Electronic Supplementary Information

Exploiting Propane-1,3-diimines as Building Blocks for Superbases: A DFT Study

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B3LYP/6-311+G//B3LYP/6-31+G* SCF energies in gas phase (E) and solution phase (E_{PCM}), B3LYP/6-31+G* zero point vibrational energies (ZPVE), and Cartesian coordinates for 2-7 and their corresponding monoprotonated cations (All energies are given in Hartee).**

2

E = -384.75171
ZPVE = 0.202860
E_{PCM} = -384.75570

C	-1.41649900	0.27562700	0.05650100
C	0.98215900	-0.26880900	-0.33887700
C	-0.00646600	0.83713700	-0.01985100
N	2.04256800	-0.46303700	0.33019100
C	0.03180800	1.86727600	-1.18104200
C	0.31509700	1.54099100	1.31294600
N	-1.69531100	-0.95852400	-0.04056300
H	1.01422400	2.35058000	-1.22511100
H	-0.16068500	1.38825000	-2.14856600
H	-0.72534100	2.64732100	-1.03259700
H	1.30900100	1.99627600	1.27236400
H	-0.42269900	2.32715900	1.51636100
H	0.31027200	0.82943200	2.14406800
H	-2.20611400	1.03528800	0.21247300
H	0.73030800	-0.88220200	-1.21859300
C	-3.08727300	-1.36207300	0.06127800
H	-3.37437400	-1.89566800	-0.85266000
H	-3.19435000	-2.06881300	0.89274000
H	-3.78142800	-0.51835600	0.21661700
C	2.93333000	-1.52933800	-0.09691700
H	3.92686800	-1.10947500	-0.29577000
H	3.04733900	-2.24899900	0.72269900
H	2.58324100	-2.06474000	-0.99565600

$2H^+$

E = -385.14376
ZPVE = 0.217371
E_{PCM} = -385.20817

C	-1.24431300	0.36361600	-0.00008000
C	1.30136100	0.17258400	0.00015100
C	0.07695600	1.07574100	0.00001600
N	1.25140100	-1.09760300	-0.00005000
C	0.11591700	1.97582700	-1.27141400
C	0.11563000	1.97592600	1.27135400
N	-1.39313900	-0.91171600	-0.00008700
H	1.04543300	2.55429100	-1.27586900
H	0.07661300	1.38104200	-2.18939300
H	-0.71751500	2.68642400	-1.27377000
H	1.04491700	2.55476400	1.27575100

H	-0.71805200	2.68623900	1.27373600
H	0.07654500	1.38121400	2.18939400
H	-2.14567700	0.98024700	-0.00024200
H	2.25915400	0.71344600	0.00036500
C	-2.66784800	-1.63538600	0.00002500
H	-2.71368900	-2.26901000	-0.88980300
H	-2.71483300	-2.26670700	0.89144600
H	-3.49947100	-0.92802600	-0.00141900
C	2.48579200	-1.87575400	0.00004300
H	2.49464600	-2.52230000	0.88337100
H	2.49466400	-2.52247900	-0.88314900
H	3.38397100	-1.24457100	0.00000100
H	-0.47550000	-1.43466400	-0.00003600

3

E = -344.19480

ZPVE = 0.151585

E_{PCM} = - -344.20079

C	-1.13568333	-0.00571667	0.02180000
C	-2.48468333	-0.01171667	0.04880000
C	-0.43068333	-1.30471667	-0.06120000
C	-0.44068333	1.30028333	0.07780000
N	0.78731667	-1.48671667	0.25380000
N	0.76231667	1.49428333	-0.28320000
C	1.28131667	2.84528333	-0.20820000
C	1.31531667	-2.83271667	0.15780000
H	-3.05268333	-0.93671667	-0.02020000
H	-3.05868333	0.90728333	0.14080000
H	-1.07068333	-2.14571667	-0.38520000
H	-1.07668333	2.13528333	0.42380000
H	2.16231667	2.85128333	0.44480000
H	1.62131667	3.15328333	-1.20520000
H	0.55131667	3.58528333	0.16580000
H	2.17131667	-2.82971667	-0.52920000
H	1.69631667	-3.13771667	1.13980000
H	0.57931667	-3.57971667	-0.19020000

3H$^+$

E = -344.59485

ZPVE = 0.166709

E_{PCM} = -344.65975

C	-1.21839344	0.36095082	0.08485246
C	-2.52739344	0.69895082	0.17085246
C	-0.89339344	-1.05404918	-0.02614754
C	-0.15839344	1.39395082	0.10085246
N	1.07660656	1.08695082	0.01885246
C	2.08360656	2.13895082	0.03885246
C	0.71560656	-2.90104918	-0.22914754
N	0.31760656	-1.49704918	-0.11314754
H	-3.31839344	-0.04604918	0.15985246
H	-2.83839344	1.73595082	0.25585246
H	-1.70539344	-1.78104918	-0.03714754

