Supplementary Information for

Computed ammonia affinity for evaluating Lewis acidity of organoboronates and organoboronamides

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1. Computational details

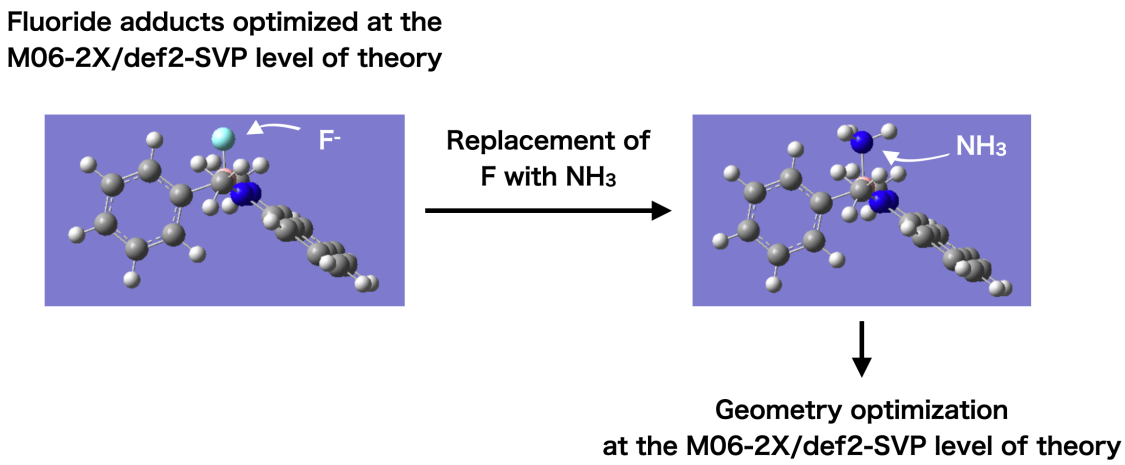


Figure S1. Geometry optimizations of ammonia adducts.

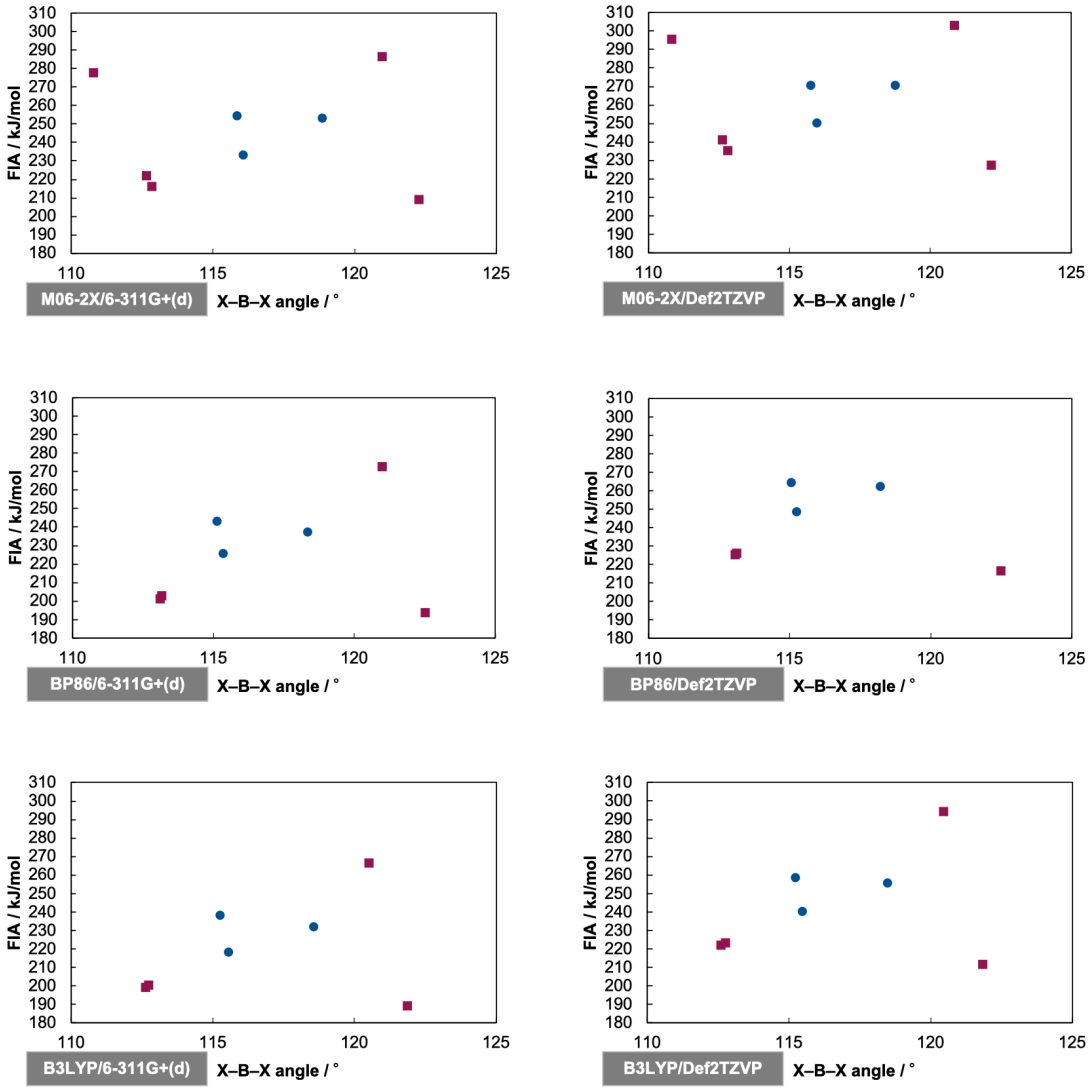


Figure S2. FIA of organoboronic acid derivatives [B(dan), B(aam), B(mdan), B(neop), B(pin), B(eg), B(cat), B(nad)] at various levels of theory.

X–B–X angle (M06-2X/def2-SVP)

●: PhB(dan), 116.1°; PhB(aam), 116.0°; PhB(mdan), 118.8°

■: PhB(neop), 121.9°; PhB(pin), 112.6°; PhB(eg), 112.8°; PhB(cat), 110.7°; PhB(nad), 120.6°

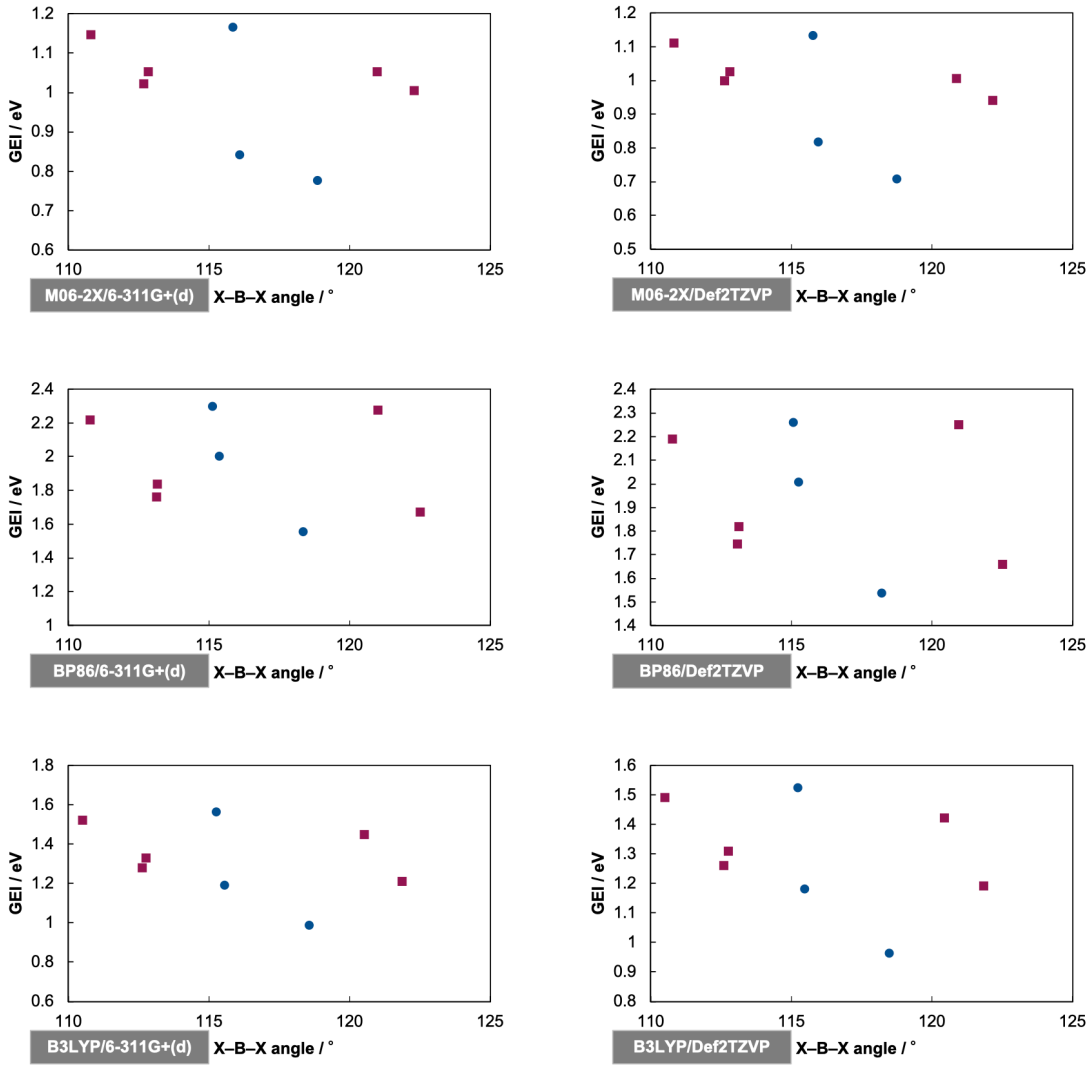


Figure S3. GEI of organoboronic acid derivatives [B(dan), B(aam), B(mdan), B(neop), B(pin), B(eg), B(cat), B(nad)] at various levels of theory.

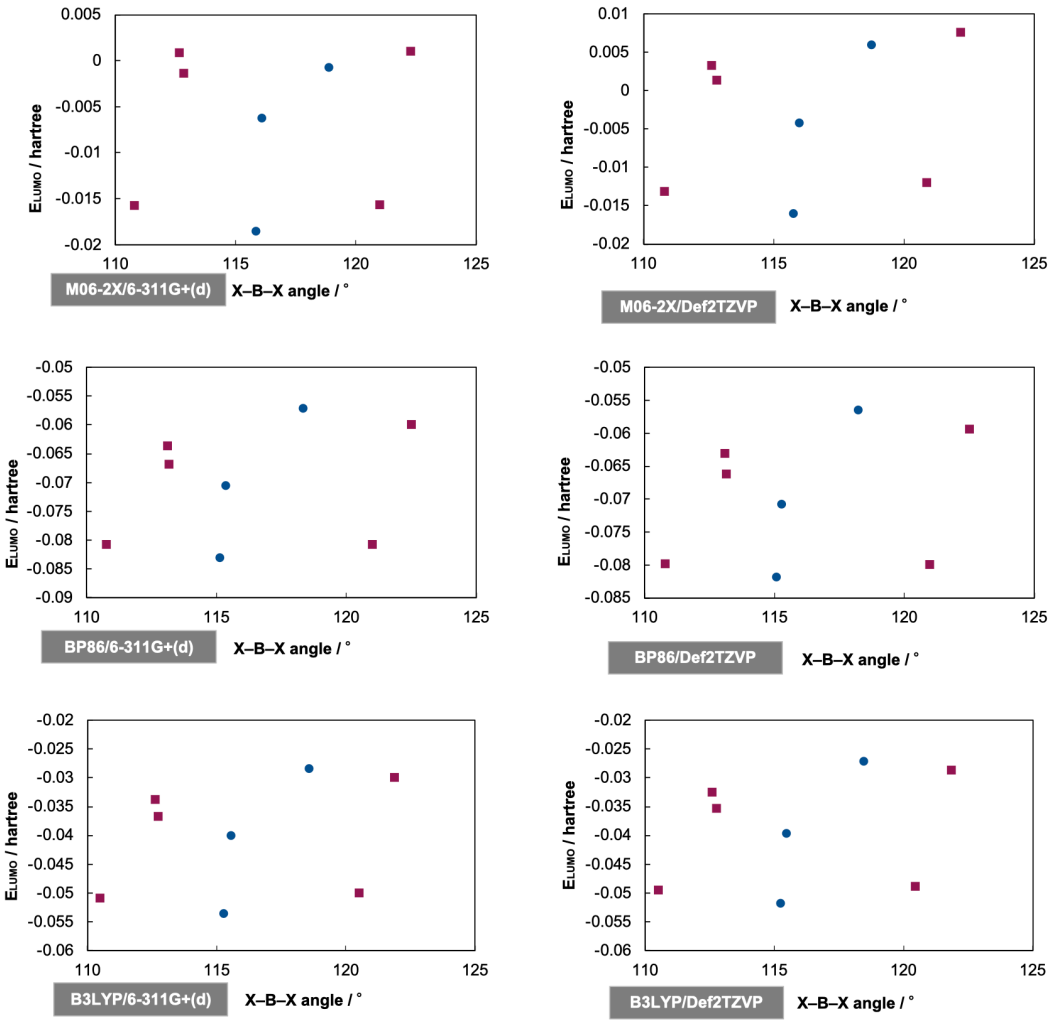


Figure S4. E_{LUMO} of organoboronic acid derivatives [B(dan), B(aam), B(mdan), B(neop), B(pin), B(eg), B(cat), B(nad)] at various levels of theory.

2. Optimized Cartesian coordinates and computed values

All calculations were conducted in the gas phase at 298 K.

E: Sum of electronic and zero-point energies

U: Sum of electronic and thermal energies

H: Sum of electronic and thermal enthalpies

G: Sum of electronic and thermal free energies

COF_2

Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

E = -312.656551 (hartree)

U = -312.653300 (hartree)

H = -312.652355 (hartree)

G = -312.682329 (hartree)

C	-0.00000134	0.13920557	0.00000000
F	1.05688788	-0.62737245	0.00000000
O	-0.00001379	1.30720872	0.00000000
F	-1.05687473	-0.62739456	0.00000000

COF_3^-

Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

E = -412.456855 (hartree)

U = -412.452879 (hartree)

H = -412.451935 (hartree)

G = -412.484015 (hartree)

C	-0.18475616	0.00160128	0.00306444
F	0.43550080	-1.05507231	-0.69359079
O	-1.40053248	0.01210656	0.02287082
F	0.45644853	1.11602840	-0.57467659
F	0.47613920	-0.07278499	1.24589480

NH_3

Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

E = -56.438783 (hartree)

U = -56.435915 (hartree)

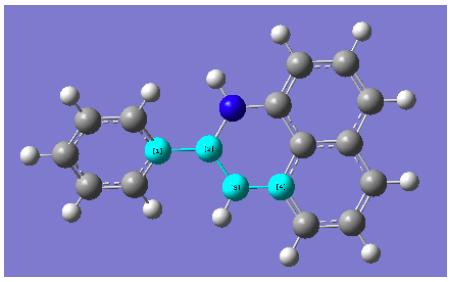
H = -56.434971 (hartree)

G = -56.456826 (hartree)

N	0.00000000	0.00000000	0.11994100
H	0.00000000	0.93767700	-0.27986200
H	-0.81205200	-0.46883900	-0.27986200
H	0.81205200	-0.46883900	-0.27986200

–Phenylboronic acid derivatives–

PhB(dan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 180.0°

N–B–N angle = 116.1°

B–N bond: 1.42327 Å, 1.42327 Å

E = -750.904925 (hartree)

U = -750.891328 (hartree)

H = -750.890383 (hartree)

G = -750.945952 (hartree)

FIA = 277.4 (kJ/mol)

AA = 12.1 (kJ/mol)

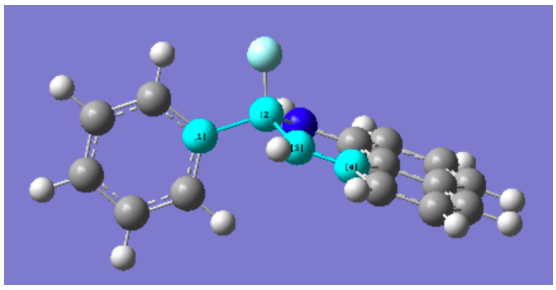
HOMO: -0.22485 (hartree)

LUMO: -0.00010 (hartree)

GEI = 0.766 (eV)

C	4.67088200	1.05815100	-0.57995500
C	5.37036500	0.00000000	0.00000100
C	4.67088100	-1.05815200	0.57995600
C	3.27712100	-1.05530500	0.57511200
C	2.55231800	0.00000000	0.00000000
C	3.27712100	1.05530500	-0.57511200
B	0.98209100	0.00000000	-0.00000100
N	0.22933400	-1.20365600	-0.10137200
N	0.22933400	1.20365700	0.10137100
C	-1.16160800	-1.24022200	-0.10532400
C	-1.16160900	1.24022300	0.10532400
C	-1.86638600	-2.42600200	-0.21159600
C	-3.27692700	-2.41571700	-0.21370400
C	-3.97983200	-1.23970200	-0.11002700
C	-3.29199600	0.00000000	0.00000000
C	-1.86827600	0.00000000	0.00000000
C	-3.97983200	1.23970100	0.11002800
C	-3.27692700	2.41571700	0.21370400
C	-1.86638600	2.42600200	0.21159700
H	5.21398200	1.88543300	-1.03974200
H	6.46160100	0.00000000	0.00000100
H	5.21398100	-1.88543300	1.03974200
H	2.74208300	-1.88478000	1.04567600
H	2.74208500	1.88478000	-1.04567700
H	0.69063900	-2.09500200	-0.23328700
H	0.69063900	2.09500200	0.23328700
H	-1.32264800	-3.36878600	-0.29352200
H	-3.81148100	-3.36333300	-0.29897700
H	-5.07066800	-1.23790200	-0.11143700
H	-5.07066800	1.23790100	0.11143700
H	-3.81148100	3.36333300	0.29897800
H	-1.32264900	3.36878700	0.29352200

PhB(dan)–F^-



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 139.9°

B–N bond: 1.52896 Å, 1.52896 Å

E = -850.732072 (hartree)

U = -850.716977 (hartree)

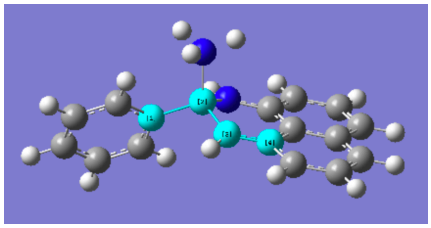
H = -850.716032 (hartree)

G = -850.775784 (hartree)

C	3.80528200	-0.00013600	-1.88169500
C	4.97882800	-0.00006200	-1.12322800
C	4.89151400	0.00004600	0.26839800
C	3.63990100	0.00008000	0.89114400
C	2.44797900	0.00000900	0.15403800
C	2.56437300	-0.00010000	-1.24522500
B	0.97632300	0.00005600	0.87363700
N	0.15998800	-1.22095100	0.44884100
N	0.15998800	1.22100600	0.44867600
C	-1.16479600	-1.24280400	0.16808200
C	-1.16481200	1.24282100	0.16798000
C	-1.87648600	-2.43972800	-0.00956500
C	-3.24506900	-2.42315900	-0.31609400
C	-3.94207400	-1.24211300	-0.45889100
C	-3.26644800	-0.00002400	-0.29904100
C	-1.87699900	-0.00000200	0.02049900
C	-3.94209700	1.24204400	-0.45896200
C	-3.24511400	2.42311100	-0.31623200
C	-1.87652800	2.43972200	-0.00971800
F	1.19312900	0.00015500	2.29042700
H	3.86295100	-0.00022200	-2.97342300
H	5.95427000	-0.00008900	-1.61589100
H	5.80419100	0.00010400	0.87064500
H	3.56849500	0.00016300	1.98178200
H	1.64731300	-0.00015600	-1.84284100
H	0.58860400	-2.13289500	0.54511100
H	0.58858300	2.13296400	0.54491000
H	-1.34569500	-3.38820700	0.09980600
H	-3.76647300	-3.37643300	-0.44259600
H	-5.00712500	-1.23918600	-0.69891700
H	-5.00714800	1.23908400	-0.69898600
H	-3.76653700	3.37636900	-0.44278000
H	-1.34575200	3.38821700	0.09959100

PhB(dan)–NH_3

The optimized structure of PhB(dan)-NH_3 obtained from the optimized structures of PhB(dan)-F was confirmed not to be local minima by verifying the presence of imaginary frequencies at the M06-2X/def2-SVP level of theory. Thus, we optimized the PhB(dan)-NH_3 structure starting from the following structure (Dihedral angle = 146.2°) at the M06-2X/def2-SVP level of theory and confirmed that the resulting structure have no imaginary frequency.

