Supporting Information

Synthesis of 3-Methoxyazetidines via an Aziridine to Azetidine Rearrangement and Theoretical Rationalization of the Reaction Mechanism

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Electronic supporting information

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Data 1: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of *N*-benzyl-*N*-(2,3-dibromo-2-methylpropyl)amine **10**.

C	-6.17123500	-0.53990000	0.14265400
C	-4.99888300	-0.11261700	0.77520400
C	-3.75424200	-0.64245200	0.41372400
C	-3.70199300	-1.60739500	-0.60434000
C	-4.86928300	-2.03441100	-1.23870300
C	-6.10912100	-1.50272800	-0.86641700
C	-2.48736000	-0.19817900	1.11579200
N	-1.45971800	0.21350400	0.15553700
C	-0.20689700	0.62441600	0.77796900
C	0.94186600	0.72075400	-0.22395400
C	1.01546100	-0.43674400	-1.20732800
Br	1.38981100	-2.19413600	-0.30088500
Br	0.46543700	2.23925600	-1.52955600
C	2.26103100	1.10070000	0.42464100
O	4.52399500	-1.08577300	-1.14783000
C	5.60036500	-1.84017400	-1.69493900
O	1.74826900	-1.41287500	3.02265800
C	2.35452400	-2.18105700	4.05668300
H	3.06564100	1.15035900	-0.31200100
H	2.16623100	2.05962500	0.93822400
H	2.52266800	0.34587500	1.17433000
H	0.07010700	-0.61578700	-1.70911700
H	1.83724200	-0.32318300	-1.91089400
H	-0.26656300	1.57456400	1.32981800
H	0.08263500	-0.14238900	1.50716200
H	-1.81782000	0.96878000	-0.42585800
H	-2.07381200	-1.03548500	1.69414800
H	-2.73411100	0.59257400	1.84553400
H	-2.73790400	-2.01078600	-0.89918700
H	-4.81381700	-2.78417400	-2.02325600
H	-7.01705300	-1.83557500	-1.36128900
H	-7.12806900	-0.11638500	0.43501500
H	-5.05124300	0.64207700	1.55642300
H	3.80697100	-1.68701000	-0.89665400
H	6.39097200	-1.12862800	-1.94415000
H	6.00114300	-2.56606100	-0.97398300
H	5.30887700	-2.37173900	-2.61149100
H	1.77469900	-1.90727700	2.19105400
H	2.29717400	-1.58339900	4.96920500
H	1.82630500	-3.12916000	4.22802900
H	3.41172900	-2.39326000	3.84571700
H	0.40557700	3.95858400	0.38246900
O	0.42636900	4.09235000	1.34160100
C	0.55759500	5.47968300	1.63205500
H	0.58294300	5.57317600	2.72023100
H	1.48746200	5.90029100	1.22488300
H	-0.29366500	6.06166000	1.25266100

Energy (B3LYP/6-31++G**) = -5973.374883 hartree

Data 2: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for the conversion of *N*-benzyl-*N*-(2,3-dibromo-2-methylpropyl)amine to 1-benzyl-2-bromomethyl-2-methylaziridine (**TS-a**).

C	4.57250600	-1.63631300	0.17929800
C	5.78243200	-1.26326400	0.76854800
C	6.16593400	0.08081200	0.78488700
C	5.33783800	1.04624400	0.20574500
C	4.12985600	0.67139400	-0.38778300
C	3.73323000	-0.67414600	-0.40063500
C	2.40329600	-1.08399600	-1.00581400
N	1.30280700	-1.07167800	-0.03518100
C	0.66988400	0.17217000	0.39547600
C	-0.51230200	-0.29600100	-0.36917500
C	-0.64760900	-0.04636500	-1.84194300
C	-1.46417600	-1.24973200	0.28228000
Br	-1.48128400	-3.02672400	-0.61223800
Br	-1.89537700	2.03899400	0.32365300
O	-1.26858200	0.28520300	3.07235400
C	-2.07849700	0.27948200	4.24265400
O	0.87840500	3.03118000	-1.26641600
C	1.01018200	4.35586100	-1.77225600
O	-4.39176400	-0.06653000	-0.23632200
C	-5.13884100	0.04992000	-1.44079300
H	-1.70965300	-0.01739700	-2.09255600
H	-0.17571700	0.89334600	-2.13221300
H	-0.21125800	-0.87509500	-2.41047900
H	-1.25173000	-1.41261100	1.33617300
H	-2.49281200	-0.91123700	0.14658200
H	0.53009000	0.24806900	1.47270100
H	1.15316000	1.05895700	-0.01037500
H	1.31014700	-1.81940200	0.64839800
H	2.13446000	-0.40657300	-1.82123600
H	2.46165200	-2.09430700	-1.42237000
H	4.28299200	-2.68488400	0.16157300
H	6.42576300	-2.01960300	1.20871100
H	7.10699000	0.37306800	1.24140200
H	5.63360500	2.09125300	0.21046000
H	3.49520500	1.42757900	-0.84327500
H	-3.89654400	0.76026000	-0.08591800
H	-1.59291800	0.97025300	2.45634400
H	0.03530000	2.96332500	-0.77737300
H	1.95297400	4.40060700	-2.32379700
H	0.19170300	4.61326600	-2.45785000
H	1.04196400	5.09926200	-0.96457700
H	-1.69801200	-0.51072800	4.89518000
H	-2.02083700	1.23440500	4.78220300
H	-3.13027600	0.06538700	4.01002800
H	-5.68276000	-0.88824800	-1.57469800
H	-5.86520400	0.87206600	-1.39011300
H	-4.49168200	0.20607500	-2.31607100

Energy (B3LYP/6-31++G**) = -5973.336950 hartree

Frequencies(cm^{-1}): -243.3829, 14.8728, 21.5367, 22.5489, 27.6793, 33.2344, 41.8192, 43.3070, 53.5581, …

Data 3: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of the protonated 1-benzyl-2-bromomethyl-2-methylaziridine **11-H**.