H	-0.50239344	2.43295082	0.18685246
H	2.76260656	1.95895082	0.87885246
H	2.67460656	2.07595082	-0.88014754
H	1.64960656	3.14395082	0.12685246
H	1.28060656	-3.03504918	-1.15514754
H	1.35460656	-3.16004918	0.61985246
H	-0.16939344	-3.54104918	-0.23714754
H	1.04260656	-0.74004918	-0.09914754

4

E = -1374.85301

ZPVE = 0.371169

E_{PCM} = -1374.86975

C	-0.47702564	-1.23349359	-0.52842949
C	0.15097436	-0.29149359	0.30757051
C	0.20497436	-2.49149359	-0.80942949
C	-1.85802564	-1.00449359	-0.94042949
N	-2.38602564	-1.36149359	-2.05442949
N	-0.30902564	-3.51449359	-1.39042949
N	1.22197436	-0.68649359	1.07057051
N	-0.25802564	1.03350641	0.42957051
P	1.97497436	0.22150641	2.14557051
P	-0.78902564	2.00250641	-0.73342949
C	0.55397436	-4.66149359	-1.58342949
C	-3.81902564	-1.21149359	-2.19242949
C	-2.59502564	2.35250641	-0.77942949
C	-0.08202564	3.66650641	-0.42542949
C	-0.31702564	1.58950641	-2.45742949
C	0.95797436	0.81050641	3.55757051
C	2.88497436	1.72250641	1.57757051
C	3.26497436	-0.83849359	2.87957051
H	1.24997436	-2.51849359	-0.46142949
H	-2.49302564	-0.51749359	-0.17142949
H	0.10797436	-5.54649359	-1.10642949
H	0.63597436	-4.89049359	-2.65542949
H	1.57597436	-4.52649359	-1.17942949
H	-4.05102564	-0.65049359	-3.10942949
H	-4.28002564	-2.20249359	-2.30542949
H	-4.30402564	-0.71049359	-1.33142949
H	-2.80102564	3.20050641	-1.44342949
H	-3.14902564	1.48150641	-1.13142949
H	-2.93302564	2.59950641	0.23157051
H	-0.49102564	4.40550641	-1.12242949
H	-0.31702564	3.97450641	0.59857051
H	1.00497436	3.63250641	-0.54142949
H	-0.59602564	2.41450641	-3.12342949
H	0.76597436	1.43750641	-2.50642949
H	-0.81502564	0.67050641	-2.77842949
H	1.56497436	1.35850641	4.28757051
H	0.16697436	1.45750641	3.16857051
H	0.49497436	-0.05249359	4.04557051
H	3.49397436	2.13950641	2.38757051

H	3.53797436	1.45050641	0.74257051
H	2.16897436	2.47450641	1.23857051
H	3.81797436	-0.30549359	3.66057051
H	2.79497436	-1.72949359	3.30557051
H	3.95897436	-1.15849359	2.09657051

$4H^+$

E = -1375.32933

ZPVE = 0.386932

E_{PCM} = -1375.37704

C	-0.04044586	-1.28763057	-0.46386624
C	0.18255414	-0.09763057	0.36513376
C	1.01355414	-2.19663057	-0.59486624
C	-1.35444586	-1.58463057	-0.99886624
N	-1.61544586	-2.59063057	-1.76186624
N	1.07355414	-0.23963057	1.35713376
N	-0.46444586	1.07836943	0.18813376
P	1.46955414	0.92236943	2.43013376
P	-1.16944586	1.78636943	-1.08386624
C	2.07355414	-4.25663057	-1.44386624
C	-2.99644586	-2.84163057	-2.13586624
C	-2.99444586	1.83436943	-0.97286624
C	-0.66644586	3.53936943	-1.06086624
C	-0.73844586	1.19136943	-2.76186624
C	0.09155414	1.43436943	3.51213376
C	2.22055414	2.45136943	1.75613376
C	2.72955414	0.17436943	3.50413376
N	0.96855414	-3.31863057	-1.30186624
H	1.95055414	-1.97563057	-0.09186624
H	-2.17244586	-0.93063057	-0.65986624
H	1.78555414	-5.24363057	-1.06786624
H	2.36155414	-4.35163057	-2.49686624
H	2.93455414	-3.89963057	-0.87186624
H	-3.08344586	-2.87163057	-3.22886624
H	-3.30544586	-3.82463057	-1.76186624
H	-3.69644586	-2.08563057	-1.74186624
H	-3.40044586	2.49836943	-1.74386624
H	-3.42444586	0.83836943	-1.10086624
H	-3.28144586	2.21536943	0.01213376
H	-1.17244586	4.09936943	-1.85386624
H	-0.92344586	3.98136943	-0.09386624
H	0.41555414	3.61536943	-1.20786624
H	-1.16044586	1.87636943	-3.50586624
H	0.35055414	1.17536943	-2.87286624
H	-1.12144586	0.18536943	-2.94286624
H	0.43955414	2.14336943	4.27013376
H	-0.69244586	1.89736943	2.90713376
H	-0.32044586	0.55136943	4.00913376
H	2.58255414	3.08636943	2.57213376
H	3.06555414	2.18736943	1.11213376
H	1.48155414	3.00136943	1.17013376
H	3.03755414	0.87236943	4.28813376