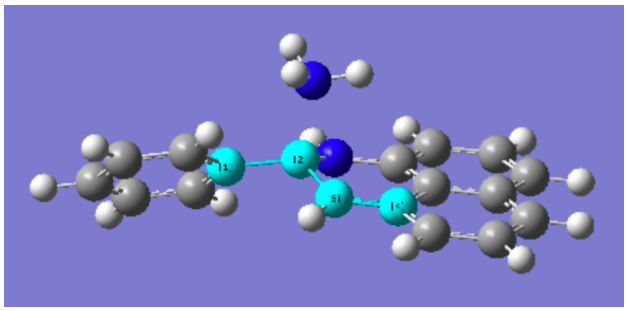


Dihedral angle = 146.2°

C	3.94290291	-0.41921022	-1.82711194
C	5.01611583	0.07867261	-1.07594708
C	4.80886412	0.51090268	0.24092264
C	3.52840031	0.44524599	0.80662891
C	2.45518823	-0.05264086	0.05546550
C	2.66243908	-0.48486684	-1.26140570
B	0.94757881	-0.12994957	0.72152647
N	0.14727528	-1.33437024	0.10394162
N	0.17260043	1.21239465	0.45686359
C	-1.17604631	-1.24177734	-0.07127164
C	-1.15179729	1.19676985	0.26665389
C	-1.90773669	-2.39862897	-0.36620695
C	-3.29915851	-2.33368822	-0.51808961
C	-3.94842354	-1.14903766	-0.39943066
C	-3.23601829	0.03137914	-0.14244949
C	-1.84491316	-0.00598551	0.02735872
C	-3.92455881	1.25086373	-0.06686053
C	-3.25198464	2.41024305	0.13930817
C	-1.85997637	2.40427795	0.29936347
H	4.10114367	-0.74922503	-2.83257208
H	5.99377853	0.12880220	-1.50787610
H	5.62828599	0.89104737	0.81445365
H	3.37015910	0.77526290	1.81208829
H	1.84301715	-0.86501123	-1.83493682
H	0.62700880	-2.17414252	-0.15029896

H	0.66931349	2.08013059	0.43924366
H	-1.40306754	-3.33619825	-0.47190885
H	-3.85299233	-3.22457434	-0.72901615
H	-5.01245780	-1.11400463	-0.50668642
H	-4.98878016	1.26708176	-0.17672361
H	-3.78775820	3.33554611	0.18006291
H	-1.33682597	3.32523206	0.45120939
H	1.73946477	-1.17324442	2.54604049
H	1.46017184	0.53194459	2.80564342
H	0.11069736	-0.57694878	2.75726264
N	1.07574095	-0.35700271	2.35079665

PhB(dan)-NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 166.1°

B–N(dan) bond: 1.48265 Å, 1.48346 Å

E = -807.347306 (hartree)

U = -807.330904 (hartree)

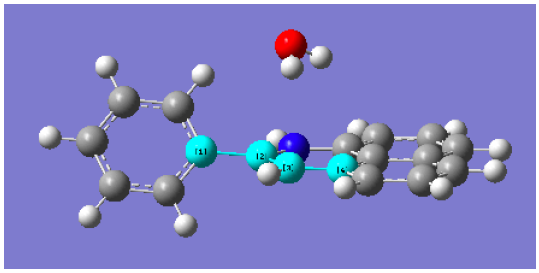
H = -807.329960 (hartree)

G = -807.391424 (hartree)

C	-4.42557000	1.04529400	-1.07856500
C	-5.26958300	0.07411400	-0.54169600
C	-4.73568600	-0.92941100	0.26629000
C	-3.36778000	-0.94687800	0.53746300
C	-2.49683200	0.02298000	0.01603700
C	-3.05824600	1.01297800	-0.80269400
B	-0.92143200	-0.01226500	0.30851100
N	-0.15939700	1.23513600	0.05564300
N	-0.18254700	-1.20272500	-0.17636800
C	1.21880900	1.24705700	0.02465900
C	1.19207400	-1.23717100	-0.24415400

C	1.95230900	2.42504000	0.10739700
C	3.35991800	2.39944900	0.07242000
C	4.04914800	1.21600900	-0.04762900
C	3.34268900	-0.01338200	-0.15248400
C	1.91752200	-0.00383900	-0.09997600
C	4.02156100	-1.24871700	-0.33742100
C	3.30584700	-2.41258800	-0.49151600
C	1.89845200	-2.41726300	-0.44679400
H	-4.83396300	1.82812500	-1.72035800
H	-6.33925400	0.09508400	-0.75655700
H	-5.38690000	-1.69973400	0.68348400
H	-2.97511800	-1.75432500	1.16604300
H	-2.40515200	1.76719500	-1.24925800
H	-0.59744300	2.14428600	0.13009200
H	-0.66183100	-2.06152900	-0.41103400
H	1.42269400	3.37566400	0.19803800
H	3.90637000	3.34217600	0.14154500
H	5.13941400	1.20185800	-0.08093800
H	5.11182100	-1.25077700	-0.37326200
H	3.83143600	-3.35666300	-0.64850100
H	1.34763800	-3.35236100	-0.56595800
H	-1.24779000	0.61108800	2.58806000
H	-1.22534700	-1.04060100	2.45785600
H	0.18473600	-0.18372900	2.32764500
N	-0.81404900	-0.17619100	2.10394500

PhB(dan)-H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

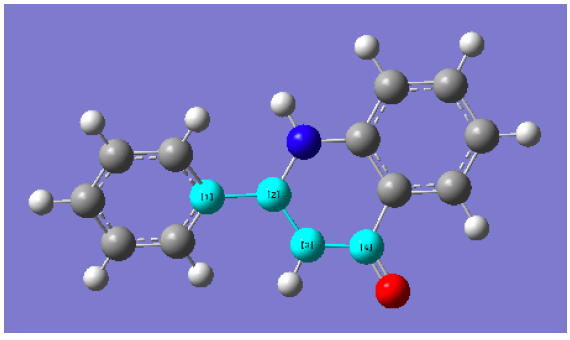
Dihedral angle = -176.7°

H = -827.200263 (hartree)

C	-4.68101900	-0.93409800	-0.96577200
C	-5.33942900	-0.02157100	-0.14160500
C	-4.60170400	0.86978100	0.63773000
C	-3.20858000	0.85484500	0.58506300

C	-2.52965000	-0.05297700	-0.24279200
C	-3.28753200	-0.95057400	-1.00965700
B	-0.96320400	-0.05752300	-0.27685400
N	-0.20915200	1.12735500	-0.50709900
N	-0.20938400	-1.25233700	-0.07498300
C	1.17763200	1.17639300	-0.44531100
C	1.18184300	-1.28175500	-0.03237400
C	1.88281500	2.35830700	-0.59592400
C	3.29165600	2.35973600	-0.52618100
C	3.99450200	1.19974900	-0.30588600
C	3.30816700	-0.03416900	-0.13891900
C	1.88554600	-0.04660400	-0.20635600
C	3.99702100	-1.25648400	0.09218700
C	3.29725200	-2.42814000	0.25012500
C	1.88788400	-2.45015700	0.19146900
H	-5.25557600	-1.63324600	-1.57572400
H	-6.43001500	-0.00858700	-0.10299400
H	-5.11476100	1.57477500	1.29400500
H	-2.62982200	1.52787300	1.22268100
H	-2.78123500	-1.66661600	-1.66289900
H	-0.67956500	2.00924200	-0.66814600
H	-0.67737200	-2.13707500	0.07945400
H	1.33921500	3.28744900	-0.77508900
H	3.82489500	3.30357900	-0.65114200
H	5.08401100	1.20687700	-0.25460900
H	5.08659700	-1.24474400	0.14156300
H	3.83282600	-3.36236300	0.42659400
H	1.34602200	-3.38842800	0.32276300
H	-0.26950000	-0.32733600	2.31566500
H	0.40241100	1.00747800	2.10904600
O	-0.35884900	0.60499100	2.54536100

PhB(aam)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 179.9°

N–B–N angle = 116.0°

B–N bond: 1.42278 Å, 1.43187 Å

H = -710.681922 (hartree)

FIA = 294.0 (kJ/mol)

AA = 18.6 (kJ/mol)

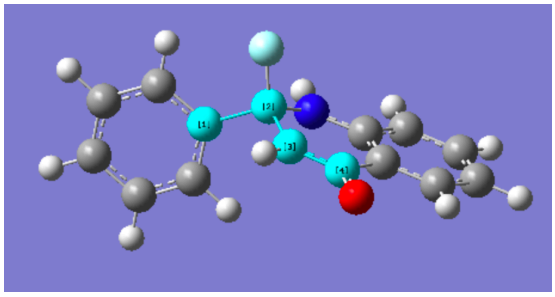
HOMO: -0.27769 (hartree)

LUMO: -0.01041 (hartree)

GEI = 1.056 (eV)

C	-4.37636700	0.78898400	0.53670800
C	-4.94800500	-0.38021100	0.03527700
C	-4.13136800	-1.38346700	-0.48625200
C	-2.74812200	-1.21507500	-0.50044800
C	-2.15092700	-0.04621400	-0.00306400
C	-2.99250300	0.95169000	0.51256200
B	-0.59347100	0.13763800	-0.02124300
N	0.29578800	-0.96633400	0.10024800
N	0.01776300	1.42502100	-0.16009500
C	1.67437300	-0.82090700	0.09201900
C	1.38201100	1.67522800	-0.18410200
C	2.52994300	-1.92720300	0.22181500
C	3.90590700	-1.75113000	0.21115000
C	4.46478000	-0.47471600	0.07094800
C	3.62527100	0.62194700	-0.05633500
C	2.23522900	0.46370300	-0.04579700
O	1.82789000	2.79319000	-0.31341100
H	-5.01127800	1.57486800	0.94876500
H	-6.03145800	-0.50922300	0.04972900
H	-4.57490400	-2.29673100	-0.88602100
H	-2.12243900	-2.00405400	-0.92703500
H	-2.55923600	1.86957600	0.91905100
H	-0.05257600	-1.90418000	0.25510800
H	-0.53467800	2.26667700	-0.29321500
H	2.10028100	-2.92512300	0.33023400
H	4.55566600	-2.62193900	0.31309300
H	5.54716600	-0.34645600	0.06302700
H	4.01150900	1.63628700	-0.16719000

PhB(aam)–F^-



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 138.2°

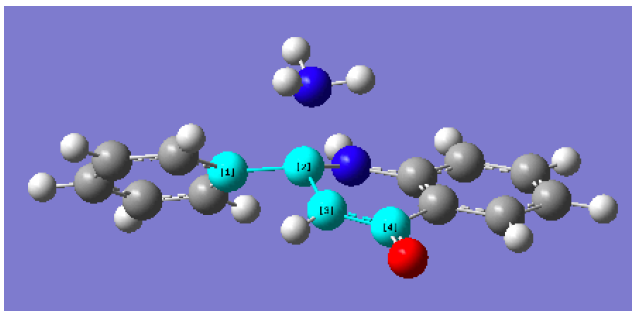
B–N bond: 1.53464 Å, 1.53226 Å

H = -810.513866 (hartree)

C	3.45742200	-0.55146800	-1.77400500
C	4.60501300	-0.56349000	-0.97699300
C	4.49033800	-0.30303000	0.38798000
C	3.23730400	-0.03407000	0.94619200
C	2.07101900	-0.01693200	0.16943900
C	2.21453800	-0.28192400	-1.20173000
B	0.59846400	0.28523000	0.81889500
N	-0.34073100	-0.90594700	0.60251700
N	-0.06437800	1.49384300	0.14434900
C	-1.64369800	-0.81768300	0.25581200
C	-1.34920000	1.65770900	-0.23673900
C	-2.50979900	-1.94195300	0.26125900
C	-3.84047300	-1.82743500	-0.11088600
C	-4.37681200	-0.59675200	-0.50879300
C	-3.53679200	0.51376800	-0.52685100
C	-2.19714300	0.42577600	-0.15494100
O	-1.80892300	2.72046200	-0.64840100
F	0.78570400	0.52926700	2.21614900
H	3.53695300	-0.75273200	-2.84557300
H	5.58179700	-0.77367000	-1.41957200
H	5.38279200	-0.30899300	1.01972300
H	3.14453100	0.17200300	2.01551200
H	1.31857400	-0.27179600	-1.83052100
H	-0.02568400	-1.82394700	0.88876900
H	0.46725300	2.35494700	0.06787100
H	-2.10579200	-2.90939600	0.57100200
H	-4.47514400	-2.71765700	-0.08965800

H	-5.42486700	-0.51283300	-0.79993700
H	-3.88723500	1.50044100	-0.83674700

PhB(aam)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 160.8°

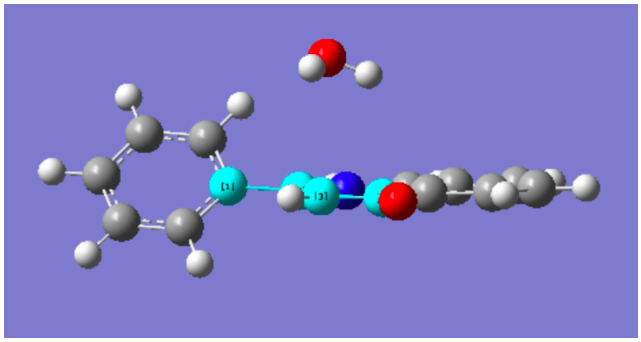
B–N(aam) bond: 1.49524 Å, 1.48634 Å

H = -767.123979 (hartree)

C	3.90275300	-1.41499600	-0.94754000
C	4.86091500	-0.51744700	-0.47885700
C	4.45593400	0.60503800	0.24285200
C	3.10090000	0.81393400	0.49757800
C	2.11592100	-0.07813200	0.04429600
C	2.55001500	-1.19130000	-0.68917200
B	0.55518500	0.17349900	0.31819500
N	-0.34440300	-0.99913400	0.16045900
N	-0.03677700	1.39985700	-0.29934600
C	-1.70593800	-0.84333500	0.05343900
C	-1.37202700	1.61260500	-0.51073800
C	-2.59591400	-1.92575400	0.20976400
C	-3.96666300	-1.73628500	0.11214400
C	-4.50153600	-0.46856100	-0.14623200
C	-3.63400300	0.60145300	-0.31869000
C	-2.24955400	0.43446200	-0.21918200
O	-1.82009500	2.66949400	-0.91439600
H	4.21049700	-2.29011000	-1.52275400
H	5.91964700	-0.68768000	-0.68086100
H	5.19757800	1.31958700	0.60443300
H	2.81372800	1.71285600	1.05496500
H	1.80883600	-1.89120500	-1.08357200
H	-0.01707700	-1.94431000	0.31195800
H	0.54014400	2.18106500	-0.59328000

H	-2.18996600	-2.91991500	0.41048400
H	-4.63198600	-2.59247200	0.23975500
H	-5.57970800	-0.32842000	-0.22325500
H	-3.99414500	1.60469600	-0.55291400
H	0.87905800	-0.22557700	2.62101900
H	0.93650100	1.40027100	2.30476500
H	-0.51789500	0.61371400	2.29722200
N	0.47329600	0.52412800	2.05863800

PhB(aam)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

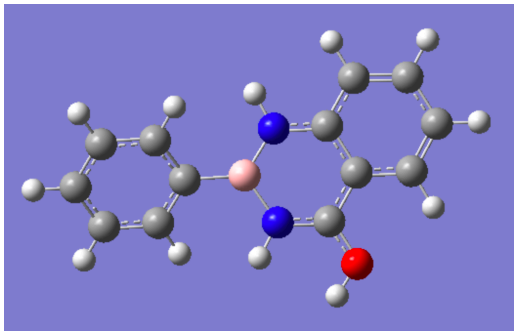
Dihedral angle = -176.7°

H = -786.991166 (hartree)

C	4.38174300	0.72202500	-0.90615900
C	4.93533300	-0.35449600	-0.21312600
C	4.10506700	-1.24318100	0.47012100
C	2.72301900	-1.06112500	0.45114100
C	2.14840600	0.01395700	-0.24522600
C	2.99980800	0.90529700	-0.91555400
B	0.59404300	0.20037800	-0.24817700
N	-0.29292400	-0.86974200	-0.55112000
N	-0.01907100	1.46463800	0.04598700
C	-1.66664100	-0.74667200	-0.45899100
C	-1.38294300	1.69983600	0.12851400
C	-2.52232400	-1.83944500	-0.68449200
C	-3.89612200	-1.68573500	-0.57645500
C	-4.45711900	-0.44611600	-0.24148600
C	-3.62063200	0.63619800	-0.01665700
C	-2.23069200	0.50105700	-0.11961500
O	-1.83428600	2.78962700	0.40208000
H	5.02912600	1.41957400	-1.44008600

H	6.01714200	-0.49772700	-0.20107300
H	4.53746600	-2.07746100	1.02496600
H	2.07501200	-1.73459300	1.01766300
H	2.57686500	1.75062100	-1.46539900
H	0.06710900	-1.78957800	-0.77323500
H	0.53869600	2.29014900	0.24464100
H	-2.09146700	-2.80790100	-0.94563200
H	-4.54391700	-2.54555000	-0.75521600
H	-5.53837100	-0.33588600	-0.16006900
H	-4.00832300	1.62231000	0.24363300
H	0.29820700	0.30539300	2.55605800
H	-0.81644300	-0.63298900	2.14738500
O	0.08069000	-0.63239200	2.50430500

PhB(aam)H$^+$



Charge = +1; Multiplicity = 1

M06-2X/def2-SVP

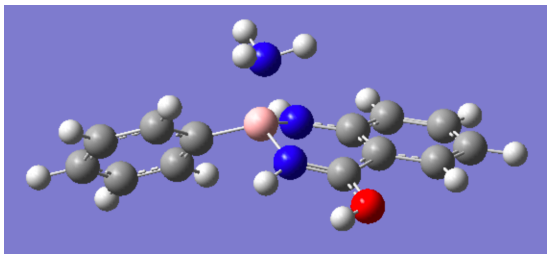
H = -711.027612 (hartree)

AA = 79.3 (kJ/mol)

C	4.37443200	0.83700500	-0.47148900
C	4.96557900	-0.34262800	-0.01811500
C	4.17074100	-1.39458600	0.43897400
C	2.78486600	-1.26627900	0.43937100
C	2.16809400	-0.08499800	-0.00828700
C	2.98821900	0.96304800	-0.46138300
B	0.62855900	0.04996500	-0.00141500
N	-0.29547600	-1.01832800	-0.10256500
N	-0.01719500	1.36984700	0.12499600
C	-1.66200400	-0.86586900	-0.08769000
C	-1.33267000	1.54802500	0.14799600
C	-2.53041100	-1.96564800	-0.19862700
C	-3.89806700	-1.76718300	-0.18128600

C	-4.45415000	-0.47751500	-0.05396900
C	-3.62266000	0.61340800	0.05456300
C	-2.21893600	0.43238100	0.03759100
H	4.99568100	1.65541000	-0.83668000
H	6.05179400	-0.44287000	-0.02156100
H	4.63417300	-2.31392300	0.79832300
H	2.18032200	-2.09505100	0.81771400
H	2.54871100	1.88930100	-0.84474100
H	0.04251400	-1.96828200	-0.22808700
H	0.58228300	2.18595900	0.23919800
H	-2.11534200	-2.96960600	-0.29735100
H	-4.55987200	-2.63027600	-0.26799900
H	-5.53575000	-0.34828400	-0.04247100
H	-4.02579600	1.62108500	0.15359000
O	-1.86530200	2.73376500	0.27594000
H	-1.22859800	3.46100600	0.34670700

PhB(aam)H$^+$–NH$_3$



Charge = +1; Multiplicity = 1

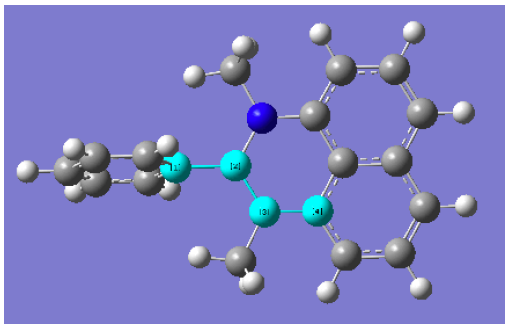
M06-2X/def2-SVP

H = -767.492776 (hartree)

C	3.81606000	-1.35521100	-1.12392200
C	4.80836300	-0.50211000	-0.64343400
C	4.46585100	0.54846500	0.20727300
C	3.13479200	0.73125200	0.57900500
C	2.11742900	-0.11947300	0.11452800
C	2.48660800	-1.15952000	-0.75059200
B	0.58986600	0.11232800	0.50656400
N	-0.35508400	-1.02352000	0.30035500
N	-0.02324600	1.37382800	-0.15896200
C	-1.69512400	-0.85864900	0.12543100
C	-1.30402300	1.49920100	-0.42659600
C	-2.60177700	-1.94065300	0.19449200
C	-3.95526700	-1.73231200	0.02334500
C	-4.48000100	-0.44833600	-0.23484000

C	-3.61774900	0.61791700	-0.34015400
C	-2.22592000	0.43081700	-0.16063600
H	4.07818800	-2.17338600	-1.79606600
H	5.84868500	-0.65260200	-0.93455500
H	5.23673900	1.22342400	0.58149800
H	2.90501400	1.57287100	1.24374900
H	1.72124600	-1.82651100	-1.15574400
H	-0.02731100	-1.98196500	0.34596000
H	0.61349600	2.08739700	-0.50891500
H	-2.21677200	-2.94178700	0.39452600
H	-4.63358600	-2.58445300	0.09158100
H	-5.55242400	-0.30861400	-0.36290400
H	-3.98831400	1.61737200	-0.56854400
H	0.96032200	-0.33863700	2.66410900
H	1.10125700	1.28204300	2.42130300
H	-0.40170500	0.58631200	2.50414700
N	0.55505100	0.45635000	2.16056800
O	-1.79796200	2.58489900	-0.97826800
H	-1.14297200	3.28277300	-1.12394800

PhB(mdan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 179.3°

N–B–N angle = 118.8°

B–N bond: 1.43066 Å, 1.43067 Å

H = -829.337202 (hartree)

FIA = 301.8 (kJ/mol)

AA = 21.5 (kJ/mol)

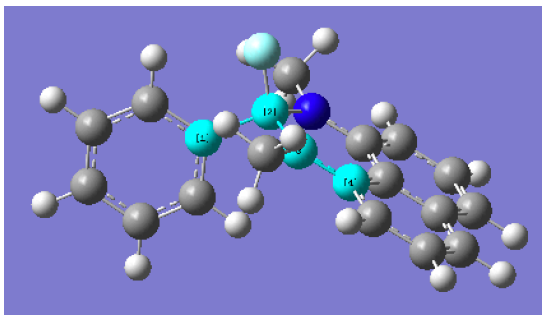
HOMO: -0.22312 (hartree)

