	1.449474761	0.477685592
C	-0.465178997	-0.959255072	-0.773639136
C	-2.379164592	0.560859899	-0.268822046
C	-1.897656485	-0.533822046	-0.909533787
H	-1.950903009	2.357524677	0.897760346
H	-0.089275780	-1.437007524	-1.685858731
H	-3.419727344	0.849996269	-0.366617628
H	-2.562424610	-1.114159680	-1.545544571
C	-0.250884320	-1.813047519	0.437638097
O	0.493920629	-1.156462747	1.200564336
H	-0.628851982	-2.801273928	0.722932770
H	0.282138679	1.984706248	1.121161169
Cl	2.182954693	0.454871687	-0.442080583

2-mercapto-1,2-dihydro-1,2-azaborine

N	-0.343059183	-1.465252057	0.784898885
B	-0.716101651	-0.188456344	0.037531712
C	0.783523501	-2.106959883	0.610505716
C	0.499861789	0.363393326	-0.909169269

C	1.826477302	-1.659296967	-0.276755617
C	1.692971831	-0.541046142	-1.032475469
H	0.913553572	-3.048750915	1.139717031
H	0.254981163	0.837807632	-1.866740733
H	2.702011490	-2.292504659	-0.367068155
H	2.472460910	-0.285530462	-1.746753076
C	0.707841119	1.374490263	0.182369273
O	-0.106265297	1.123478183	1.090089112
H	1.425671812	2.199966771	0.263395410
H	-1.032720276	-1.921387164	1.378526094
S	-2.455330505	0.049996236	-0.468350888
H	-3.035234144	-0.275570664	0.707279500

2-ethynyl-1,2-dihydro-1,2-azaborine

N	-0.147666164	-1.292800165	-0.603399962
B	0.622195394	-0.095827626	-0.030228843
C	-1.427909471	-1.489551029	-0.443075638
C	-0.370823629	0.926685127	0.809801213
C	-2.285476069	-0.598924483	0.299908200
C	-1.802320257	0.494050301	0.941097426
H	-1.855832773	-2.399544625	-0.859498078
H	-0.004624100	1.398801140	1.728264208
H	-3.326789840	-0.885660884	0.396155629
H	-2.469364694	1.075596375	1.573909155
C	-0.187033365	1.797618438	-0.393461955
O	0.509216791	1.151497806	-1.204960546
H	-0.557340887	2.801453176	-0.633711275
H	0.377332739	-2.030128776	-1.070183321
C	2.074023211	-0.371520659	0.327567085
C	3.224401168	-0.623172157	0.626154865
H	4.239389737	-0.835830065	0.888819515

2-formyl-1,2-dihydro-1,2-azaborine

N	-0.220757892	1.187949518	-0.492626763
B	-0.552909799	-0.196922706	0.029370052
C	0.975740661	1.701724518	-0.479824113
C	0.698461051	-0.917136775	0.847922225
C	2.113195318	1.024761324	0.098267753
C	1.985589092	-0.135868143	0.788179296
H	1.104623573	2.712108121	-0.864102914
H	3.063827738	1.545977358	0.070319731
H	2.841940306	-0.520681167	1.337754211
C	0.626801709	-1.846237360	-0.317903677
O	-0.203584275	-1.334230638	-1.109769986
H	1.125379504	-2.794010546	-0.550098530
H	-1.010607763	1.783086781	-0.754686728
C	-2.107650456	-0.271151159	0.441364274
O	-2.765225082	0.756611644	0.371070874
H	-2.592301245	-1.208281973	0.786402089
H	0.585718551	-1.420068628	1.814314653

Intermediates of the reaction of methyleneiminium cation with benzene derivatives at the *orto*-position

Aniline

C	-0.326326913	0.546406000	0.368907144
C	0.023797383	-0.902483398	0.106863298
C	0.823817532	1.495821315	0.212906065
C	1.379141040	-1.286330142	-0.113811911
C	2.083570129	1.078593488	-0.030809514
C	2.356266783	-0.330944970	-0.182409050
H	1.616130206	-2.336052239	-0.258578887
H	2.901560635	1.785723993	-0.113192407
H	3.379743679	-0.642697555	-0.371591725
H	0.602379577	2.551667186	0.341563046
C	-1.592499934	1.034054221	-0.412013211
H	-1.699261946	2.110243761	-0.230306473
H	-1.418436184	0.900129221	-1.483491144
N	-2.782233859	0.260472483	-0.029545950
H	-3.500038015	0.317847273	-0.747619830
H	-3.196050294	0.612448620	0.831826455
H	-0.594263782	0.589706580	1.441322235
N	-0.954902421	-1.784267330	0.107921249
H	-0.775062967	-2.768291263	-0.055848746
H	-1.922472060	-1.417644438	0.156657295

Intermediates of the reaction of methyleneiminium cation with benzene derivatives at the *para*-position

Styrene

C	0.981049687	1.107367099	-0.137102443
C	1.446466806	-0.244088458	-0.044970454
C	-0.338055844	1.373392312	-0.355148596
C	0.507577154	-1.309984077	-0.190881268
C	-1.349386959	0.311244069	-0.482402959
C	-0.818948267	-1.055126233	-0.399215622
H	0.863908471	-2.332985468	-0.119683303
H	-1.873442097	0.431080545	-1.446412344
H	-1.536716111	-1.866927991	-0.478506645
H	-0.670925742	2.405834555	-0.432792913
C	-2.588343312	0.513386747	0.563238987
H	-2.181692090	0.391118113	1.568967203
H	-2.896211393	1.556773177	0.440748182

N	-3.633005530	-0.427463117	0.307521519
H	-4.423632501	-0.064326400	-0.210024542
H	-3.944438086	-0.950962085	1.115027229
H	1.684300381	1.926415223	-0.043378376
C	2.834736850	-0.586584324	0.193999245
H	3.059655213	-1.649492064	0.230999685
C	3.845624769	0.292345631	0.367037266
H	3.712441309	1.369351169	0.348864143
H	4.857540377	-0.062540886	0.533501743

Thiophenol

C	0.812798403	1.279258572	-0.067039233
C	1.367643580	-0.042863838	-0.040171224
C	-0.522294635	1.451044920	-0.266628272
C	0.522163950	-1.182021997	-0.216726697
C	-1.452615685	0.319169278	-0.446904920
C	-0.816567005	-1.009566221	-0.406501507
H	0.948959912	-2.179503009	-0.185475812
H	-1.936668250	0.431414952	-1.434662302
H	-1.475782596	-1.866957157	-0.511537015
H	-0.931739096	2.458012965	-0.296884356
C	-2.717857361	0.389320613	0.550110378
H	-2.344790131	0.249899769	1.567239241
H	-3.105590773	1.411479361	0.469526997
N	-3.674755010	-0.631235226	0.220053863
H	-4.434796764	-0.315222091	-0.371318200
H	-4.049215116	-1.118682329	1.024573186
H	1.468525994	2.134435370	0.064446548
S	3.063441924	-0.165895059	0.223680142
H	3.154542631	-1.511336230	0.163651808

Phenol

C	1.309501438	1.209214732	-0.009306189
C	1.795926181	-0.132571480	0.058159027
C	-0.010896730	1.420758510	-0.251953941
C	0.932280123	-1.254341936	-0.117924647
C	-0.973984699	0.314801978	-0.440372027
C	-0.391950852	-1.037954216	-0.350502688
H	1.337109634	-2.260554580	-0.047947672
H	-1.407025632	0.418878964	-1.452807135
H	-1.082874612	-1.869721203	-0.457494838
H	-0.387788289	2.438839823	-0.314062150
C	-2.271637696	0.450696587	0.497895046
H	-1.950680947	0.313383219	1.533097721
H	-2.616734816	1.485666402	0.387773661
N	-3.250549671	-0.543027465	0.141461578
H	-3.956819683	-0.212550799	-0.506727659
H	-3.703107993	-0.970378252	0.940543921
H	2.016945394	2.019387569	0.131134944
O	3.081272848	-0.263720264	0.302168734