H	2.32055414	-0.73063057	3.96313376
H	3.60155414	-0.10463057	2.90513376
H	0.06655414	-3.50663057	-1.75886624

5

E = -1601.58014

ZPVE = 0.396261

E_{PCM} = -1601.60213

C	-1.05308152	0.08780435	-1.89961413
O	-0.18808152	1.05480435	-2.43661413
C	-0.83308152	1.55880435	-3.62561413
C	-2.00308152	0.57580435	-3.84961413
C	-1.17008152	-1.94819565	-0.53161413
O	-1.91408152	-2.15719565	0.62038587
C	-1.87408152	-4.02819565	-0.78961413
C	-2.21008152	-3.56719565	0.64638587
N	-2.12308152	-0.14119565	-2.58361413
N	-1.06308152	-2.93419565	-1.33861413
C	-0.63108152	-0.58619565	-0.70161413
C	0.33891848	-0.15219565	0.22338587
N	0.77291848	1.13580435	0.45138587
N	0.91191848	-1.13719565	0.98438587
P	2.04891848	-0.90519565	2.08238587
P	0.10691848	2.56680435	0.22438587
C	2.44591848	-2.55819565	2.74038587
C	1.64291848	0.10080435	3.57138587
C	3.64691848	-0.22819565	1.47638587
C	0.37091848	3.54680435	1.75538587
C	0.93591848	3.59680435	-1.04661413
C	-1.70508152	2.68680435	-0.04361413
H	-1.17508152	2.58680435	-3.43361413
H	-0.09308152	1.57480435	-4.43061413
H	-2.93808152	1.08980435	-4.10361413
H	-1.78808152	-0.13319565	-4.66361413
H	-2.77408152	-4.15819565	-1.40761413
H	-1.31708152	-4.97119565	-0.81061413
H	-3.25808152	-3.69319565	0.93238587
H	-1.56808152	-4.04019565	1.40238587
H	2.75291848	-3.20519565	1.91338587
H	3.24791848	-2.50819565	3.48438587
H	1.54891848	-2.98719565	3.19638587
H	1.48891848	1.14080435	3.27738587
H	0.71691848	-0.28119565	4.01438587
H	2.44691848	0.04580435	4.31438587
H	4.39291848	-0.18819565	2.27838587
H	4.01591848	-0.86819565	0.66838587
H	3.47491848	0.77380435	1.07538587
H	-0.19108152	3.10180435	2.58138587
H	1.43591848	3.53980435	2.01038587
H	0.04591848	4.58480435	1.62038587
H	0.90791848	3.07880435	-2.00561413
H	0.45391848	4.57680435	-1.13061413

H	1.98091848	3.73880435	-0.75161413
H	-2.02008152	3.73280435	0.04938587
H	-1.99808152	2.30080435	-1.02061413
H	-2.21208152	2.08880435	0.72038587

