

Supporting Information

Theoretical Insight into the Ring-Expansions of Bicyclic Aziridinium Ions

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1) Table S1. Gibbs free energy profiles for the ring-expansion of 1-azoniabicyclo[n.1.0]alkane 1 and 5 with different nucleophiles. (Energies in kJ/mol at 298 K and 1 atm)

		B3LYP/6-31++G(d,p)				B3LYP-D/6-31++G(d,p) ^[f]				M062X/6-31+G(d,p)					
		Path i	Path ii	Path i	Path ii	Path i	Path ii	Path i	Path ii	Path i	Path ii	Path i	Path ii	Expt ^[g]	
	Nu	ΔG^\ddagger		ΔG_{rxn}		ΔG^\ddagger		ΔG_{rxn}		ΔG^\ddagger		ΔG_{rxn}			
Explicit Solvent ^[a,b]	1	CN	24.2	16.4	-230.8	-220.0	28.5	19.7	-211.5	-204.8	37.7	30.3	-204.2	-201.1	0:100
	1	N₃	30.7	28.1	-129.7	-127.3	31.8	28.5	-123.4	-105.4	50.9	43.0	-127.0	-112.4	36:64
	1	Cl	23.7	19.3	-77.9	-65.5	27.9	21.8	-68.5	-50.7	51.3	41.1	-63.5	-46.5	100:0
	5	CN	27.3	18.6	-199.4	-209.4	32.7	23.8	-180.7	-193.3	49.6	38.2	-178.7	-196.8	8:92
	5	N₃	25.2	20.4	-113.1	-132.6	28.2	26.2	-92.0	-109.6	66.6	63.1	-79.2	-81.4	59:41
	5	NH₂	35.5	23.3	-277.8	-279.7	40.1	28.8	-250.1	-253.3	26.6	16.6	-286.4	-292.1	65:35
	Implicit solvent (IEFPCM) ^[c,d]	1	CN	78.1	71.1	-140.7	-133.8	70.0	61.6	-151.4	-140.0	89.6	77.4	-150.2	-139.4
1		N₃	73.5	71.2	-59.6	-48.6	59.5	58.4	-75.9	-57.0	82.0	78.6	-83.0	-63.7	36:64
1		Cl	81.6	78.0	6.2	19.3	75.2	69.5	-1.5	15.0	96.7	90.8	-7.7	11.4	100:0
5		CN	77.2	72.7	-120.2	-131.3	67.9	63.8	-127.0	-139.2	90.5	78.2	-124.3	-136.8	8:92
5		N₃	73.9	72.9	-42.9	-51.3	59.1	59.8	-54.0	-57.6	87.3	78.2	-61.6	-62.8	59:41
5		NH₂	50.0	41.1	-228.7	-230.0	38.2	31.0	-239.5	-242.0	54.9	43.1	-249.9	-252.5	65:35
Implicit solvent (CPCM) ^[c,e]		1	CN	77.2	70.6	-140.9	-134.0	69.1	61.1	-151.6	-140.1	88.8	77.6	-150.6	-139.7
	1	N₃	73.3	70.9	-59.7	-50.8	59.3	58.2	-76.0	-59.2	81.3	77.8	-83.4	-64.1	36:64
	1	Cl	81.0	76.9	6.0	20.4	74.7	68.5	-1.6	16.3	96.0	89.9	-8.0	11.2	100:0
	5	CN	75.8	72.1	-119.8	-131.7	66.4	63.3	-127.1	-139.5	90.4	77.9	-125.4	-137.0	8:92
	5	N₃	73.3	72.6	-42.8	-50.1	58.5	59.4	-53.8	-56.4	87.4	78.4	-60.6	-62.9	59:41
	5	NH₂	48.9	41.0	-228.6	-233.5	37.1	30.8	-239.4	-245.5	54.9	43.1	-249.3	-252.2	65:35

- [a] All energies relative to the pre-reactive complex (PRC) of path **ii**.
- [b] Optimizations with two explicit acetonitrile molecules in gas phase.
- [c] All energies relative to the separate reactants.
- [d] Optimizations with IEFPCM in acetonitrile ($\epsilon = 35.688$).
- [e] Optimizations with CPCM in acetonitrile ($\epsilon = 35.688$).
- [f] Energy refinement with DFT-D dispersion correction.
- [g] Experimental results **3:4** for aziridinium **1**, **7:8** for aziridinium **5**.

2)Transition states for the ring opening of 1-azoniabicyclo[3.1.0]hexane 1 with different nucleophiles (M062X/6-31+G(d,p) level of theory, 298 K and 1 atm, gas phase, explicit solvent)

TS-CN-1 Imaginary freq: -521.27

C	0.656140	-2.577110	1.461793
C	-0.773666	-2.028290	1.344982
C	1.559980	-1.405225	1.875392
H	0.700354	-3.392305	2.187740
H	0.995167	-2.972204	0.502058
H	-1.288747	-2.072284	2.308281
H	-1.366750	-2.572560	0.598608
H	2.599555	-1.611673	1.624716
H	1.498516	-1.213318	2.951940
C	1.083954	-0.169040	1.136312
C	0.322622	-0.336179	-0.103954
H	1.040436	0.803001	1.608737
H	0.558270	-1.181403	-0.747844
H	0.094577	0.578446	-0.645181
C	-1.729798	0.356872	1.175714
H	-1.249028	1.334457	1.065394
N	-0.634615	-0.616536	0.980715
C	-2.762330	0.228274	0.070072
C	-2.759493	1.157247	-0.973972
C	-3.693373	-0.815607	0.046985
C	-3.668954	1.044759	-2.024920
H	-2.041022	1.974220	-0.953355
C	-4.601511	-0.930064	-1.002745
H	-3.717009	-1.544650	0.853344
C	-4.590172	0.000207	-2.041950
H	-3.657889	1.774862	-2.828160
H	-5.320475	-1.743482	-1.008877
H	-5.299014	-0.089082	-2.859137
C	-2.310773	0.271196	2.582939
H	-2.895696	-0.637260	2.746978
H	-1.509785	0.311542	3.327778
H	-2.976100	1.123032	2.740990
C	2.578579	4.040927	-0.536606
H	3.319085	3.240048	-0.633714
H	2.888162	4.737765	0.244327
H	2.470124	4.578605	-1.480362
C	1.299992	3.437988	-0.170611
N	0.282445	2.966905	0.114789
C	4.794295	-1.499859	-2.044894
H	5.611242	-2.085780	-1.619642
H	4.827078	-0.478281	-1.652662
H	4.882223	-1.493322	-3.132857
C	3.516450	-2.093674	-1.661620
N	2.502998	-2.565460	-1.364410
C	3.058196	0.607170	0.311165
N	3.901781	1.093671	-0.340987