H	3.378630058	-1.189326340	0.336194711

Aniline

C	1.316511332	1.215229072	-0.010235725
C	1.833640916	-0.129940368	0.059450572
C	-0.001515352	1.419975876	-0.237881138
C	0.946566009	-1.251548854	-0.103578354
C	-0.970683743	0.311933307	-0.430724850
C	-0.372702136	-1.041265739	-0.328083525
H	1.350825682	-2.257046507	-0.030310792
H	-1.373619226	0.408540687	-1.456809627
H	-1.059483387	-1.876756914	-0.428790689
H	-0.381538488	2.437484201	-0.290138719
C	-2.255405050	0.452800170	0.487851210
H	-1.948359147	0.314070340	1.528024774
H	-2.610495905	1.486877924	0.384534252
N	-3.235421800	-0.552251787	0.131205998
H	-3.894635851	-0.235419179	-0.572367421
H	-3.757451410	-0.890711743	0.931381791
H	2.000838738	2.048426843	0.120545803
N	3.125852988	-0.329471770	0.284403418
H	3.516425969	-1.262170129	0.337397915
H	3.769187528	0.442520834	0.407859059

Intermediates of the reaction of methyleneiminium cation with substituted 1,2-dihydro-1,2-azaborines on C3

1,2-dihydro-1,2-azaborine

N	-1.950968894	0.893973474	0.033408385
B	-0.594322328	1.402432716	-0.124003122
C	-2.235216303	-0.412385306	0.104159565
C	0.521643052	0.321988987	-0.273619377
C	-1.247880005	-1.416157190	0.044229743
C	0.075651695	-1.073419542	-0.096129827
H	0.725777023	0.406352683	-1.369715795
H	-1.561344846	-2.449067617	0.144026817
H	0.850181022	-1.839206883	-0.083284730
H	-3.280622165	-0.683631590	0.233698320
C	1.933580061	0.602835302	0.371304278
H	2.192247204	1.642503663	0.134084050
H	1.832153975	0.535405905	1.457914330
N	2.905232339	-0.375807613	-0.075669476
H	3.596632921	-0.596442541	0.632418350
H	3.391504793	-0.099463893	-0.923077541
H	-2.738794862	1.531525007	0.113349778
H	-0.436386951	2.573952344	-0.182996297

1-phenyl-1,2-dihydro-1,2-azaborine

N	0.114625179	-0.285383845	0.196833416
B	-0.879852793	0.779615207	0.009325650
C	-0.287343108	-1.544700936	0.423967632
C	-2.382546886	0.390655713	0.153654450
C	-1.639121248	-1.958222954	0.459778618
C	-2.652850156	-1.053962817	0.288678387
H	-2.540214857	0.792858344	1.187661985
H	-1.836417575	-3.014035431	0.608520430
H	-3.692965639	-1.373235693	0.261816697
H	0.501272407	-2.278328760	0.572130667
C	-3.440636097	1.149877960	-0.716407357
H	-3.176851481	2.215628086	-0.704641862
H	-3.340518040	0.807650916	-1.750606367
N	-4.788982081	0.856579800	-0.257603273
H	-5.469750307	0.894450836	-1.008582714
H	-5.099588563	1.483527870	0.478844579
H	-0.491315766	1.879891133	-0.183175262
C	1.536445357	-0.021073594	0.055882435
C	2.300470943	-0.806912241	-0.813419288
C	2.114151670	1.019664909	0.788187451
C	3.667697576	-0.552496028	-0.935881871
C	3.481832574	1.262425484	0.657598910
C	4.258747984	0.478548451	-0.201145441
H	1.833688552	-1.583347830	-1.412772521
H	1.512681162	1.618297877	1.464516099
H	4.264067454	-1.150920587	-1.616688909
H	3.939453330	2.061027246	1.232085968
H	5.320950929	0.675663241	-0.302359626

1-methyl-1,2-dihydro-1,2-azaborine

N	1.722493283	-0.322598352	-0.014485671
B	0.475685345	-1.079922626	-0.162506253
C	1.690667559	1.008665415	0.078050157
C	-0.849538686	-0.270338448	-0.277276010
C	0.507190356	1.785369106	0.056633396
C	-0.716213238	1.185889401	-0.075414156
H	-1.033602680	-0.383055714	-1.375051981
H	0.607919029	2.858208575	0.176598782
H	-1.633598825	1.770672591	-0.039773712
H	2.648871283	1.511341348	0.194862485
C	-2.151993537	-0.868756161	0.370884797
H	-2.174082142	-1.939528078	0.130221921
H	-2.062570555	-0.784563950	1.457650996
N	-3.323851080	-0.128774455	-0.061271021
H	-4.052789759	-0.106002543	0.643435211
H	-3.725980819	-0.489045295	-0.921447622

H	0.555837428	-2.259206943	-0.247073014
C	3.023234596	-1.032839727	0.062472922
H	3.016543582	-1.705426941	0.922289758
H	3.169229023	-1.616881317	-0.847690532
H	3.837642245	-0.315512098	0.169609495

1-vinyl-1,2-dihydro-1,2-azaborine

N	1.432680017	0.149774708	0.028345159
B	0.336637138	-0.830626301	-0.070983836
C	1.137367154	1.459969464	0.062635279
C	-1.109729613	-0.283026997	-0.243469237
C	-0.166725858	1.997458744	0.004353761
C	-1.258397638	1.178251542	-0.105624913
H	-1.224801247	-0.472139421	-1.341334700
H	-0.267316438	3.074634858	0.076654028
H	-2.268776709	1.582432832	-0.097144180
H	1.982029011	2.138651701	0.160365183
C	-2.292373982	-1.091131428	0.399012564
H	-2.102561461	-2.156827407	0.214600014
H	-2.259273117	-0.941368926	1.482024781
N	-3.568516153	-0.607846266	-0.098434565
H	-4.317769641	-0.726595529	0.574955982
H	-3.850322277	-1.055816849	-0.965522776
H	0.599853309	-1.982112248	-0.070886341
C	2.818726865	-0.222195977	0.154794131
H	3.450320959	0.588657020	0.503148947
C	3.318988109	-1.423945767	-0.128957459
H	2.729265069	-2.256397768	-0.492700694
H	4.381841673	-1.588940399	0.005471772

1-chloro-1,2-dihydro-1,2-azaborine

N	1.237031761	-0.002689959	-0.041376681
B	0.118484339	-0.932690940	-0.209470330
C	1.077716904	1.322256472	0.078635833
C	-1.288683512	-0.266612521	-0.303165911
C	-0.190640365	1.940144440	0.060195977
C	-1.330467945	1.190372710	-0.086147889
H	-1.494008683	-0.395967626	-1.393800940
H	-0.223628373	3.015979031	0.191980872
H	-2.313036692	1.657640470	-0.047978882
H	1.978930047	1.915605766	0.210354292
C	-2.504867410	-1.024985754	0.371033938
H	-2.404609689	-2.085059627	0.107781364
H	-2.393225324	-0.947244729	1.455724829
N	-3.760470577	-0.423126693	-0.023936943
H	-4.453620152	-0.429392174	0.715806557
H	-4.167639546	-0.845173673	-0.852444583
H	0.349488133	-2.085653843	-0.314231534
Cl	2.862960673	-0.614897385	0.048624046