5H$^+$

E = -1602.04857

ZPVE = 0.411374

E_{PCM} = -1602.09836

C	-0.35036757	-0.17325946	-2.06690270
O	0.78163243	0.44174054	-2.49290270
C	0.69363243	0.61574054	-3.93590270
C	-0.40336757	-0.36725946	-4.36690270
C	-1.71236757	-1.24125946	-0.35990270
O	-1.86336757	-1.47625946	0.98409730
C	-3.58636757	-2.43925946	-0.30890270
C	-2.95536757	-2.43125946	1.10209730
N	-2.60336757	-1.74025946	-1.14990270
C	-0.57936757	-0.42425946	-0.73390270
C	0.47063243	-0.09125946	0.29209730
N	0.50163243	1.07874054	0.95109730
N	1.36063243	-1.04825946	0.50709730
P	2.56363243	-0.93025946	1.62209730
P	-0.55436757	2.31874054	0.77909730
C	3.46463243	-2.50225946	1.51009730
C	1.98763243	-0.76525946	3.34609730
C	3.77563243	0.39974054	1.31009730
C	-0.12036757	3.48874054	2.10109730
C	-0.39936757	3.24574054	-0.78790270
C	-2.32936757	1.94074054	0.99409730
N	-1.15636757	-0.46725946	-3.11790270
H	0.42063243	1.65674054	-4.13690270
H	1.67863243	0.40274054	-4.35390270
H	-1.02236757	0.02674054	-5.17690270
H	0.00863243	-1.33925946	-4.67090270
H	-4.54736757	-1.90925946	-0.34090270
H	-3.75836757	-3.45425946	-0.68090270
H	-3.61936757	-2.08525946	1.89609730
H	-2.52236757	-3.39725946	1.38309730
H	3.84863243	-2.62625946	0.49309730
H	4.29663243	-2.52725946	2.22009730
H	2.77863243	-3.32725946	1.72209730
H	1.47663243	0.19174054	3.47009730
H	1.28763243	-1.57525946	3.57009730
H	2.83563243	-0.82225946	4.03709730
H	4.60563243	0.33274054	2.02109730
H	4.16763243	0.29774054	0.29309730
H	3.28463243	1.36974054	1.40709730
H	-0.25336757	3.00774054	3.07509730
H	0.92663243	3.78774054	1.99809730
H	-0.75536757	4.37974054	2.05209730
H	-0.73136757	2.62474054	-1.62390270

H	-1.01036757	4.15374054	-0.74890270
H	0.64763243	3.52074054	-0.94590270
H	-2.89236757	2.87674054	1.08309730
H	-2.70636757	1.37274054	0.14109730
H	-2.46636757	1.34674054	1.90209730
H	-1.91636757	-1.12925946	-2.93790270

6

E = -1680.22006

ZPVE = 0.454050

E_{PCM} = -1680.23702

C	4.32228500	0.39027700	-0.20335200
C	4.45094500	-1.02756000	-0.77615600
C	3.28071000	-1.24422900	-1.72512100
C	1.94761400	0.12916900	-0.28687800
C	0.75498500	4.33523200	-0.50620700
C	0.45299300	2.06263200	0.10578900
C	-0.45672100	3.72580500	1.55529400
C	0.58603300	4.67532500	0.97987600
N	0.79206000	2.90480800	-0.78976400
C	-0.59902300	-0.14684600	-0.17092600
C	0.58717100	0.59296700	-0.07911800
N	2.96873600	0.77256600	0.15924900
N	-1.74726000	0.58208000	-0.38833300
N	-0.75500700	-1.51778600	-0.06281600
P	0.06010600	-2.61835100	0.74793000
P	-3.19728800	-0.04114900	-0.60717400
C	-4.30519000	1.37300400	-0.92252700
C	-4.00317600	-0.94843600	0.78263100
C	-3.40563000	-1.14878000	-2.06047000
C	-1.14109500	-3.64550300	1.68767900
C	0.90291300	-3.87187000	-0.29367700
C	1.25845400	-2.08094700	2.02936300
O	2.03335000	-1.04589000	-1.04714200
O	-0.05396100	2.36674700	1.35679400
H	4.70126800	1.11887800	-0.93821500
H	4.95779000	0.50285500	0.68499300
H	4.40971300	-1.77593400	0.02768800
H	5.40462200	-1.16184800	-1.30416900
H	3.33226600	-0.54513500	-2.57208000
H	3.24338000	-2.26291000	-2.12675800
H	-0.06618900	4.77829400	-1.09005900
H	1.68024400	4.77790800	-0.89814900
H	-1.43191200	3.87642400	1.06639200
H	-0.58594200	3.84118900	2.63587400
H	1.53346400	4.52851000	1.51386600
H	0.27824300	5.72032700	1.11956200
H	-5.32881900	1.03944500	-1.12411500
H	-4.30376400	2.03387800	-0.05039600
H	-3.92776800	1.93677000	-1.77966800
H	-3.95794600	-0.32901300	1.68456400
H	-5.05144100	-1.17211600	0.55130200

H	-3.46473300	-1.88018200	0.96846800
H	-3.07631300	-0.61544600	-2.95852300
H	-2.76855200	-2.02552800	-1.92482600
H	-4.44926100	-1.45782400	-2.18295700
H	-1.90552200	-4.02647900	1.00325200
H	-0.64414300	-4.49338100	2.17178300
H	-1.62975700	-3.03302600	2.45315600
H	0.16210900	-4.33066500	-0.95630700
H	1.66392100	-3.38264300	-0.90006200
H	1.36036100	-4.65268700	0.32565700
H	0.78188200	-1.32656800	2.66304700
H	1.55134800	-2.93960500	2.64304400
H	2.14475300	-1.63094500	1.57954700