TS-CN-2 Imaginary freq : -551.14

C	-0.86948600	-0.08015600	0.16250200
N	0.61454900	-0.06150700	-0.75393300
C	1.01358200	-1.30439700	-1.44791500
C	-0.28679000	-1.85569200	-2.04650400
C	-1.14539200	-0.60648500	-2.31300600
C	-0.73213500	0.35854900	-1.22158000
C	1.64057600	0.96732800	-0.47010100
C	2.02425300	1.72891500	-1.73526800
C	2.79387900	0.30194800	0.26340600
C	2.55125600	-0.25796300	1.52349700
C	3.56424800	-0.90514900	2.22239000
C	4.84283800	-1.00008600	1.66991600
C	5.09500000	-0.44350900	0.42030800
C	4.07459900	0.20359300	-0.27992100
C	-3.07876600	0.32978900	0.51783900
N	-4.20959600	0.63527100	0.47823100
H	-0.09214300	-2.42871800	-2.95532200
H	-0.78597700	-2.51689200	-1.33459000
H	1.73879200	-1.04526200	-2.22999100
H	1.49452600	-1.98636600	-0.74263800
H	-2.21840300	-0.80856100	-2.26096800
H	-0.91740900	-0.16762400	-3.29013600
H	-0.84436800	1.42594400	-1.39813200
H	-1.06596500	-1.11802400	0.39956800
H	-0.68560200	0.63508900	0.95172900
H	1.15756500	1.67934500	0.20888500
H	1.55505700	-0.18804600	1.95410300
H	4.29098900	0.63277100	-1.25330800
H	3.35923400	-1.33376300	3.19844000
H	6.08664300	-0.51170900	-0.01623100
H	5.63601700	-1.50389100	2.21318600
H	1.14618200	2.23513400	-2.14364200
H	2.76736700	2.49449400	-1.49783000
H	2.44057600	1.07382400	-2.50657500
C	-3.27561500	3.78110200	0.95231500
H	-3.89739500	2.90374500	0.74611600
H	-3.61241200	4.63904500	0.36764700
H	-3.33002500	4.02249700	2.01544600
C	-1.89517600	3.46089200	0.59787900
N	-0.80195700	3.21081200	0.31230300
C	-4.82277800	-2.60047100	1.01071000
H	-5.00636600	-2.82137500	2.06374400
H	-5.48641200	-3.20751800	0.39233600
H	-4.99311100	-1.53557500	0.82473300
C	-3.43255200	-2.90750300	0.68401200
N	-2.33251000	-3.15497400	0.42490600

TS-N₃-1 Imaginary frequency: -503.72

C	0.55077300	-2.56596200	1.34385800
C	-0.85419800	-1.94359800	1.34613300
C	1.56015700	-1.42921900	1.56988500
H	0.63640900	-3.33403600	2.11605900
H	0.75163100	-3.04454100	0.38298900
H	-1.26103400	-1.89909000	2.35984600
H	-1.54821900	-2.50833800	0.70923700
H	2.55051200	-1.72320000	1.21598800
H	1.64104100	-1.16691500	2.62937800
C	1.08535000	-0.21377900	0.79874800
C	0.15574700	-0.40919800	-0.31924900
H	1.11135900	0.77776100	1.24227400
H	0.26349500	-1.30126500	-0.93429900
H	-0.08673700	0.48383900	-0.89036000
C	-1.71649000	0.46980500	1.10987400
H	-1.20443900	1.41339300	0.89219900
N	-0.69729300	-0.57075600	0.86967500
C	-2.86388500	0.33423200	0.12466700
C	-2.95548800	1.22400400	-0.94877600
C	-3.81489400	-0.68500200	0.24530200
C	-3.97965300	1.09707400	-1.88723700
H	-2.21918200	2.01970900	-1.04146100
C	-4.83566200	-0.81491300	-0.69271900
H	-3.76491600	-1.38141300	1.07892500
C	-4.91968700	0.07699700	-1.76199200
H	-4.04192700	1.79644900	-2.71519700
H	-5.56831900	-1.60911900	-0.58781100
H	-5.71640700	-0.02341200	-2.49232500
C	-2.15587900	0.49681000	2.57020600
H	-2.76299400	-0.36942400	2.84551000
H	-1.28273900	0.53810500	3.22885500
H	-2.76229900	1.38962900	2.73893500
N	3.47493600	0.89558300	0.76269100
N	2.91958300	0.34107400	-0.14348300
N	3.96277600	1.44303100	1.65982500
C	2.78404000	3.49485700	-0.69333400
H	3.31496400	3.41634100	0.25964200
H	2.87045700	4.50836800	-1.08818200
H	3.21483900	2.77351300	-1.39027000
C	1.37657700	3.16362100	-0.48910200
N	0.25800400	2.91566300	-0.32857100
C	4.19441200	-1.70181700	-2.24722900
H	5.03579500	-2.29202800	-1.87956900
H	4.16394400	-0.73642400	-1.73353300
H	4.29367800	-1.56267000	-3.32529200
C	2.94216400	-2.39305400	-1.95287800
N	1.94639200	-2.93465000	-1.72277800