1-mercapto-1,2-dihydro-1,2-azaborine

N	1.280821396	-0.020671478	-0.000538677
B	0.142423950	-0.929443479	-0.177539133
C	1.101494123	1.307646518	0.097917150
C	-1.267364075	-0.271112770	-0.287600975
C	-0.163183312	1.933513726	0.059968618
C	-1.306002499	1.188611349	-0.084772008
H	-1.456481315	-0.406378732	-1.380969076
H	-0.194336499	3.010649099	0.181184871
H	-2.286559189	1.661310741	-0.057554684
H	1.999637005	1.906929793	0.229793798
C	-2.490288259	-1.017281701	0.374993946
H	-2.383183536	-2.083251611	0.137675239
H	-2.404608199	-0.916770915	1.460457299
N	-3.741623088	-0.426306374	-0.056762091
H	-4.459171673	-0.457307719	0.659074152
H	-4.113779460	-0.850217365	-0.901053889
H	0.357168453	-2.088181927	-0.274385524
S	2.956053319	-0.621055952	-0.014886934
H	2.919161318	-1.114798947	1.242486412

1-hydroxy-1,2-dihydro-1,2-azaborine

N	1.655290241	-0.324992148	-0.020856131
B	0.433830311	-1.099311345	-0.186373940
C	1.673531238	1.002513415	0.089288763
C	-0.875513155	-0.267862625	-0.303153708
C	0.495077101	1.782631652	0.054244375
C	-0.729014440	1.188239159	-0.102529858
H	-1.090757890	-0.381789709	-1.393503737
H	0.601279168	2.854332213	0.177881032
H	-1.642209143	1.779596955	-0.086510466
H	2.655388081	1.449779926	0.225262448
C	-2.179617121	-0.856053190	0.374265244
H	-2.216379842	-1.924146826	0.125539925
H	-2.062264719	-0.778874921	1.458396977
N	-3.347817504	-0.104139150	-0.032959659
H	-4.041599053	-0.022773659	0.701730639
H	-3.798496289	-0.477490232	-0.862406015
H	0.534321086	-2.277688443	-0.272119581
O	2.915466519	-0.902725987	0.092691850
H	2.803548261	-1.850975342	-0.096637053

1-amino-1,2-dihydro-1,2-azaborine

N	-1.691092119	0.333656997	-0.019516363
B	-0.452147302	1.095303585	-0.154557627
C	-1.687465193	-1.004138849	0.038432174
C	0.865426638	0.269332107	-0.259737220
C	-0.508114950	-1.781161799	0.058089696
C	0.721211839	-1.183640716	-0.044386625
H	1.025348749	0.363307168	-1.364257625

H	-0.614753804	-2.854663974	0.166139134
H	1.636097533	-1.770505194	0.012614424
H	-2.669336355	-1.468640057	0.092201376
C	2.179685275	0.867515414	0.358578808
H	2.212487898	1.932634271	0.094460120
H	2.100814576	0.809277781	1.447934749
N	3.338187597	0.103361090	-0.068095887
H	4.075172193	0.091670153	0.628513562
H	3.734085241	0.436852620	-0.941963796
H	-0.532082166	2.274123714	-0.244674609
N	-2.982874093	0.931509103	0.045998430
H	-2.951223444	1.821844382	-0.444307313
H	-3.220234106	1.105653847	1.022242871

1-ethynyl-1,2-dihydro-1,2-azaborine

N	1.422031818	-0.021748716	-0.047321273
B	0.277105085	-0.942823044	-0.216777003
C	1.228412638	1.313399946	0.072464264
C	-1.133929207	-0.291793179	-0.299447041
C	-0.040950419	1.917734176	0.065644824
C	-1.180805523	1.163188011	-0.068792336
H	-1.334734908	-0.405229629	-1.393492848
H	-0.083945241	2.992455550	0.202936802
H	-2.165226759	1.624536219	-0.010624120
H	2.126056646	1.912829224	0.199335217
C	-2.345145766	-1.060221509	0.361681559
H	-2.249404861	-2.115338120	0.076750239
H	-2.231382479	-1.006881389	1.447782408
N	-3.604100611	-0.448145986	-0.014268188
H	-4.298512839	-0.490651587	0.723326739
H	-4.007364571	-0.845988059	-0.856848351
H	0.516491777	-2.094442247	-0.327661289
C	2.698964002	-0.513506164	0.026347151
C	3.814919688	-0.965042377	0.094289196
H	4.805185750	-1.362580387	0.159521019

1-formyl-1,2-dihydro-1,2-azaborine

N	1.387294027	0.169162747	-0.014922290
B	0.316773520	-0.831298837	-0.181110132
C	1.104459549	1.482281069	0.080999031
C	-1.135761969	-0.274048782	-0.293008080
C	-0.195215784	2.012152716	0.050167293
C	-1.280675941	1.176026665	-0.086622772
H	-1.324149240	-0.421717217	-1.384432175
H	-0.313158581	3.083211060	0.170241326
H	-2.294716159	1.572083606	-0.045275810
H	1.954114548	2.152382034	0.210157637
C	-2.307350617	-1.106906588	0.369350885
H	-2.133460280	-2.157906994	0.108456314
H	-2.213692952	-1.023232682	1.455385595

N	-3.596363440	-0.589533267	-0.040016098
H	-4.297536785	-0.649879635	0.689877008
H	-3.962308360	-1.035642025	-0.875399818
H	0.620771807	-1.967516917	-0.268129589
C	2.797981163	-0.228889425	0.078429370
O	3.139741093	-1.367599271	0.005587579
H	3.471424189	0.632520443	0.218971806

2-phenyl-1,2-dihydro-1,2-azaborine

N	-0.810673285	-1.893442673	-0.063848737
B	-0.336217703	-0.500862057	0.100889994
C	-2.083858365	-2.258461103	0.033032478
C	-1.491735591	0.557628237	0.312113514
C	-3.134271649	-1.338447596	0.265473459
C	-2.858897523	-0.005301101	0.398202626
H	-1.306177330	1.090324673	1.262279359
H	-4.146822789	-1.721765853	0.317325617
H	-3.672548906	0.705494537	0.530504908
C	1.174559932	-0.222470441	0.066416110
C	1.702436497	0.956593676	0.645899967
C	2.092742689	-1.120167698	-0.531700292
C	3.069603099	1.220936274	0.638148671
C	3.458557538	-0.852202284	-0.558990315
C	3.949135092	0.317497371	0.031987052
H	1.038135626	1.664808851	1.133765384
H	1.743254265	-2.028591270	-1.018222778
H	3.452208907	2.123894639	1.103147698
H	4.140660306	-1.548353668	-1.036429561
H	5.015064350	0.523456668	0.020543819
H	-2.306072989	-3.317655998	-0.078150847
C	-1.497624170	1.748842418	-0.755909447
H	-0.458955600	2.090059274	-0.840032905
H	-1.785124951	1.341356356	-1.729208056
N	-2.438764004	2.780306563	-0.375223440
H	-2.874958050	3.233462979	-1.170225362
H	-2.033542149	3.492975304	0.222887344
H	-0.143148463	-2.646657987	-0.205006910

2-methyl-1,2-dihydro-1,2-azaborine

N	1.957758162	-0.331963104	0.062329289
B	0.660135813	-1.018677067	-0.076951388
C	2.099576143	0.993196935	0.100185911
C	-0.562793225	-0.042141557	-0.264898625
C	1.009584123	1.886640479	0.017206615
C	-0.264723498	1.399011477	-0.115634624
H	-0.762554002	-0.159646343	-1.356361027
H	1.210484079	2.949111390	0.092646576
H	-1.117498174	2.076504755	-0.120970577
H	3.109468792	1.379139844	0.222161540

C	-1.932691341	-0.431814806	0.402604415
H	-2.091493852	-1.503909971	0.230536912
H	-1.839466422	-0.292062647	1.483740992
N	-3.002668718	0.420154116	-0.086236257
H	-3.736807293	0.556193677	0.600331685
H	-3.428933650	0.070818649	-0.939465937
H	2.811484574	-0.875899109	0.161605173
C	0.611001244	-2.574183944	-0.063386278
H	0.219678450	-2.914728853	0.907928557
H	-0.079780048	-2.977528203	-0.812371884
H	1.582553477	-3.059330273	-0.202847118