LUMO: 0.00971 (hartree)

GEI = 0.665 (eV)

C	4.56067500	-0.35520300	1.15223800
C	5.26129800	0.00000000	0.00000100
C	4.56067500	0.35520300	-1.15223600
C	3.16580600	0.35745000	-1.14764800
C	2.44214700	-0.00000400	-0.00000100
C	3.16580600	-0.35745100	1.14764900
B	0.85925900	-0.00000400	-0.00000100
N	0.13137700	1.23041000	0.05541300
N	0.13137100	-1.23041600	-0.05541500
C	-1.26732000	1.24889400	0.04100000
C	-1.26732500	-1.24889200	-0.04099800
C	-1.98802600	2.43528900	0.07214700
C	-3.39851500	2.41825700	0.06739900
C	-4.09341900	1.23708300	0.03433200
C	-3.39514800	0.00000400	0.00000200
C	-1.96969400	0.00000300	0.00000100
C	-4.09342200	-1.23707200	-0.03432900
C	-3.39852200	-2.41824900	-0.06739800
C	-1.98803300	-2.43528400	-0.07214800
C	0.80008900	-2.51473500	-0.15417900
C	0.80011200	2.51472200	0.15417300
H	5.10297900	-0.63289000	2.05770500
H	6.35248400	0.00000100	0.00000200
H	5.10298000	0.63289200	-2.05770100
H	2.62987700	0.64555400	-2.05612200
H	2.62987500	-0.64555500	2.05612200
H	-1.47763900	3.39421400	0.09985700
H	-3.93522100	3.36816600	0.09231500
H	-5.18420200	1.22504600	0.03356500
H	-5.18420600	-1.22503300	-0.03356200
H	-3.93523000	-3.36815600	-0.09231700
H	-1.47764600	-3.39421000	-0.09986100
H	1.88207100	-2.36550900	-0.20552100
H	0.57134200	-3.14842000	0.71766500
H	0.47521100	-3.05329600	-1.05832600
H	1.88209100	2.36547800	0.20551100
H	0.57137100	3.14840800	-0.71767100
H	0.47524600	3.05328800	1.05832100

PhB(mdan)–F$^-$



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 118.2°

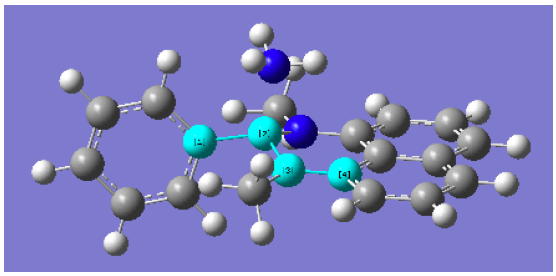
B–N bond: 1.53255 Å, 1.53255 Å

H = -929.172122 (hartree)

C	3.22388600	0.00000300	2.22504500
C	4.51515900	0.00000100	1.69052500
C	4.68067900	-0.00000200	0.30619600
C	3.56147300	-0.00000200	-0.53195000
C	2.25612300	0.00000000	-0.02167200
C	2.11798700	0.00000300	1.37577100
B	0.92151200	0.00000000	-0.98233800
N	0.07246900	1.24780200	-0.71621900
N	0.07246900	-1.24780300	-0.71621800
C	-1.20331300	1.25168500	-0.25283100
C	-1.20331300	-1.25168600	-0.25283000
C	-1.90296500	2.44489200	0.00259100
C	-3.22220300	2.41918600	0.48467800
C	-3.87981800	1.23650800	0.72685800
C	-3.21711400	0.00000000	0.48609700
C	-1.87910900	0.00000000	-0.00214200
C	-3.87981800	-1.23650800	0.72685900
C	-3.22220300	-2.41918600	0.48468000
C	-1.90296400	-2.44489200	0.00259300
F	1.37553000	-0.00000100	-2.33819400
C	0.72197700	-2.50803700	-0.95661300
C	0.72197600	2.50803700	-0.95661500
H	3.08373200	0.00000500	3.30912900
H	5.38551100	0.00000100	2.35120400
H	5.68711000	-0.00000400	-0.12129400
H	3.69021000	-0.00000400	-1.61814100
H	1.10864800	0.00000500	1.80166700

H	-1.42286700	3.40508700	-0.17146400
H	-3.72984100	3.37017100	0.66991900
H	-4.90527300	1.22219300	1.10132700
H	-4.90527200	-1.22219200	1.10132800
H	-3.72984100	-3.37017100	0.66992100
H	-1.42286700	-3.40508800	-0.17146200
H	1.72881600	-2.31746400	-1.34802200
H	0.81601100	-3.11334900	-0.03445100
H	0.17528000	-3.11838300	-1.69906300
H	1.72881500	2.31746300	-1.34802400
H	0.17527900	3.11838100	-1.69906600
H	0.81601100	3.11334800	-0.03445400

PhB(mdan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 167.5°

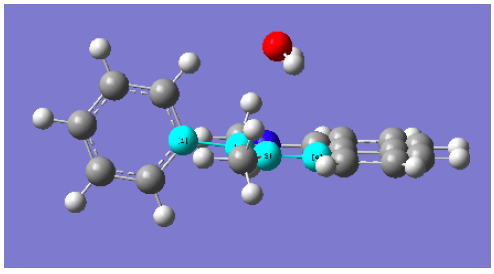
B–N(mdan) bond: 1.49835 Å, 1.49835 Å

H = -885.780344 (hartree)

C	4.16298400	-0.00000300	-1.61044500
C	5.14354600	-0.00000100	-0.61543600
C	4.76047300	0.00000200	0.72244200
C	3.40344900	0.00000300	1.05936300
C	2.40118400	0.00000100	0.08235200
C	2.81530000	-0.00000300	-1.26131300
B	0.81702400	0.00000100	0.36143400
N	0.10181000	-1.24700900	-0.06102800
N	0.10180900	1.24701000	-0.06102900
C	-1.27984700	-1.25549900	-0.10860500
C	-1.27984800	1.25549900	-0.10860600
C	-2.01484700	-2.44023300	-0.15592100
C	-3.42340800	-2.41787800	-0.18798300
C	-4.11732600	-1.23491400	-0.17363100
C	-3.41415800	0.00000000	-0.14093400

C	-1.98842500	0.00000000	-0.09918100
C	-4.11732600	1.23491300	-0.17363300
C	-3.42340900	2.41787700	-0.18798500
C	-2.01484800	2.44023200	-0.15592300
C	0.77118900	2.52661300	-0.07208900
C	0.77119000	-2.52661200	-0.07208800
H	4.45427300	-0.00000500	-2.66243000
H	6.20099200	-0.00000100	-0.88472300
H	5.51760600	0.00000400	1.50871000
H	3.14535700	0.00000500	2.12313800
H	2.05326700	-0.00000400	-2.04580900
H	-1.50738600	-3.40152600	-0.16920100
H	-3.96250800	-3.36668900	-0.22373300
H	-5.20772400	-1.21890600	-0.20182900
H	-5.20772400	1.21890400	-0.20183000
H	-3.96250900	3.36668800	-0.22373500
H	-1.50738700	3.40152600	-0.16920400
H	1.85632100	2.37799200	-0.06611400
H	0.51166600	3.10450500	-0.97432000
H	0.49835300	3.15395300	0.79973200
H	1.85632200	-2.37799000	-0.06611300
H	0.49835500	-3.15395200	0.79973500
H	0.51166800	-3.10450500	-0.97431800
H	0.98926200	-0.83080500	2.57259100
H	0.98926300	0.83080800	2.57259100
H	-0.40956500	0.00000200	2.25876300
N	0.60520100	0.00000100	2.11900400

PhB(mdan)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

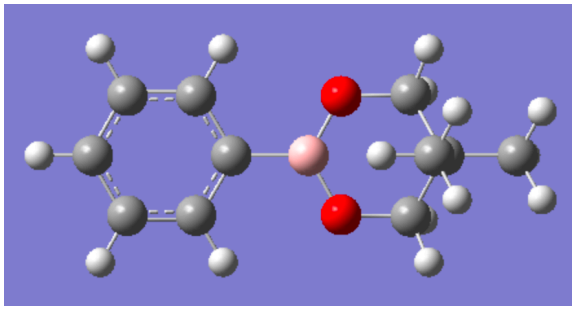
Dihedral angle = -173.4°

H = -905.650709 (hartree)

C	4.64704800	-0.00029900	-1.23759400
C	5.24530700	-0.00002500	0.02222800

C	4.44865500	0.00028100	1.16728200
C	3.05807200	0.00031200	1.05430600
C	2.44136600	0.00002000	-0.20732300
C	3.25621600	-0.00026600	-1.34873400
B	0.86500700	0.00002200	-0.28787800
N	0.13479200	-1.23250800	-0.31448000
N	0.13473200	1.23249700	-0.31455400
C	-1.25960800	-1.25068600	-0.24718900
C	-1.25966700	1.25064400	-0.24736300
C	-1.98012300	-2.43766600	-0.19456500
C	-3.38812100	-2.41964300	-0.10901500
C	-4.08159100	-1.23762600	-0.06986400
C	-3.38462600	-0.00005100	-0.11468000
C	-1.96186800	-0.00003400	-0.20523300
C	-4.08163100	1.23751000	-0.07009300
C	-3.38821400	2.41955100	-0.10945700
C	-1.98021400	2.43761200	-0.19497700
C	0.81073100	2.51675000	-0.31934200
C	0.81080000	-2.51674500	-0.31938100
H	5.26598500	-0.00053600	-2.13657500
H	6.33300900	-0.00004500	0.11116100
H	4.91321600	0.00050400	2.15496400
H	2.42944400	0.00055900	1.94922700
H	2.80028100	-0.00048200	-2.34258100
H	-1.46957000	-3.39659500	-0.22371100
H	-3.92404300	-3.36953200	-0.07258500
H	-5.17017600	-1.22537300	-0.00225800
H	-5.17021700	1.22522600	-0.00248700
H	-3.92418800	3.36941800	-0.07322000
H	-1.46967300	3.39654200	-0.22428800
H	1.89176300	2.36244700	-0.37600400
H	0.49288700	3.12270000	-1.18220800
H	0.58462800	3.08686400	0.59706100
H	1.89182100	-2.36244300	-0.37629200
H	0.58495100	-3.08685100	0.59709400
H	0.49274500	-3.12272000	-1.18214900
H	-0.42465200	0.75416400	2.21189200
H	-0.42395900	-0.75398600	2.21174100
O	0.04610700	0.00028500	2.58872500

PhB(neop)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

O–B–O angle = 121.9°

B–O bond: 1.36554 Å, 1.36554 Å

H = -602.650973 (hartree)

FIA = 252.8 (kJ/mol)

AA = 23.7 (kJ/mol)

HOMO: -0.29583 (hartree)

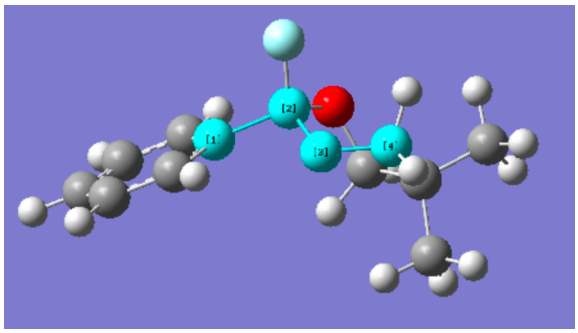
LUMO: 0.01213 (hartree)

GEI = 0.889 (eV)

C	-1.55028000	0.00000000	-0.12116100
B	0.00676800	0.00000000	-0.28938200
O	0.66673900	1.19380100	-0.35252500
C	2.07111300	1.22806300	-0.49348300
C	2.74225900	-0.00000100	0.12731800
C	2.07110900	-1.22803800	-0.49353100
O	0.66674000	-1.19380200	-0.35251300
C	2.54479000	-0.00003000	1.64606700
C	-2.26291800	1.20516000	-0.04306500
C	-3.64820400	1.20877400	0.10897400
C	-4.34138900	0.00000000	0.18513600
C	-3.64820500	-1.20877400	0.10896700
C	-2.26291800	-1.20516000	-0.04307200
C	4.22917500	0.00000500	-0.21606800
H	2.43696600	2.14802100	-0.01119000
H	2.32770800	1.28925600	-1.56594000
H	2.43699400	-2.14802000	-0.01130900
H	2.32766600	-1.28916000	-1.56600200
H	1.48068900	-0.00001400	1.92191300
H	3.00920500	-0.89091900	2.09436400
H	3.00924300	0.89082000	2.09440100

H	-1.71407600	2.14754400	-0.10382100
H	-4.19116200	2.15364100	0.16851500
H	-5.42651100	0.00000000	0.30411500
H	-4.19116300	-2.15364100	0.16850300
H	-1.71407700	-2.14754300	-0.10383400
H	4.72438300	-0.88873300	0.20284200
H	4.39089700	0.00000600	-1.30467900
H	4.72437700	0.88874600	0.20284200

PhB(neop)–F^-



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 156.6°

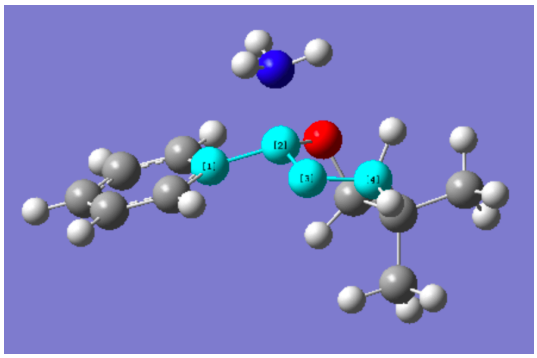
B–O bond: 1.47581 Å, 1.48081 Å

H = -702.467232 (hartree)

C	1.48174700	-0.29395200	-0.02137500
B	-0.01932700	-0.94616700	-0.07481700
O	-0.77969600	-0.44952500	-1.24443000
C	-1.42711600	0.74029900	-0.96372000
C	-2.57745100	0.52813500	0.05251300
C	-2.10128200	-0.61384300	0.98505400
O	-0.72766100	-0.56934300	1.16385000
C	-3.85155700	0.09502000	-0.66732500
C	2.18518500	-0.14871600	1.18422700
C	3.47360400	0.38688500	1.22605300
C	4.09618600	0.80451000	0.04757700
C	3.41319600	0.68327000	-1.16334600
C	2.12462400	0.14398300	-1.18800800
C	-2.79903600	1.81234300	0.84629800
F	0.04953800	-2.35460200	-0.20105600
H	-1.84135700	1.17392400	-1.89587100
H	-0.72404700	1.49250000	-0.54459600

H	-2.41409100	-1.58228300	0.54441700
H	-2.61269900	-0.52261000	1.96396100
H	-3.62099200	-0.74279600	-1.34315600
H	-4.62216700	-0.23923100	0.04869600
H	-4.27665000	0.91942700	-1.26409300
H	1.69136600	-0.46030900	2.10897900
H	3.99732700	0.48617100	2.18130800
H	5.10425200	1.22664200	0.07426200
H	3.88864800	1.01515900	-2.09094500
H	1.58026900	0.05762500	-2.13301200
H	-3.67778400	1.72963400	1.50776600
H	-1.91305000	2.01701300	1.46677700
H	-2.95798500	2.67472900	0.17605500

PhB(neop)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 156.5°

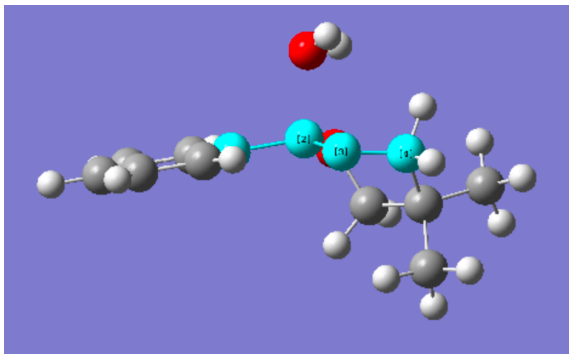
B–O bond: 1.43391 Å, 1.44128 Å

H = -659.094975 (hartree)

C	-1.47520000	0.15521300	0.04231600
B	0.01804800	0.74774500	0.15840800
O	0.79121700	0.79326700	-1.05708500
C	1.52399200	-0.39581000	-1.20593000
C	2.61239100	-0.53112300	-0.10976500
C	2.13409200	0.29210700	1.10563300
O	0.74656400	0.21913700	1.27462000
C	3.94367000	0.03886500	-0.59701700
C	-2.13681500	-0.38674100	1.15372500
C	-3.44750100	-0.85563500	1.05878200
C	-4.12310300	-0.79396500	-0.16091000
C	-3.47991100	-0.26859000	-1.28177300

C	-2.16922900	0.19922000	-1.17528200
C	2.75800800	-2.00237600	0.27609200
H	1.99025400	-0.40344300	-2.20420600
H	0.84144800	-1.26609800	-1.15473100
H	2.46278800	1.34460300	0.96649000
H	2.62426400	-0.07411200	2.02237400
H	3.80270600	1.05608700	-0.99432400
H	4.67921800	0.08805800	0.22205200
H	4.37069700	-0.58557600	-1.39647000
H	-1.59898400	-0.45488900	2.10342500
H	-3.94386200	-1.27827500	1.93480300
H	-5.14751200	-1.16289300	-0.23953000
H	-4.00047900	-0.23104800	-2.24093400
H	-1.65681100	0.59295800	-2.05849800
H	3.59377500	-2.14762500	0.97802400
H	1.83410000	-2.36065700	0.75443000
H	2.94947100	-2.62564900	-0.61178500
H	-0.66255300	2.82154000	-0.33987800
H	-0.75981400	2.53193600	1.29510300
H	0.71903700	2.84448700	0.58184600
N	-0.19037000	2.39509300	0.45918000

PhB(neop)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

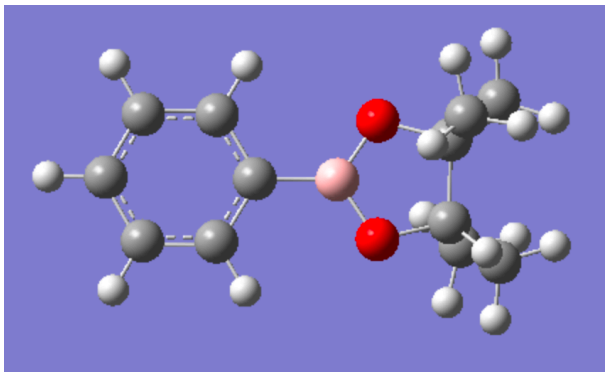
Dihedral angle = 165.9°

H = -678.943999 (hartree)

C	-1.52969900	0.10101100	0.05569900
B	-0.01390500	0.52912300	0.21680500
O	0.75100400	0.87325800	-0.93016400
C	1.61486800	-0.18284000	-1.28791900
C	2.66733900	-0.47000000	-0.18596200

C	2.10271200	0.07850700	1.13977400
O	0.71163400	-0.09872900	1.23972200
C	3.98160000	0.24874900	-0.49027100
C	-2.19795000	-0.61224200	1.06006300
C	-3.53272800	-0.98739300	0.90960800
C	-4.22095900	-0.65632200	-0.25817200
C	-3.56921400	0.04566700	-1.27271900
C	-2.23463000	0.41723500	-1.11329100
C	2.88708700	-1.97899300	-0.07962800
H	2.11413200	0.08416600	-2.23171100
H	1.02022100	-1.09539200	-1.47844600
H	2.35781900	1.15507200	1.21478100
H	2.58187500	-0.42701800	1.99231800
H	3.80197800	1.31717800	-0.68692900
H	4.68376500	0.16819800	0.35474200
H	4.46952900	-0.18475400	-1.37610000
H	-1.65333200	-0.88266000	1.96817600
H	-4.03888900	-1.54347800	1.70111800
H	-5.26526600	-0.95023800	-0.37972100
H	-4.10387100	0.29938800	-2.19013600
H	-1.71803300	0.95883700	-1.90987000
H	3.69991400	-2.21102900	0.62543300
H	1.96930500	-2.47403500	0.27136800
H	3.15537100	-2.40717400	-1.05807400
H	0.16073900	2.28506500	1.75332700
H	0.53591400	2.71845700	0.30453700
O	-0.15166300	2.29091300	0.83770200

PhB(pin)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

O–B–O angle = 112.6°

B–O bond: 1.36931 Å, 1.36931 Å

H = -641.895641 (hartree)

FIA = 265.6 (kJ/mol)

AA = 36.2 (kJ/mol)

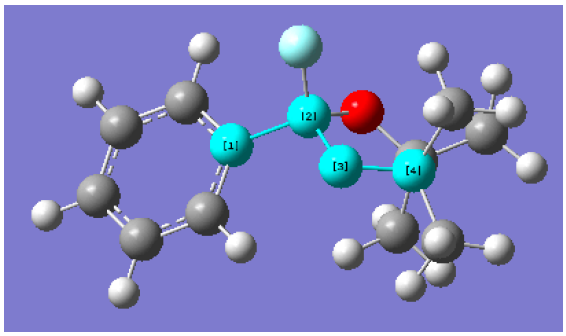
HOMO: -0.30065 (hartree)

LUMO: 0.00806 (hartree)

GEI = 0.943 (eV)