C	-3.72007000	0.03300200	-0.50103500
C	-4.62881700	0.99576400	-0.03881600
C	-5.81940300	0.60598100	0.57885700
C	-6.11100800	-0.75133700	0.73784100
C	-5.21242800	-1.71689200	0.27476900
C	-4.02327500	-1.32729000	-0.34456900
C	-2.42197000	0.45888700	-1.14309100
N	-1.34705300	0.59981400	-0.11671100
C	-0.45886600	-0.54547500	0.29582900
C	0.15380200	0.59292300	-0.43254800
C	0.92749300	1.59224400	0.38796600
Br	0.59016400	3.43373000	-0.25110600
C	0.54336800	0.47318700	-1.88887000
Br	2.58089800	-1.95920100	0.44720100
O	1.15841700	-0.40655700	2.96693800
C	1.61617300	-0.72370100	4.27628000
O	3.71043100	0.79609500	-0.88862800
C	5.07838700	0.97041600	-1.23153200
O	0.21271800	-2.91347800	-1.64376400
C	0.39796100	-4.18359800	-2.25786700
H	1.63554700	0.43813400	-1.92998100
H	0.16391200	-0.44386600	-2.34247000
H	0.21562400	1.34953200	-2.45530500
H	0.67699100	1.56804900	1.44787400
H	1.99632800	1.42885400	0.24934700
H	-0.31378800	-0.63387400	1.36818500
H	-0.64808700	-1.45991600	-0.25766100
H	-1.60291100	1.23432200	0.63841800
H	-2.07338700	-0.27458100	-1.87013100
H	-2.51580600	1.42796200	-1.64052000
H	-4.41265000	2.05338300	-0.17352900
H	-6.51843300	1.35939900	0.92901200
H	-7.03759900	-1.05579900	1.21504600
H	-5.43922300	-2.77242100	0.38971700
H	-3.33142200	-2.08144900	-0.71047900
H	3.57873700	-0.10677200	-0.52320700
H	1.69309900	-0.91337900	2.31443100
H	0.99034900	-2.72785200	-1.06973800
H	-0.47716200	-4.37695700	-2.88490400
H	1.29350200	-4.19842300	-2.89334400
H	0.48227800	-4.98684900	-1.51375500
H	1.02336300	-0.13655500	4.98321800
H	1.48412300	-1.78941800	4.50686500
H	2.67498900	-0.46381900	4.40740400
H	5.19326500	1.98917800	-1.61171900
H	5.73609600	0.84603200	-0.36046800
H	5.39384500	0.26672500	-2.01433100

Energy (B3LYP/6-31++G**) = -5973.353258 hartree

Data 4: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for the conversion of *N*-benzyl-*N*-(2,3-dibromo-2-methylpropyl)amine to 1-benzyl-3-bromo-3-methylazetidine (**TS-b**).

C	-4.88101000	-0.54736100	0.55114400
C	-6.13990300	-0.46011700	-0.04467500
C	-6.58217500	0.75737200	-0.57248800
C	-5.76093600	1.88445900	-0.49853000
C	-4.49906600	1.79303500	0.09623400
C	-4.04518900	0.57757300	0.62540500
C	-2.66009100	0.46551900	1.23300500
N	-1.69592900	-0.23751500	0.36582800
C	-1.37888700	0.33244300	-0.96190000
C	0.09240300	-0.08162100	-1.03228700
C	0.29806500	-0.16358700	0.48250300
C	0.97128900	0.82004600	-1.87727400
Br	0.15342000	-1.94761300	-1.75132000
Br	2.83861700	-0.20724000	0.68572300
H	0.49159100	0.97885600	-2.84868900
H	1.09528800	1.78329800	-1.37083000
H	1.96026400	0.39966700	-2.04550500
H	0.40519500	-1.09227800	1.02157700
H	0.33327300	0.76981900	1.03206900
H	-2.02255600	-0.00222100	-1.77922700
H	-1.43791800	1.42337700	-0.88406300
H	-1.91312200	-1.22988400	0.28758000
H	-2.24923700	1.45904900	1.43755900
H	-2.69009800	-0.08098900	2.18121500
H	-4.54982700	-1.49585300	0.96882800
H	-6.77771100	-1.33787500	-0.09155000
H	-7.56315900	0.82673900	-1.03295100
H	-6.10099400	2.83453000	-0.89981400
H	-3.86787100	2.67602000	0.15900200
H	4.02816700	0.99737600	-1.08061200
H	2.11749700	1.99463500	1.34658600
H	2.00714300	-2.28300500	1.78110400
O	1.43913500	2.68740400	1.45716600
O	4.33499700	1.53674000	-1.83013300
O	1.25413000	-2.73730800	2.19863200
C	2.06013800	3.88168300	1.91833700
H	1.27731500	4.63917300	2.01111200
H	2.52875300	3.74379900	2.90242400
H	2.81657900	4.24631300	1.21076900
C	5.75041100	1.45583000	-1.90830600
H	6.06132400	2.07354300	-2.75522600
H	6.23838200	1.84197700	-1.00154700
H	6.09839200	0.42750000	-2.08225300
C	1.46310500	-2.74040500	3.60694100
H	0.58544600	-3.20653600	4.06232000
H	2.35006400	-3.32571100	3.88466900
H	1.57303300	-1.72275200	4.00659300

Energy (B3LYP/6-31++G**) = -5973.333422 hartree

Frequencies(cm^{-1}): -363.3609, 9.0934, 14.3878, 20.2282, 23.9882, 25.4307, 26.9040, 35.3985, 39.7306, …

Data 5: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of the protonated 1-benzyl-3-bromo-3-methylazetidine **12-H**.

C	2.90167900	-0.52911800	0.70304800
C	3.75347400	-0.11213100	1.73718000
C	5.13274300	-0.03570800	1.53183900
C	5.67273600	-0.38836500	0.29162400
C	4.83155900	-0.81659100	-0.73949000
C	3.45092300	-0.88546600	-0.53853800
C	1.41121900	-0.58449700	0.91739700
N	0.78149400	0.75210400	0.59704200
C	0.77414600	1.24704800	-0.84639100
C	-0.66371600	1.76507900	-0.65258900
Br	-0.55046200	3.68876200	-0.10337300
C	-0.74400400	0.88974700	0.60696000
C	-1.66470200	1.57516100	-1.76561900
Br	-1.68622500	-2.43580500	-0.36928300
O	0.60316700	-1.51305600	-2.50604600
C	0.66607900	-2.24310000	-3.72787800
O	-0.95732800	-1.52082400	2.74343800
C	-1.90454100	-1.80688900	3.76574300
O	-3.80703400	0.05848100	0.28069300
C	-5.21102100	-0.14392800	0.19735300
H	-1.40250200	2.18926500	-2.63148500
H	-1.66308600	0.51911600	-2.05630700
H	-2.67039200	1.82512800	-1.42307700
H	-1.14515000	1.29525900	1.53188600
H	-1.16656500	-0.09585800	0.39644300
H	1.57084100	1.95723000	-1.06057700
H	0.81588700	0.38229300	-1.51654000
H	1.19909100	1.46910700	1.19564000
H	0.91928300	-1.31366200	0.27175300
H	1.12926400	-0.81172200	1.94828200
H	3.33853500	0.13508500	2.71218600
H	5.78402900	0.28314500	2.34019000
H	6.74610800	-0.33904300	0.13330900
H	5.25108100	-1.10368500	-1.69925500
H	2.79254000	-1.22912100	-1.33274500
H	-3.35073200	-0.77129300	0.03454700
H	-0.11169500	-1.89376700	-1.94646500
H	-1.24361200	-1.95853200	1.91459900
H	1.45248400	-1.79288800	-4.33999100
H	0.91435400	-3.29825900	-3.55433100
H	-0.28137500	-2.18997400	-4.27966400
H	-5.69263400	0.79198600	0.49429700
H	-5.53100900	-0.39141500	-0.82483100
H	-5.55272300	-0.94009200	0.87334500
H	-1.55922500	-1.31309400	4.67849700
H	-2.90218100	-1.42238600	3.51466400
H	-1.97690100	-2.88530200	3.96079900