2-vinyl-1,2-dihydro-1,2-azaborine

N	-1.386690650	1.364782399	0.284131380
B	0.020573471	0.999578086	0.018823680
C	-2.406588665	0.520653898	0.160335137
C	0.248415202	-0.521459487	-0.339690145
C	-2.239825315	-0.835129786	-0.206196584
C	-0.985606460	-1.333864140	-0.435368352
H	0.737201454	-0.567405427	-1.329800741
H	-3.123378699	-1.459731339	-0.270601017
H	-0.855642381	-2.391304694	-0.659082692
H	-3.401774034	0.909980284	0.364146090
C	1.294771601	-1.291298247	0.598758023
H	2.164963157	-0.630737129	0.691874566
H	0.856590250	-1.391016803	1.595640640
N	1.589771839	-2.604744044	0.074258427
H	1.760793446	-3.295428851	0.796090212
H	2.364384401	-2.616067256	-0.581036356
H	-1.624995469	2.318095170	0.546631941
C	1.061799429	2.124033247	0.109607428
H	0.772121093	3.081004623	0.549282351
C	2.320525087	2.037641251	-0.367939691
H	2.697230642	1.141278110	-0.855791898
H	3.018367895	2.868920785	-0.311409911

2-chloro-1,2-dihydro-1,2-azaborine

N	1.392385847	1.231299271	0.174006959
B	0.826823120	-0.096302902	-0.069829675
C	0.646423212	2.338162860	0.176037464
C	-0.713353844	-0.166929437	-0.341213126
C	-0.748479794	2.325380129	-0.043247974
C	-1.399938409	1.140796559	-0.273965755
H	-0.825905425	-0.521281171	-1.384787983
H	-1.280094209	3.269084123	-0.002593463
H	-2.481451230	1.125817614	-0.400521257
H	1.160279803	3.276754794	0.370954778
C	-1.529218418	-1.275637318	0.476214721
H	-0.947434293	-2.200616254	0.395194318
H	-1.540993529	-0.983814270	1.529464195

N	-2.882080979	-1.375814523	-0.015348238
H	-3.566959004	-1.529173665	0.715573158
H	-3.003435878	-2.079944732	-0.735625012
H	2.388170186	1.344569496	0.351336223
Cl	1.912250453	-1.457642936	-0.063610805

2-mercapto-1,2-dihydro-1,2-azaborine

N	1.366888008	1.238126742	0.198760650
B	0.845571873	-0.117013221	-0.073403898
C	0.601542966	2.323464000	0.187547065
C	-0.703767020	-0.214691148	-0.359309020
C	-0.792175339	2.282604935	-0.062024043
C	-1.413007622	1.089061432	-0.303133700
H	-0.816546709	-0.571671335	-1.400792799
H	-1.342587084	3.215822675	-0.031410407
H	-2.491887133	1.053559356	-0.444262086
H	1.089163050	3.272798325	0.397719222
C	-1.504752962	-1.296874660	0.485808474
H	-0.928543652	-2.230449841	0.441804175
H	-1.516619020	-0.979769653	1.532302132
N	-2.865570905	-1.416459511	0.007892720
H	-3.526078440	-1.635949760	0.745055832
H	-2.973294350	-2.097403485	-0.737062501
H	2.352868751	1.388914369	0.399420872
S	2.076389780	-1.419262254	-0.063163477
H	1.259558836	-2.448352826	-0.359876162

2-hydroxy-1,2-dihydro-1,2-azaborine

N	1.954026937	-0.285325252	0.099337775
B	0.658459494	-0.981777760	-0.091007625
C	2.060258509	1.033089438	0.140476942
C	-0.599387299	-0.059481592	-0.327418386
C	0.943010658	1.900928728	0.009083483
C	-0.311030256	1.393250872	-0.177901215
H	-0.842428566	-0.181922025	-1.404252624
H	1.118026235	2.967630059	0.088690711
H	-1.170634965	2.059396358	-0.226409360
H	3.052641804	1.448124602	0.303328666
C	-1.926361912	-0.462713294	0.416742982
H	-2.078528707	-1.542402422	0.267889314
H	-1.785910539	-0.308521800	1.490668531
N	-3.034980385	0.358146193	-0.032715026
H	-3.746286283	0.476587232	0.680631378
H	-3.482085999	-0.000328839	-0.871224184
H	2.802141707	-0.833817656	0.227592508
O	0.757464748	-2.320664485	-0.065727584
H	-0.044569470	-2.847518082	-0.171422190

2-amino-1,2-dihydro-1,2-azaborine

N	1.964834037	-0.307105675	0.109597023

B	0.662007136	-1.007237835	-0.094420533
C	2.073914283	1.010669235	0.146214402
C	-0.588150882	-0.063397376	-0.340751271
C	0.965153330	1.886720939	0.003570696
C	-0.289326752	1.386813489	-0.195233558
H	-0.852723945	-0.185379934	-1.410573907
H	1.148336149	2.952040854	0.083282716
H	-1.143006969	2.059956098	-0.251096540
H	3.067252877	1.421454763	0.313853737
C	-1.906956329	-0.439056459	0.429178754
H	-2.069555159	-1.519623463	0.305877641
H	-1.752420288	-0.263930868	1.498151608
N	-3.017392394	0.381868725	-0.022807650
H	-3.730719792	0.494904899	0.689620020
H	-3.462867411	0.016528757	-0.859416364
H	2.824732698	-0.829689792	0.254316816
N	0.651750457	-2.396061370	-0.082266216
H	1.467948207	-2.980806356	0.042525816
H	-0.191545855	-2.938284065	-0.209697784

2-ethynyl-1,2-dihydro-1,2-azaborine

N	1.308356169	1.388464314	0.133958684
B	0.935264084	-0.019865259	-0.063417003
C	0.421977269	2.383332731	0.138209113
C	-0.594845828	-0.285929244	-0.305972294
C	-0.965881337	2.178084793	-0.029460907
C	-1.456797514	0.910999405	-0.212034742
H	-0.646378231	-0.597004393	-1.371714179
H	-1.619302331	3.041625002	0.017977317
H	-2.530231144	0.744111190	-0.289437004
H	0.807945680	3.387649806	0.298220206
C	-1.237314641	-1.526343594	0.446283744
H	-0.536923277	-2.361243121	0.326228497
H	-1.284815331	-1.293013764	1.513444324
N	-2.573341506	-1.788497441	-0.046561695
H	-3.208672530	-2.107459547	0.675942625
H	-2.596630012	-2.450495550	-0.815461340
H	2.281991028	1.642233534	0.282390713
C	2.023715639	-1.055916715	-0.061285369
C	2.902356061	-1.898165467	-0.066900522
H	3.675833799	-2.638157890	-0.073720433

Intermediates of the reaction of methyleneiminium cation with substituted 1,2-dihydro-1,2-azaborines on C5