C	-3.78284500	-1.19675900	0.17440400
C	-4.47932000	0.00000000	0.00000000
C	-3.78284500	1.19676000	-0.17440400
C	-2.38942000	1.19383200	-0.17308500
C	-1.67425600	0.00000000	0.00000000
C	-2.38942000	-1.19383200	0.17308500
B	-0.11730900	0.00000100	0.00000300
O	0.64234200	1.11970500	-0.21025200
C	2.00561500	0.77847200	0.09579300
C	2.00561400	-0.77847200	-0.09579500
O	0.64234100	-1.11970400	0.21025300
C	2.25632800	-1.19216500	-1.54382900
C	2.93288800	-1.53406900	0.84048500
C	2.25633100	1.19216000	1.54382800
C	2.93289000	1.53407200	-0.84048600
H	-4.32956600	-2.13136300	0.31046400
H	-5.57090700	0.00000000	0.00000000
H	-4.32956600	2.13136400	-0.31046400
H	-1.83788600	2.12707100	-0.30779200
H	-1.83788700	-2.12707000	0.30779200
H	1.60199200	-0.63425700	-2.22889100
H	3.30153100	-1.02264000	-1.83731400
H	2.02958100	-2.26186000	-1.64773600
H	2.86650300	-2.61046100	0.63090500
H	3.97545100	-1.21625500	0.69120800
H	2.65769600	-1.37290800	1.88957400
H	1.60199400	0.63425100	2.22888800
H	3.30153300	1.02263100	1.83731100
H	2.02958600	2.26185500	1.64773800
H	3.97545300	1.21626000	-0.69120700
H	2.65770000	1.37291300	-1.88957400
H	2.86650100	2.61046300	-0.63090300

PhB(pin)–F^-



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 140.3°

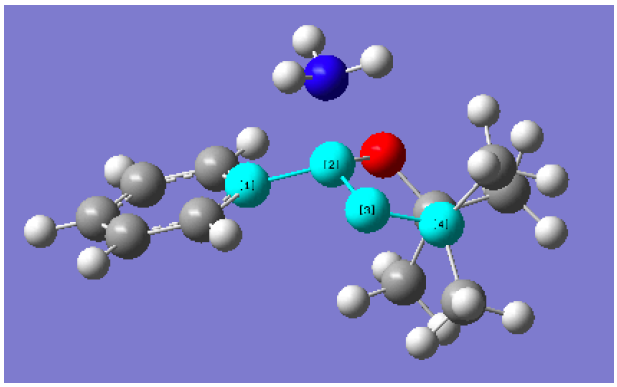
B–O bond: 1.47617 Å, 1.48314 Å

H = -741.716778 (hartree)

C	-3.30392400	1.41370700	-0.49695900
C	-4.24639100	0.60220400	0.13489500
C	-3.85683400	-0.65503000	0.60303400
C	-2.53971500	-1.08498000	0.43801100
C	-1.56859400	-0.28538400	-0.18572900
C	-1.98781700	0.96934400	-0.64999000
B	-0.02108300	-0.79486000	-0.32938100
O	0.70671000	-0.78624500	0.96288700
C	1.71956700	0.17450500	0.91395900
C	2.02241700	0.27736600	-0.62072900
O	0.74836100	0.13220900	-1.18236000
C	2.62391100	1.60843900	-1.06076400
C	2.91905700	-0.87698800	-1.09216700
C	2.90419400	-0.28572400	1.76014200
C	1.18009200	1.50219400	1.46641600
F	-0.01426000	-2.12078600	-0.83775100
H	-3.59889200	2.39734800	-0.87373300
H	-5.27717500	0.94400900	0.25957600
H	-4.58827400	-1.30162900	1.09633500
H	-2.24576700	-2.07524000	0.79800500
H	-1.24765300	1.59860400	-1.15301300
H	1.92344400	2.43121200	-0.86542100
H	3.57375500	1.81323000	-0.53991600
H	2.82016600	1.58085400	-2.14351600
H	2.90211600	-0.89448300	-2.19195500
H	3.96161900	-0.76824100	-0.75171800

H	2.50792200	-1.83046200	-0.73240800
H	3.20519700	-1.30184700	1.47446700
H	3.76688900	0.39241200	1.65137900
H	2.60941100	-0.30584600	2.82048900
H	1.95728700	2.27957900	1.54509200
H	0.36584000	1.86506300	0.82258500
H	0.76152500	1.31116600	2.46548000

PhB(pin)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 138.9°

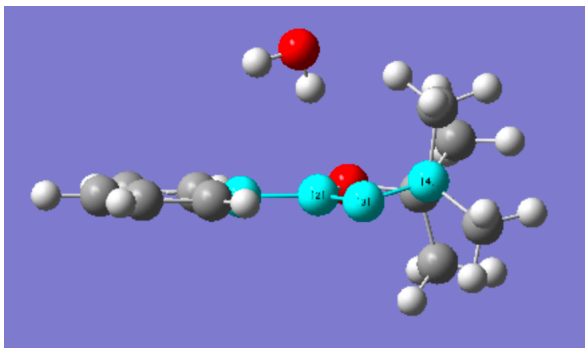
B–O bond: 1.43500 Å, 1.43962 Å

H = -698.344395 (hartree)

C	3.58867400	-0.82734900	0.99677600
C	4.27107300	0.27053800	0.47079300
C	3.60156300	1.16524900	-0.36440200
C	2.25756600	0.95394600	-0.67627000
C	1.55623500	-0.14833700	-0.16764800
C	2.24502000	-1.02913600	0.67910500
B	0.01862300	-0.40587300	-0.56489200
O	-0.76325300	0.72212200	-0.99941600
C	-1.75720700	0.93125000	-0.00555800
C	-2.04203700	-0.53169500	0.48107300
O	-0.75881600	-1.13549700	0.39555300
C	-2.54737100	-0.63780500	1.91236600
C	-3.00383200	-1.26509400	-0.46001000
C	-2.95182400	1.63888600	-0.62657200
C	-1.15798400	1.79070300	1.11027500
H	4.10548100	-1.52140200	1.66284300

H	5.32139700	0.43369000	0.71942900
H	4.12847000	2.03325400	-0.76610300
H	1.72615800	1.66768100	-1.31283800
H	1.70431600	-1.87596600	1.11224800
H	-1.79593300	-0.26110500	2.61664000
H	-3.48158700	-0.07108600	2.04487100
H	-2.74434900	-1.69147400	2.15713100
H	-2.94996900	-2.34279400	-0.24860300
H	-4.04367900	-0.93402200	-0.32610200
H	-2.73609900	-1.09169000	-1.51400800
H	-3.30262700	1.11482600	-1.52460700
H	-3.78227800	1.71162300	0.09194500
H	-2.66106600	2.65720300	-0.92081300
H	-1.90666400	2.05855700	1.86971300
H	-0.32562000	1.26439500	1.59989700
H	-0.76184900	2.71343900	0.66351100
H	0.53524500	-0.84579100	-2.71439700
H	0.69810900	-2.19997300	-1.76807300
H	-0.81958800	-1.68332100	-2.22513700
N	0.11661500	-1.38094600	-1.95167900

PhB(pin)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

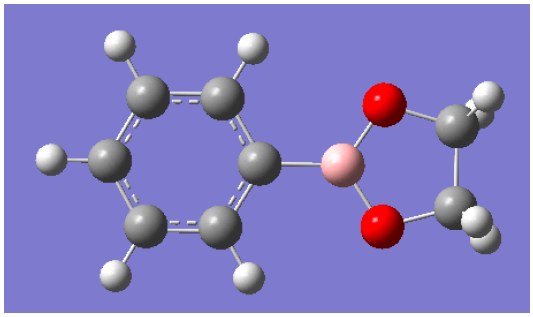
Dihedral angle = -166.2°

H = -718.210221 (hartree)

C	3.74879200	-1.31754800	-0.21230800
C	4.44385500	-0.17669000	0.19193000
C	3.74661300	0.95106900	0.62782100
C	2.35332500	0.93371700	0.66044600
C	1.63938500	-0.20468000	0.25561100
C	2.35555200	-1.32822700	-0.18198500

B	0.08180000	-0.20258200	0.25205100
O	-0.65691000	0.91924600	0.54209500
C	-2.04750700	0.53160100	0.56007900
C	-2.03613800	-0.80071400	-0.27369100
O	-0.68987100	-1.27771600	-0.07088400
C	-3.01427900	-1.85601700	0.21283100
C	-2.19837300	-0.56444400	-1.77304400
C	-2.87501200	1.64888400	-0.05217100
C	-2.42567400	0.31699600	2.02207000
H	4.29645900	-2.19739900	-0.55376800
H	5.53495800	-0.16590600	0.16627100
H	4.29193000	1.84158100	0.94446800
H	1.80337100	1.81280900	1.00615200
H	1.80457900	-2.21507400	-0.50274100
H	-2.80598900	-2.15242900	1.24781900
H	-4.04650000	-1.48116500	0.14897700
H	-2.93205500	-2.74792800	-0.42296700
H	-1.99838900	-1.50976400	-2.29608800
H	-3.21903700	-0.23940300	-2.01856700
H	-1.47981000	0.18752300	-2.13079300
H	-2.50031200	1.92002500	-1.04735100
H	-3.92791000	1.34345600	-0.14142900
H	-2.82726300	2.53758900	0.59225400
H	-3.49130200	0.07239500	2.12968100
H	-1.83037800	-0.49368300	2.46576100
H	-2.21793400	1.24046300	2.57937500
H	0.04086900	1.90305100	-1.12819000
H	1.19364200	1.36619900	-1.94827300
O	0.31663400	1.75683000	-2.04325900

PhB(eg)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

O–B–O angle = 112.8°

B–O bond: 1.36835 Å, 1.36835 Å

H = -484.935047 (hartree)

FIA = 258.4 (kJ/mol)

AA = 36.3 (kJ/mol)

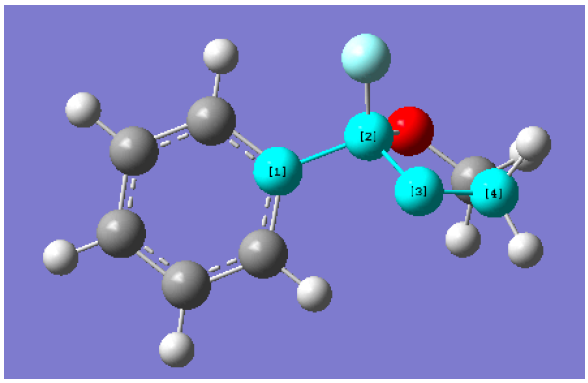
HOMO: -0.30237 (hartree)

LUMO: 0.00641 (hartree)

GEI = 0.965 (eV)

C	2.68979400	-1.20934100	0.01237600
C	3.38612400	0.00000000	-0.00002000
C	2.68979400	1.20934100	-0.01239400
C	1.29640200	1.20649800	-0.01200100
C	0.58180600	0.00000100	0.00002100
C	1.29640100	-1.20649700	0.01202000
B	-0.97357200	0.00000100	0.00006100
O	-1.73097000	1.13928300	-0.02739900
C	-3.09834000	0.77067900	0.06525700
C	-3.09833600	-0.77067900	-0.06529500
O	-1.73097000	-1.13928400	0.02740600
H	3.23633400	-2.15381200	0.02206400
H	4.47770900	-0.00000100	-0.00003500
H	3.23633500	2.15381100	-0.02209300
H	0.74551300	2.14969900	-0.02121300
H	0.74551200	-2.14969800	0.02125600
H	-3.49924200	1.10628400	1.03370700
H	-3.67071000	1.26344800	-0.73269100
H	-3.49920600	-1.10627500	-1.03376200
H	-3.67073400	-1.26345700	0.73262800

PhB(eg)–F^-



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

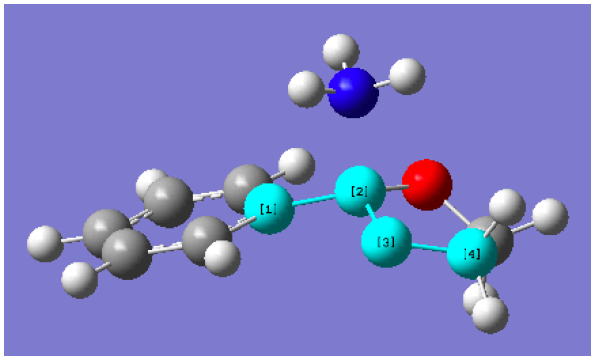
Dihedral angle = 140.9°

B–O bond: 1.47626 Å, 1.48356 Å

H = -584.753477 (hartree)

C	2.46897000	-1.46343400	-0.13144700
C	3.40769200	-0.45942700	0.11413400
C	2.97272700	0.86052600	0.24517800
C	1.61379100	1.16330900	0.13511900
C	0.64859300	0.17315700	-0.10027800
C	1.11423900	-1.14303100	-0.23737300
B	-0.94836500	0.51784300	-0.16413100
O	-1.60812300	0.33890300	1.15255500
C	-2.57159500	-0.65019900	1.04106500
C	-2.86324900	-0.73421100	-0.46321100
O	-1.64129000	-0.43627300	-1.05231600
F	-1.12106900	1.86150600	-0.58730300
H	2.79965600	-2.49999000	-0.24553800
H	4.47018800	-0.70308400	0.19714000
H	3.70007500	1.65646800	0.43012100
H	1.27683300	2.19983200	0.22462400
H	0.37967200	-1.92531400	-0.44865600
H	-2.19635600	-1.63484400	1.40384500
H	-3.47613900	-0.41082100	1.63444600
H	-3.64747900	0.00596100	-0.73672100
H	-3.22669700	-1.73215100	-0.77391600

PhB(eg)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

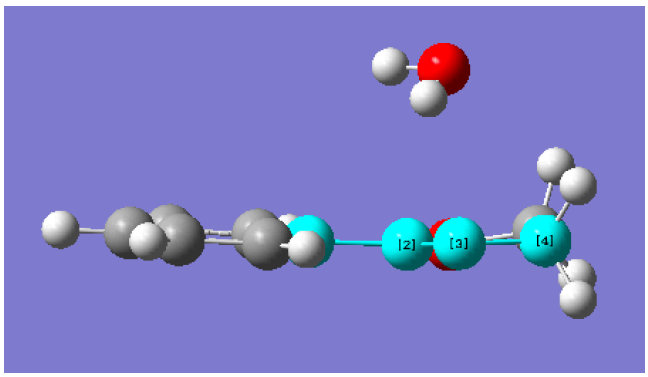
Dihedral angle = 146.7°

B–O bond: 1.43238 Å, 1.43828 Å

H = -541.383851 (hartree)

C	2.78017300	-1.17559900	0.35266200
C	3.47295100	0.03476600	0.30064100
C	2.77311700	1.22378300	0.09431100
C	1.38700400	1.19677100	-0.06699900
C	0.67345600	-0.00917000	-0.02849300
C	1.39453700	-1.19189600	0.19019600
B	-0.91160200	-0.03623900	-0.26693800
O	-1.65238900	1.17495600	-0.03696300
C	-2.68342800	0.87074100	0.87146800
C	-2.89457500	-0.63946400	0.70015000
O	-1.62584600	-1.12262400	0.33417500
H	3.32307600	-2.10650500	0.52866400
H	4.55675700	0.05186800	0.42990700
H	3.31019400	2.17411200	0.06708000
H	0.83498400	2.13079100	-0.20613700
H	0.85037000	-2.13874000	0.25521700
H	-2.37091600	1.10397800	1.90546900
H	-3.58724500	1.45821900	0.64715800
H	-3.64250400	-0.83922700	-0.09545600
H	-3.24660200	-1.13513300	1.61699700
H	-0.66212300	0.53939400	-2.44893900
H	-0.55156100	-1.10519900	-2.25409600
H	-2.04188400	-0.35801600	-2.22345300
N	-1.05829500	-0.26751500	-1.96414700

PhB(eg)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

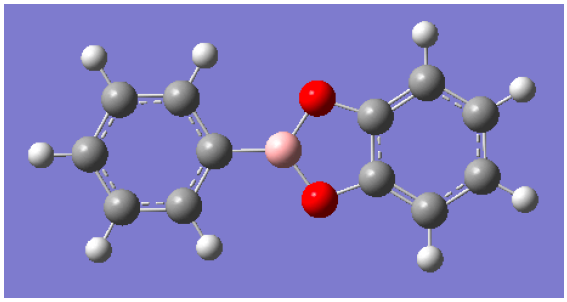
Dihedral angle = -176.2°

H = -561.247805 (hartree)

C	2.84965200	-1.19550500	0.19630000
C	3.54803700	-0.01194100	-0.04696500

C	2.86400000	1.20217600	-0.12456000
C	1.48054700	1.23004200	0.04142800
C	0.76360600	0.04972000	0.28765800
C	1.46620600	-1.16223100	0.36136000
B	-0.78578700	0.08285000	0.43845900
O	-1.52460600	1.22717700	0.41389100
C	-2.89507000	0.85905400	0.32709800
C	-2.91088800	-0.66394100	0.59258600
O	-1.54183000	-1.05342800	0.56675200
H	3.38692400	-2.14330000	0.25806400
H	4.63157800	-0.03584200	-0.17638900
H	3.41259600	2.12626600	-0.31396600
H	0.93831300	2.17672900	-0.01651100
H	0.91456700	-2.08533500	0.55517300
H	-3.47749300	1.42718400	1.06518300
H	-3.25774600	1.09193100	-0.68355100
H	-3.46121900	-1.21107100	-0.18517700
H	-3.33826900	-0.91926600	1.57365300
H	-1.22693900	-1.15099500	-1.73405500
H	-0.73858000	0.13656500	-2.36440600
O	-1.53998000	-0.38266900	-2.22811000

PhB(cat)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

O–B–O angle = 110.7°

B–O bond: 1.38647 Å, 1.38647 Å

H = -637.185510 (hartree)

FIA = 322.8 (kJ/mol)

AA = 54.7 (kJ/mol)

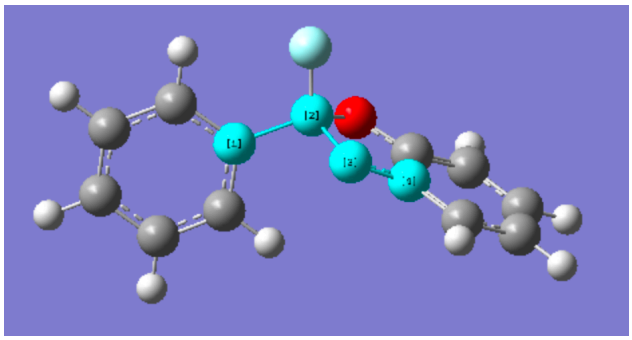
HOMO: -0.28380 (hartree)

LUMO: -0.01009 (hartree)

GEI = 1.073 (eV)

C	3.88615400	1.20968300	-0.00000200
C	4.58223300	0.00000000	-0.00002000
C	3.88615500	-1.20968300	-0.00003500
C	2.49332200	-1.20765700	-0.00003100
C	1.77915900	0.00000000	-0.00001300
C	2.49332200	1.20765700	0.00000200
B	0.23268500	-0.00000100	-0.00001100
O	-0.55605800	-1.14025400	-0.00001700
C	-1.84906700	-0.69830900	-0.00000400
C	-1.84906600	0.69830900	0.00002000
O	-0.55605700	1.14025400	0.00002200
C	-3.02269400	-1.43031200	-0.00000900
C	-4.21722300	-0.69883300	0.00001400
C	-4.21722300	0.69883400	0.00003800
C	-3.02269400	1.43031200	0.00004100
H	4.43225800	2.15440000	0.00000900
H	5.67379900	0.00000100	-0.00002300
H	4.43225900	-2.15439900	-0.00004900
H	1.94484400	-2.15240200	-0.00004300
H	1.94484200	2.15240100	0.00001600
H	-3.00663100	-2.51962000	-0.00002700
H	-5.16775500	-1.23347100	0.00001300
H	-5.16775500	1.23347200	0.00005600
H	-3.00663000	2.51962000	0.00006000

PhB(cat)–F^-



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 125.1°

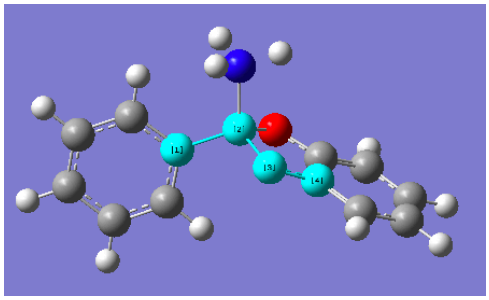
B–O bond: 1.50504 Å, 1.50504 Å

H = -737.028447 (hartree)

C	2.96561200	-1.87960600	0.00010300
C	4.16804200	-1.16846900	0.00012000
C	4.13732900	0.22570000	0.00005800
C	2.91198500	0.89751600	-0.00002000
C	1.69385900	0.20727500	-0.00003600
C	1.75119000	-1.19432000	0.00002600
B	0.26179300	0.97202200	-0.00010800
O	-0.57966000	0.55460400	1.17584300
C	-1.74791000	0.12087500	0.70972000
C	-1.74791900	0.12073000	-0.70973600
O	-0.57967300	0.55436200	-1.17596200
C	-2.85985500	-0.30552600	1.41771300
C	-3.99017700	-0.74023600	0.69465600
C	-3.99018600	-0.74037800	-0.69446900
C	-2.85987300	-0.30581500	-1.41762900
F	0.43721200	2.36135700	-0.00024800
H	2.97985400	-2.97271600	0.00015000
H	5.12302700	-1.69983000	0.00018100
H	5.07349200	0.79061700	0.00006900
H	2.88564700	1.99028100	-0.00007200
H	0.81325900	-1.75814800	0.00001000
H	-2.84375000	-0.29923700	2.50860900
H	-4.87476100	-1.08074700	1.23764600
H	-4.87477600	-1.08099900	-1.23737900
H	-2.84378100	-0.29974900	-2.50852600

PhB(cat)–NH_3

The optimized structure of PhB(cat)-NH_3 obtained from the optimized structures of PhB(cat)-F was confirmed not to be local minima by verifying the presence of imaginary frequencies at the M06-2X/def2-SVP level of theory. Thus, we optimized the PhB(cat)-NH_3 structure starting from the following structure (Dihedral angle = 128.1°) at the M06-2X/def2-SVP level of theory and confirmed that the resulting structure have no imaginary frequency.