Energy (B3LYP/6-31++G**) = -5973.367200 hartree

Data 6: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-2-bromomethyl-2-methylaziridine **11**.

N	-0.72290500	0.00017700	-0.87670800
C	-0.51349900	-0.04790300	-2.32617500
C	0.62785800	-0.31831900	-1.38349600
C	1.20985400	-1.71876500	-1.27618900
H	0.54266600	-2.47420500	-1.69539900
H	2.15921000	-1.76555000	-1.81754700
H	1.41140100	-1.98316300	-0.23311100
H	-0.91497200	-0.90528600	-2.86554500
H	-0.59517000	0.90246800	-2.84919700
C	-1.53536300	-1.05396300	-0.25666000
H	-1.38670500	-2.02629200	-0.74799300
H	-1.18356600	-1.16781400	0.77536400
C	-3.02211600	-0.74099100	-0.27222500
C	-3.54234600	0.50005100	-0.65880200
H	-2.87439300	1.29515700	-0.97166300
C	-4.92305200	0.72992000	-0.63903800
H	-5.30652300	1.69915000	-0.94562800
C	-5.80238700	-0.27306600	-0.22943800
H	-6.87325900	-0.09190100	-0.21475600
C	-5.29158200	-1.51602500	0.15982700
H	-5.96445200	-2.30718400	0.47881000
C	-3.91584000	-1.74539500	0.13403000
H	-3.52813100	-2.71688600	0.43361800
C	1.61182500	0.81142700	-1.23547300
H	1.15762800	1.79385300	-1.34639200
H	2.46855700	0.68570400	-1.89771300
Br	2.44219200	0.88819800	0.59560500
H	-0.82281200	1.82085700	-0.29254000
O	-0.72372300	2.79753500	-0.25883600
C	-0.96168300	3.25912500	1.06281100
H	-2.00847900	3.11577600	1.36790200
H	-0.74109000	4.33014300	1.08019600
H	-0.31105600	2.76085800	1.79599600
H	1.10088800	-0.66901200	2.06159900
O	0.52688600	-1.35532900	2.43438200
C	0.57447800	-1.29097100	3.85625500
H	-0.08715600	-2.07530200	4.23113200
H	0.21878400	-0.32389600	4.23703100
H	1.58640200	-1.47719200	4.24139700
H	4.22860700	-0.55605700	-0.44644600
O	4.58728700	-1.10498400	-1.16030100
H	6.25029900	-1.70870700	-0.03359500
C	5.99530100	-1.23097900	-0.98948700
H	6.35822900	-1.86602100	-1.80104900
H	6.50644400	-0.26033200	-1.05132100

Energy (B3LYP/6-31++G**) = -3400.997221 hartree

Data 7: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for the conversion of 1-benzyl-2-bromomethyl-2-methylaziridine to 1-benzyl-3-methyl-1-azoniabicyclo[1.1.0]butane (**TS (11-13)**).

C	-4.77957800	-0.37398600	-0.78767700
C	-3.60080700	-0.49261600	-0.04249200
C	-3.60235200	-0.09982700	1.30427200
C	-4.76334000	0.40412100	1.89069000
C	-5.93893900	0.51697000	1.14004100
C	-5.94604300	0.12598500	-0.19992200
C	-2.34502500	-1.04813400	-0.67837900
N	-1.26342800	-0.04962100	-0.68115600
C	-0.97557700	0.92093800	-1.75382000
C	-0.02207600	-0.19207000	-1.52683900
C	0.28044400	-1.32016100	-2.46403100
C	0.47828500	-0.05525100	-0.17178400
Br	3.12703500	0.07765900	-0.54937400
O	1.96234200	0.39273400	2.51584500
C	2.69286400	0.61734600	3.71143300
O	1.47504800	2.95792600	-0.81980800
C	2.06343000	4.19116500	-0.42489900
O	1.90415600	-2.95861500	0.00520300
C	2.54322000	-3.94233300	0.81031000
H	-2.55420300	-1.38273800	-1.70265500
H	-1.96908700	-1.91017300	-0.11682900
H	-2.69040900	-0.18183800	1.88931600
H	-4.75274200	0.70632500	2.93376900
H	-6.84267600	0.90699100	1.59888300
H	-6.85445800	0.21035900	-0.78912400
H	-4.79029700	-0.67780600	-1.83182800
H	-1.60997600	0.83092600	-2.63363600
H	-0.73322600	1.93061700	-1.43110700
H	0.58003400	0.91069000	0.30064400
H	0.66540600	-0.95286700	0.40620500
H	2.51990600	-2.21542300	-0.14501200
H	1.82513300	-4.75244600	0.96300800
H	2.83285900	-3.54252000	1.79150400
H	3.43375700	-4.35538000	0.31726800
H	2.15985500	2.26184800	-0.81710500
H	1.27288300	4.94639400	-0.43557900
H	2.85391100	4.50543800	-1.12009700
H	2.48234600	4.13908000	0.58928900
H	2.57582400	0.34971700	1.75789900
H	1.97037100	0.63371200	4.53221700
H	3.42201700	-0.18182600	3.90807900
H	3.22360600	1.58030300	3.69814600
H	1.17951200	-1.05717300	-3.02958300
H	0.49412400	-2.24129600	-1.91464100
H	-0.53610100	-1.48086000	-3.17419400

Energy (B3LYP/6-31++G**) = -3400.960639 hartree

Frequencies(cm^{-1}): -358.2073, 18.4640, 23.0087, 24.7944, 26.6925, 35.1069, 43.7949, 47.0613, 56.1905, …

Data 8: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-3-methyl-1-azoniabicyclo[1.1.0]butane **13** (product of **TS (11-13)** and reactant **TS (13-12)** and **TS (13-9)**).