1-phenyl-1,2-dihydro-1,2-azaborine

N	-0.056456878	-0.396578227	-0.127730389

B	0.400076337	-1.836115750	-0.195394223
C	0.812036078	0.580725993	-0.202166676
C	1.883908681	-2.070920318	-0.398567838
C	2.262241293	0.394251466	-0.365480724
C	2.729579091	-1.013525226	-0.473734362
H	2.292172759	-3.075026387	-0.474309137
H	2.527268079	0.933564288	-1.294099872
H	3.804235899	-1.126730281	-0.595968793
H	0.422710850	1.595301915	-0.125398126
C	3.071849780	1.213965579	0.752781040
H	2.637372365	2.220588471	0.796590798
H	2.888106540	0.728327275	1.714489724
N	4.478749807	1.202686373	0.445842991
H	4.810472519	2.044187493	-0.010851241
H	5.068126121	0.993896706	1.241940667
H	-0.446435655	-2.652386404	-0.086280417
C	-1.473896810	-0.081117520	-0.034414916
C	-2.245438807	-0.692005834	0.957645997
C	-2.035064891	0.823745207	-0.941031495
C	-3.598366406	-0.366103612	1.054814524
C	-3.392299445	1.133812069	-0.837023604
C	-4.171907599	0.543984840	0.160993051
H	-1.798685018	-1.395223242	1.652579594
H	-1.436296966	1.249902512	-1.740840578
H	-4.202963135	-0.824565381	1.830276361
H	-3.839309838	1.822870143	-1.545904355
H	-5.227390632	0.784106641	0.236091108

1-methyl-1,2-dihydro-1,2-azaborine

N	-1.618399540	-0.354773573	-0.001006767
B	-1.696473759	1.126925028	-0.270546789
C	-0.495099365	-0.913298364	0.355411039
C	-0.422165452	1.921573322	-0.076837970
C	0.778160543	-0.192635578	0.491400140
C	0.718699602	1.276835023	0.276318666
H	-0.390583208	2.996218819	-0.233023245
H	1.143096359	-0.403056234	1.511801335
H	1.668786615	1.791974483	0.398533598
H	-0.505250389	-1.986515258	0.548731457
C	1.922256239	-0.884369498	-0.422273645
H	1.880173850	-1.961470664	-0.224090012
H	1.646289606	-0.720145546	-1.466812723
N	3.200968426	-0.303717318	-0.130290588
H	3.806616118	-0.877698238	0.442987982
H	3.702716116	0.034859302	-0.940851033
H	-2.756529031	1.524281495	-0.615525000
C	-2.852461820	-1.165831808	-0.132034035
H	-3.604968571	-0.776491742	0.556283979
H	-3.227414344	-1.074460878	-1.153069971
H	-2.645044934	-2.211871914	0.096760296

1-vinyl-1,2-dihydro-1,2-azaborine

N	1.282142607	-0.186277937	-0.082724752
B	1.236941547	1.298277725	0.213669508
C	0.176814044	-0.813677948	-0.415395286
C	-0.101760808	1.988339166	0.063460759
C	-1.151131519	-0.196812323	-0.497583655
C	-1.202685322	1.268245187	-0.265829771
H	-0.205077973	3.055526665	0.239022744
H	-1.538895181	-0.428634790	-1.504755683
H	-2.191913453	1.711855341	-0.352008787
H	0.259300556	-1.879328241	-0.629243843
C	-2.205124545	-0.985901534	0.451059692
H	-2.079628495	-2.054633364	0.244194679
H	-1.907124270	-0.801998686	1.486128997
N	-3.535448594	-0.512825901	0.205430238
H	-4.111702547	-1.130498212	-0.352294509
H	-4.035836690	-0.213474596	1.032002255
H	2.244441174	1.809240454	0.550666268
C	2.500682704	-0.954139763	-0.029550325
H	2.350093870	-2.005589454	-0.253070001
C	3.709106492	-0.469437928	0.253879712
H	3.912881125	0.568751961	0.480761590
H	4.549527399	-1.154393462	0.258109222

1-hydroxy-1,2-dihydro-1,2-azaborine

N	-1.567940989	-0.328500686	-0.002269495
B	-1.683321231	1.140585693	-0.274886345
C	-0.470357946	-0.918621468	0.375208910
C	-0.411269334	1.927675466	-0.073848329
C	0.795506543	-0.187408224	0.509505402
C	0.727330847	1.278415537	0.289526283
H	-0.376579025	3.001406859	-0.234522668
H	1.180358733	-0.395500689	1.521292881
H	1.674767893	1.797996706	0.413094450
H	-0.529644014	-1.989176739	0.564164696
C	1.947590387	-0.872339283	-0.425614733
H	1.912779496	-1.946459965	-0.216884198
H	1.650147127	-0.712821102	-1.464580220
N	3.219060334	-0.284778540	-0.147543426
H	3.850122850	-0.856038811	0.399529356
H	3.693319013	0.112948889	-0.947228854
H	-2.755949649	1.507831965	-0.620563834
O	-2.662799456	-1.164379135	-0.125573099
H	-3.416086570	-0.597377520	-0.371461993

1-amino-1,2-dihydro-1,2-azaborine

N	1.603279235	-0.372288057	0.015888773
B	1.709204049	1.122443051	0.235460372
C	0.470639432	-0.938648354	-0.301864137
C	0.438037025	1.915076812	0.069858943

C	-0.796366030	-0.196224787	-0.451212574
C	-0.716705956	1.273217162	-0.246480590
H	0.418701125	2.991465952	0.214830441
H	-1.136166995	-0.383603159	-1.486608409
H	-1.665380976	1.794231129	-0.353021714
H	0.474217604	-2.015202224	-0.470346050
C	-1.960060728	-0.855896921	0.430024857
H	-1.914932159	-1.940620531	0.267812169
H	-1.728984274	-0.666316976	1.481449239
N	-3.228875719	-0.267741144	0.083192690
H	-3.769477103	-0.811865517	-0.579379890
H	-3.805495717	-0.044360980	0.884963926
H	2.788222632	1.504971857	0.536700744
N	2.783102762	-1.103251843	0.042242832
H	2.644630918	-2.078901772	0.289713111
H	3.475357431	-0.648137224	0.627675338

2-phenyl-1,2-dihydro-1,2-azaborine

N	0.581866704	1.263788751	-0.274256392
B	-0.155498093	-0.060347636	-0.200865265
C	1.870349008	1.389380544	-0.394233012
C	0.786825991	-1.265785046	-0.299694380
C	2.787147766	0.241562908	-0.439242724
C	2.124746860	-1.097367452	-0.406578481
H	0.412352334	-2.285304309	-0.270663142
H	3.357058494	0.351643567	-1.379673347
H	2.814251941	-1.936570145	-0.453029163
C	-1.678147424	-0.036755093	-0.039361256
C	-2.395968477	-1.258919110	-0.033363086
C	-2.428814793	1.156563979	0.109187053
C	-3.780067671	-1.287617197	0.108757830
C	-3.811973517	1.134311175	0.253962110
C	-4.489930031	-0.090700203	0.253029036
H	-1.862480573	-2.197446456	-0.144876056
H	-1.941386659	2.129793730	0.121224506
H	-4.307293810	-2.236200849	0.107840167
H	-4.363955327	2.061756018	0.367262033
H	-5.569700465	-0.110692753	0.365217766
H	2.280965184	2.397681639	-0.452601013
C	3.923913529	0.383979117	0.683215799
H	4.315262715	1.408428428	0.630710576
H	3.442892030	0.258780806	1.656681109
N	4.928045442	-0.630533485	0.489634692
H	5.749812545	-0.309933900	-0.008990504
H	5.208219082	-1.094204738	1.344659045
H	0.048271950	2.130844418	-0.249268003

2-methyl-1,2-dihydro-1,2-azaborine

N	1.241171911	1.159124624	0.043343830
B	1.876179252	-0.210486525	-0.087716963

C	-0.014453894	1.367622895	0.326838831
C	0.892989798	-1.353224449	0.167059935
C	-0.978780678	0.279297147	0.495559805
C	-0.410629376	-1.096833352	0.432087628
H	1.214365966	-2.390882326	0.122921785
H	-1.473212979	0.444911867	1.467385188
H	-1.138352174	-1.889976584	0.587579028
H	-0.353807145	2.399769652	0.415930615
C	-2.221372849	0.462985992	-0.540513796
H	-2.559824194	1.500780330	-0.449168278
H	-1.821213971	0.319379414	-1.547101214
N	-3.247266724	-0.489943190	-0.248459588
H	-4.067194248	-0.114319545	0.210198296
H	-3.508979810	-1.086817667	-1.021525128
H	1.824378968	1.986544501	-0.078143798
C	3.392748190	-0.271590242	-0.418211162
H	3.963951934	-0.222419335	0.523431702
H	3.677394888	-1.215246403	-0.892400861
H	3.756329787	0.553663992	-1.041686006