6H$^+$

E = -1680.69884

ZPVE = 0.469734

E_{PCM} = -1680.74650

C	3.57384100	-2.39253100	-1.10751600
C	2.85573200	-3.61952700	-0.54905300
C	1.37917200	-3.51085000	-0.89753100
C	1.49558300	-1.14150500	-0.50468300
C	3.20590200	2.84397700	-0.94026500
C	1.39560200	1.33961300	-0.48919100
C	0.89550500	3.67721300	-0.67395300
C	2.34546400	3.93228900	-0.29280300
N	2.63743600	1.50439200	-0.80444500
C	-0.71227100	-0.04570600	-0.14950300
C	0.78479100	0.03388600	-0.29775100
N	-1.39012500	-0.05816200	-1.29089900
N	-1.33368800	-0.08673000	1.04095900
P	-0.61309800	-0.12972800	2.50866000
P	-3.03190000	-0.08550000	-1.35834800
C	-3.43153900	-0.08232700	-3.12994700
C	-3.85199300	1.37230000	-0.62726600
C	-3.81948200	-1.57308400	-0.64726700
C	0.68781500	1.10115000	2.87423200
C	-1.94979100	0.19108000	3.70043200
C	0.07318400	-1.76479900	2.94489800
O	0.81144300	-2.30427000	-0.33644300
O	0.49106100	2.35277000	-0.26679200
N	2.80691500	-1.18652900	-0.80616400
H	3.69613400	-2.49169100	-2.19552600
H	4.57283700	-2.28590200	-0.67231100
H	2.97269800	-3.67447700	0.54034500
H	3.27780800	-4.53541700	-0.97748100
H	1.22329800	-3.49315000	-1.98366500
H	0.78401400	-4.31993000	-0.46808000
H	3.33815200	3.05783200	-2.01139200
H	4.21111000	2.83181000	-0.50363900
H	0.75055000	3.76127900	-1.75856800
H	0.19805900	4.35432400	-0.17458800

H	2.44620000	3.90258200	0.80051700
H	2.65451900	4.93038900	-0.62507200
H	-4.51457600	-0.09632200	-3.28674500
H	-3.00703900	0.81282700	-3.59423700
H	-2.98401900	-0.96069600	-3.60382500
H	-3.43678200	2.28007700	-1.07661100
H	-4.93000300	1.33909800	-0.81710800
H	-3.66716200	1.39163100	0.44846700
H	-3.37835400	-2.46616400	-1.09931100
H	-3.64492200	-1.59713100	0.43108500
H	-4.89639400	-1.56619100	-0.84687000
H	0.33918100	2.09458300	2.57901100
H	0.89872000	1.09347900	3.95016800
H	1.60159300	0.87063200	2.32229100
H	-2.35664700	1.19299500	3.53348200
H	-2.75126100	-0.53979400	3.55945600
H	-1.57628300	0.12255100	4.72723100
H	0.87115200	-2.02788700	2.24618800
H	0.46578100	-1.75248800	3.96740700
H	-0.71593700	-2.52009400	2.87096100
H	3.20364800	-0.24621600	-0.96354600

7

E = -1835.11524

ZPVE = 0.525566

E_{PCM} = -1835.12510

C	1.17841800	2.54407900	-2.16331600
H	2.22369700	2.85601700	-2.28801900
O	0.00000000	2.39581200	-0.11494800
N	1.14277300	1.17177100	-1.65566300
C	-0.82525500	3.97362000	-1.81276500
C	-1.04701700	3.05196100	-3.02825300
H	-0.58006500	4.99043600	-2.15224900
H	-1.68756400	4.04697700	-1.14144700
C	0.38604500	2.71928900	-3.48198000
H	-1.56428400	2.13419800	-2.72340100
H	-1.64558100	3.52577900	-3.81497200
H	0.45237900	1.81953500	-4.10121600
H	0.80348700	3.55939200	-4.05619200
C	0.39901500	3.38213200	-1.09321400
H	0.99215200	4.14263100	-0.57281600
C	0.43377400	1.15533100	-0.57814300
C	-1.17841800	-2.54407900	-2.16331600
H	-2.22369700	-2.85601700	-2.28801900
O	0.00000000	-2.39581200	-0.11494800
N	-1.14277300	-1.17177100	-1.65566300
C	0.82525500	-3.97362000	-1.81276500
C	1.04701700	-3.05196100	-3.02825300
H	0.58006500	-4.99043600	-2.15224900
H	1.68756400	-4.04697700	-1.14144700
C	-0.38604500	-2.71928900	-3.48198000
H	1.56428400	-2.13419800	-2.72340100