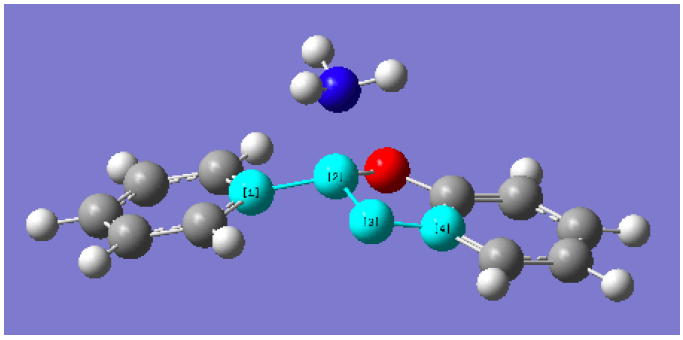


Dihedral angle = 128.1°

C	3.06137361	-1.84720942	-0.00016920
C	4.23483755	-1.09727926	0.00022841
C	4.15176143	0.29077395	0.00045416
C	2.90651874	0.91629143	0.00028354
C	1.71197465	0.18824999	-0.00010730
C	1.82597303	-1.20800594	-0.00033182
B	0.26064131	0.91558095	-0.00025169
O	-0.58802736	0.49603514	1.18159864
C	-1.77435507	0.09596384	0.70592698
C	-1.77439507	0.09562350	-0.70591327
O	-0.58808858	0.49545774	-1.18184375
C	-2.89536444	-0.29688927	1.41388712
C	-4.03455611	-0.69781540	0.69402434
C	-4.03459516	-0.69814851	-0.69350543
C	-2.89544263	-0.29756836	-1.41362341
H	3.11225837	-2.93127377	-0.00035524
H	5.20109267	-1.59025646	0.00035547
H	5.05891855	0.88682867	0.00075852
H	2.85062984	1.99870844	0.00044784
H	0.92224429	-1.80816061	-0.00065276
H	-2.88608754	-0.29265394	2.49738393
H	-4.92195262	-1.00961581	1.23341466
H	-4.92202128	-1.01020879	-1.23269658

H	-2.88622522	-0.29385355	-2.49712269
H	0.97196941	2.85872029	0.87302993
H	0.97227030	2.85827750	-0.87427299
H	-0.53279201	3.01673867	-0.00092078
N	0.43318523	2.55653447	-0.00063781

PhB(cat)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 147.0°

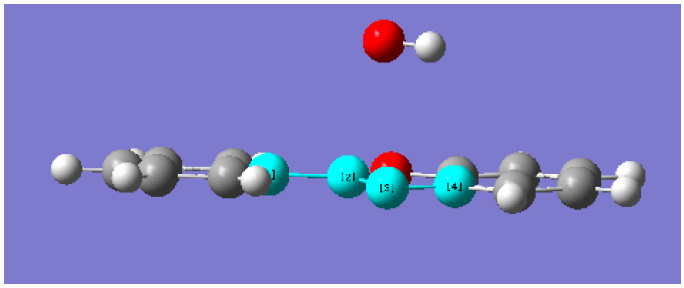
B–O bond: 1.45372 Å, 1.45375 Å

H = -693.641305 (hartree)

C	3.79717100	-1.20650200	0.48795500
C	4.47697200	0.00059700	0.65283900
C	3.79653100	1.20736900	0.48825900
C	2.44252700	1.20264700	0.15232900
C	1.74467400	-0.00003500	-0.02638600
C	2.44318000	-1.20239500	0.15201700
B	0.21548300	-0.00043000	-0.46318400
O	-0.58295100	1.17093500	-0.14101200
C	-1.83345500	0.70349600	0.09522200
C	-1.83347900	-0.70345500	0.09623100
O	-0.58296200	-1.17125700	-0.13923000
C	-2.99381800	1.42275200	0.31899600
C	-4.17484700	0.69669200	0.54645000
C	-4.17486000	-0.69594800	0.54748000
C	-2.99385100	-1.42236300	0.32105800
H	4.32347000	-2.15229700	0.62996300
H	5.53553700	0.00083600	0.91879500
H	4.32231400	2.15341600	0.63049200
H	1.90612400	2.14981500	0.04614800
H	1.90724800	-2.14981900	0.04564400

H	-2.97629600	2.51260000	0.32216800
H	-5.10568100	1.23584200	0.72692800
H	-5.10570200	-1.23481300	0.72876500
H	-2.97634100	-2.51220600	0.32583100
H	0.70394600	0.82894700	-2.52789300
H	0.70431300	-0.83204200	-2.52737800
H	-0.73896100	-0.00184100	-2.52187300
N	0.22420800	-0.00154800	-2.17634600

PhB(cat)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

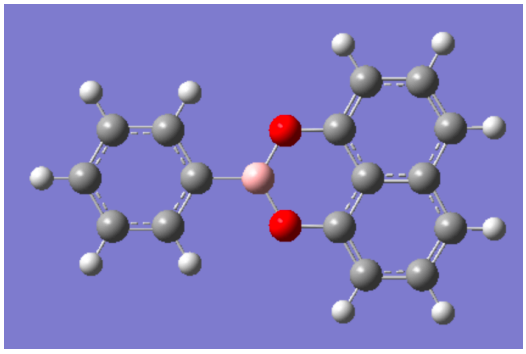
Dihedral angle = 179.3°

H = -713.495645 (hartree)

C	-3.93299700	-1.22349600	-0.07161600
C	-4.62617800	-0.01621700	-0.17098300
C	-3.92708400	1.18619600	-0.28358900
C	-2.53409200	1.17863400	-0.29621500
C	-1.82344700	-0.02631100	-0.19670600
C	-2.54029000	-1.22644200	-0.08490200
B	-0.27801400	-0.03255800	-0.20959500
O	0.51095400	1.11370000	-0.30252000
C	1.80009900	0.66985100	-0.29643000
C	1.79940200	-0.72924200	-0.25707800
O	0.51318800	-1.17330000	-0.23972400
C	2.97511000	1.40002500	-0.31380000
C	4.17145400	0.67011000	-0.28707300
C	4.17135200	-0.72621700	-0.24582400
C	2.97580700	-1.45752200	-0.22990900
H	-4.48186400	-2.16229100	0.01740400
H	-5.71759800	-0.01254400	-0.16055100
H	-4.47093900	2.12887200	-0.36215400
H	-1.98387100	2.11801700	-0.38701800

H	-1.99367900	-2.16851400	-0.00526400
H	2.95910200	2.48895700	-0.34928900
H	5.12148900	1.20518000	-0.29976500
H	5.12163600	-1.26066000	-0.22566300
H	2.95968100	-2.54640300	-0.19850500
H	1.27117200	-0.12041100	2.34737200
H	0.44677300	1.14555300	2.21050000
O	0.36377600	0.20345200	2.40045100

PhB(nad)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

O–B–O angle = 120.6°

B–O bond: 1.37387 Å, 1.37387 Å

H = -790.616097 (hartree)

FIA = 334.7 (kJ/mol)

AA = 64.8 (kJ/mol)

HOMO: -0.25591 (hartree)

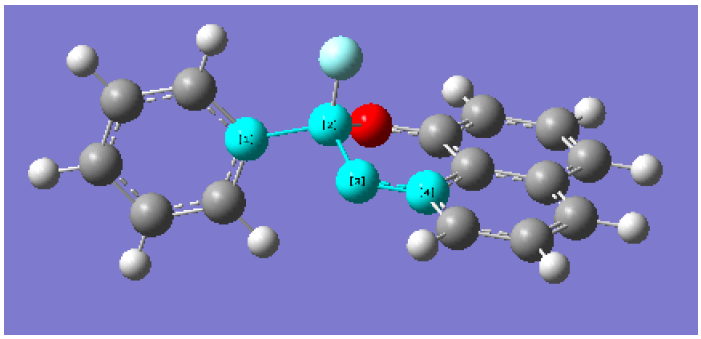
LUMO: -0.01030 (hartree)

GEI = 0.981 (eV)

C	-4.59106100	-1.20941600	-0.00001100
C	-5.28753000	0.00000000	0.00000300
C	-4.59106100	1.20941600	0.00001500
C	-3.19807500	1.20665600	0.00001200
C	-2.48250500	0.00000000	-0.00000200
C	-3.19807500	-1.20665600	-0.00001400
B	-0.92720800	0.00000000	-0.00000600
O	-0.24666900	1.19347400	0.00002100
C	1.11759900	1.22833900	-0.00000600
C	1.82870100	0.00000000	-0.00000100

C	1.11759900	-1.22833900	0.00000400
O	-0.24666900	-1.19347400	-0.00002600
C	1.78461800	2.42837100	-0.00003000
C	3.20068900	2.42735000	-0.00003800
C	3.91873100	1.25432400	-0.00001900
C	3.24872100	0.00000000	0.00000100
C	3.91873100	-1.25432400	0.00002300
C	3.20068900	-2.42735000	0.00004000
C	1.78461800	-2.42837100	0.00003000
H	-5.13704800	-2.15428800	-0.00002100
H	-6.37916600	0.00000000	0.00000500
H	-5.13704800	2.15428800	0.00002600
H	-2.64860000	2.15066400	0.00002100
H	-2.64860000	-2.15066400	-0.00002500
H	1.21290200	3.35582700	-0.00003400
H	3.72683100	3.38322000	-0.00005600
H	5.00970900	1.27050000	-0.00001900
H	5.00970900	-1.27050000	0.00002500
H	3.72683100	-3.38322000	0.00006100
H	1.21290200	-3.35582700	0.00003400

PhB(nad)–F$^-$



Charge = -1; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 160.1°

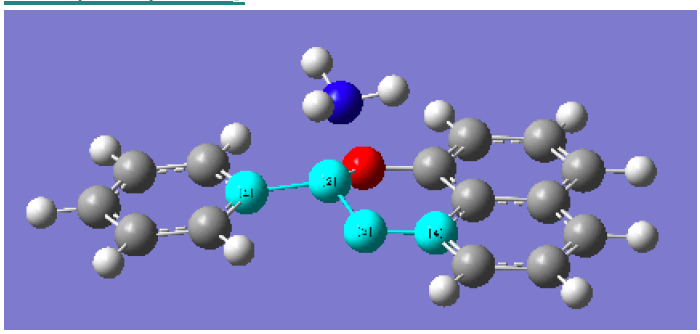
B–O bond: 1.48777 Å, 1.48776 Å

H = -890.463572 (hartree)

C	3.22300100	-2.42352800	-0.21175000
C	3.94476600	-1.24968000	-0.23308300
C	3.26896500	-0.00003800	-0.16161000
C	1.85150200	-0.00002000	-0.03838300
C	1.12047600	-1.23062100	-0.01350100

C	1.81755500	-2.42936700	-0.10757700
C	3.94483900	1.24959200	-0.23261900
C	3.22314400	2.42347500	-0.21084900
C	1.81769800	2.42935500	-0.10667100
C	1.12055100	1.23061500	-0.01304900
O	-0.20006200	-1.21631800	0.06694000
O	-0.19999500	1.21636200	0.06736300
B	-0.87545300	-0.00004100	0.59418300
F	-0.76356200	-0.00030800	1.99621500
C	-2.42385500	0.00006600	0.12130100
C	-2.77563700	0.00101600	-1.23610100
C	-4.10831800	0.00104500	-1.64763000
C	-5.13234700	0.00011700	-0.69783100
C	-4.80685800	-0.00082600	0.65818400
C	-3.46732900	-0.00083600	1.05472600
H	3.74957800	-3.37952800	-0.27558200
H	5.03341700	-1.26029800	-0.31812000
H	1.24787300	-3.35858000	-0.09040000
H	5.03349000	1.26017600	-0.31765700
H	3.74977600	3.37946800	-0.27432500
H	1.24807000	3.35859400	-0.08915100
H	-1.97868100	0.00177800	-1.98510600
H	-4.35420800	0.00180700	-2.71278200
H	-6.17815500	0.00013100	-1.01482900
H	-5.60171300	-0.00156200	1.40879800
H	-3.20859100	-0.00155500	2.11654000

PhB(nad)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

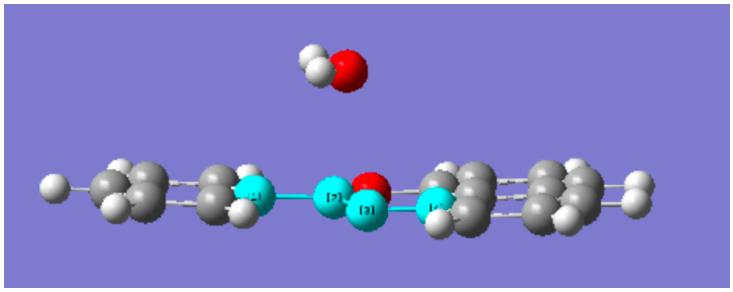
Dihedral angle = 169.8°

B–O bond: 1.44109 Å, 1.44110 Å

H = -847.075741 (hartree)

C	-3.25465800	2.42511300	-0.17309600
C	-3.96822800	1.24931400	-0.14709600
C	-3.28998600	-0.00007400	-0.13212500
C	-1.86690900	-0.00002700	-0.12360400
C	-1.15154500	1.23634200	-0.14768900
C	-1.84119800	2.43101200	-0.17333700
C	-3.96814000	-1.24951200	-0.14681200
C	-3.25449000	-2.42526900	-0.17254600
C	-1.84102800	-2.43107800	-0.17273900
C	-1.15146600	-1.23635700	-0.14731600
O	0.19479700	1.21999600	-0.14247200
O	0.19489600	-1.21993000	-0.14197500
B	0.85733400	0.00014300	0.24450900
C	2.42796200	0.00009800	-0.02711400
C	3.14229300	-1.20214600	-0.12563600
C	4.52552700	-1.20682700	-0.30689200
C	5.22028700	-0.00020400	-0.39389200
C	4.52586900	1.20657000	-0.30600000
C	3.14262100	1.20212400	-0.12474000
H	-3.78483400	3.37887500	-0.19509200
H	-5.05920500	1.25797000	-0.15102700
H	-1.27486600	3.36179500	-0.20102000
H	-5.05911600	-1.25824600	-0.15074200
H	-3.78460900	-3.37906800	-0.19434200
H	-1.27463400	-3.36182900	-0.20015400
H	2.59646300	-2.14837400	-0.07924800
H	5.06402100	-2.15291700	-0.38871900
H	6.30214600	-0.00030600	-0.53863400
H	5.06459400	2.15258100	-0.38713200
H	2.59712100	2.14853700	-0.07765500
H	1.14317900	-0.82956600	2.33614200
H	1.14357300	0.83050100	2.33585200
H	-0.29558400	0.00077900	2.22608400
N	0.69086700	0.00050700	1.94893000

PhB(nad)–H_2O



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

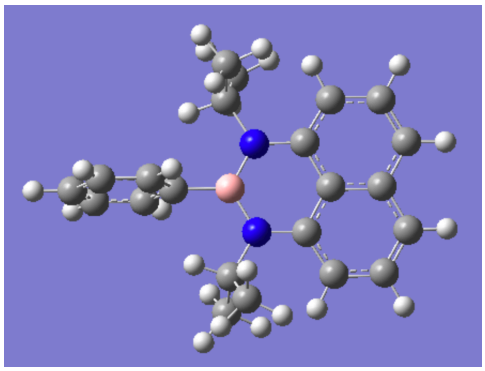
Dihedral angle = -177.0°

H = -866.928006 (hartree)

C	-3.25794200	2.42574800	-0.09719400
C	-3.97365000	1.25259200	-0.05207500
C	-3.30287500	-0.00122600	-0.08515900
C	-1.88525100	-0.00210800	-0.15889600
C	-1.17491900	1.22721700	-0.20254600
C	-1.84434100	2.42628500	-0.17442700
C	-3.97525200	-1.25409700	-0.05471700
C	-3.26071700	-2.42797600	-0.10224800
C	-1.84726400	-2.43020200	-0.17959200
C	-1.17612100	-1.23204400	-0.20528700
O	0.18449500	1.19639600	-0.27752600
O	0.18271200	-1.20256900	-0.28190500
B	0.85366700	-0.00447600	-0.21461400
C	2.41575300	-0.00395900	-0.23232300
C	3.13281900	-1.20923700	-0.20341300
C	4.52661000	-1.21159000	-0.18723300
C	5.22356200	-0.00264200	-0.20162500
C	4.52593500	1.20558100	-0.23430000
C	3.13219400	1.20188200	-0.24951800
H	-3.78362700	3.38154500	-0.07379400
H	-5.06296800	1.26708800	0.00637100
H	-1.27461000	3.35424700	-0.21228700
H	-5.06457700	-1.26743600	0.00372700
H	-3.78752400	-3.38320000	-0.08055100
H	-1.27857100	-3.35869500	-0.21860200
H	2.58298300	-2.15343700	-0.20020200
H	5.07297400	-2.15601800	-0.16711600
H	6.31495100	-0.00213300	-0.19059900
H	5.07185800	2.15032600	-0.25137900

H	2.58200300	2.14529600	-0.28236600
H	1.33886600	-0.66909500	2.38919400
H	1.16957200	0.83958200	2.35154000
O	0.67017900	0.01729200	2.27473900

PhB(*i*Pdan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 120.4°

B–N bond: 1.43354 Å, 1.43354 Å

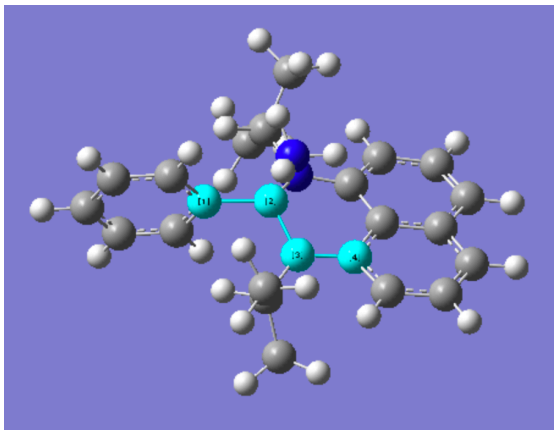
H = -986.263149 (hartree)

AA = 21.6 (kJ/mol)

C	-4.41122000	-0.14409200	-1.19674400
C	-5.11222900	0.00004900	0.00022900
C	-4.41107600	0.14417900	1.19710000
C	-3.01601400	0.14533300	1.19363400
C	-2.29207600	0.00003500	0.00005500
C	-3.01617500	-0.14526100	-1.19345000
B	-0.70457900	0.00000200	-0.00003200
N	0.00781300	1.24365800	-0.02915100
N	0.00778900	-1.24367000	0.02897900
C	1.40907600	1.25613500	0.04982700
C	1.40907000	-1.25617000	-0.04977300
C	2.14893700	2.42671000	0.16056500
C	3.55713700	2.40655500	0.18488100
C	4.24553900	1.22661500	0.09448100
C	3.53717100	-0.00001500	0.00009400
C	2.10767100	-0.00001900	0.00003000
C	4.24555000	-1.22664500	-0.09418800
C	3.55715400	-2.40659700	-0.18447000
C	2.14895200	-2.42676000	-0.16023700

H	-4.95365500	-0.25611500	-2.13717000
H	-6.20337700	0.00005200	0.00029100
H	-4.95338000	0.25620200	2.13760100
H	-2.48048600	0.25695200	2.14064900
H	-2.48075200	-0.25690100	-2.14052200
H	1.65317400	3.38724500	0.22408700
H	4.09399000	3.35295000	0.26900800
H	5.33608700	1.20468800	0.09686000
H	5.33609700	-1.20471700	-0.09652400
H	4.09401200	-3.35300400	-0.26842900
H	1.65322600	-3.38732000	-0.22359600
C	-0.75516900	-2.50364900	0.15009800
C	-0.41499400	-3.31128800	1.40677900
C	-0.79962300	-3.31678300	-1.14671400
H	-1.78793200	-2.17803200	0.30949200
H	-0.45348800	-2.65537800	2.28830100
H	-1.17218400	-4.09785500	1.53634900
H	0.56919400	-3.79242700	1.39034500
H	-1.19884600	-2.69185300	-1.95845300
H	0.17436000	-3.70167800	-1.47126100
H	-1.47701000	-4.17299400	-1.01547800
C	-0.75508400	2.50364200	-0.15067500
C	-0.41421700	3.31130300	-1.40714900
C	-0.80013900	3.31674300	1.14612900
H	-1.78776300	2.17802400	-0.31063600
H	-0.45198200	2.65537300	-2.28868600
H	-1.17148500	4.09771000	-1.53722600
H	0.56985400	3.79265700	-1.39005900
H	-1.20025700	2.69196400	1.95754300
H	0.17382300	3.70110200	1.47139200
H	-1.47699300	4.17330900	1.01446300

PhB(*i*Pdan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 176.3°

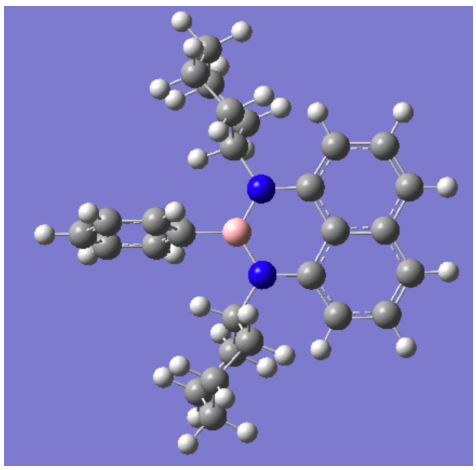
B–N bond: 1.50945 Å, 1.50171 Å

H = -1042.706337 (hartree)