2-vinyl-1,2-dihydro-1,2-azaborine

N	0.708541653	1.397528580	0.049455369
B	1.509913301	0.111337261	0.030894103
C	-0.574439528	1.464461850	0.259478826
C	0.660565336	-1.132221346	0.300892577
C	-1.409905878	0.275368640	0.461418545
C	-0.674558470	-1.023453951	0.495418398
H	1.096892342	-2.127224444	0.331303876
H	-1.941499164	0.432355042	1.416199234
H	-1.308500957	-1.890276013	0.665534459
H	-1.040741693	2.449842795	0.265636289
C	-2.623560792	0.253136315	-0.604830679
H	-3.080019792	1.250171631	-0.597299972
H	-2.185305091	0.089016288	-1.592432896
N	-3.544883551	-0.796941017	-0.274006307
H	-4.393595713	-0.486439725	0.182393340
H	-3.767280666	-1.414854388	-1.043467903
H	1.192847683	2.283114176	-0.094506757
C	3.007378274	0.242187861	-0.252219361
H	3.452428178	1.223730810	-0.428565134
C	3.840080704	-0.820283913	-0.297981520
H	3.487682110	-1.835891145	-0.135333429
H	4.902814534	-0.713913216	-0.499331563

2-chloro-1,2-dihydro-1,2-azaborine

N	0.698531692	1.230234184	0.137435558
B	1.332087635	-0.124575967	0.075195379
C	-0.569236467	1.414092009	0.407430989
C	0.409015632	-1.293094443	0.376537206
C	-1.505962978	0.310039161	0.560542965

C	-0.904618865	-1.049538237	0.606432622
H	0.771341824	-2.316636793	0.401856982
H	-2.137940054	0.508579557	1.436540531
H	-1.610192411	-1.854188430	0.800352379
H	-0.927961060	2.440672064	0.472591699
C	-2.650150586	0.392431455	-0.660544857
H	-3.031488429	1.416414541	-0.639199252
H	-2.103499859	0.228862312	-1.591609136
N	-3.662853363	-0.569342743	-0.452720347
H	-4.568925426	-0.231143608	-0.161583415
H	-3.719223545	-1.330495888	-1.113750289
H	1.276032142	2.059255929	-0.001770142
Cl	3.021922080	-0.174403848	-0.328807140

2-mercapto-1,2-dihydro-1,2-azaborine

N	0.739994201	1.214414414	0.131498215
B	1.389078093	-0.144228736	0.056473536
C	-0.532212963	1.392602905	0.350352195
C	0.436631153	-1.316344427	0.279238006
C	-1.483513448	0.285327529	0.492359577
C	-0.880208710	-1.081332855	0.479071448
H	0.781632499	-2.346934274	0.271059424
H	-2.019575326	0.454618523	1.441554482
H	-1.595418665	-1.888039610	0.619533227
H	-0.895968251	2.418456828	0.406044659
C	-2.673738883	0.424967579	-0.598867353
H	-3.041967565	1.455700603	-0.544105971
H	-2.227190131	0.274015690	-1.584939403
N	-3.690894472	-0.551075956	-0.336749066
H	-4.536691137	-0.182659815	0.079645749
H	-3.915824048	-1.145787335	-1.123374112
H	1.305748242	2.056684582	0.028224604
S	3.144613759	-0.118962882	-0.284760497
H	3.331099860	-1.453334627	-0.257504505

2-hydroxy-1,2-dihydro-1,2-azaborine

N	1.237175919	1.152545579	0.044266591
B	1.845703848	-0.228240077	-0.074873402
C	-0.017516920	1.365125271	0.301973965
C	0.867465099	-1.385708853	0.128593610
C	-0.991329752	0.274841069	0.469893479
C	-0.431858253	-1.110783499	0.379499620
H	1.175365359	-2.426771271	0.068581546
H	-1.437674630	0.425673447	1.469129037
H	-1.173079926	-1.894989207	0.512051742
H	-0.356146560	2.398302135	0.381240226
C	-2.245540655	0.484543097	-0.511776003
H	-2.570907758	1.527661218	-0.410781196
H	-1.890315701	0.342544516	-1.535781244
N	-3.273002427	-0.473273574	-0.198642161

H	-4.029946412	-0.102816369	0.363690733
H	-3.650536001	-0.947862873	-1.009018569
H	1.849872443	1.961173686	-0.068848421
O	3.159142830	-0.175523426	-0.347522693
H	3.632552625	-1.012879608	-0.438619413

2-amino-1,2-dihydro-1,2-azaborine

N	1.241160939	1.174493196	0.046334518
B	1.874044379	-0.201447328	-0.073819365
C	-0.019338148	1.364683008	0.298050290
C	0.891455171	-1.363121521	0.132827134
C	-0.987117930	0.267922148	0.464350679
C	-0.410350357	-1.112878341	0.379513915
H	1.215718649	-2.399614062	0.077992063
H	-1.433727017	0.423314360	1.463412319
H	-1.139786402	-1.907075199	0.514373435
H	-0.370924106	2.393787745	0.374759396
C	-2.231538658	0.469273088	-0.520412007
H	-2.556796613	1.515346564	-0.442301350
H	-1.875588151	0.305468904	-1.541052540
N	-3.264037786	-0.483908455	-0.196997341
H	-4.003507723	-0.109094267	0.385711099
H	-3.668577211	-0.933545156	-1.008736942
H	1.812108463	2.012643153	-0.055936820
N	3.232844662	-0.260769917	-0.354077968
H	3.850178149	0.528720641	-0.489034412
H	3.713262524	-1.146770140	-0.441430917

2-ethynyl-1,2-dihydro-1,2-azaborine

N	0.851962174	1.210118297	0.131314652
B	1.503405337	-0.147895781	0.064938620
C	-0.419433222	1.395007702	0.355360002
C	0.552388539	-1.314358684	0.307502110
C	-1.366209322	0.288510593	0.498440720
C	-0.766708680	-1.075415171	0.509200827
H	0.905376244	-2.341437634	0.311718921
H	-1.936897551	0.469130861	1.423461557
H	-1.482062146	-1.880359626	0.661002330
H	-0.782959421	2.421034577	0.408297787
C	-2.541899824	0.409897779	-0.635460748
H	-2.912290705	1.439259893	-0.592134359
H	-2.061782416	0.253749883	-1.604377199
N	-3.560102796	-0.559118127	-0.392825430
H	-4.428621668	-0.198788665	-0.020517162
H	-3.725342606	-1.214283025	-1.144560867
H	1.431571343	2.040852499	0.016315182
C	2.974798021	-0.177065507	-0.226517562
C	4.168880703	-0.212489508	-0.461504419
H	5.218526944	-0.251745931	-0.666982176

Mannich reaction on 1-phenyl-2-vinyl-azaborine

methyleneiminium addition to C3 (intermediate)