H	1.64558100	-3.52577900	-3.81497200
H	-0.45237900	-1.81953500	-4.10121600
H	-0.80348700	-3.55939200	-4.05619200
C	-0.39901500	-3.38213200	-1.09321400
H	-0.99215200	-4.14263100	-0.57281600
C	-0.43377400	-1.15533100	-0.57814300
C	0.00000000	0.00000000	0.18508900
C	0.00000000	0.00000000	1.61972600
N	-0.95703500	-0.61794300	2.36371300
P	-2.51389000	-0.79221300	2.04044900
C	-3.01327100	-2.51011200	1.63728200
C	-3.42640800	-0.42057600	3.58303000
C	-3.27076900	0.27388400	0.75459600
H	-2.61027300	-3.18301800	2.40065000
H	-4.10483500	-2.60217800	1.61160900
H	-2.60176700	-2.79684500	0.66777500
H	-3.03222900	-1.04800900	4.38808100
H	-3.25862700	0.62682700	3.85211700
H	-4.50078200	-0.60211800	3.46855900
H	-2.91961000	-0.02000000	-0.23898900
H	-4.36290900	0.19033700	0.80424800
H	-2.97764100	1.31291300	0.93488900
N	0.95703500	0.61794300	2.36371300
P	2.51389000	0.79221300	2.04044900
C	3.01327100	2.51011200	1.63728200
C	3.42640800	0.42057600	3.58303000
C	3.27076900	-0.27388400	0.75459600
H	2.61027300	3.18301800	2.40065000
H	4.10483500	2.60217800	1.61160900
H	2.60176700	2.79684500	0.66777500
H	3.03222900	1.04800900	4.38808100
H	3.25862700	-0.62682700	3.85211700
H	4.50078200	0.60211800	3.46855900
H	2.91961000	0.02000000	-0.23898900
H	4.36290900	-0.19033700	0.80424800
H	2.97764100	-1.31291300	0.93488900

7H$^+$

E = -1835.58021

ZPVE = 0.539686

E_{PCM} = -1835.62821

C	2.69856200	-0.58839000	-2.42235000
H	2.84297800	-1.55869900	-2.91055300
O	2.35273900	-0.27151400	-0.08988500
N	1.27691100	-0.42799700	-2.08445600
C	4.33014200	0.78352500	-1.14167800
C	3.71055600	1.62847400	-2.27232100
H	5.34267600	0.46772800	-1.42587600
H	4.40601400	1.29936000	-0.17892300
C	3.24758800	0.56899300	-3.28890400
H	2.85023000	2.19889000	-1.89755300
H	4.41668900	2.34859700	-2.69792300