TS-N₃-2

Imaginary frequency: -532.93

C	0.56715900	-2.02381700	-0.40121500
C	3.27583000	-0.45797200	-0.13105200
H	-0.14718800	-2.60354600	0.18552100
H	0.22287600	-2.04251300	-1.44325400
H	3.99348600	0.17906100	-0.65609200
H	3.70809000	-0.69071600	0.84774700
C	2.05044500	0.38903200	0.07787000
C	0.94101400	0.41431200	-0.86939300
H	1.89421600	0.88174800	1.03114800
H	1.14470800	0.03687600	-1.86927100
H	0.29247800	1.28897000	-0.86504000
C	-0.48715900	-0.20179900	1.06060500
H	-0.17307600	0.81103200	1.35023800
N	0.54292700	-0.63550000	0.08346100
C	-1.84655100	-0.06121200	0.39987900
C	-2.26946800	1.20950800	-0.00554400
C	-2.67758000	-1.16130600	0.16305800
C	-3.49532100	1.37409000	-0.64895700
H	-1.63504100	2.07298700	0.19428100
C	-3.90158700	-0.99707800	-0.48149000
H	-2.38272300	-2.15416500	0.49268200
C	-4.31122900	0.27134100	-0.89144300
H	-3.81230500	2.36590700	-0.95542200
H	-4.53894600	-1.85813900	-0.65771600
H	-5.26730600	0.39922600	-1.38932800
C	-0.46154300	-1.07780700	2.30695400
H	0.55251500	-1.11679600	2.71630200
H	-1.12623400	-0.64802100	3.05964600
H	-0.79811200	-2.10098900	2.11900300
C	1.96070800	-2.63705800	-0.28037300
C	3.04279000	-1.75986900	-0.90904200
H	1.94239600	-3.62273100	-0.75727000
H	2.19106300	-2.79288100	0.78175500
H	3.98971300	-2.30714300	-0.93431100
H	2.78793700	-1.54431100	-1.95462900
N	0.86748100	3.25924800	0.57245600
N	1.86887500	2.91674200	0.08009700
N	2.84020300	2.42579200	-0.39817700

TS-Cl-i

Imaginary frequency: -440.47

C	0.75697300	-2.41379500	1.47920900
C	-0.69080800	-1.91211700	1.36321100
C	1.64202800	-1.21881800	1.86414300
H	0.83200300	-3.21482800	2.21882800
H	1.09254000	-2.82154500	0.52315900
H	-1.19578600	-1.95092900	2.33276300
H	-1.26477900	-2.51101800	0.64209900
H	2.69012700	-1.43293800	1.65167100
H	1.55629300	-0.98485400	2.93074900
C	1.19568600	-0.00939700	1.06594000
C	0.34868700	-0.22755300	-0.11524100
H	1.10761500	0.96316700	1.53426100
H	0.58491800	-1.06961500	-0.76611900
H	0.09988100	0.67464900	-0.66997300
C	-1.74801900	0.41554000	1.11115900
H	-1.31317500	1.40952600	0.96260600
N	-0.61606200	-0.51336200	0.95436500
C	-2.78416600	0.19965500	0.02108800
C	-2.86038200	1.10000200	-1.04485500
C	-3.64881400	-0.90033700	0.04021700
C	-3.78156900	0.90522800	-2.07395000
H	-2.19669700	1.96205600	-1.05908700
C	-4.56648200	-1.09878100	-0.98791700
H	-3.61350800	-1.60767200	0.86525000
C	-4.63522400	-0.19504200	-2.04813200
H	-3.83263100	1.61501100	-2.89387700
H	-5.23068000	-1.95712200	-0.96098000
H	-5.35353100	-0.34775000	-2.84747100
C	-2.32436300	0.36234300	2.52288800
H	-2.85788100	-0.56933800	2.72815100
H	-1.52424700	0.47688000	3.26068000
H	-3.03570500	1.18207000	2.64731200
Cl	3.22804700	0.75482200	0.16333500
C	2.62891100	3.95604100	-0.32874200
H	3.04026900	3.42183000	-1.18618600
H	3.26001800	3.73211000	0.53224200
H	2.60091600	5.03066700	-0.51871800
C	1.27641600	3.46826300	-0.06989100
N	0.19541300	3.10837600	0.13091300
C	4.60877400	-1.68928200	-1.92061000
H	5.36835800	-2.38542300	-1.56037900
H	4.64754300	-0.76015000	-1.34504000
H	4.78000600	-1.48228600	-2.97840100
C	3.28231400	-2.27446100	-1.74315500
N	2.23230000	-2.73921800	-1.60419300