C	-2.82875900	0.92620000	-0.19960200
C	-2.57800500	-0.45432100	-0.20920100
C	-3.65779600	-1.35133800	-0.18443200
C	-4.97048400	-0.87992900	-0.12839700
C	-5.21528000	0.49708400	-0.10746500
C	-4.14542000	1.39503600	-0.14848700
C	-1.16507900	-0.97422900	-0.26123000
N	-0.65127400	-1.35568200	1.09771100
C	-1.28692900	-1.36602600	2.43626700
C	-0.05812500	-0.55226300	2.23014100
C	0.75408900	-1.58646200	1.54535100
C	0.14150900	0.92210300	2.31687600
O	1.21330700	-2.64402900	-1.60276200
C	1.86234500	-3.32931800	-2.66690800
O	3.44682000	0.18501000	1.86200300
C	4.81679000	0.52788300	2.01955300
Br	2.12046000	0.51530100	-1.15631200
O	-0.11898700	2.89393600	-0.60455100
C	0.08011800	4.05492200	-1.40164200
H	5.00006500	1.59052700	1.80718400
H	5.46788800	-0.07597900	1.37199300
H	5.08544300	0.33110400	3.06146200
H	3.18945000	0.35666100	0.93239500
H	0.57841600	2.24329600	-0.83090200
H	-0.69471900	4.77703400	-1.12857600
H	-0.00809900	3.83478600	-2.47448700
H	1.06246800	4.51063300	-1.21741300
H	1.55884800	-1.72731300	-1.57311000
H	1.67629900	-2.84625700	-3.63593700
H	1.45575500	-4.34415200	-2.69903200
H	2.94787700	-3.39283400	-2.50953900
H	-0.81253600	1.45401000	2.33774200
H	0.74482000	1.28034800	1.48102300
H	0.69268100	1.13652300	3.23776500
H	0.92496400	-2.55919100	2.00408200
H	1.50053700	-1.23898300	0.83753600
H	-2.23305100	-0.83385000	2.47952000
H	-1.25168700	-2.32466300	2.95437500
H	-1.07196800	-1.88616200	-0.85584200
H	-0.45701300	-0.24432600	-0.66254700
H	-3.46873600	-2.42197400	-0.21923500
H	-5.79869600	-1.58240200	-0.11381400
H	-6.23614600	0.86654500	-0.07144100
H	-4.33279100	2.46484100	-0.15092300
H	-2.00020100	1.63063800	-0.25779300

Energy (B3LYP/6-31++G**) = -3400.973849 hartree

Data 9: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-2-(bromomethyl)aziridine **8**.

C	-4.51988400	-1.30375400	-1.18942500
C	-5.89577200	-1.08901700	-1.06760300
C	-6.39785000	-0.37665500	0.02403200
C	-5.51490400	0.11727900	0.98944300
C	-4.14122000	-0.10520300	0.86974700
C	-3.62909500	-0.82206400	-0.22121900
C	-2.14551100	-1.11431400	-0.34124400
N	-1.32117500	-0.01098200	0.15768000
C	-0.94610900	1.02767600	-0.80651000
C	0.05613100	0.02827300	-0.33393100
C	1.08502700	0.35709000	0.70460700
Br	2.72588100	1.11562600	-0.15549400
O	2.34453100	-2.55195000	1.36343300
C	2.16497400	-3.85391600	1.89995900
O	3.74480800	-2.07843700	-1.03331600
C	5.11197300	-2.36442500	-1.33407900
O	0.67510400	3.81323100	0.44116900
C	0.94660200	5.20948200	0.38010200
H	0.35041200	-0.74767300	-1.04157100
H	-4.13523600	-1.85221700	-2.04656900
H	-6.57130100	-1.47105400	-1.82795700
H	-7.46591800	-0.20277500	0.11903400
H	-5.89661500	0.67772600	1.83846200
H	-3.45358800	0.28318500	1.61428000
H	-1.91033300	-1.36110700	-1.39187600
H	-1.89107300	-1.99925700	0.25743400
H	0.75054300	1.13686500	1.38636300
H	1.44363200	-0.52063100	1.24187700
H	-0.91810900	2.04407500	-0.42213100
H	-1.30612900	0.91839500	-1.82974200
H	1.46756100	3.32221300	0.17795100
H	2.88629400	-2.59191200	0.55192900
H	3.62799200	-1.11727700	-0.95046200
H	5.19613800	-3.44903000	-1.42877400
H	5.41550700	-1.90563500	-2.28298100
H	5.78357100	-2.02470200	-0.53539300
H	0.02982400	5.72335900	0.67831900
H	1.74972500	5.50267200	1.07012900
H	1.21236700	5.53236600	-0.63594200
H	1.53955500	-3.75506200	2.79116200
H	1.65697500	-4.52571100	1.19322400
H	3.11889400	-4.31232000	2.19821000

Energy (B3LYP/6-31++G**) = -3361.706931 hartree

Data 10: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for the conversion of 1-benzyl-2-(bromomethyl)aziridine to 1-benzyl-1-azoniabicyclo[1.1.0]butane (**TS (8-27)**).