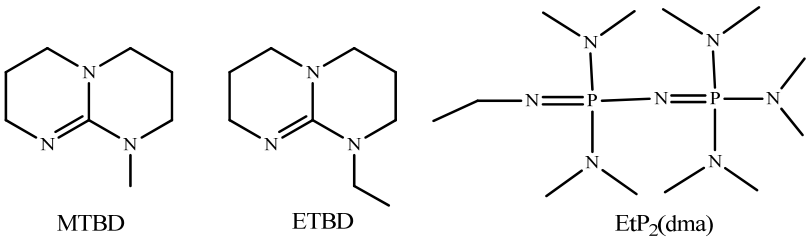
H	2.49545900	0.93052200	-3.99669400
H	4.10758800	0.21129400	-3.87035500
C	3.43888800	-0.46295900	-1.05041600
H	3.97982300	-1.35846400	-0.73257100
C	1.18276500	-0.24408900	-0.80680700
C	-2.82456400	-0.09049800	-2.45064000
H	-3.01375800	0.67058100	-3.21458800
O	-2.40341600	0.29458400	-0.11661400
N	-1.41678000	-0.07459000	-2.06955000
C	-4.43448100	-0.94597500	-0.77194100
C	-3.83428300	-2.13071100	-1.55218800
H	-5.43447700	-0.71028400	-1.15919500
H	-4.52871000	-1.11028500	0.30585700
C	-3.36199600	-1.48107200	-2.86682800
H	-2.98312900	-2.55771100	-1.00584200
H	-4.55344900	-2.93931400	-1.71402000
H	-2.60857600	-2.06530200	-3.40497600
H	-4.21461600	-1.34292400	-3.54383500
C	-3.50524600	0.23166900	-1.08268600
H	-4.00086200	1.20444800	-1.04256400
C	-1.22636300	0.07085400	-0.74594900
C	-0.02732200	0.00524800	-0.05473500
C	-0.00042900	0.17395100	1.43945300
N	-0.33916800	1.31936400	2.02065900
P	-0.61245600	2.82618100	1.53528700
C	-2.33382100	3.28170600	1.92240200
C	0.45311700	3.92155500	2.52836400
C	-0.31782000	3.31989600	-0.20866400
H	-2.52211000	3.08856100	2.98254200
H	-2.51509600	4.34012600	1.70831800
H	-3.01382400	2.66419500	1.32945500
H	0.28814500	3.71147200	3.58892400
H	1.50306600	3.71982800	2.29428200
H	0.23258000	4.97463600	2.32458900
H	-1.00963100	2.81628500	-0.88751900
H	-0.45346400	4.40342100	-0.30228000
H	0.70507600	3.06537600	-0.50082200
N	0.34486900	-0.81485300	2.25336700
P	0.73277500	-2.36783700	2.10427000
C	2.49884100	-2.59621900	2.49000500
C	-0.20090300	-3.27389500	3.37993500
C	0.41133900	-3.27307300	0.53993300
H	2.70444000	-2.16539100	3.47433700
H	2.76232700	-3.65902800	2.49680300
H	3.09908500	-2.06879400	1.74445600
H	-0.01133000	-2.81351500	4.35367600
H	-1.27250100	-3.20692400	3.16792800
H	0.09686500	-4.32727200	3.40887400
H	0.99258100	-2.86008700	-0.28715900
H	0.68046700	-4.32692400	0.67454200
H	-0.65127100	-3.21108600	0.28693100
H	-0.60692100	-0.30045400	-2.65368700

Cartesian coordinates of B3LYP/6-31+G* optimized transition state geometries of 3 with HCl including electronic energy (E), zero point energy (ZPVE).

3.HCl

E = -804.92654
ZPVE = 0.159178

C	2.12809200	-1.75786000	0.89056900
C	-0.16005200	-1.65371400	0.25095700
C	-1.37272500	2.52862400	0.83367500
C	-1.64932100	0.41514200	-0.12941900
N	-1.07268500	1.11410200	0.75999600
C	-2.28197400	-1.82896200	-0.90391500
N	0.96083500	-1.05689400	0.38073800
H	2.93312200	-1.68112700	0.15255700
H	2.46589000	-1.25358600	1.80244300
H	-0.44766400	3.07784500	0.62270300
H	-1.67796100	2.77683800	1.85694300
H	1.30887200	0.16680300	-0.16971500
Cl	1.92587500	1.33310500	-0.87063500
H	1.91740300	-2.81266900	1.10784700
H	-0.23389600	-2.71793500	0.51047300
H	-2.39850000	0.83579200	-0.82045100
H	-2.15558100	2.85401600	0.12862800
C	-1.38932800	-1.03421900	-0.27992800
H	-2.13069700	-2.90111300	-0.99833600
H	-3.18607900	-1.42216200	-1.34905700



Scheme S1

Table S1 Comparison of experimental and calculated (B3LYP/6-311+G**//B3LYP/6-31+G*) gas phase basicities (GB) of some organic superbases.

	Gas phase basicity (kcal/mol)	
Compounds	Experimental[a]	Calculated
MTBD	246.2	247.3
ETBD	247.5	248.2
EtP$_2$(dma)	264.6	265.7

[a] I. Kaljurand, I. A. Koppel, A. Kütt, E.-I. Rõõm, T. Rodima, I. Koppel, M. Mishima and I. Leito, *J. Phys. Chem. A* 2007, **111**, 1245 and references therein.

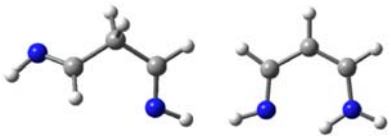


Fig. S1 B3LYP/6-31+G* optimized geometries of **1** and **1a** (relative energies are in kcal/mol) [Gray = carbon; blue = nitrogen; white = hydrogen].