C	4.09432700	-0.20494200	-1.48006500
C	5.03679400	-0.02846600	-0.46351700
C	4.60274500	0.16598400	0.84391700
C	3.23392000	0.17907200	1.13108000
C	2.26831200	0.00043200	0.13341800
C	2.73522500	-0.18933300	-1.18035200
B	0.67308000	0.01192900	0.36770300
N	-0.02938400	-1.26737200	-0.01748400
N	-0.02196400	1.24977300	-0.12199200
C	-1.40555700	-1.24972100	-0.18003500
C	-1.40518400	1.26939000	-0.01272700
C	-2.16518000	-2.39948300	-0.40772300
C	-3.57074300	-2.36511500	-0.44633300
C	-4.25815200	-1.19412300	-0.25874100
C	-3.54116500	0.01776100	-0.08187900
C	-2.11114200	0.01002200	-0.07146200
C	-4.24638000	1.24350200	0.05996700
C	-3.55494900	2.41958600	0.18494800
C	-2.14741400	2.43904100	0.14919400
H	4.42479900	-0.35347600	-2.50977200
H	6.10338700	-0.04084500	-0.69339300
H	5.32905000	0.30804400	1.64625700
H	2.93628000	0.33616700	2.17278300
H	2.00340200	-0.31658800	-1.98359100
H	-1.67761800	-3.35709400	-0.54626800

H	-4.11165800	-3.29836300	-0.61528500
H	-5.34848700	-1.16642700	-0.26593000
H	-5.33707600	1.22418200	0.05927600
H	-4.09135500	3.36301000	0.30421400
H	-1.64319800	3.39521700	0.23951800
H	0.83426200	-0.69421000	2.61979800
H	0.73395700	0.96573400	2.51428500
H	-0.60188700	0.03492000	2.22241600
N	0.41535500	0.08411100	2.10804700
C	0.70659900	-2.53202800	0.11493300
C	0.87243400	-3.29513200	-1.20419000
C	0.24783700	-3.42927200	1.27632100
H	1.72542800	-2.22804700	0.38795500
H	1.36440700	-2.64865400	-1.94320500
H	1.50936800	-4.17800400	-1.04623400
H	-0.07654100	-3.63329500	-1.63763300
H	0.16438800	-2.84890600	2.20886500
H	-0.72040100	-3.91615400	1.11525500
H	0.99751400	-4.21656600	1.44184200
C	0.74332000	2.47056600	-0.39397600
C	0.97822100	3.34220200	0.84878300
C	0.25386200	3.25861900	-1.61395700
H	1.73794300	2.11372400	-0.68559400
H	1.60499400	2.79934500	1.57556300
H	1.52601600	4.25756500	0.58039200
H	0.04603400	3.63788600	1.34959800
H	0.06008700	2.56529300	-2.44443300
H	-0.65762600	3.84291700	-1.44472200
H	1.04471600	3.95602300	-1.92609800

PhB(Cydan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 120.4°

B–N bond: 1.43348 Å, 1.43348 Å

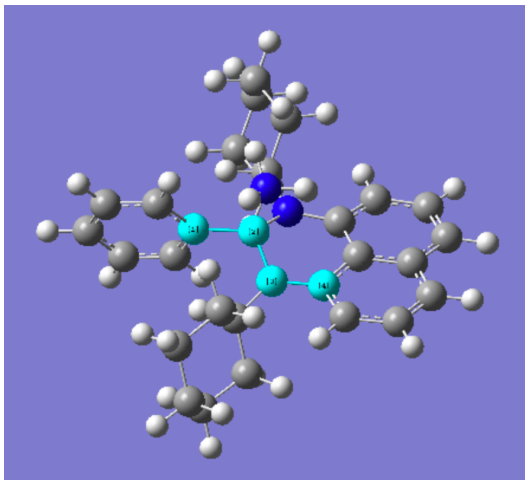
H = -1219.331159 (hartree)

AA = 22.1 (kJ/mol)

C	-0.14695200	4.07400000	-1.19663000
C	-0.00000300	4.77517500	-0.00001100
C	0.14693700	4.07403900	1.19662600
C	0.14807800	2.67884300	1.19323400
C	0.00000700	1.95486200	0.00002900
C	-0.14809200	2.67880800	-1.19319800
B	0.00001300	0.36727900	0.00003700
N	1.24381700	-0.34483400	0.02670100
N	-1.24379700	-0.34481500	-0.02663500
C	1.25120900	-1.74553900	0.12211700
C	-1.25121400	-1.74551800	-0.12205500
C	2.41153800	-2.48424200	0.31374100
C	2.38954600	-3.89234000	0.34217300
C	1.21816000	-4.58121300	0.17455200
C	-0.00002000	-3.87339700	-0.00000900
C	-0.00001000	-2.44394800	0.00001700
C	-1.21821100	-4.58118800	-0.17458600
C	-2.38959100	-3.89228900	-0.34215800
C	-2.41156200	-2.48419300	-0.31367400
H	-0.26052800	4.61636500	-2.13692800
H	-0.00000300	5.86633000	-0.00003000
H	0.26050400	4.61642900	2.13691000
H	0.26153800	2.14334800	2.14000300
H	-0.26156600	2.14327600	-2.13994300
H	3.36538300	-1.98619700	0.43659000
H	3.32820100	-4.42892400	0.49023400
H	1.19654000	-5.67177900	0.17628000
H	-1.19660800	-5.67175400	-0.17636400
H	-3.32825800	-4.42885300	-0.49021300
H	-3.36540800	-1.98613500	-0.43647900
C	-2.49989100	0.42024500	0.06378700
C	-3.28510600	0.52224900	-1.25217200
C	-3.37749900	0.06805700	1.27411100
H	-2.18001700	1.45039400	0.26385100
C	-4.44128700	1.51198000	-1.09343200

H	-3.67970500	-0.45090900	-1.57815400
H	-2.59551900	0.85957600	-2.04163300
C	-4.52881300	1.07020700	1.38708700
H	-3.78975400	-0.94818700	1.21082300
H	-2.74927500	0.09501500	2.17809400
C	-5.33483800	1.13767200	0.08943900
H	-5.02809900	1.55888300	-2.02278400
H	-4.02953600	2.52299600	-0.92740800
H	-5.17914500	0.80067900	2.23242600
H	-4.12131300	2.07214200	1.60808200
H	-6.16022100	1.85854300	0.18847800
H	-5.79619700	0.15265800	-0.10203900
C	2.49992300	0.42021300	-0.06377200
C	3.28516500	0.52228500	1.25216400
C	3.37750500	0.06797900	-1.27409900
H	2.18004100	1.45034800	-0.26388400
C	4.44132900	1.51202400	1.09335400
H	3.67978100	-0.45085300	1.57818200
H	2.59559200	0.85963900	2.04162700
C	4.52879600	1.07014500	-1.38714500
H	3.78977800	-0.94825600	-1.21078200
H	2.74926400	0.09489400	-2.17807100
C	5.33485800	1.13768100	-0.08952300
H	5.02815900	1.55897600	2.02269200
H	4.02956000	2.52302800	0.92729600
H	5.17910700	0.80059300	-2.23249300
H	4.12127100	2.07206300	-1.60817000
H	6.16022300	1.85856400	-0.18861900
H	5.79624200	0.15268600	0.10198600

PhB(Cydan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 177.6°

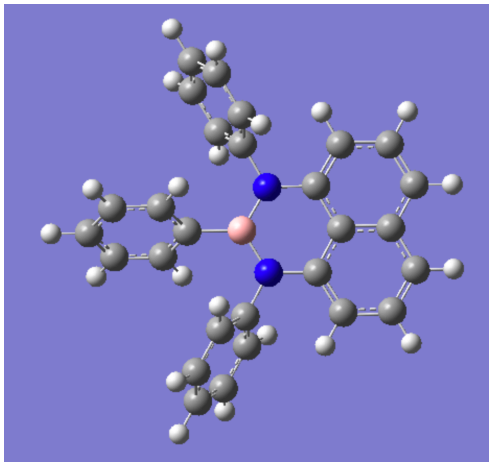
B–N bond: 1.51168 Å, 1.50449 Å

H = -1275.774539 (hartree)

C	-0.00733200	-3.83985100	-1.23656400
C	0.18736700	-4.72661700	-0.17351900
C	0.31649400	-4.22615600	1.11778300
C	0.24755800	-2.84697300	1.34338500
C	0.05175400	-1.93686300	0.29876700
C	-0.07159200	-2.47056700	-0.99797300
B	-0.00272600	-0.33410900	0.46770500
N	-1.27233300	0.31879800	-0.02927500
N	1.24718900	0.37799700	0.02711800
C	-1.28477500	1.69731400	-0.17735100
C	1.22691500	1.76273100	0.10679700
C	-2.44342700	2.42966600	-0.44598900
C	-2.44323900	3.83546500	-0.48171900
C	-1.29774800	4.55152000	-0.25020700
C	-0.07643300	3.86495900	-0.02471000
C	-0.04813000	2.43435400	-0.01049300
C	1.12370200	4.60300100	0.15954200
C	2.31290600	3.94372700	0.32823100
C	2.36984700	2.53766500	0.30315700
H	-0.10628300	-4.22206600	-2.25424500
H	0.23909900	-5.80127200	-0.35530300
H	0.47116900	-4.90792900	1.95605800
H	0.35689300	-2.49677200	2.37461800
H	-0.21347600	-1.78241400	-1.83669300
H	-3.38292700	1.91925900	-0.61996600
H	-3.38288900	4.35283400	-0.68530100
H	-1.29641800	5.64219600	-0.25825700
H	1.07504900	5.69273900	0.15419000
H	3.23707600	4.50545200	0.47772500
H	3.33390600	2.05751000	0.43310600
H	-0.84886600	-0.43489000	2.66091300
H	0.81097200	-0.27351200	2.66433500
H	-0.14610200	1.01289400	2.25972300
N	-0.05205700	-0.00534700	2.18797600
C	-2.50841400	-0.46670600	-0.04197900
C	-3.52591800	-0.13877200	1.06900100
C	-3.17680000	-0.59350500	-1.42139800

H	-2.18943800	-1.49225000	0.19099600
C	-4.65003100	-1.17726300	1.08256400
H	-3.95932700	0.86390000	0.95103700
H	-3.00860900	-0.13138900	2.04402000
C	-4.30620600	-1.62327800	-1.37410700
H	-3.57540300	0.36904600	-1.77326000
H	-2.40876900	-0.89502000	-2.14893000
C	-5.32396200	-1.28070200	-0.28592600
H	-5.38868900	-0.92523200	1.85839700
H	-4.23254000	-2.16390800	1.34997500
H	-4.79948100	-1.69051800	-2.35532000
H	-3.87795100	-2.61975100	-1.16609100
H	-6.12750700	-2.03210400	-0.25943300
H	-5.80136900	-0.31468300	-0.52741600
C	2.48377000	-0.36899200	-0.19844600
C	3.29115700	0.08096100	-1.42536100
C	3.36780800	-0.57044900	1.04626500
H	2.15616700	-1.38409900	-0.46025900
C	4.42953500	-0.90367100	-1.69814900
H	3.71252800	1.08762900	-1.29748300
H	2.60537500	0.13638800	-2.28461000
C	4.51916600	-1.53070700	0.74065300
H	3.76933900	0.38502200	1.41862100
H	2.74710900	-0.99402400	1.85541600
C	5.32674700	-1.06395000	-0.47045800
H	5.01933800	-0.56735400	-2.56393900
H	4.00822900	-1.88861100	-1.96527100
H	5.16944700	-1.63963800	1.62179800
H	4.10070600	-2.53042500	0.52920200
H	6.14344700	-1.77137300	-0.67934900
H	5.79991700	-0.09327200	-0.23903600

PhB(Phdan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 117.8°

B–N bond: 1.43507 Å, 1.43507 Å

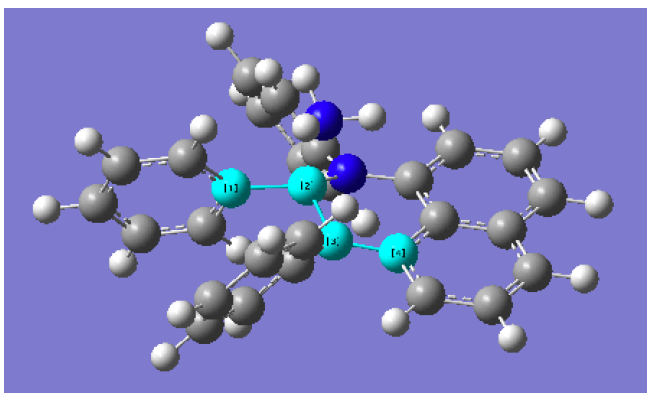
H = -1212.279056 (hartree)

AA = 29.1 (kJ/mol)

C	-0.67818200	-4.03220300	0.99690600
C	-0.00059500	-4.73302400	-0.00007600
C	0.67711000	-4.03230700	-0.99704900
C	0.68152700	-2.63839000	-0.98942700
C	-0.00036500	-1.91350400	-0.00006000
C	-0.68236900	-2.63828500	0.98930200
B	-0.00014300	-0.33442600	-0.00006000
N	1.22777100	0.40698400	0.04425100
N	-1.22778200	0.40744700	-0.04434400
C	1.24691800	1.81325800	0.09885900
C	-1.24639700	1.81373400	-0.09894500
C	2.42397000	2.52824500	0.25161100
C	2.40534900	3.93849100	0.27233200
C	1.23123600	4.63461400	0.13885000
C	0.00066800	3.93809300	-0.00001800
C	0.00039200	2.51181200	-0.00003500
C	-1.22963200	4.63509000	-0.13886200
C	-2.40401500	3.93942200	-0.27234400
C	-2.42318000	2.52918200	-0.25165600
H	-1.21082600	-4.57334900	1.78072000
H	-0.00067500	-5.82438000	-0.00007400
H	1.20967200	-4.57353400	-1.78086300

H	1.23340700	-2.10538400	-1.76749800
H	-1.23414600	-2.10519600	1.76739000
H	3.37124100	2.00246700	0.35219100
H	3.34867100	4.47416800	0.39085400
H	1.22000800	5.72543100	0.14104100
H	-1.21798300	5.72590200	-0.14101500
H	-3.34713300	4.47546600	-0.39083400
H	-3.37065500	2.00376600	-0.35222000
C	-2.48251000	-0.28104700	-0.05986500
C	-2.87914200	-0.98953300	-1.19305500
C	-3.30026100	-0.26520000	1.07334300
C	-4.07978000	-1.69846100	-1.18683900
H	-2.22871000	-0.99438000	-2.06888500
C	-4.50350300	-0.96589100	1.07328400
H	-2.97831700	0.29924600	1.95084500
C	-4.89355100	-1.68835200	-0.05563800
H	-4.37846000	-2.26230800	-2.07157600
H	-5.13618100	-0.95525500	1.96206000
H	-5.83247400	-2.24355300	-0.05179100
C	2.48227600	-0.28191200	0.05985900
C	3.30006900	-0.26635500	-1.07332000
C	2.87871100	-0.99036900	1.19313500
C	4.50318700	-0.96726200	-1.07314100
H	2.97828600	0.29809400	-1.95088000
C	4.07922100	-1.69951300	1.18704100
H	2.22825300	-0.99497200	2.06894800
C	4.89305400	-1.68966200	0.05587800
H	5.13591600	-0.95681500	-1.96188300
H	4.37776600	-2.26331600	2.07185200
H	5.83188700	-2.24501500	0.05214400

PhB(Phdan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 166.0°

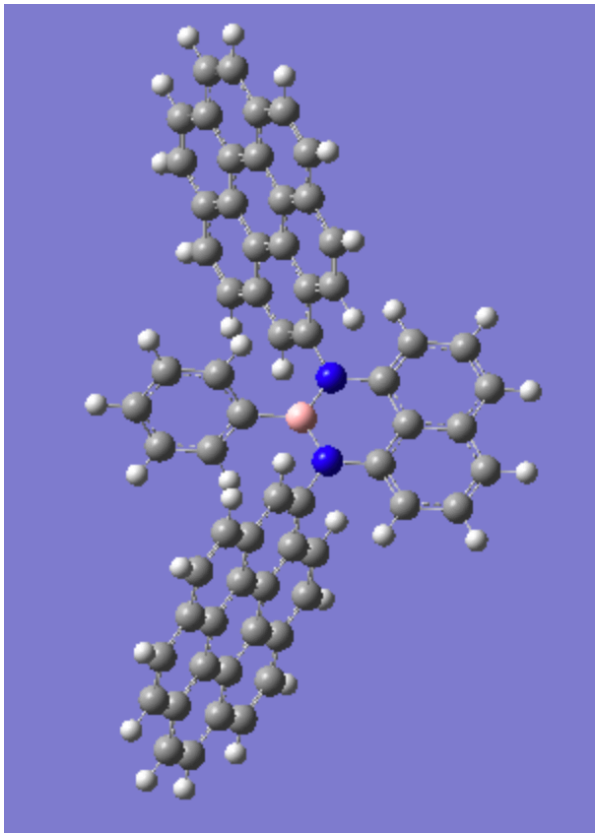
B–N bond: 1.50863 Å, 1.51867 Å

H = -1268.725116 (hartree)

C	1.84827300	-3.30367700	-1.30973500
C	2.85445700	-3.68355800	-0.41903600
C	3.00567500	-2.98988800	0.77823000
C	2.15334200	-1.92449600	1.07759500
C	1.13746900	-1.52288800	0.20239200
C	1.00623400	-2.23958700	-0.99841000
B	0.20151100	-0.23890000	0.44764800
N	-1.27186800	-0.42326000	0.18096900
N	0.73024800	1.03100400	-0.19589800
C	-2.09135600	0.70879700	0.18346800
C	-0.09206900	2.14360700	-0.32429200
C	-3.45500200	0.63076800	0.44815000
C	-4.26487000	1.78223400	0.42619800
C	-3.73375000	3.01574700	0.14202300
C	-2.34450200	3.14965700	-0.12066600
C	-1.50180800	1.99641500	-0.06877200
C	-1.78838100	4.41277900	-0.45692200
C	-0.45237800	4.51473700	-0.75417700
C	0.39780800	3.39385700	-0.69037600
H	1.72031600	-3.84221100	-2.25045900
H	3.51699600	-4.51669500	-0.65958800
H	3.79231300	-3.27253900	1.48007100
H	2.32427700	-1.39084100	2.01832800
H	0.22243500	-1.95288900	-1.70478700
H	-3.90360700	-0.33788200	0.66371100
H	-5.33148500	1.67996600	0.63465900
H	-4.36337400	3.90589000	0.10476300
H	-2.44367700	5.28410600	-0.49176600
H	-0.02776300	5.47941600	-1.03853800
H	1.45479200	3.50874100	-0.92458700
H	0.02062800	-0.64912300	2.72953200
H	1.21144300	0.46523300	2.39607500
H	-0.38847000	0.89847800	2.29170900
N	0.27898300	0.13766000	2.13187000
C	-1.86952200	-1.69974000	0.04789200
C	-1.63067100	-2.72055100	0.97400200
C	-2.68911500	-1.97939900	-1.05737100

C	-2.17946800	-3.99034300	0.79557200
H	-0.98651500	-2.53070900	1.83382100
C	-3.24870800	-3.24069100	-1.22546100
H	-2.87548900	-1.18671000	-1.78430100
C	-2.99383200	-4.25684700	-0.30139900
H	-1.96769100	-4.77415600	1.52445200
H	-3.87901000	-3.43758000	-2.09430900
H	-3.42577400	-5.24870700	-0.43947900
C	2.14190900	1.21707300	-0.18922900
C	2.76273900	1.95164500	0.83185100
C	2.93945100	0.61129500	-1.16438200
C	4.15141200	2.05644600	0.88947700
H	2.14188300	2.47294900	1.56651900
C	4.32801500	0.70958200	-1.10150700
H	2.45203800	0.04427000	-1.95755900
C	4.93934500	1.42742700	-0.07409700
H	4.61914800	2.63280500	1.68953200
H	4.93675400	0.21957600	-1.86288400
H	6.02655200	1.50286700	-0.02785500

PhB(cordan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 117.6°

B–N bond: 1.43587 Å, 1.43588 Å

H = -2589.687462 (hartree)

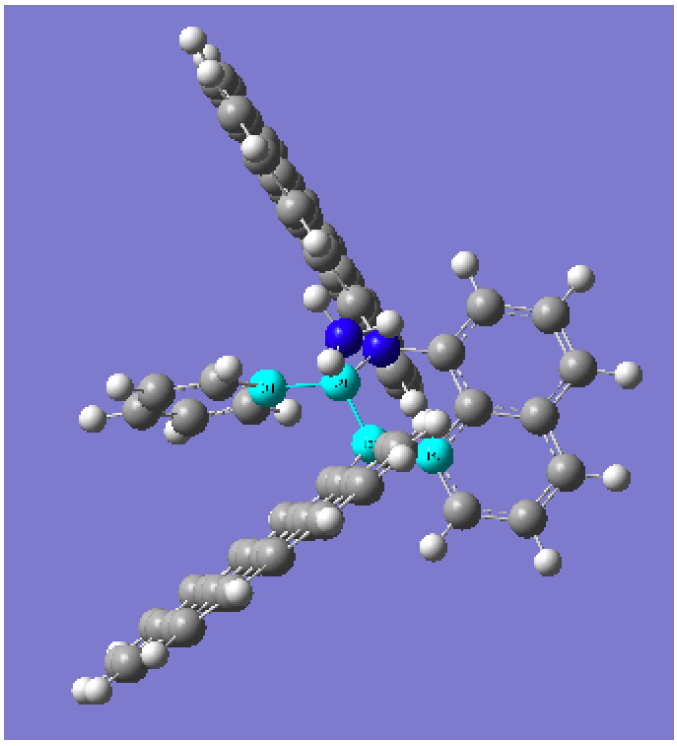
AA = 29.7 (kJ/mol)