C	5.79548100	0.27623700	1.04080200
C	6.23824100	0.46118900	-0.27052200
C	5.38103200	0.18113600	-1.34001700
C	4.08750300	-0.28172200	-1.09707200
C	3.63319900	-0.46751000	0.21672000
C	4.49785900	-0.18502900	1.28124700
C	2.22856000	-0.95906900	0.47775700
N	1.23060900	0.10311800	0.23321900
C	-0.20215000	-0.08197400	0.64274100
C	-0.24847000	0.16097600	-0.77817500
C	0.61938500	0.97257500	1.26306900
Br	-2.94893200	0.15796300	-1.15484700
H	-0.55836000	-0.98077100	1.12938800
H	4.15951000	-0.33250800	2.30413800
H	6.45704200	0.48826100	1.87551300
H	7.24635400	0.81770300	-0.46001200
H	5.72210900	0.31912000	-2.36176700
H	3.42523200	-0.49948100	-1.93100600
H	2.12664700	-1.31439100	1.51151800
H	1.96574900	-1.78812900	-0.18703700
H	-0.25549300	1.16744600	-1.17319800
H	-0.23138000	-0.68925200	-1.44685600
H	0.47471400	2.01274300	0.98368100
H	0.95568100	0.77844500	2.27883200
H	-2.16156400	2.29842000	-0.39228200
H	-1.99012300	-2.07480200	-1.02152900
H	-3.08155900	-0.42583800	1.15047200
O	-1.57457900	3.02284800	-0.09816000
O	-1.29621000	-2.74465600	-0.86705300
O	-2.87918400	-0.73598700	2.05555000
C	-4.03542600	-0.58371900	2.86642400
H	-3.79298100	-0.97988000	3.85655300
H	-4.32499100	0.47120500	2.97634400
H	-4.89352700	-1.14411600	2.46958200
C	-2.26865000	4.25826200	-0.22349900
H	-1.58715200	5.04832300	0.10333400
H	-2.56364600	4.45873300	-1.26242400
H	-3.16552200	4.28811000	0.41022400
C	-1.91647500	-3.99885100	-0.60452400
H	-1.11858400	-4.72122700	-0.41198300
H	-2.56820800	-3.95119200	0.27784700
H	-2.50233200	-4.35009900	-1.46463100

Energy (B3LYP/6-31++G**) = -3361.660865 hartree

Frequencies(cm^{-1}): - 363.4611, 15.0889, 17.4976, 21.3611, 26.8782, 29.2058, 35.0359, 44.4153, 54.9300, …

Data 11: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-1-azoniabicyclo[1.1.0]butane **8**.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.39800128
C	1.21157538	0.00000000	2.09535086
C	2.42241649	0.01311178	1.39889369
C	2.42880367	0.02120201	-0.00379330
C	1.21026101	0.00988884	-0.69692901
C	3.74083378	0.06540656	-0.74472646
N	4.16250911	1.48366532	-0.96846067
C	5.51133353	2.06870730	-1.28199109
C	4.81789674	2.43677930	-0.02872981
C	4.39141744	2.23023148	-2.23519754
O	5.98599033	0.33389229	2.02261830
C	6.85950410	0.35836487	3.14807541
O	5.46009072	-0.49291715	-3.42058132
C	5.81825430	-1.23308546	-4.58366286
Br	7.11151696	-1.21103869	-0.65553117
O	8.69063952	1.61461615	-1.14201430
C	10.04855703	1.66281284	-1.55420274
H	6.40396405	1.46551914	-1.39039683
H	1.20862602	-0.00220922	-1.78438978
H	-0.93910385	-0.01385512	-0.54543521
H	-0.94070571	-0.01306722	1.94096240
H	1.21455014	-0.01342074	3.18134287
H	3.36854208	0.00092024	1.93540166
H	3.68836189	-0.38430873	-1.73776410
H	4.54863760	-0.42776610	-0.20084476
H	4.31030274	3.39670224	0.05859966
H	5.17954301	1.96508128	0.88610097
H	3.85499845	3.17554755	-2.31021403
H	4.42258327	1.58492583	-3.10997119
H	6.40229009	-0.20950797	1.31656941
H	8.43234972	0.68134292	-0.98950491
H	6.03055798	-0.78588611	-2.67446564
H	5.15192368	-0.91809019	-5.39165822
H	6.85464604	-1.03469077	-4.88709555
H	5.69621577	-2.31286482	-4.42821665
H	6.39650401	0.99222455	3.90946226
H	7.00300658	-0.64548697	3.56849419
H	7.84029370	0.77789204	2.88889130
H	10.31283530	2.71611304	-1.68454399
H	10.72005573	1.22722830	-0.80112186
H	10.20929647	1.14272029	-2.50942337

Energy (B3LYP/6-31++G**) = -3361.678130 hartree

Data 12: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-2-bromomethyl-2-methylaziridine **11-*trans*** (without explicit methanol molecules).

C	3.42814300	0.81997200	-0.78500400
C	2.29398000	0.12264600	-0.34964700
C	2.46838900	-1.08413800	0.34303000
C	3.74969800	-1.58243300	0.58732100
C	4.87658000	-0.88184900	0.14500800
C	4.71224500	0.32216400	-0.54337700
C	0.90560100	0.65308400	-0.65833800
N	-0.01606300	0.41426000	0.45260200
C	-1.30664200	1.09795000	0.51540200
C	-2.41618400	0.23527900	1.05503500
Br	-3.18267400	-0.93078900	-0.36700700
C	-0.19366300	1.44910300	1.46718600
C	-1.74522800	2.11319500	-0.52670200
H	1.59192700	-1.62095000	0.69190800
H	3.86921700	-2.51867300	1.12567700
H	5.87266000	-1.26996300	0.33774000
H	5.58034500	0.87787900	-0.88678100
H	3.30836500	1.76184200	-1.31601100
H	0.49492800	0.12684900	-1.52984200
H	0.98613800	1.71670200	-0.93268700
H	-2.56001400	2.72551300	-0.12475300
H	-0.93747400	2.79100300	-0.81110600
H	-2.11481100	1.61421500	-1.42748200
H	-2.05656100	-0.46207900	1.80907200
H	-3.25436800	0.82369400	1.43001000
H	-0.20564100	1.10901600	2.50090300
H	0.29382800	2.41291500	1.31090400

Energy (B3LYP/6-31++G**) = -3054.0807135 hartree

Data 13: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-2-bromomethyl-2-methylaziridine **11-*cis*** (without explicit methanol molecules).

C	4.15967100	-1.19747200	0.70425100
C	4.87658700	-0.30928800	-0.10004200
C	4.18649600	0.59128000	-0.91876200
C	2.79055800	0.60158500	-0.93558400
C	2.06202300	-0.28667400	-0.13052600
C	2.76159200	-1.17960000	0.69097600
C	0.54680600	-0.30947200	-0.16157600
N	-0.01002800	1.04846900	-0.12470700
C	-1.35387600	1.30428500	0.41223800
C	-2.16643000	2.33008600	-0.35494900
C	-0.11795200	1.72150400	1.16448800
C	-2.16012100	0.19329200	1.03256300
Br	-2.92167900	-1.04935800	-0.32698000
H	2.20715600	-1.87217100	1.32018300
H	4.68450000	-1.89921200	1.34638700
H	5.96277000	-0.31663800	-0.08926400
H	4.73779100	1.28600300	-1.54646400
H	2.25436900	1.30431900	-1.56621800
H	0.19045600	-0.95117500	0.65931700
H	0.19426000	-0.76850300	-1.09240500
H	0.14882800	1.15933200	2.06089500
H	0.17255500	2.77007400	1.18531500
H	-2.90219500	2.81344900	0.29948200
H	-1.50840800	3.09970900	-0.76539900
H	-2.70197300	1.85605600	-1.18351100
H	-1.59779700	-0.44432200	1.71027800
H	-3.02546400	0.59417000	1.56018700

Energy (B3LYP/6-31++G**) = -3054.0814375 hartree

Data 14: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-2-(bromomethyl)aziridine **8-*trans*** (without explicit methanol molecules).