TS-CI-2

Imaginary frequency: -493.43

C	0.31615500	-1.63024900	2.26251000
C	-0.98682300	-1.16158300	1.60350200
C	1.13466200	-0.34045300	2.43935800
H	0.12412000	-2.13722500	3.21044700
H	0.83811500	-2.33273500	1.60828600
H	-1.73020300	-0.86148600	2.35483000
H	-1.43858600	-1.91571900	0.95419600
H	2.21431200	-0.50905900	2.43944500
H	0.85767200	0.17890400	3.36313500
C	0.72613400	0.50711300	1.24998100
C	1.00460200	-0.02187700	-0.08413900
H	0.80917600	1.58816100	1.34801000
H	1.15919800	-1.08368600	-0.23046800
H	0.78065200	0.60884200	-0.93484700
C	-1.63943200	1.00672300	0.43861400
H	-1.15863400	1.68115100	-0.27964100
N	-0.60427900	0.02583300	0.81599600
C	-2.76462500	0.27241900	-0.27426800
C	-2.46751800	-0.42241500	-1.45320200
C	-4.07363000	0.24802900	0.20571400
C	-3.45401300	-1.12608200	-2.13457500
H	-1.44771600	-0.41638800	-1.83068500
C	-5.06776600	-0.45695900	-0.47681700
H	-4.33376700	0.78076200	1.11490200
C	-4.76173400	-1.14543600	-1.64594500
H	-3.20418700	-1.66042200	-3.04582600
H	-6.08200400	-0.46509200	-0.08961100
H	-5.53489800	-1.69312800	-2.17553600
C	-2.07067800	1.85214400	1.63510600
H	-1.20660300	2.38495300	2.04019000
H	-2.80265000	2.60116800	1.32147700
H	-2.51459600	1.24844400	2.43277300
Cl	3.30223700	0.35652600	-0.39089800
C	1.76011400	3.49705000	-0.80817300
N	0.66588100	3.30203600	-0.48685600
C	3.14299400	3.74046900	-1.21018700
H	3.69344300	2.80160400	-1.09876200
H	3.17003100	4.07099500	-2.24996600
H	3.57974400	4.51059400	-0.57199400
C	4.44158500	-2.87743600	-1.00921100
H	5.09774900	-3.35852700	-0.28173800
H	4.60580800	-1.79630400	-1.00187900
H	4.64096500	-3.28357700	-2.00241400
C	3.04699000	-3.12199500	-0.64995600
N	1.94164500	-3.31643200	-0.36898800

3)Transition states for the ring-expansion of 1-azoniabicyclo[3.1.0]hexane 1 with different nucleophiles (M062X/6-31+G(d,p) level of theory, 298 K and 1 atm, IEFPCM in acetonitrile)

TS-CN-1 Imaginary frequency: -564.20

C	2.027631	-1.725511	-1.303106
C	0.598298	-1.622837	-0.753352
C	2.959841	-1.148131	-0.231321
H	2.280723	-2.761457	-1.535185
H	2.123168	-1.155053	-2.230852
H	0.354487	-2.498891	-0.148412
H	-0.145839	-1.522418	-1.552641
H	3.943333	-0.929697	-0.644045
H	3.088541	-1.857290	0.592179
C	2.312201	0.108981	0.323982
C	1.220387	0.746471	-0.424631
H	2.366286	0.332732	1.381087
H	1.275071	0.781951	-1.511545
H	0.831725	1.670650	-0.003098
C	-0.476510	-0.262074	1.140637
H	-0.139323	0.589371	1.742750
N	0.584340	-0.451765	0.129843
C	-1.784313	0.129383	0.472950
C	-2.192060	1.466551	0.473942
C	-2.581110	-0.818661	-0.180194
C	-3.368766	1.854096	-0.167889
H	-1.589457	2.211251	0.988591
C	-3.754909	-0.434242	-0.825046
H	-2.291003	-1.866049	-0.186946
C	-4.151495	0.904035	-0.821226
H	-3.672633	2.896184	-0.154334
H	-4.361966	-1.180687	-1.327747
H	-5.067446	1.202050	-1.321732
C	-0.582328	-1.471247	2.064030
H	-0.997111	-2.349364	1.564293
H	0.405091	-1.727043	2.459099
H	-1.241518	-1.222710	2.898824
N	4.792359	2.393613	-0.116351
C	3.973294	1.572107	0.047104

TS-CN-2 Imaginary frequency: -604.48

C	-1.861224	0.874235	-0.041281
N	-0.594204	-0.393134	-0.032493
C	-0.351183	-1.094940	1.247443
C	-1.747493	-1.343773	1.830467
C	-2.653565	-1.471889	0.595079
C	-2.018384	-0.533456	-0.411617
C	0.442798	-0.443704	-1.085792
C	0.530676	-1.833135	-1.713007
C	1.746319	0.088469	-0.508189
C	1.797349	1.421225	-0.080645
C	2.959705	1.947730	0.474036
C	4.094943	1.144838	0.608264
C	4.054434	-0.180032	0.182970
C	2.885081	-0.706202	-0.372358
C	-3.885455	1.733066	-0.323082
N	-4.999876	2.048100	-0.499647
H	-1.763600	-2.239533	2.452665
H	-2.058901	-0.503773	2.456628
H	0.161537	-2.040102	1.035920
H	0.288697	-0.486645	1.890240
H	-3.693708	-1.204236	0.793950
H	-2.624874	-2.489856	0.195530
H	-2.193839	-0.737566	-1.466643
H	-1.906689	1.178992	0.994035
H	-1.483458	1.574664	-0.772288
H	0.106457	0.258810	-1.858824
H	0.915778	2.049943	-0.180631
H	2.875886	-1.740852	-0.699181
H	2.982263	2.983419	0.798479
H	4.932447	-0.811123	0.279662
H	5.004275	1.552938	1.038155
H	-0.438232	-2.120545	-2.128659
H	1.259161	-1.828034	-2.527606
H	0.831354	-2.595852	-0.990180