N	1.178108899	1.279254080	-0.066534721
B	0.356439907	0.038486058	0.078403860
C	2.504473150	1.200720901	-0.023935246
C	1.158789826	-1.307418907	0.280246534
C	3.257108576	0.008255524	0.137942218
C	2.630103160	-1.191061732	0.295551841
H	0.857970259	-1.710357736	1.266824019
H	4.337794839	0.096481248	0.136939548
H	3.204439077	-2.108483149	0.406340348
C	-1.192876437	0.060490252	0.063035246
C	-1.897418582	-0.708975557	1.019653356
C	-1.959527038	0.750080007	-0.905406012
C	-3.290827644	-0.759093213	1.031424801
C	-3.351517588	0.671953178	-0.918930726
C	-4.020952885	-0.072756422	0.057127564
H	-1.352383712	-1.254305967	1.786199637
H	-1.468828901	1.328680968	-1.682546621
H	-3.805731769	-1.337072744	1.792469775
H	-3.914475791	1.194295937	-1.686167503
H	-5.105573410	-0.119755180	0.056271880
H	3.051053808	2.134002759	-0.115830188
C	0.538338787	2.633111403	-0.206997065
H	0.298690028	2.770701878	-1.266188583
H	-0.405351004	2.569718063	0.333647116
C	1.357727302	3.811290873	0.309067900
H	2.229974837	4.042822747	-0.308795948
H	1.680019463	3.662365154	1.344922352
H	0.715909493	4.696456179	0.288856313
C	0.730092677	-2.483261446	-0.707962381
H	-0.365627858	-2.491177453	-0.723954494
H	1.071586141	-2.231008528	-1.716086909
N	1.331594203	-3.739044620	-0.304418379
H	1.558867336	-4.338196832	-1.090014929
H	0.755635310	-4.264931327	0.345118028

methyleneiminium addition to C3 (product)

N	-0.981541849	1.449022075	0.284281923
B	-0.455397315	0.107638485	0.137744439
C	-2.334297259	1.680618435	0.331032259
C	-1.485464126	-1.017728402	0.043494081
C	-3.248934199	0.666647945	0.244639538
C	-2.822522790	-0.682684425	0.101534829
H	-4.305482968	0.907672286	0.295865505
H	-3.576176965	-1.465521197	0.049493703

C	1.112971709	-0.131970560	0.096596676
C	1.827852968	-0.156478031	-1.117045905
C	1.844938559	-0.372814158	1.276231088
C	3.204636140	-0.398842347	-1.153843375
C	3.221725144	-0.616276216	1.249561603
C	3.907546239	-0.628764490	0.031990594
H	1.299976777	0.013087975	-2.053453383
H	1.330505563	-0.372814514	2.235214738
H	3.727041089	-0.409361102	-2.106957102
H	3.757015530	-0.798408521	2.177835413
H	4.977051568	-0.818371246	0.007165893
H	-2.643896712	2.715401289	0.447298043
C	-0.118323333	2.647610585	0.352285888
H	-0.545192217	3.335075343	1.091684365
H	0.859860976	2.336723652	0.721598853
C	0.029554831	3.350172934	-0.999400219
H	-0.943917949	3.648876374	-1.402398837
H	0.513459239	2.692094436	-1.727226392
H	0.644576625	4.250213567	-0.890632948
C	-1.059846403	-2.470858309	-0.085044509
H	-0.181088968	-2.524598348	-0.746825486
H	-0.709809558	-2.826319271	0.894468327
N	-2.151499689	-3.363314872	-0.500979564
H	-1.855785476	-4.333924722	-0.451837452
H	-2.419815246	-3.177295984	-1.464846013

methyleneiminium addition to C5 (intermediate)

N	-0.611565104	0.958533445	0.100973952
B	0.217561230	-0.338474683	0.095444563
C	-1.900439296	0.915734320	0.265467318
C	-0.620235946	-1.620176495	0.121847074
C	-2.703253282	-0.307216838	0.474154727
C	-1.953049707	-1.587771888	0.336464550
H	-0.139911630	-2.592074475	0.043757612
H	-3.081208406	-0.226664115	1.512466614
H	-2.560215290	-2.484747134	0.426577719
C	1.759928308	-0.332147167	0.053686093
C	2.393724618	-1.345859038	-0.707438232
C	2.596870043	0.555385776	0.772268444
C	3.781985385	-1.437575304	-0.786304738
C	3.984192844	0.440920994	0.727984792
C	4.580512433	-0.546788924	-0.063630236
H	1.791493793	-2.059527239	-1.262378070
H	2.167927536	1.320164416	1.412190986
H	4.240122817	-2.209059283	-1.397107337
H	4.601752390	1.118408864	1.309317062
H	5.662362438	-0.626639479	-0.108348859
H	-2.442114730	1.858574034	0.236602746
C	0.060762408	2.280162247	-0.154944303
H	0.560256026	2.562706872	0.775052710
H	0.840725438	2.071674143	-0.888144287

C	-0.841732783	3.407736592	-0.636649129
H	-1.540858155	3.762869873	0.126344748
H	-1.398890245	3.134746336	-1.539136168
H	-0.200724520	4.255743664	-0.893070043
C	-4.016629633	-0.271106983	-0.408625310
H	-4.465182322	0.728582777	-0.311327862
H	-3.726043327	-0.399458876	-1.455248270
N	-4.896374147	-1.352909092	-0.018898781
H	-5.562713682	-1.090188236	0.699680314
H	-5.402164553	-1.749550889	-0.802136214

methyleneiminium addition to C5 (product)

N	0.644897553	0.888036072	-0.170761130
B	-0.115243431	-0.328456203	0.049779385
C	2.017359171	0.885882152	-0.105471791
C	0.721171267	-1.556667160	0.375514441
C	2.764283023	-0.230120138	0.174863575
C	2.091976806	-1.467434188	0.416573101
H	0.266369316	-2.527713497	0.562558442
H	2.712732151	-2.338043117	0.622177748
C	-1.693762444	-0.365996509	-0.043443258
C	-2.456330129	-0.793425996	1.061959349
C	-2.398777865	-0.059118351	-1.225165473
C	-3.849886676	-0.887661555	1.002047965
C	-3.790702717	-0.161313636	-1.298796069
C	-4.523004860	-0.570568958	-0.180727970
H	-1.949903879	-1.056736187	1.987930810
H	-1.850031262	0.247363507	-2.113660600
H	-4.408521572	-1.214539190	1.875210995
H	-4.302629084	0.075046764	-2.228017119
H	-5.605449081	-0.648368627	-0.233298468
H	2.503403630	1.841222489	-0.290750010
C	0.021703645	2.213371618	-0.374460328
H	0.604293660	2.758045158	-1.126771727
H	-0.977204875	2.061243077	-0.781059171
C	-0.065928640	3.025251906	0.920930081
H	0.925221387	3.193901278	1.355114436
H	-0.678790943	2.503137299	1.662102566
H	-0.522891550	4.001175318	0.723834327
C	4.273558367	-0.149466493	0.224044148
H	4.578631002	0.903044509	0.096470061
H	4.626024012	-0.459419722	1.216603068
N	4.883918528	-1.067226436	-0.749304784
H	4.639036417	-0.803570962	-1.700362848
H	5.897622188	-1.061773194	-0.674248803

N,N-dimethylmethyleneiminium addition to C3 (intermediate)