H	-3.29587700	1.49019500	1.01887400
C	-2.54272100	0.72166900	0.84389100
H	-2.28437100	0.21237100	1.77153800
Br	-3.44487900	-0.65450700	-0.27002200
C	-1.32559800	1.25593500	0.15633000
H	-1.50257400	1.68645800	-0.83090200
H	0.34729700	2.67662900	0.48498600
C	-0.19835900	1.85339700	0.94716400
H	-0.24226700	1.88329800	2.03326300
N	-0.08396200	0.52472700	0.35039900
C	0.79284900	0.38265200	-0.81680400
H	0.36095700	-0.41288100	-1.43687300
H	0.81235500	1.29886600	-1.43295000
C	2.20533500	0.01631500	-0.40999400
C	3.30508100	0.70892500	-0.93001900
H	3.14249300	1.53622900	-1.61712600
C	4.61028800	0.34742300	-0.57906800
H	5.45220000	0.89584000	-0.99216200
C	4.82763900	-0.71077100	0.30514800
H	5.83951600	-0.99323100	0.58127900
C	3.73384800	-1.40470800	0.83475500
H	3.89573000	-2.22801400	1.52499900
C	2.43327600	-1.04357700	0.48099200
H	1.58322300	-1.57465100	0.89868800

Energy (B3LYP/6-31++G**) = -3014.7600902 hartree

Data 15: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-2-(bromomethyl)aziridine **8-*cis*** (without explicit methanol molecules).

C	3.94672900	-1.10878500	0.90854500
C	4.71539100	-0.41805700	-0.03036900
C	4.08038200	0.35907100	-1.00541700
C	2.68734300	0.44175900	-1.04359300
C	1.90723800	-0.24938600	-0.10453700
C	2.55182100	-1.01740700	0.87311600
C	0.39407100	-0.19883300	-0.15665900
N	-0.09141100	1.17374400	-0.35091600
C	-1.41471400	1.56031200	0.14766700
H	-1.94904100	2.22683400	-0.52729900
C	-0.15855300	2.05487800	0.80705000
C	-2.30577500	0.62524100	0.90869600
Br	-3.14967600	-0.72589000	-0.28030500
H	1.95674600	-1.55566100	1.60743400
H	4.42889300	-1.71299300	1.67180700
H	5.79940800	-0.48257100	-0.00343500
H	4.67234600	0.90018800	-1.73844500
H	2.19365900	1.04844400	-1.79672000
H	-0.00368600	-0.67658400	0.75187200
H	0.02346400	-0.78486800	-1.00557800
H	0.08765400	1.63690900	1.78477200
H	0.17514500	3.07854200	0.65388800
H	-1.79448800	0.05173500	1.67905100
H	-3.13516300	1.16719900	1.36275500

Energy (B3LYP/6-31++G**) = -3014.7573908 hartree

Data 16: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-3-methyl-1-azoniabicyclo[1.1.0]butane **13** (reactant of **TS (13-14)**, without explicit methanol molecules).

C	3.07399700	-0.60338400	-0.36399000
H	3.35947400	-0.26145100	-1.35656800
H	3.66864700	-1.41708300	0.04816100
C	2.37537500	0.37163500	0.51354400
C	1.59339000	-0.60623200	1.31480900
H	2.08031800	-1.42318100	1.84511000
H	0.64440600	-0.26654600	1.72027500
C	2.22739600	1.84977900	0.37884700
H	3.00004200	2.32956000	0.98862900
H	2.37250500	2.17281900	-0.65582800
H	1.25259400	2.18641500	0.73838200
N	1.60285300	-0.72706200	-0.17076200
C	0.49833800	-0.73129000	-1.19332300
H	0.48222800	-1.75253600	-1.58339300
H	0.82019800	-0.05764700	-1.99264900
C	-0.83246400	-0.33206200	-0.61544100
C	-1.28555600	0.99220200	-0.71325300
H	-0.68514200	1.73772000	-1.22889000
C	-2.52322700	1.35398300	-0.17701000
H	-2.87287700	2.37750900	-0.26734700
C	-3.31650200	0.39461900	0.45889000
H	-4.28133600	0.67493200	0.86948700
C	-2.87669500	-0.92958700	0.54991400
H	-3.49998700	-1.67957600	1.02624100
C	-1.64171300	-1.29336500	0.01047200
H	-1.31507200	-2.32928900	0.06297400

Energy (B3LYP/6-31++G**) = -481.887453 hartree

Data 17: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for the equilibration of 1-benzyl-3-methyl-1-azoniabicyclo[1.1.0]butane and 1-benzyl-3-methylazetidine carbenium ion (**TS (13-14)**).

C	2.70810500	1.21296300	-0.56997300
C	3.24721200	0.00015600	-1.01383700
C	2.70809300	-1.21277800	-0.57033200
C	1.62588100	-1.21383800	0.30904200
C	1.06892500	-0.00009600	0.76293800
C	1.62589100	1.21377400	0.30940100
C	-0.10988500	-0.00024200	1.68455900
N	-1.43370300	-0.00019300	0.94594500
C	-1.73188000	1.06585600	-0.06045100
C	-2.63398100	0.00005300	-0.54921800
C	-4.00712700	0.00022800	-1.01575100
C	-1.73186700	-1.06594300	-0.06066900
H	-3.91715300	0.00050300	-2.12291200
H	-4.55181600	0.91008400	-0.75096000
H	-4.55197400	-0.90966600	-0.75142700
H	-2.17499900	1.99304900	0.31234000
H	-0.88936600	1.27429200	-0.74860300
H	-2.17508700	-1.99318400	0.31187300
H	-0.13892000	-0.88599000	2.32363100
H	-0.13895200	0.88534700	2.32385200
H	1.23445400	2.15803000	0.68072200
H	3.14138700	2.15287000	-0.89705100
H	4.09564900	0.00025200	-1.69093300
H	3.14136400	-2.15259300	-0.89769000
H	1.23443900	-2.15820100	0.68009200
H	-0.88930800	-1.27422600	-0.74879800

Energy (B3LYP/6-31++G**) = -481.854617 hartree

Frequencies(cm^{-1}): -165.4546, 56.8767, 73.4646, 76.5356, 81.2963, 217.6661, 222.7067, 274.1120, 353.5951, …

Data 18: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) 1-benzyl-3-methylazetidine carbenium ion **14**.