TS-N3-1

Imaginary frequency: -571.46

C	-1.89039500	1.42712200	-1.41031000
C	-0.41353600	1.46072300	-0.99389500
C	-2.72184400	1.19693800	-0.14247400
H	-2.17309700	2.35752300	-1.90618200
H	-2.06892200	0.61697600	-2.12246100
H	-0.12177900	2.47079800	-0.69733800
H	0.24272500	1.12382200	-1.80627200
H	-3.73175500	0.87766500	-0.41298700
H	-2.81016500	2.11593500	0.44422300
C	-2.02480300	0.15354000	0.70658200
C	-0.98901500	-0.68851600	0.08441100
H	-1.96623300	0.27183200	1.78113300
H	-1.14405700	-1.05688800	-0.92974200
H	-0.55826500	-1.45089400	0.72957400
C	0.87760300	0.66940900	1.07941600
H	0.59785600	0.06870300	1.95267800
N	-0.29063900	0.59596900	0.18085300
C	2.09022500	0.01650800	0.43582400
C	2.49130000	-1.26061600	0.83820000
C	2.80132500	0.65623500	-0.58728700
C	3.57696700	-1.89252300	0.22988600
H	1.95600700	-1.76338800	1.64034600
C	3.88242600	0.02603900	-1.19977700
H	2.51715600	1.65406000	-0.91102600
C	4.27274500	-1.25100900	-0.79309500
H	3.87787300	-2.88282000	0.55718000
H	4.42212100	0.53356000	-1.99321300
H	5.11666900	-1.74000500	-1.26932700
C	1.12205300	2.09689600	1.55736000
H	1.49427800	2.74869800	0.76386900
H	0.19614800	2.52187600	1.95538200
H	1.87177600	2.08041700	2.35172000
N	-4.01649200	-1.46292700	-0.01425000
N	-3.58080500	-1.21792800	1.06766500
N	-4.42187000	-1.65973400	-1.08521400

TS-N3-2 Imaginary frequency: -619.19

C	1.641369	0.968256	1.837801
C	0.191625	0.790739	1.367163
C	2.377122	1.503579	0.599383
H	1.702570	1.653102	2.684795
H	2.064383	0.012320	2.157601
H	-0.382944	1.713710	1.507384
H	-0.332780	-0.025271	1.869467
H	3.444863	1.269839	0.599249
H	2.257962	2.587962	0.514793
C	1.653576	0.841695	-0.558905
C	1.623562	-0.622260	-0.612811
H	1.687449	1.353419	-1.519775
H	1.770641	-1.199962	0.293166
H	1.166771	-1.103409	-1.467429
C	-0.861894	0.795056	-0.954404
H	-0.597116	0.375088	-1.933670
N	0.294461	0.510855	-0.082227
C	-2.071833	0.030935	-0.433975
C	-1.981173	-1.359695	-0.288014
C	-3.269018	0.664205	-0.098302
C	-3.060954	-2.099269	0.183210
H	-1.053452	-1.866540	-0.541335
C	-4.355963	-0.076304	0.374410
H	-3.370960	1.739352	-0.202636
C	-4.255922	-1.457155	0.517083
H	-2.972155	-3.176111	0.288796
H	-5.279706	0.433323	0.630204
H	-5.100843	-2.031791	0.883504
C	-1.071616	2.298112	-1.127327
H	-0.154996	2.764009	-1.497660
H	-1.861871	2.484649	-1.858694
H	-1.350611	2.785590	-0.189591
N	3.501508	-1.186460	-1.298253
N	4.156134	-1.289200	-0.305999
N	4.763542	-1.383286	0.679331

TS-CI-1 Imaginary frequency: -501.56

C	1.954313	-1.686996	-1.333064
C	0.536427	-1.663755	-0.744020
C	2.911739	-1.129673	-0.273838
H	2.235597	-2.701544	-1.621729
H	2.002078	-1.072594	-2.236262
H	0.344437	-2.576236	-0.174276
H	-0.221271	-1.573943	-1.534228
H	3.880948	-0.895864	-0.714681
H	3.076019	-1.857830	0.526523
C	2.293292	0.114760	0.332383
C	1.099871	0.691654	-0.314573
H	2.371446	0.279115	1.400214
H	1.106487	0.804273	-1.399539
H	0.709242	1.584481	0.170163
C	-0.615177	-0.395751	1.160359
H	-0.290109	0.405203	1.834642
N	0.477580	-0.533197	0.181624
C	-1.894630	0.065738	0.478882
C	-2.282277	1.406188	0.564899
C	-2.680505	-0.816042	-0.273815
C	-3.426474	1.863271	-0.089950
H	-1.687954	2.098050	1.157277
C	-3.822022	-0.362243	-0.931633
H	-2.406959	-1.865321	-0.347656
C	-4.197602	0.979141	-0.842262
H	-3.714479	2.906886	-0.009610
H	-4.421406	-1.056873	-1.512016
H	-5.088998	1.330041	-1.352877
C	-0.780691	-1.662242	1.993672
H	-1.186857	-2.496387	1.416960
H	0.184244	-1.963174	2.411519
H	-1.472312	-1.459626	2.814731
Cl	3.921130	1.730554	-0.027221

TS-CI-2 Imaginary frequency: -546.76

C	-1.642019	-1.394019	1.856681
C	-0.245288	-1.153397	1.273479
C	-2.538166	-1.537333	0.616704
H	-1.663139	-2.280615	2.492028
H	-1.954905	-0.543489	2.468536
H	0.260208	-2.104900	1.066498
H	0.398710	-0.552111	1.919389
H	-3.584215	-1.285695	0.804303
H	-2.487594	-2.555894	0.220237
C	-1.905684	-0.590489	-0.387301
C	-1.880693	0.838728	-0.052015
H	-2.069913	-0.818952	-1.440454
H	-1.907135	1.140377	0.986057
H	-1.461718	1.528103	-0.772685
C	0.543678	-0.492237	-1.051987
H	0.198097	0.198971	-1.831893
N	-0.489172	-0.449537	-0.001364
C	1.842738	0.065774	-0.485712
C	1.850605	1.374096	0.015068
C	3.023265	-0.676926	-0.441682
C	3.010673	1.927386	0.547606
H	0.935407	1.960418	-0.008893
C	4.190537	-0.124257	0.092957
H	3.049139	-1.691969	-0.823833
C	4.188382	1.176343	0.588364
H	2.998290	2.943769	0.928854
H	5.100013	-0.716428	0.118837
H	5.095631	1.605118	1.002322
C	0.656836	-1.884046	-1.673670
H	-0.314555	-2.201088	-2.061569
H	1.362810	-1.867662	-2.507893
H	0.996906	-2.631478	-0.952102
Cl	-4.005706	1.637796	-0.411127