C	0.85214500	-2.91710300	-0.85581400
C	-0.00001000	-3.61794000	-0.00320700
C	-0.85215900	-2.91821800	0.85031500
C	-0.85428000	-1.52411600	0.84475500
C	-0.00003000	-0.80041300	-0.00139400
C	0.85425300	-1.52300800	-0.84845000
B	-0.00001500	0.77580800	-0.00038200
N	-1.19404000	1.51966400	-0.28796100
N	1.19402200	1.51924700	0.28828900
C	-1.20579800	2.92707500	-0.32984200
C	1.20577900	2.92660600	0.33218900
C	-2.34045200	3.64050100	-0.67774600
C	-2.32172900	5.05109300	-0.68378000
C	-1.18841500	5.74668700	-0.34721000
C	-0.00002200	5.05084500	0.00265600
C	-0.00000400	3.62449600	0.00163300
C	1.18834100	5.74621600	0.35355900
C	2.32162900	5.05016200	0.68925600
C	2.34037000	3.63957900	0.68125900
H	1.52216600	-3.45771200	-1.52630600
H	-0.00000600	-4.70923200	-0.00392000
H	-1.52215800	-3.45970400	1.52012300
H	-1.53719000	-0.99229500	1.51284800
H	1.53719600	-0.99029700	-1.51580200
H	-3.25456800	3.11281800	-0.94438500
H	-3.23168400	5.58686900	-0.95853200
H	-1.17821400	6.83752100	-0.34434900
H	1.17811800	6.83705200	0.35223900
H	3.23154900	5.58556000	0.96486200
H	3.25446600	3.11155900	0.94728300
C	2.41436100	0.83014600	0.57339400
C	3.43159000	0.76046500	-0.43491600
C	2.58641900	0.21708300	1.78540600
C	4.61352300	0.03649400	-0.15494900
C	3.28357700	1.37814800	-1.71170800

C	3.76664200	-0.51949500	2.08572000
H	1.79037500	0.28283800	2.52942100
C	5.63922700	-0.06306200	-1.14547900
C	4.78334200	-0.60793400	1.10887500
C	4.26905800	1.28132100	-2.65760800
H	2.37112000	1.93664600	-1.92485900
C	3.95298800	-1.17120700	3.33984100
C	5.47244500	0.56226000	-2.40257100
C	6.83328000	-0.79693100	-0.86795900
C	5.97583700	-1.34218300	1.38596900
H	4.14305000	1.76161700	-3.62985400
C	5.09750700	-1.87331800	3.60612200
H	3.16136800	-1.10069400	4.08799100
C	6.51068800	0.45030900	-3.37369600
C	7.00236300	-1.43577400	0.39800300
C	7.84825800	-0.89331900	-1.84822800
C	6.13922400	-1.97840700	2.63853400
H	5.22841200	-2.36795000	4.57051900
C	7.65552000	-0.25015300	-3.10633600
H	6.37481500	0.93713700	-4.34136800
C	8.18356500	-2.16315100	0.67227700
C	9.03030600	-1.63138800	-1.54639400
C	7.34022700	-2.70497000	2.89025700
H	8.44287300	-0.32788300	-3.85866200
C	9.19202600	-2.24286900	-0.33240200
C	8.32482700	-2.79362300	1.94365500
H	9.81040400	-1.70140200	-2.30698500
H	7.46130900	-3.19390700	3.85886500
H	10.10228100	-2.80528600	-0.11542300
H	9.23890800	-3.35380700	2.15005300
C	-2.41455800	0.83105000	-0.57346500
C	-3.43116200	0.75984200	0.43537200
C	-2.58742000	0.21997600	-1.78636200
C	-4.61329800	0.03635900	0.15502200
C	-3.28227800	1.37545300	1.71306500
C	-3.76792700	-0.51598100	-2.08712700
H	-1.79183900	0.28687200	-2.53077100
C	-5.63831800	-0.06482100	1.14609400
C	-4.78398800	-0.60596900	-1.10975200
C	-4.26709700	1.27705900	2.65949300
H	-2.36968500	1.93361200	1.92650800
C	-3.95519400	-1.16554800	-3.34222200
C	-5.47064900	0.55840000	2.40411000

C	-6.83258000	-0.79820100	0.86818200
C	-5.97672500	-1.33967500	-1.38726200
H	-4.14041800	1.75576000	3.63243700
C	-5.09996400	-1.86709800	-3.60891400
H	-3.16409000	-1.09383000	-4.09080400
C	-6.50819800	0.44481200	3.37578700
C	-7.00257000	-1.43488900	-0.39874200
C	-7.84686700	-0.89622500	1.84900400
C	-6.14102100	-1.97375700	-2.64079000
H	-5.23158400	-2.36006000	-4.57406800
C	-7.65322300	-0.25519500	3.10806400
H	-6.37162600	0.93000600	4.34418000
C	-8.18399700	-2.16174800	-0.67342200
C	-9.02915200	-1.63374400	1.54675200
C	-7.34224700	-2.69981500	-2.89291800
H	-8.44003900	-0.33419200	3.86082000
C	-9.19175000	-2.24314500	0.33183000
C	-8.32618600	-2.79003700	-1.94578000
H	-9.80871500	-1.70502800	2.30777300
H	-7.46404100	-3.18708200	-3.86227800
H	-10.10217900	-2.80515700	0.11453000
H	-9.24044200	-3.34981600	-2.15249800

PhB(cordan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 153.4°

B–N bond: 1.50806 Å, 1.52237 Å

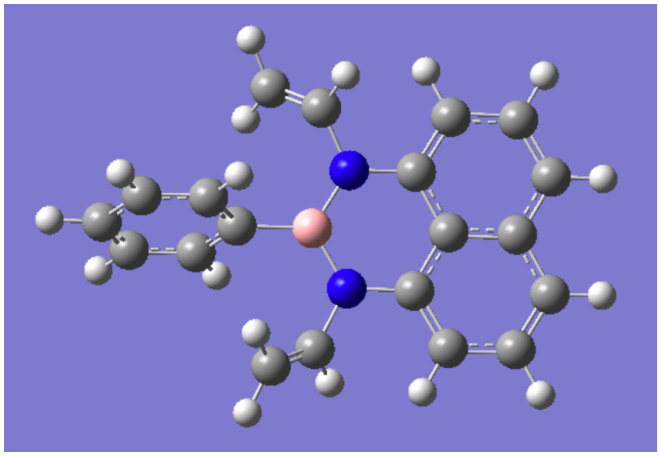
H = -2646.133752 (hartree)

C	0.82702100	-2.81666600	1.24138800
C	0.04890000	-3.75414800	0.55937300
C	-0.76499700	-3.33435600	-0.48948200
C	-0.79550500	-1.98523000	-0.84905500
C	-0.02865700	-1.02346700	-0.17929300
C	0.78398800	-1.47369500	0.87387100
B	-0.13476000	0.55823300	-0.46007200
N	1.17512500	1.30533600	-0.47694400
N	-1.16485400	1.27291800	0.40349200
C	1.17949700	2.70208900	-0.39522000
C	-1.05778100	2.61989900	0.72343700
C	2.23941300	3.46115400	-0.87450800
C	2.25997200	4.85986900	-0.69948100
C	1.24100900	5.50700700	-0.04614600
C	0.12992000	4.77251900	0.45019700
C	0.07583600	3.36115900	0.24348600
C	-0.91494200	5.41521100	1.16632200
C	-1.95227600	4.67323200	1.67598200
C	-2.03165800	3.28329800	1.46262000
H	1.47076800	-3.13495700	2.06334300
H	0.07768200	-4.80674800	0.84579300
H	-1.38485300	-4.05542600	-1.02508600
H	-1.47447900	-1.69371900	-1.65765100
H	1.38986300	-0.75118200	1.42731400
H	3.07529200	2.96530000	-1.36722800
H	3.11143100	5.42582700	-1.08148900
H	1.26969000	6.58615300	0.11163600
H	-0.86530800	6.49447800	1.31640600
H	-2.74321600	5.16163000	2.24816100
H	-2.87884900	2.72399800	1.85832100
H	-0.28766100	0.10685400	-2.72338000
H	-1.77041400	0.52977300	-2.10499900
H	-0.61776100	1.69122800	-2.35509200
N	-0.76471300	0.72182400	-2.06195800
C	2.41122000	0.65689300	-0.71891500
C	3.43854000	0.70489400	0.29222400
C	2.64070700	-0.03974800	-1.87925100

C	4.66930200	0.05146400	0.05601700
C	3.24073700	1.37101800	1.53765700
C	3.86271700	-0.72559300	-2.12955300
H	1.87137200	-0.06649500	-2.65285000
C	5.70203500	0.09254100	1.04467900
C	4.88697400	-0.66820100	-1.15982600
C	4.23005500	1.40626400	2.48362300
H	2.28176300	1.85266500	1.73139900
C	4.09354900	-1.45042000	-3.33493000
C	5.48926900	0.77924600	2.26176000
C	6.94969700	-0.56273600	0.80715700
C	6.13008300	-1.32794400	-1.39557800
H	4.06148900	1.92162800	3.43112700
C	5.28691700	-2.08187400	-3.56279700
H	3.29729200	-1.49436900	-4.08075500
C	6.53600500	0.81364800	3.23008200
C	7.16537400	-1.27171900	-0.41352000
C	7.97264400	-0.51289100	1.78290300
C	6.33794100	-2.03762800	-2.60151200
H	5.45017300	-2.63285100	-4.49113400
C	7.73329800	0.19345100	2.99850000
H	6.36288100	1.34832000	4.16605600
C	8.39915000	-1.92145200	-0.64823700
C	9.20891900	-1.17254900	1.52041900
C	7.59133100	-2.68432100	-2.81360900
H	8.52715300	0.22856000	3.74724100
C	9.41502000	-1.85087500	0.34936400
C	8.58440700	-2.62755400	-1.87376900
H	9.99492100	-1.12772100	2.27690600
H	7.74571400	-3.23010700	-3.74656200
H	10.36672000	-2.35232100	0.16271900
H	9.53919400	-3.12711700	-2.04929100
C	-2.39996300	0.60623800	0.63461200
C	-3.55358800	0.92074400	-0.17158000
C	-2.47197300	-0.40766700	1.55733100
C	-4.72928600	0.14394900	-0.02432200
C	-3.56036200	1.98950200	-1.12140800
C	-3.64059400	-1.20057000	1.71927600
H	-1.58676300	-0.63328700	2.15314300
C	-5.87816200	0.41861600	-0.83200800
C	-4.77300000	-0.92586000	0.92129500
C	-4.66212900	2.24991200	-1.89279800
H	-2.68132900	2.63027000	-1.20439600

C	-3.69537700	-2.27783800	2.65218700
C	-5.84908700	1.47236400	-1.77449100
C	-7.06027100	-0.37261600	-0.69106300
C	-5.95256300	-1.71731100	1.06147900
H	-4.64825700	3.07891500	-2.60335200
C	-4.82671900	-3.03618000	2.78706700
H	-2.81015600	-2.48951300	3.25466900
C	-7.00574500	1.72875100	-2.56774200
C	-7.09804400	-1.44065400	0.25599400
C	-8.19495700	-0.09931600	-1.49072200
C	-5.98604900	-2.77655100	1.99824900
H	-4.85666000	-3.85855500	3.50451200
C	-8.13672600	0.97100900	-2.43091700
H	-6.97314500	2.54732100	-3.28941600
C	-8.26729400	-2.22375200	0.39549600
C	-9.36177400	-0.90293700	-1.33052600
C	-7.17735200	-3.55063200	2.11969100
H	-9.01683500	1.17725500	-3.04310300
C	-9.39678000	-1.92600800	-0.42189200
C	-8.27644600	-3.28448700	1.34834000
H	-10.23403200	-0.68584900	-1.95014800
H	-7.19775800	-4.36638600	2.84502600
H	-10.29741200	-2.53287200	-0.30971100
H	-9.18196600	-3.88538200	1.45256100

PhB(eedan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 117.7°

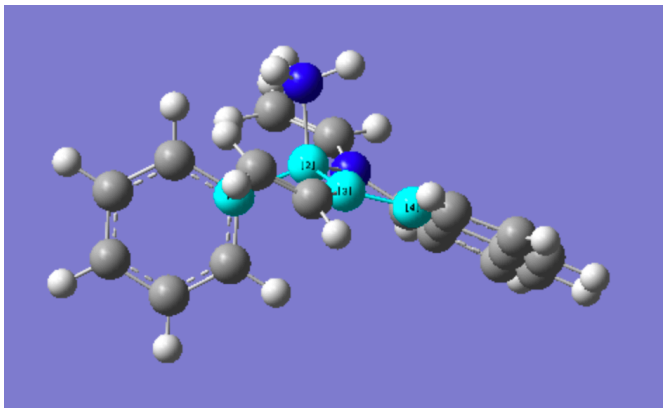
B–N bond: 1.43990 Å, 1.43989 Å

H = -905.402093 (hartree)

AA = 49.2 (kJ/mol)

C	-4.41512300	-0.40926300	-1.13361100
C	-5.11571300	0.00003400	0.00068900
C	-4.41446300	0.40934600	1.13458200
C	-3.02026100	0.41630100	1.12707700
C	-2.29867600	0.00002900	-0.00014700
C	-3.02091300	-0.41622800	-1.12693400
B	-0.72028200	0.00001800	-0.00028900
N	0.02432500	1.23082700	0.06279300
N	0.02430400	-1.23080000	-0.06326600
C	1.43065700	1.24615400	-0.00004500
C	1.43061600	-1.24616400	-0.00009800
C	2.14441300	2.43200600	-0.07229300
C	3.55532900	2.41833000	-0.08723300
C	4.25210200	1.23818200	-0.03903400
C	3.55641000	-0.00004300	0.00018600
C	2.13108100	-0.00001800	0.00001500
C	4.25205400	-1.23829200	0.03956200
C	3.55522900	-2.41841800	0.08756100
C	2.14431500	-2.43204300	0.07228200
H	-4.95734700	-0.73038500	-2.02464500
H	-6.20696800	0.00003200	0.00100200
H	-4.95616600	0.73047800	2.02592900
H	-2.48419400	0.75918100	2.01612000
H	-2.48537600	-0.75910600	-2.01629600
H	1.62002900	3.38292500	-0.13724700
H	4.08987800	3.36821700	-0.13825300
H	5.34294200	1.22830200	-0.03976600
H	5.34289300	-1.22845400	0.04056500
H	4.08973400	-3.36832500	0.13867700
H	1.61988300	-3.38294900	0.13707000
C	-0.59948000	-2.49177500	-0.25601200
C	-1.59214900	-2.98179300	0.48147100
H	-0.18877500	-3.06729800	-1.09309500
H	-2.03864100	-3.94142400	0.22038600
H	-2.00176300	-2.43273000	1.33054400
C	-0.59946500	2.49183800	0.25523800
C	-1.59198700	2.98177700	-0.48249600
H	-0.18897300	3.06744800	1.09236100
H	-2.03854600	3.94142000	-0.22157000
H	-2.00145600	2.43263000	-1.33158300

PhB(eedan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 139.7°

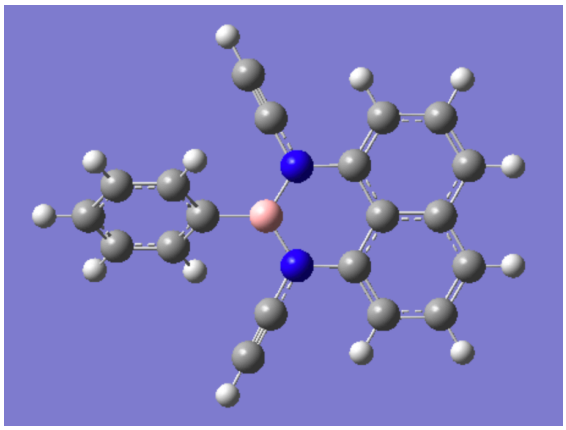
B–N bond: 1.53350 Å, 1.52431 Å

H = -961.855812 (hartree)

C	-3.20477700	0.38593400	-2.31357600
C	-4.47534700	0.23902300	-1.75647500
C	-4.59880300	-0.03821200	-0.39657400
C	-3.45409500	-0.16997600	0.39095100
C	-2.16759500	-0.03050700	-0.14403000
C	-2.07162600	0.25531200	-1.51296800
B	-0.77293000	-0.13300500	0.66920300
N	0.03733000	1.16869800	0.64349000
N	0.08443100	-1.32821600	0.26928100
C	1.30513900	1.24247300	0.06093900
C	1.47571400	-1.24023500	0.13802300
C	1.86869400	2.45230000	-0.32345300
C	3.21456700	2.52073600	-0.74166900
C	4.00048700	1.39677900	-0.77886300
C	3.44439700	0.12968300	-0.45353200
C	2.07178500	0.04301300	-0.08547300
C	4.23338600	-1.05221500	-0.48433600
C	3.67106300	-2.25798300	-0.15144900
C	2.29832700	-2.36034400	0.16083200
H	-3.09829500	0.60697700	-3.37716700
H	-5.36545800	0.34263400	-2.37909600
H	-5.58720900	-0.15354700	0.05188600
H	-3.59402300	-0.38448300	1.45769100
H	-1.08088800	0.37889500	-1.96046800
H	1.26773600	3.36024200	-0.30571700

H	3.62927600	3.48935100	-1.02600300
H	5.05032200	1.45190100	-1.07031900
H	5.28628200	-0.97680600	-0.75971500
H	4.28142700	-3.16267300	-0.13900300
H	1.88723500	-3.33563600	0.41472700
H	-1.57552300	0.46958300	2.67138200
H	-1.65525000	-1.19591900	2.45921200
H	-0.20268300	-0.46247200	2.76835800
N	-1.09968000	-0.35581100	2.28973200
C	-0.44044800	2.31459200	1.26634700
C	-1.70394200	2.62711000	1.61043400
H	0.35422700	3.01095700	1.55519300
H	-1.87426100	3.54841900	2.16587900
H	-2.57315800	2.05020700	1.29627800
C	-0.49089000	-2.57528300	0.03464300
C	-1.67261200	-3.05115700	0.45406700
H	0.11685100	-3.22414800	-0.60200700
H	-1.98948900	-4.03715400	0.11753200
H	-2.38756000	-2.49025800	1.05478600

PhB(eydan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 116.6°

B–N bond: 1.44486 Å, 1.44486 Å

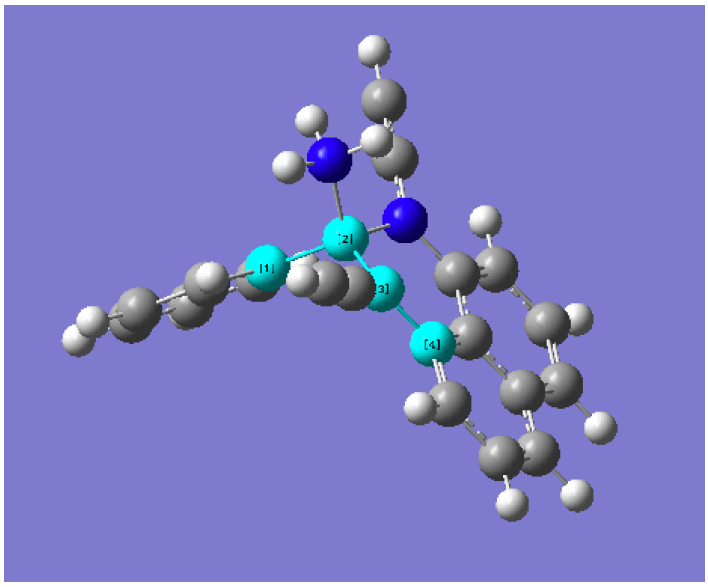
H = -902.956180 (hartree)

AA = 71.4 (kJ/mol)

C	-4.48244000	0.74991800	0.94554000
C	-5.18120000	0.00000400	0.00003600
C	-4.48248600	-0.74991900	-0.94549600

C	-3.08914300	-0.75685100	-0.93650000
C	-2.36846300	-0.00002200	-0.00001300
C	-3.08909800	0.75682700	0.93649400
B	-0.80229600	-0.00002000	-0.00002500
N	-0.04307500	-1.22827000	0.05088800
N	-0.04310100	1.22824700	-0.05093900
C	1.37919700	-1.24966500	0.03566800
C	1.37917100	1.24967200	-0.03569100
C	2.08346400	-2.43477700	0.06468700
C	3.49523200	-2.42134800	0.06060200
C	4.18857400	-1.23863700	0.03064700
C	3.49324100	0.00002600	0.00000800
C	2.06750600	0.00001100	-0.00000600
C	4.18855000	1.23870200	-0.03061700
C	3.49518300	2.42139800	-0.06058300
C	2.08341500	2.43479900	-0.06469400
H	-5.02495400	1.33582200	1.68912200
H	-6.27257300	0.00001400	0.00005500
H	-5.02503500	-1.33581000	-1.68906100
H	-2.55389200	-1.36317600	-1.67086000
H	-2.55381000	1.36314900	1.67083000
H	1.54404700	-3.37969600	0.09352100
H	4.03102300	-3.37122800	0.08385700
H	5.27939500	-1.22727600	0.03031800
H	5.27937100	1.22736400	-0.03026700
H	4.03095600	3.37129000	-0.08382500
H	1.54398000	3.37970700	-0.09353700
C	-0.68793000	2.41785000	-0.16563600
C	-1.23972700	3.48760700	-0.26888500
H	-1.74867000	4.42697300	-0.36531600
C	-0.68787600	-2.41789000	0.16556400
C	-1.23961100	-3.48767100	0.26891300
H	-1.74848000	-4.42707200	0.36539900

PhB(eydan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 91.4°

B–N bond: 1.53355 Å, 1.53757 Å

H = -959.418340 (hartree)

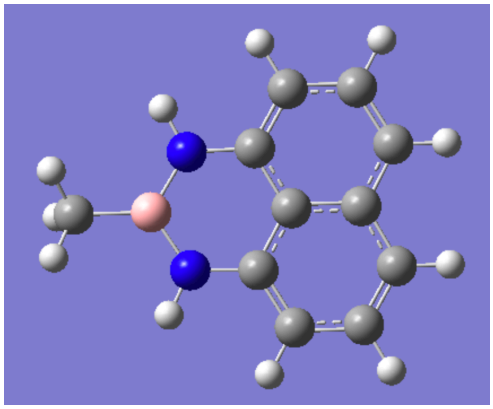
C	-2.93458300	1.34129500	-2.17537900
C	-3.88039600	0.34101600	-2.39205200
C	-3.88572500	-0.79024600	-1.57568700
C	-2.95057000	-0.91073500	-0.54899400
C	-1.99393200	0.08975100	-0.30441000
C	-2.00549600	1.21437700	-1.14169900
B	-0.91279200	-0.05831200	0.88327500
N	0.01875800	1.14785700	1.05398000
N	-0.04584800	-1.32742300	0.83975400
C	1.25693500	1.18566800	0.38843100
C	1.18946600	-1.31415200	0.16826300
C	1.92877200	2.37489100	0.17685500
C	3.17123300	2.38419900	-0.49169100
C	3.73735300	1.21854100	-0.94221900
C	3.08166700	-0.02506300	-0.73239800
C	1.82143600	-0.05022600	-0.06545900
C	3.67301900	-1.24571500	-1.15573100
C	3.04442700	-2.44074400	-0.91035100
C	1.80049100	-2.48203400	-0.24707900
H	-2.91841700	2.22534300	-2.81525700
H	-4.60855100	0.43873800	-3.19911900

H	-4.61527000	-1.58406700	-1.74612700
H	-2.95507700	-1.82194200	0.05788800
H	-1.26963200	2.00782800	-0.98715300
H	1.48596800	3.30633500	0.52956100
H	3.67915600	3.33706400	-0.64885600
H	4.69856500	1.22370000	-1.45816900
H	4.63524700	-1.21197700	-1.66869200
H	3.50280500	-3.37729500	-1.23193200
H	1.30590700	-3.43545000	-0.06211000
H	-2.23660800	0.71730400	2.44325400
H	-2.39703600	-0.93963800	2.25092500
H	-1.08459200	-0.31804500	3.06256400
N	-1.73265800	-0.16125900	2.28493200
C	-0.50528600	2.26686200	1.57219600
C	-1.03845000	3.23288900	2.08098500
H	-1.49199500	4.10732400	2.50471500
C	-0.59234700	-2.48757800	1.22417600
C	-1.12854200	-3.50053500	1.62917600
H	-1.58510200	-4.41265100	1.95986100

–Methylboronic acid derivatives–

All the structures of methylboronic acid derivatives and their ammonia adducts were optimized starting from the geometries based on the respective phenylboronic acid derivatives and ammonia adducts optimized at the M06-2X/def2-SVP level of theory.