C	1.80720500	0.21752200	-1.03337200
H	2.37242100	0.52858100	-1.92088400
H	0.90217900	-0.33970300	-1.37587900
C	2.46463200	-0.59401200	-0.00070800
C	1.80782900	0.21589400	1.03349400
H	0.90292400	-0.34230400	1.37500100
H	2.37289300	0.52539300	1.92163500
C	3.52051300	-1.59101500	-0.00177200
H	3.52262300	-2.20133900	-0.90942800
H	3.52323300	-2.20275800	0.90493000
H	4.47504900	-1.02684500	-0.00151700
N	1.46037000	1.22417700	0.00100100
C	0.09040800	1.80511600	0.00189100
H	0.04088900	2.45308200	-0.87855700
H	0.04113800	2.45110900	0.88380300
C	-1.03820300	0.80032500	0.00091700
C	-1.56546400	0.31003100	1.21198800
H	-1.21960500	0.72294700	2.15740800
C	-2.56949900	-0.66047200	1.21053600
H	-2.97675500	-1.01871600	2.15087100
C	-3.06766900	-1.14988400	-0.00102400
H	-3.85826600	-1.89360600	-0.00176700
C	-2.57038600	-0.65710000	-1.21158400
H	-2.97835200	-1.01271600	-2.15260600
C	-1.56635400	0.31339500	-1.21110000
H	-1.22104200	0.72882500	-2.15561100

Energy (B3LYP/6-31++G**) = -481.863368 hartree

Data 19: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for the conversion of 1-benzyl-3-methyl-1-azoniabicyclo[1.1.0]butane to 1-benzyl-3-bromo-3-methylazetidine (**TS (13-12)**).

C	-5.38527100	-0.98926300	1.01280800
C	-4.15764700	-1.24950200	0.40401600
C	-3.65080600	-0.37990100	-0.57281300
C	-4.39374000	0.75106000	-0.93027200
C	-5.62591200	1.01245800	-0.32300700
C	-6.12244800	0.14338000	0.65000100
C	-2.31456800	-0.65624800	-1.23169800
N	-1.20294100	-0.49552700	-0.28430700
C	-0.48144500	0.78147300	0.04091100
C	0.35250400	-0.13449300	-0.75991600
C	0.73763300	0.03949100	-2.19312300
C	-0.01134800	-1.39396600	-0.08871800
Br	3.12697100	0.33000000	0.24916300
O	2.56227200	-2.58001000	-1.21072500
C	3.63808900	-3.50130500	-1.33319100
O	1.46932000	2.99587900	-0.77952800
C	2.09951500	4.26813800	-0.70972500
O	1.07839300	-0.23647300	2.74038100
C	1.53633300	-0.21664000	4.08618900
H	1.21416100	1.01344700	-2.31379100
H	-0.14365500	0.01176200	-2.84927600
H	1.42327600	-0.75667400	-2.48674600
H	-0.27672400	0.89195300	1.10496200
H	-0.85133600	1.67225100	-0.46184000
H	0.24199400	-1.52690900	0.96239200
H	0.00908800	-2.29484700	-0.69810300
H	-2.26489500	-1.68374200	-1.60524600
H	-2.17352300	0.01846000	-2.08557300
H	-4.01064400	1.43107200	-1.68730500
H	-6.19288900	1.89310400	-0.60965200
H	-7.07866100	0.34476600	1.12356500
H	-5.76800900	-1.66923100	1.76805200
H	-3.58812800	-2.12944700	0.69206200
H	2.88422200	-1.77756800	-0.74795600
H	1.83359300	-0.04966200	2.14060300
H	2.08254100	2.31909700	-0.42268200
H	3.26187600	-4.37195000	-1.87784100
H	4.47990500	-3.07448600	-1.89536500
H	4.00452900	-3.83490200	-0.35242100
H	1.40699200	4.99935000	-1.13635300
H	2.31924500	4.55978300	0.32672400
H	3.03397900	4.29433100	-1.28693800
H	0.67262300	-0.41128400	4.72817100
H	2.29148800	-0.99286100	4.27177500
H	1.96032400	0.75962400	4.35844100

Energy (B3LYP/6-31++G**) = -3400.969751 hartree

Frequencies(cm^{-1}): -84.2294, 13.8393, 17.4317, 21.8609, 27.3958, 34.1817, 57.2487, 58.3925, 62.3209,…

Data 20: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-3-bromo-3-methylazetidine **12**.

C	-5.54860500	0.60592300	0.28973400
C	-4.84345500	-0.35556800	1.02167200
C	-3.69108400	-0.94142000	0.49439200
C	-3.22540400	-0.56940600	-0.77724800
C	-3.93802900	0.39471400	-1.50248600
C	-5.09451900	0.97934700	-0.97656400
C	-1.96867100	-1.18818700	-1.35563100
N	-0.75809500	-0.75669100	-0.64309100
C	0.54958000	-1.10399500	-1.26463200
C	1.06456200	0.31057700	-0.93332900
C	1.90992800	1.06958800	-1.93026800
C	-0.41031800	0.68964500	-0.69417000
Br	2.03320600	0.27392300	0.84290200
O	4.10381900	-1.57437400	-1.16755600
C	5.34012000	-2.24029900	-0.93112300
O	1.53581600	3.63265200	0.35025900
C	1.62842300	4.74257900	1.23745300
O	-0.97422100	-2.54005300	1.61581300
C	0.01301000	-2.60530500	2.63234100
H	2.07394000	2.10017500	-1.60489900
H	1.37905700	1.09349900	-2.88967000
H	2.87109700	0.57212000	-2.08478700
H	-0.66978600	1.26747600	0.19436900
H	-0.81589300	1.19824200	-1.58278100
H	1.06135600	-1.96659400	-0.83234000
H	0.48318100	-1.23570200	-2.35668500
H	-2.01143400	-2.28148100	-1.28493500
H	-1.89552700	-0.92682800	-2.42724000
H	-3.59403200	0.68322200	-2.49290600
H	-5.63640200	1.72199800	-1.55532100
H	-6.44661600	1.05666700	0.70271200
H	-5.19406500	-0.65351400	2.00593300
H	-3.14622500	-1.68471900	1.07008800
H	3.83171200	-1.10534100	-0.36452300
H	-0.78425400	-1.79906900	0.99991000
H	1.84297100	2.83245200	0.80201000
H	5.60631500	-2.75246100	-1.85866200
H	6.14491200	-1.53594800	-0.67948900
H	5.25798300	-2.98947100	-0.13175400
H	1.26708500	5.61622900	0.69002000
H	1.00310600	4.60888800	2.13081500
H	2.66398900	4.93277800	1.55138300
H	-0.24868800	-3.44208900	3.28632900
H	1.01790800	-2.78710100	2.22427100
H	0.04622200	-1.68886500	3.23925100