N	1.189748261	1.731665943	0.073124058
B	0.420340769	0.463053473	-0.100313268

C	0.558693858	2.901772007	0.019741305
C	-1.128621535	0.618858322	-0.367349664
C	-0.832948459	3.076931873	-0.187563027
C	-1.645653232	1.999775074	-0.382270525
H	-1.317534774	0.187197673	-1.369235594
H	-1.215106234	4.091599741	-0.185562889
H	-2.716328011	2.134424131	-0.522580998
C	1.098848143	-0.929873731	-0.047527923
C	0.753151137	-1.900558218	-1.017182554
C	2.000716349	-1.321911698	0.969130610
C	1.305210411	-3.180933175	-0.995499790
C	2.525036074	-2.613097345	1.015571847
C	2.188289736	-3.541772380	0.025857044
H	0.063714221	-1.646201156	-1.818324600
H	2.274451504	-0.625853931	1.756866231
H	1.042234022	-3.897401812	-1.767459263
H	3.198461829	-2.894266162	1.819258156
H	2.609822387	-4.541885819	0.052753790
H	1.168902272	3.791008170	0.142663068
C	2.681403562	1.730014620	0.264445954
H	2.873572594	1.630500325	1.337699056
H	3.038905311	0.820827599	-0.216435048
C	3.419405611	2.940699787	-0.299630941
H	3.247162271	3.861817188	0.264098630
H	3.173336160	3.112746424	-1.352572982
H	4.491803404	2.734621355	-0.240775946
C	-2.055126994	-0.283449707	0.571913017
H	-1.584543345	-1.277872270	0.611401225
H	-2.024741859	0.134153592	1.582459611
N	-3.423528571	-0.316948013	0.113344128
C	-4.408027355	-0.425430940	1.193479038
H	-4.357770695	-1.391257831	1.724647709
H	-4.255038166	0.377877828	1.920038394
H	-5.412913843	-0.317708379	0.777016414
C	-3.660814162	-1.286952888	-0.953725642
H	-3.518885564	-2.329572564	-0.619357013
H	-4.682725134	-1.178701577	-1.325035267
H	-2.985511534	-1.106271222	-1.797035544

N,N-dimethylmethyleneiminium addition to C3 (product)

N	0.208801687	2.006421121	-0.156298375
B	0.140978785	0.564123401	-0.327143118
C	1.393093967	2.684208660	-0.286589916
C	1.462452723	-0.141155933	-0.647280738
C	2.567608221	2.052077122	-0.594252366
C	2.590729789	0.645066407	-0.784102239
H	3.470457481	2.642610505	-0.706491193
H	3.543173334	0.190360010	-1.059297572
C	-1.265990129	-0.166747757	-0.253381145
C	-1.955025922	-0.388890195	0.954945950
C	-1.874325081	-0.644472656	-1.431841348

C	-3.186721079	-1.049555808	0.989183648
C	-3.108899591	-1.300460153	-1.409279452
C	-3.770232134	-1.506507866	-0.195685103
H	-1.518253939	-0.051482444	1.892247731
H	-1.374130796	-0.499439825	-2.387094757
H	-3.688848049	-1.208576248	1.939946166
H	-3.550901996	-1.654043492	-2.337085016
H	-4.727177334	-2.020389760	-0.172935048
H	1.351693789	3.761467796	-0.152981652
C	-0.973588741	2.845731457	0.139339272
H	-0.934410104	3.731066082	-0.506048540
H	-1.863014157	2.279711666	-0.138460533
C	-1.055448799	3.270808800	1.607441900
H	-0.178819217	3.855044759	1.906443203
H	-1.121568469	2.398603561	2.264250581
H	-1.945686119	3.888304712	1.768749444
C	1.600945516	-1.652639747	-0.835726275
H	0.645176543	-2.076091080	-1.160101031
H	2.329910520	-1.854212750	-1.632043730
N	2.033643857	-2.442558564	0.332706766
C	1.085340565	-2.455322286	1.437114985
H	1.008173674	-1.488694024	1.970158540
H	0.089828544	-2.717830162	1.068766834
H	1.393082350	-3.214104249	2.165595160
C	3.390172320	-2.169003537	0.780770705
H	4.082833638	-2.244424014	-0.064870782
H	3.520616664	-1.173240707	1.245062617
H	3.680360275	-2.922666640	1.521552522

N,N-dimethylmethyleneiminium addition to C5 (intermediate)

N	0.170526548	1.110692539	0.068106553
B	0.872118206	-0.256092281	0.123563800
C	-1.117970406	1.197254635	0.225741841
C	-0.082632176	-1.450383987	0.218861003
C	-2.033645291	0.068943605	0.484258512
C	-1.406723614	-1.281749963	0.422661762
H	0.305515189	-2.465398838	0.195287538
H	-2.412896451	0.243542637	1.509909863
H	-2.094795472	-2.113078891	0.552921782
C	2.407878544	-0.400874171	0.070620049
C	2.932634123	-1.501718240	-0.651174292
C	3.334116068	0.430337267	0.745407491
C	4.304643034	-1.731133480	-0.734819732
C	4.703568491	0.181067862	0.695751860
C	5.193201580	-0.892266763	-0.056465118
H	2.258184837	-2.175680896	-1.171715320
H	2.987581366	1.258610591	1.355521294
H	4.679667304	-2.568932219	-1.314169661
H	5.390069246	0.819811703	1.242626246
H	6.261714949	-1.078727725	-0.104490471
H	-1.568320412	2.184230687	0.150331718

C	0.964854631	2.349685842	-0.245861253
H	1.506983362	2.612802877	0.665590333
H	1.707740137	2.038467686	-0.981499923
C	0.170778525	3.544351769	-0.754697430
H	-0.480902957	3.988810804	0.003550998
H	-0.421812776	3.300396878	-1.642805026
H	0.888266028	4.317294841	-1.043757313
C	-3.320985940	0.185384371	-0.428361287
H	-3.669459441	1.235534026	-0.406399670
H	-3.023254517	-0.041361314	-1.456276367
N	-4.337265381	-0.753446929	-0.010577922
C	-5.115729834	-0.287597338	1.136707130
H	-5.807978914	-1.072881714	1.448680228
H	-4.463898898	-0.074083137	1.990704270
H	-5.698768532	0.623558150	0.912254898
C	-5.198202820	-1.188073995	-1.115883142
H	-5.874499662	-1.967572224	-0.756570380
H	-5.808387480	-0.368456776	-1.533170144
H	-4.588515245	-1.614174354	-1.917418761

N,N-dimethylmethyleneiminium addition to C5 (product)

N	0.072807682	0.990332684	0.106340950
B	0.766786431	-0.257332564	-0.154987358
C	-1.289959528	1.085733510	-0.039570406
C	-0.124530583	-1.402007288	-0.612873842
C	-2.087587436	0.044505356	-0.440463588
C	-1.481165873	-1.215326385	-0.731968582
H	0.278215364	-2.387187583	-0.840874215
H	-2.141783381	-2.025471896	-1.037638841
C	2.331075357	-0.407309891	0.023080058
C	3.130373192	-0.812270327	-1.064649734
C	2.981175165	-0.226848469	1.261009018
C	4.508865241	-1.004417128	-0.933136864
C	4.356570613	-0.428159912	1.405694705
C	5.127712476	-0.812118915	0.304846206
H	2.665264352	-0.979427833	-2.033646907
H	2.400000051	0.057069910	2.136240145
H	5.097574711	-1.309989541	-1.794157505
H	4.825184959	-0.288932190	2.376468084
H	6.197774144	-0.966541322	0.412684627
H	-1.725428136	2.056960835	0.184028375
C	0.766195528	2.255344132	0.432754688
H	0.161494209	2.801226549	1.166191253
H	1.714964268	2.011314014	0.909125333
C	1.015842670	3.121675172	-0.804506090
H	0.077771496	3.382205083	-1.305820669
H	1.653162826	2.594985922	-1.521372597
H	1.519665378	4.051276083	-0.517826862
C	-3.580053727	0.234517823	-0.600112309
H	-3.843613162	1.290075049	-0.380644427

H	-3.855675356	0.057009079	-1.647699791
N	-4.374392165	-0.694711474	0.209655747
C	-4.217995170	-0.463798352	1.641211627
H	-4.772178519	-1.226323023	2.197098388
H	-3.163918869	-0.535212059	1.920150781
H	-4.592805543	0.531691775	1.955321288
C	-5.778970081	-0.673289417	-0.179070438
H	-6.330223987	-1.427682650	0.390967347
H	-6.262005623	0.308857143	-0.001571868
H	-5.875433346	-0.912639316	-1.242936312