4)Transition states for the ring-expansion of 1-azoniabicyclo[3.1.0]hexane 1 with different nucleophiles (M062X/6-31+G(d,p) level of theory, 298 K and 1 atm, CPCM in acetonitrile)

TS-CN-1 Imaginary frequency: -564.20

C	2.02728300	-1.72769900	-1.30187500
C	0.59788300	-1.62396100	-0.75241000
C	2.95936400	-1.14858700	-0.23087300
H	2.28034200	-2.76402300	-1.53232800
H	2.12302000	-1.15877000	-2.23052400
H	0.35402200	-2.49893700	-0.14588400
H	-0.14632100	-1.52480200	-1.55179300
H	3.94281400	-0.93043600	-0.64378300
H	3.08816600	-1.85652800	0.59368400
C	2.31133800	0.10916700	0.32250900
C	1.22032300	0.74592000	-0.42782300
H	2.36461800	0.33444400	1.37930000
H	1.27552400	0.77918700	-1.51474400
H	0.83145000	1.67094400	-0.00839900
C	-0.47578900	-0.26005200	1.14012100
H	-0.13795200	0.59237400	1.74058300
N	0.58421200	-0.45139600	0.12875000
C	-1.78409800	0.13025700	0.47288400
C	-2.19180500	1.46738800	0.47183100
C	-2.58135900	-0.81894500	-0.17794500
C	-3.36896500	1.85380500	-0.16978100
H	-1.58879300	2.21296500	0.98473600
C	-3.75561800	-0.43566700	-0.82256700
H	-2.29126800	-1.86636500	-0.18297600
C	-4.15215400	0.90260500	-0.82083300
H	-3.67280700	2.89591400	-0.15783000
H	-4.36311100	-1.18298100	-1.32344500
H	-5.06846800	1.19975300	-1.32118500
C	-0.58079500	-1.46772400	2.06557300
H	-0.99602200	-2.34660700	1.56757500
H	0.40692200	-1.72294000	2.46032500
H	-1.23937200	-1.21796100	2.90046200
N	4.79307200	2.39346600	-0.11526300
C	3.97376500	1.57187300	0.04649300

TS-CN-2 Imaginary frequency: -603.90

C	-1.86095600	0.87328100	-0.03971300
N	-0.59395500	-0.39327400	-0.03358900
C	-0.34959800	-1.09700600	1.24506200
C	-1.74530900	-1.34659900	1.82908800
C	-2.65242900	-1.47357100	0.59434700
C	-2.01840500	-0.53383200	-0.41182500
C	0.44257800	-0.44153100	-1.08760400
C	0.53033900	-1.82968300	-1.71767700
C	1.74609600	0.08967400	-0.50926700
C	1.79866700	1.42325900	-0.08468900
C	2.96059700	1.94874700	0.47180100
C	4.09383400	1.14391700	0.61075400
C	4.05187100	-0.18176700	0.18818400
C	2.88296900	-0.70687200	-0.36896300
C	-3.88652000	1.73275600	-0.31915300
N	-5.00054300	2.04996900	-0.49432400
H	-1.76083100	-2.24290500	2.45050900
H	-2.05631700	-0.50729400	2.45635900
H	0.16276700	-2.04193500	1.03147700
H	0.29128100	-0.48988800	1.88795600
H	-3.69242900	-1.20630300	0.79428600
H	-2.62390700	-2.49111200	0.19366500
H	-2.19474500	-0.73667800	-1.46692100
H	-1.90649100	1.17684700	0.99592400
H	-1.48435100	1.57496800	-0.77009300
H	0.10580800	0.26251000	-1.85905700
H	0.91865500	2.05354200	-0.18869500
H	2.87261100	-1.74216400	-0.69378600
H	2.98438900	2.98514000	0.79389400
H	4.92845100	-0.81429600	0.28846200
H	5.00286400	1.55119200	1.04205900
H	-0.43818900	-2.11569900	-2.13519600
H	1.25986500	-1.82323400	-2.53133000
H	0.82966100	-2.59419300	-0.99619400

TS-N3-1

Imaginary frequency: -570.77

C	-1.88805600	1.42794200	-1.41192500
C	-0.41135200	1.45963600	-0.99467000
C	-2.72061100	1.19788100	-0.14472700
H	-2.16954400	2.35887000	-1.90751900
H	-2.06710400	0.61844600	-2.12463500
H	-0.11834600	2.46931200	-0.69791500
H	0.24507500	1.12175900	-1.80651600
H	-3.73020600	0.87846500	-0.41617000
H	-2.80962000	2.11688700	0.44186300
C	-2.02435800	0.15448600	0.70495900
C	-0.98983800	-0.68921100	0.08301100
H	-1.96592200	0.27288500	1.77948200
H	-1.14496500	-1.05698800	-0.93130000
H	-0.56004900	-1.45220300	0.72803200
C	0.87693900	0.66720100	1.07997800
H	0.59646500	0.06481300	1.95188500
N	-0.29044500	0.59474400	0.18016500
C	2.09027200	0.01573200	0.43640400
C	2.48969700	-1.26292200	0.83542200
C	2.80343100	0.65805400	-0.58359100
C	3.57569900	-1.89386400	0.22683500
H	1.95279000	-1.76774100	1.63520200
C	3.88493700	0.02885000	-1.19633600
H	2.52061900	1.65714800	-0.90464800
C	4.27357000	-1.24974300	-0.79303300
H	3.87519800	-2.88545000	0.55148300
H	4.42629700	0.53833800	-1.98737100
H	5.11780400	-1.73797000	-1.26949500
C	1.12007800	2.09390900	1.56085400
H	1.49299400	2.74749900	0.76918700
H	0.19344400	2.51764100	1.95854900
H	1.86885200	2.07643900	2.35606900
N	-4.01835700	-1.46121200	-0.01345400
N	-3.58272400	-1.21483800	1.06816400
N	-4.42364900	-1.65953000	-1.08420000