MeB(dan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 115.4°

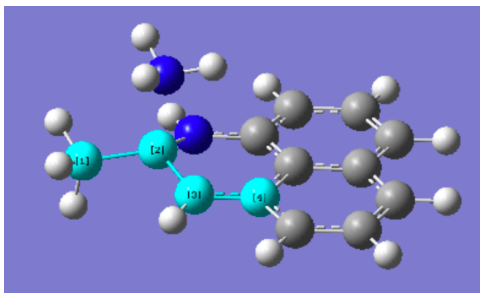
B–N bond: 1.42565 Å, 1.42566 Å

H = -559.423684 (hartree)

AA = 10.1 (kJ/mol)

B	2.45848100	0.00005500	-0.01262000
N	1.69691300	-1.20515300	-0.01420500
N	1.69687900	1.20522600	-0.01429900
C	0.30688900	-1.24343300	-0.00655000
C	0.30684700	1.24345200	-0.00657000
C	-0.39787500	-2.43455100	-0.00349900
C	-1.80829800	-2.42495700	0.00335700
C	-2.51223500	-1.24479900	0.00718800
C	-1.82488000	-0.00002300	0.00409700
C	-0.40106900	-0.00000100	-0.00251700
C	-2.51227300	1.24473300	0.00720900
C	-1.80837400	2.42491400	0.00340100
C	-0.39795000	2.43454900	-0.00347200
H	2.15424600	-2.10778900	-0.01752200
H	2.15416400	2.10788500	-0.01782100
H	0.14597600	-3.38088500	-0.00648000
H	-2.34240700	-3.37670800	0.00567700
H	-3.60307200	-1.24383300	0.01245700
H	-3.60311000	1.24373200	0.01247600
H	-2.34251100	3.37664800	0.00575300
H	0.14587200	3.38089900	-0.00644900
C	4.03674500	0.00001000	0.02122200
H	4.39185300	-0.00051300	1.06421100
H	4.46238200	-0.88852200	-0.46685200
H	4.46249900	0.88894200	-0.46601500

MeB(dan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

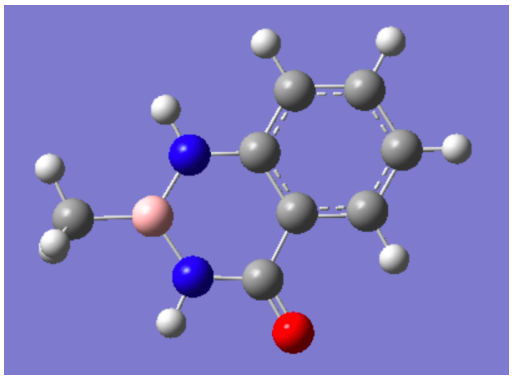
Dihedral angle = 167.3°

B–N bond: 1.48521 Å, 1.48517 Å

H = -615.862503 (hartree)

B	-2.23895500	0.00000800	-0.15374200
N	-1.43294800	1.22307600	-0.39931100
N	-1.43294500	-1.22281200	-0.40030300
C	-0.06730700	1.24917100	-0.23369400
C	-0.06738000	-1.24908200	-0.23396800
C	0.65451900	2.43714800	-0.18279400
C	2.05050300	2.42242400	-0.00053000
C	2.74173600	1.24085900	0.12959100
C	2.05117500	-0.00004500	0.06142800
C	0.63529500	0.00001600	-0.11042100
C	2.74160900	-1.24103000	0.12968600
C	2.05027300	-2.42253000	-0.00035700
C	0.65429600	-2.43712400	-0.18280100
H	-1.86994600	2.12057600	-0.56098600
H	-1.87001100	-2.12034800	-0.56161200
H	0.12363300	3.38598300	-0.28394400
H	2.58712300	3.37261300	0.03842300
H	3.82393400	1.23514700	0.26682500
H	3.82380500	-1.23540700	0.26694600
H	2.58678700	-3.37277300	0.03875500
H	0.12334300	-3.38591100	-0.28404800
H	-2.85517300	0.83019800	2.02142600
H	-2.85598700	-0.83003500	2.02220200
H	-1.42455900	-0.00056900	2.01558500
N	-2.38444900	-0.00031700	1.66046900
C	-3.75235300	0.00020900	-0.67330500
H	-4.31556800	-0.88737500	-0.34029700
H	-4.31551000	0.88768000	-0.33989400
H	-3.76890400	0.00046000	-1.77366400

MeB(aam)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 115.4°

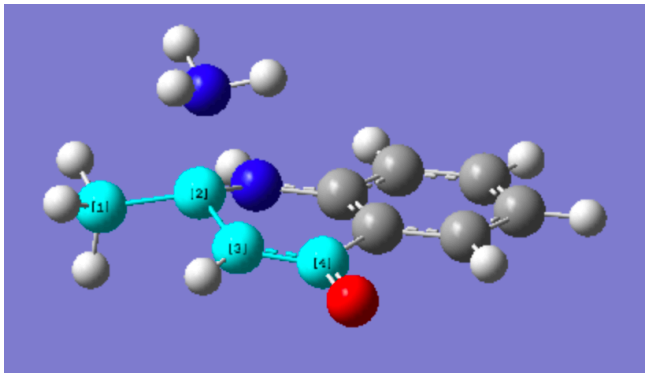
B–N bond: 1.42372 Å, 1.43498 Å

H = -519.215609 (hartree)

AA = 16.7 (kJ/mol)

B	-2.05780400	-0.51137300	-0.00047800
N	-0.90799900	-1.35096900	-0.00059900
N	-1.79122600	0.89862400	-0.00038000
C	0.38763700	-0.85799800	-0.00027600
C	-0.53912000	1.49252700	-0.00014100
C	1.50019500	-1.71547400	-0.00016500
C	2.78531700	-1.19283700	0.00016800
C	2.99674000	0.19150200	0.00037400
C	1.90221900	1.04350800	0.00026200
C	0.59925000	0.53411200	-0.00004200
O	-0.39659900	2.69522200	-0.00003900
H	-0.99777600	-2.35891900	-0.00080200
H	-2.54161200	1.58255700	-0.00046000
H	1.34228000	-2.79595100	-0.00032500
H	3.63796400	-1.87399300	0.00026600
H	4.01018400	0.59280800	0.00062500
H	2.01387400	2.12884700	0.00041600
C	-3.52885300	-1.07749300	0.00068500
H	-3.56586100	-2.17548200	-0.01005400
H	-4.07669400	-0.73173300	0.89084800
H	-4.08628400	-0.71371900	-0.87615100

MeB(aam)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

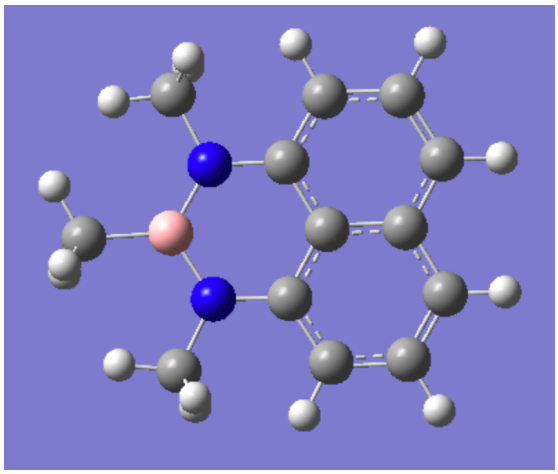
Dihedral angle = 161.7°

B–N bond: 1.48900 Å, 1.49744 Å

H = -575.656935 (hartree)

B	1.87317600	-0.35918400	-0.14040900
N	0.71286900	-1.25246700	-0.41034900
N	1.49017700	1.07982000	-0.29825600
C	-0.58043600	-0.82995600	-0.23163100
C	0.22378700	1.58086600	-0.17504300
C	-1.66760900	-1.72900800	-0.22147800
C	-2.96174100	-1.27488900	-0.01482100
C	-3.22425900	0.08567400	0.18665200
C	-2.16498800	0.98249000	0.15773600
C	-0.85214200	0.54704800	-0.04636400
O	-0.02223800	2.77350900	-0.18044700
H	0.83465300	-2.22599000	-0.65472200
H	2.18180600	1.80543000	-0.45561800
H	-1.47486500	-2.79317400	-0.37589500
H	-3.78300500	-1.99438700	-0.00958100
H	-4.24432900	0.43435800	0.34769300
H	-2.31536600	2.05731700	0.27296400
H	2.35274400	-1.44578700	1.91795800
H	2.77964500	0.15758400	1.98436800
H	1.18610800	-0.27786400	2.05432700
N	2.08818000	-0.50358400	1.62724800
C	3.28413000	-0.80197000	-0.75439900
H	4.11744400	-0.16917000	-0.40671200
H	3.54405300	-1.84615100	-0.51212500
H	3.25409900	-0.72222800	-1.85145200

MeB(mdan)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

N–B–N angle = 117.7°

B–N bond: 1.43654 Å, 1.43793 Å

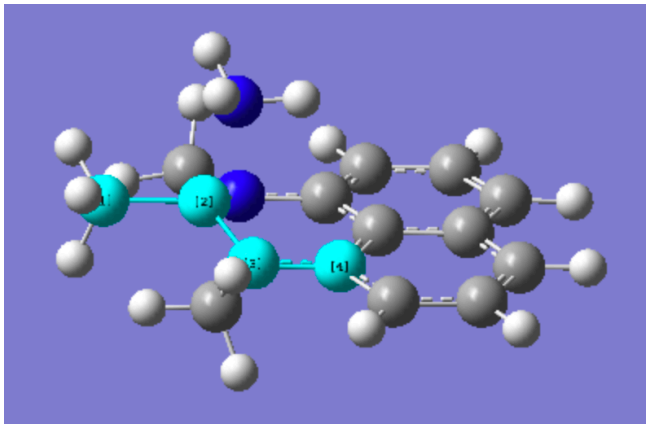
H = -637.869867 (hartree)

AA = 18.3 (kJ/mol)

B	2.10481500	0.04719100	-0.00003200
N	1.38197900	-1.19585500	-0.00003200
N	1.34061500	1.26359200	0.00012800
C	-0.01387700	-1.24349700	0.00007600
C	-0.05995200	1.25097800	-0.00001600
C	-0.71242300	-2.44461500	0.00017600
C	-2.12274600	-2.45541800	0.00017700
C	-2.84104800	-1.28796800	0.00006900
C	-2.16643800	-0.03755600	-0.00002600
C	-0.74099800	-0.00954100	0.00001000
C	-2.88915600	1.18539200	-0.00015400
C	-2.21623500	2.37936100	-0.00024900
C	-0.80647300	2.42309500	-0.00017300
C	1.95392600	2.57728500	0.00048800
C	2.06448700	-2.47453900	-0.00015800
H	-0.18569000	-3.39489400	0.00024300
H	-2.64024000	-3.41631400	0.00025600
H	-3.93184800	-1.29693700	0.00004900
H	-3.97951100	1.15226700	-0.00018100
H	-2.77007300	3.31975200	-0.00037200
H	-0.31993700	3.39420100	-0.00025400
H	3.04100700	2.49135000	0.00096200

H	1.65239600	3.15208200	-0.88949200
H	1.65164400	3.15185500	0.89035600
H	3.14651800	-2.32686400	-0.00035700
H	1.79527900	-3.06555100	0.88992400
H	1.79494800	-3.06555100	-0.89014100
C	3.69302600	0.01444800	-0.00028200
H	4.06309300	-0.53098400	0.88211600
H	4.06269400	-0.53119600	-0.88271800
H	4.18493000	0.99212000	-0.00054500

MeB(mdan)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 178.9°

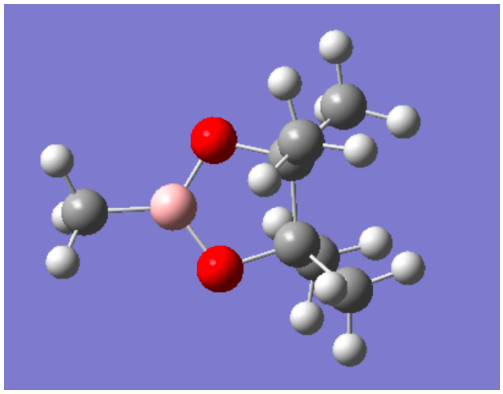
B–N bond: 1.50127 Å, 1.50127 Å

H = -694.311818 (hartree)

B	-1.93269400	0.00000000	0.07373700
N	-1.19380700	1.24110400	-0.33554300
N	-1.19380700	-1.24110500	-0.33554300
C	0.18026000	1.25612400	-0.20518500
C	0.18026000	-1.25612400	-0.20518500
C	0.91612500	2.44113200	-0.16810600
C	2.31546700	2.41843200	-0.00608800
C	3.00049700	1.23573100	0.11522700
C	2.29984800	0.00000000	0.05919900
C	0.88111600	0.00000000	-0.08925000
C	3.00049700	-1.23573000	0.11522700
C	2.31546700	-2.41843100	-0.00608800
C	0.91612500	-2.44113200	-0.16810500
C	-1.85614600	-2.49888700	-0.57188000

C	-1.85614700	2.49888700	-0.57188000
H	0.41306000	3.40143100	-0.25519900
H	2.85578000	3.36682400	0.02435600
H	4.08469100	1.22086500	0.23503500
H	4.08469200	-1.22086400	0.23503500
H	2.85578000	-3.36682300	0.02435700
H	0.41306100	-3.40143100	-0.25519900
H	-2.90942900	-2.32628800	-0.81524800
H	-1.39842500	-3.02836500	-1.42292800
H	-1.80955500	-3.18581900	0.29741500
H	-2.90943000	2.32628700	-0.81524800
H	-1.80955600	3.18581800	0.29741500
H	-1.39842600	3.02836500	-1.42292900
H	-2.10867400	0.83032500	2.29372300
H	-2.10867400	-0.83032500	2.29372400
H	-0.70070200	0.00000000	2.02578200
N	-1.71076000	0.00000000	1.85311800
C	-3.52656000	0.00000000	-0.11266000
H	-4.00191800	0.88281900	0.34302300
H	-3.79913400	-0.00000100	-1.18040700
H	-4.00191800	-0.88281800	0.34302500

MeB(pin)



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

O–B–O angle = 112.0°

B–O bond: 1.37133 Å, 1.37170 Å

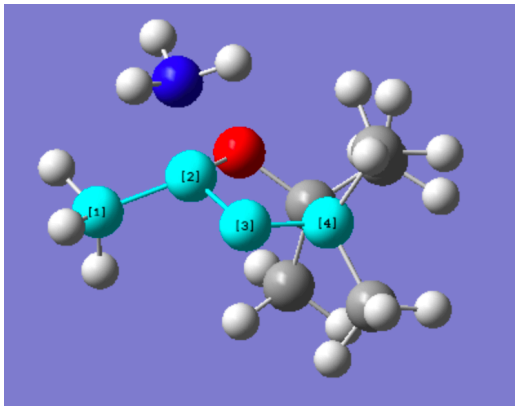
H = -450.427582 (hartree)

AA = 28.8 (kJ/mol)

B	1.56737900	0.01513700	-0.01927000

O	0.79563300	1.06824100	0.40015700
C	-0.56902000	0.77963900	0.05668500
C	-0.55641500	-0.78415500	-0.05492900
O	0.80459900	-1.04807700	-0.43071900
C	-0.79141300	-1.47103300	1.28849500
C	-1.48813400	-1.35521300	-1.11046000
C	-0.84809600	1.46219500	-1.28043100
C	-1.48577700	1.33392600	1.13414500
H	-0.13518500	-1.04923800	2.06333800
H	-1.83485300	-1.37048000	1.61794500
H	-0.55569100	-2.53865700	1.18287700
H	-1.41024200	-2.45109700	-1.11267900
H	-2.53176400	-1.08281300	-0.89367900
H	-1.22586400	-0.99276500	-2.11156500
H	-0.20313500	1.05208300	-2.07074200
H	-1.89730800	1.34337200	-1.58458000
H	-0.62868700	2.53378300	-1.17996300
H	-2.52911800	1.04247200	0.94217100
H	-1.19334700	0.97688600	2.12882300
H	-1.42792100	2.43105100	1.13454300
C	3.13305300	0.01223500	-0.00502500
H	3.48658200	-0.36976700	0.96577700
H	3.53831100	-0.64956900	-0.78188600
H	3.54429400	1.02219100	-0.13042100

MeB(pin)–NH_3



Charge = 0; Multiplicity = 1

M06-2X/def2-SVP

Dihedral angle = 142.9°

B–N bond: 1.44503 Å, 1.43778 Å

H = -506.873520 (hartree)

B	1.37856400	0.12428500	0.08878400
O	0.52552300	0.69348100	-0.92927800
C	-0.80621900	0.64833900	-0.44481900
C	-0.78444600	-0.62915800	0.46220700
O	0.52867400	-0.59816100	0.99595400
C	-1.78693800	-0.61540000	1.60777600
C	-0.97342400	-1.91085000	-0.35964300
C	-1.77248300	0.58042400	-1.61891300
C	-1.07444100	1.91464800	0.37309800
H	-1.57047700	0.20580100	2.30146500
H	-2.81638400	-0.50865100	1.23300900
H	-1.71864400	-1.55882200	2.16849600
H	-0.65295900	-2.76917900	0.24891900
H	-2.02320200	-2.06150800	-0.64988500
H	-0.38181300	-1.88343700	-1.28783300
H	-1.50968200	-0.23366300	-2.30622500
H	-2.80620500	0.43340100	-1.27065100
H	-1.72988500	1.52360300	-2.18187500
H	-2.12462300	1.98530300	0.69146400
H	-0.43302200	1.93962200	1.26534800
H	-0.83360700	2.78728200	-0.24991900
H	2.61300000	-0.64900600	-1.64836800
H	3.04156600	-1.43381900	-0.24334800
H	1.63086400	-1.83375500	-1.02252100
N	2.25988400	-1.06595200	-0.78600600
C	2.50506000	1.05223300	0.75883100
H	3.10344100	0.51110200	1.51063800
H	3.19683700	1.48556800	0.01721000
H	2.02656600	1.89642000	1.27756800

3. Stability test of PhB(mdan) towards hydrolysis

We conducted the stability test of PhB(mdan) towards hydrolysis according to Krempner's procedure.[1] A standard NMR tube was charged with PhB(mdan) (0.0082 g, 0.03 mmol) and 0.6 mL of a DMSO-D_6/water mixture (10 vol% H_2O). The progress of the hydrolysis was monitored periodically by ^{1}H NMR spectroscopy, and we confirmed that PhB(mdan) did not decompose after 24 days.

4. Reference

1. C. P. Manankandayalage, D. K. Unruh and C. Krempner, *Dalton Trans.*, 2020, **49**, 4834–4842.