Energy (B3LYP/6-31++G**) = -3401.003905 hartree

Data 21: Cartesian coordinates, energy, imaginary and low frequencies of the optimized geometry (B3LYP/6-31++G**) of the transition state for conversion of 1-benzyl-3-methyl-1-azoniabicyclo[1.1.0]butane to 1-benzyl-3-methoxy-3-methylazetidine (**TS (13-9)**).

C	-4.59453000	0.87256300	0.46367100
C	-5.65953400	0.28258300	-0.22327900
C	-5.48904700	-0.96088600	-0.83633800
C	-4.25242900	-1.60976600	-0.75905100
C	-3.18753300	-1.02860900	-0.06691100
C	-3.35885800	0.21984600	0.55148600
C	-2.22560200	0.84801600	1.34354900
N	-0.94702600	0.65198400	0.67060000
C	-0.53041700	1.32748300	-0.59523900
C	0.30278000	1.91484600	0.48477700
C	0.09960400	3.27759200	1.05691200
C	0.41098300	0.68357100	1.30141300
O	2.34414600	2.24670900	-0.27252100
C	2.60506400	3.18196600	-1.31889700
Br	2.41594700	-0.68603900	-1.45347100
O	3.26288200	-1.03533700	1.73745200
C	4.58544700	-1.40966300	2.09312300
O	-0.07145000	-2.49936100	-0.07326900
C	0.47603700	-3.61407800	0.62374900
H	2.43492400	4.18636200	-0.92197900
H	1.95332000	3.01389000	-2.18621300
H	3.64850500	3.10518800	-1.64404900
H	0.07246000	4.02932800	0.26512100
H	-0.85086000	3.33204000	1.60488100
H	0.90931800	3.51109300	1.75076800
H	1.04633400	-0.12315100	0.94505500
H	0.42831600	0.80748300	2.38527000
H	-0.05384000	0.63752300	-1.29390500
H	-1.28474700	1.97496300	-1.04698400
H	-2.44477100	1.91453900	1.52178200
H	-2.12823400	0.36842300	2.32387800
H	-4.72878800	1.84466300	0.93336300
H	-6.61419800	0.79698600	-0.28469800
H	-6.31261600	-1.41901300	-1.37631600
H	-4.11122400	-2.57253000	-1.24141400
H	-2.22416300	-1.53357900	-0.02267100
H	2.49653500	1.32836500	-0.63511400
H	3.18998700	-1.01640000	0.76176200
H	4.63409800	-1.43487700	3.18560900
H	4.84788500	-2.40668000	1.71152500
H	5.33062000	-0.68777100	1.72915300
H	0.64568300	-2.07285400	-0.58348400
H	-0.32733700	-4.04406700	1.22926100
H	0.83951800	-4.38705700	-0.06747900
H	1.29791200	-3.31426800	1.28705400

Energy (B3LYP/6-31++G**) = -3400.957831 hartree

Frequencies(cm^{-1}): -212.4874, 13.4941, 20.5770, 27.6504, 32.3206, 42.7703, 44.2466, 48.2932, 55.1154,…

Data 22: Cartesian coordinates and energy of the optimized geometry (B3LYP/6-31+G(d,p)) of 1-benzyl-3-methoxy-3-methylazetidine **9**.

N	-1.16927400	1.08114100	0.56890600
H	1.59235300	-0.97096400	2.08723200
O	1.59700500	-0.56116900	2.97238000
C	2.13389000	-1.48173000	3.91096800
H	3.17535100	-1.74663600	3.67925500
H	1.53888400	-2.40411200	3.96942000
H	2.11218900	-0.99444000	4.88962000
C	-2.48603100	0.85286200	1.12555100
H	-3.03442800	1.80173100	1.29843100
H	-2.33691600	0.39112000	2.11108000
C	-3.32733400	-0.06494200	0.25579100
C	-2.73619100	-1.13455600	-0.43417500
H	-1.66156800	-1.27960800	-0.37150600
C	-3.52518200	-2.00316400	-1.19209500
H	-3.05575600	-2.82949300	-1.71876400
C	-4.90841300	-1.81504400	-1.27567300
H	-5.51795900	-2.49270500	-1.86687000
C	-5.50112100	-0.74643500	-0.59828400
H	-6.57398500	-0.58693000	-0.66194300
C	-4.71194500	0.12472500	0.15832900
H	-5.17810900	0.95791200	0.67994000
C	-0.98866800	1.92728500	-0.62056900
H	-0.96021700	1.39074600	-1.57543900
H	-1.71035400	2.75956000	-0.69849100
C	-0.15778700	1.84107000	1.32490300
H	-0.57900500	2.65269800	1.94357900
H	0.52978900	1.24172800	1.93020200
C	0.35218800	2.41519100	-0.01623600
C	0.74493100	3.87449100	-0.09682500
H	-0.03788000	4.47804500	0.36915400
H	0.85321000	4.22030700	-1.12927800
H	1.68169600	4.05414200	0.44034500
O	1.49572800	1.58105000	-0.46951900
C	2.02143700	1.80526500	-1.81331800
H	1.21159900	1.75873400	-2.54563300
H	2.75414200	1.01595500	-1.98239400
H	2.51284300	2.77668500	-1.82776400
H	1.35921100	0.45110500	-0.31977000
Br	1.31343800	-1.33399700	-0.25994400
H	3.56907800	-0.97267900	-1.03732800
O	4.33054900	-0.52862500	-1.45481200
C	5.36240900	-1.48103000	-1.67770000
H	5.74693700	-1.89440100	-0.73494000
H	6.17906500	-0.96099200	-2.18527300
H	5.02507000	-2.30958300	-2.31558000

Energy (B3LYP/6-31++G**) = -3400.992562 hartree