TS-N3-2

Imaginary frequency: -618.55

C	1.63850300	0.97448200	1.83642600
C	0.18934500	0.79620800	1.36445900
C	2.37633700	1.50485800	0.59707900
H	1.69908800	1.66234300	2.68101600
H	2.06041100	0.01951000	2.16042500
H	-0.38469400	1.72017700	1.50027900
H	-0.33666100	-0.01737400	1.86900600
H	3.44387800	1.27033000	0.59924600
H	2.25808900	2.58907700	0.50855600
C	1.65391600	0.83953300	-0.55993900
C	1.62237700	-0.62451100	-0.60857600
H	1.68936000	1.34787800	-1.52251900
H	1.76947400	-1.19929200	0.29923000
H	1.16615600	-1.10843500	-1.46189400
C	-0.86141000	0.79153000	-0.95827500
H	-0.59573800	0.36758500	-1.93557500
N	0.29409300	0.51076100	-0.08368700
C	-2.07162700	0.02950400	-0.43563000
C	-1.98377700	-1.36162500	-0.29320900
C	-3.26568800	0.66505600	-0.09339000
C	-3.06324900	-2.09954500	0.18122300
H	-1.05860300	-1.87031800	-0.55221300
C	-4.35233300	-0.07375900	0.38256000
H	-3.36533600	1.74067700	-0.19511000
C	-4.25505600	-1.45514400	0.52181800
H	-2.97678100	-3.17685200	0.28388000
H	-5.27371200	0.43755800	0.64345800
H	-5.09979100	-2.02846300	0.89071700
C	-1.07077900	2.29386100	-1.13750500
H	-0.15451800	2.75789700	-1.51106300
H	-1.86200600	2.47739700	-1.86859400
H	-1.34838600	2.78567200	-0.20164500
N	3.50051900	-1.19286200	-1.29310900
N	4.15712900	-1.29012500	-0.30162900
N	4.76688900	-1.37892500	0.68279000

TS-CI-1

Imaginary frequency: -501.17

C	1.95399600	-1.68801100	-1.33274800
C	0.53630800	-1.66476000	-0.74330200
C	2.91124000	-1.13007100	-0.27373000
H	2.23541800	-2.70254200	-1.62137500
H	2.00149200	-1.07373800	-2.23603300
H	0.34493900	-2.57664700	-0.17234400
H	-0.22185900	-1.57606400	-1.53318700
H	3.88042100	-0.89591600	-0.71438900
H	3.07571800	-1.85789400	0.52692700
C	2.29203900	0.11428000	0.33188100
C	1.09955000	0.69133600	-0.31633800
H	2.37004400	0.27967600	1.39953600
H	1.10660100	0.80287400	-1.40135600
H	0.70860000	1.58459200	0.16730900
C	-0.61475900	-0.39493400	1.16036200
H	-0.28936900	0.40663300	1.83382700
N	0.47759500	-0.53325100	0.18119900
C	-1.89432800	0.06609500	0.47892100
C	-2.28215900	1.40648100	0.56449900
C	-2.68009200	-0.81607200	-0.27334600
C	-3.42643500	1.86314500	-0.09044400
H	-1.68775700	2.09872800	1.15635400
C	-3.82168900	-0.36270200	-0.93125500
H	-2.40649500	-1.86538600	-0.34664700
C	-4.19741600	0.97865700	-0.84239600
H	-3.71452600	2.90676600	-0.01054600
H	-4.42105200	-1.05766700	-1.51125600
H	-5.08881800	1.32924400	-1.35320700
C	-0.78007100	-1.66064800	1.99489600
H	-1.18564800	-2.49547300	1.41874200
H	0.18474000	-1.96093200	2.41354400
H	-1.47218100	-1.45761600	2.81540800
Cl	3.92114400	1.73101900	-0.02715900

TS-Cl-2

Imaginary frequency: -546.09

C	-1.64233600	-1.39398600	1.85751100
C	-0.24560200	-1.15499800	1.27370600
C	-2.53905100	-1.53730500	0.61791900
H	-1.66409600	-2.28007400	2.49354700
H	-1.95428800	-0.54278300	2.46888800
H	0.25873500	-2.10709200	1.06649500
H	0.39954900	-0.55440700	1.91908900
H	-3.58476200	-1.28439900	0.80559900
H	-2.48974500	-2.55624000	0.22222700
C	-1.90611300	-0.59176600	-0.38698600
C	-1.87902800	0.83742700	-0.05226600
H	-2.07068200	-0.82071800	-1.43995100
H	-1.90634200	1.13972400	0.98556400
H	-1.45963100	1.52616500	-0.77326000
C	0.54350300	-0.49319100	-1.05165900
H	0.19755700	0.19796400	-1.83149000
N	-0.48945100	-0.45109000	-0.00110700
C	1.84224500	0.06548700	-0.48533600
C	1.84880100	1.37293800	0.01766200
C	3.02382300	-0.67562200	-0.44376000
C	3.00856900	1.92692500	0.55002700
H	0.93281000	1.95807200	-0.00450000
C	4.19081300	-0.12223500	0.09068600
H	3.05076900	-1.68993400	-0.82776700
C	4.18732500	1.17746000	0.58834900
H	2.99512300	2.94265600	0.93297700
H	5.10114400	-0.71316300	0.11467600
H	5.09437600	1.60678800	1.00216400
C	0.65723800	-1.88488300	-1.67351300
H	-0.31406400	-2.20249800	-2.06119600
H	1.36285800	-1.86806100	-2.50801500
H	0.99808400	-2.63216000	-0.95214200
Cl	-4.00366800	1.64001700	-0.41289400