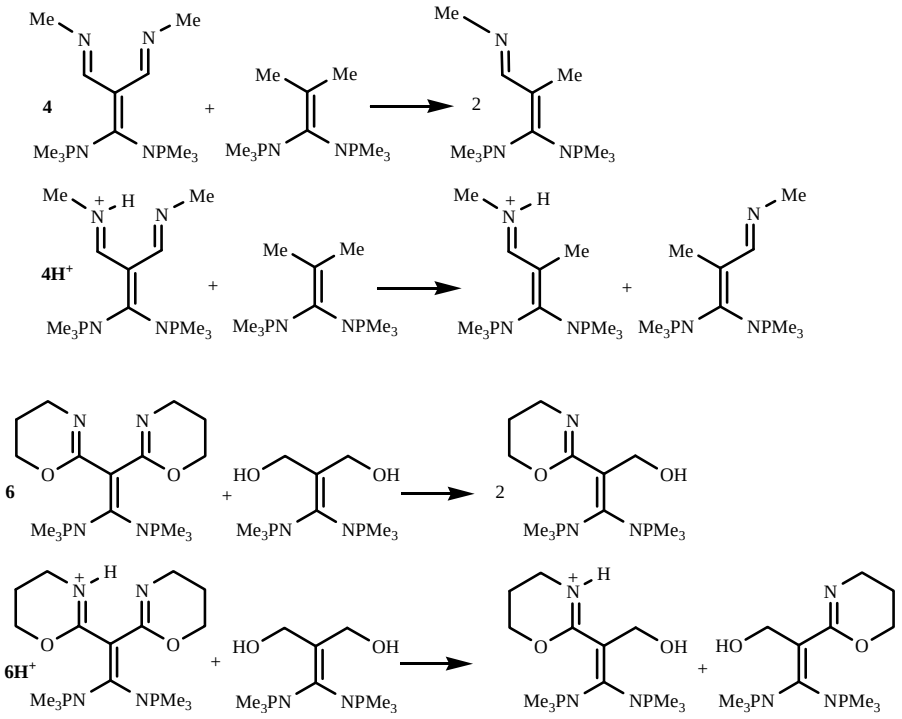


Fig. S2 Isodesmic reactions used to obtain strain energy of unprotonated bases and the sum of the cation strain and the H-bond energies $(SE+HB)^+$ for their corresponding monoprotonated cations.

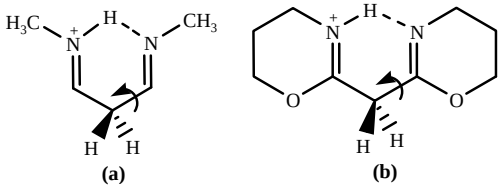
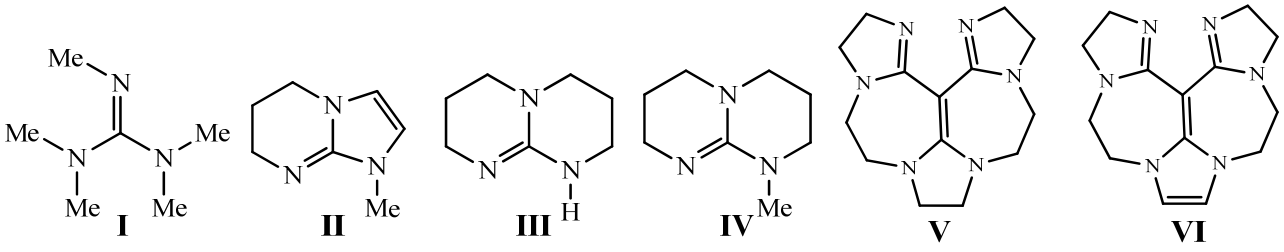


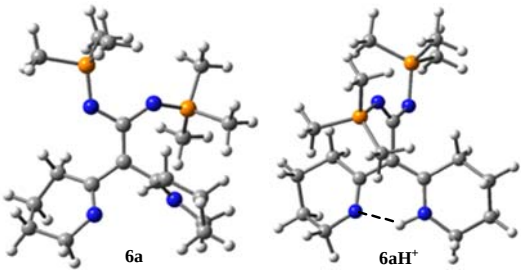
Fig. S3 The model systems used to estimate cationic hydrogen bond energies for (a) **4H**$^+$ and (b) **6H**$^+$



Scheme S2

Table S2 Comparison of experimental and calculated (B3LYP/6-311+G**//B3LYP/6-31+G*) p*K*a(MeCN) of imine bases.

	p*K*a(MeCN)		
Compounds	Experimental	Calculated	
		UAHF	Bondi
I	25.0	24.1	27.6
II	24.5	23.0	26.1
III	26.0	26.5	28.0
IV	25.4	25.9	28.4
V	29.2	33.5	32.4
VI	31.9	35.9	34.8



PA = 288.7 kcal/mol
p*K*a = 42.3

Fig. S4 B3LYP/6-31+G* optimized geometries of **6a** and its conjugate acids [Gray = carbon; blue = nitrogen; white = hydrogen; orange = phosphorus].