5. Transition states for the ring-expansion of 1-azoniabicyclo[4.1.0]heptane 5 with different nucleophiles (M062X/6-31+G(d,p) level of theory, 298 K and 1 atm, gas phase, explicit solvent)

TS-CN-1 Imaginary frequency: -537.56

C	0.29862700	-1.00699000	-1.10499500
C	3.00306100	-0.87631400	0.18266900
H	-0.68227100	-1.48096000	-1.02380200
H	0.25186000	-0.32218400	-1.95929100
H	3.91200900	-0.26984200	0.26488900
H	3.09063200	-1.73153700	0.86384100
C	1.87619100	0.00499000	0.66619600
C	1.43681900	1.19832200	-0.04785800
H	1.84941600	0.11281900	1.74998000
H	1.60678900	1.30858700	-1.10974300
H	0.96080400	2.00494200	0.48912500
C	-0.59796100	-0.22384800	1.12975300
H	-0.34890300	0.57263100	1.84319700
N	0.49178400	-0.18569500	0.11997800
C	-1.92912500	0.12999800	0.48279400
C	-2.05127700	1.34870200	-0.19633800
C	-3.03794700	-0.71511400	0.54675100
C	-3.25063400	1.71174500	-0.79876700
H	-1.20019300	2.02117100	-0.25533200
C	-4.24379200	-0.35202700	-0.05589500
H	-2.97760300	-1.66385700	1.07025300
C	-4.35339800	0.85965400	-0.73025600
H	-3.32639400	2.66199200	-1.31770200
H	-5.09639800	-1.02094900	0.00541500
H	-5.29136300	1.14238600	-1.19731000
C	-0.56707500	-1.56052000	1.86390600
H	0.42291500	-1.72511200	2.29756400
H	-1.29867900	-1.57276700	2.67548600
H	-0.78665600	-2.39382300	1.18855700
C	1.39907200	-2.03822300	-1.32248300
C	2.77842200	-1.38881800	-1.23672400
H	1.23264200	-2.50346400	-2.29902800
H	1.31932300	-2.82956100	-0.56502700
H	3.56129900	-2.10762600	-1.49196800
H	2.85910700	-0.56622400	-1.95910300
C	3.39500300	2.39047700	0.15247300
N	4.50903600	2.11014800	0.38611600

TS-CN-2 Imaginary frequency: -563.08

C	0.35774200	-1.49561900	-0.80047500
C	3.21939100	-0.70763400	0.10500000
H	-0.53183900	-2.02167800	-0.44738100
H	0.14362700	-1.15334900	-1.81995100
H	4.14085600	-0.16433500	-0.10407100
H	3.38382000	-1.29246100	1.01781200
C	2.17338600	0.33996400	0.40507300
C	1.21700500	0.86244600	-0.56095900
H	2.06497200	0.68822500	1.42371000
H	1.44306800	0.73191700	-1.61680300
H	0.78109500	1.83234500	-0.33833300
C	-0.47154100	-0.02366300	1.09249800
H	-0.16805000	0.93254300	1.53387600
N	0.55515900	-0.30538100	0.05319900
C	-1.84120600	0.17302400	0.46247700
C	-2.16773500	1.41935000	-0.08443800
C	-2.78413900	-0.85665700	0.39374200
C	-3.39540000	1.62510600	-0.70850700
H	-1.46376400	2.24413700	-0.00764600
C	-4.01535800	-0.65267700	-0.22749700
H	-2.57252100	-1.82502700	0.83867100
C	-4.32173100	0.58639300	-0.78487600
H	-3.63090700	2.59995200	-1.12346800
H	-4.73736900	-1.46218300	-0.26930400
H	-5.28211200	0.74577700	-1.26459400
C	-0.40131300	-1.09408400	2.17544700
H	0.58729500	-1.08258100	2.64235100
H	-1.15624900	-0.90587300	2.94245000
H	-0.56931300	-2.09764000	1.77339400
C	3.42242200	2.30239600	0.27894000
C	1.57182500	-2.41676900	-0.78254100
C	2.87096700	-1.65760400	-1.04322700
H	1.41844200	-3.19722800	-1.53492200
H	1.63459800	-2.91312800	0.19497800
H	3.69596000	-2.36693000	-1.15549700
H	2.80679800	-1.11023700	-1.99247700
N	3.07422800	3.36165700	-0.08416200

TS-N₃-1

Imaginary frequency: -550.69

C	-0.03108000	-1.58377200	-0.78704500
C	2.79583200	-1.29449000	0.15387200
H	-1.03613000	-1.87657100	-0.47358500
H	-0.10390300	-1.26610500	-1.83420000
H	3.74632700	-0.80265600	-0.07891200
H	2.91791500	-1.83918700	1.09738000
C	1.79304300	-0.18342300	0.36314000
C	1.42171300	0.72290400	-0.71688200
H	1.89410200	0.31083200	1.32959100
H	1.48624400	0.40733400	-1.75055600
H	1.01813400	1.69916400	-0.47251800
C	-0.61115500	0.06668500	1.04662200
H	-0.21809100	1.03883500	1.37639000
N	0.35480000	-0.40346500	0.02313600
C	-1.97522100	0.29894900	0.41286100
C	-2.07381500	1.14073100	-0.70214400
C	-3.13767900	-0.29462200	0.90694000
C	-3.30141500	1.37857200	-1.31041500
H	-1.18070400	1.61400000	-1.09999300
C	-4.37200300	-0.05525300	0.29967600
H	-3.09776200	-0.94690900	1.77305600
C	-4.45764100	0.77867200	-0.81004700
H	-3.35587700	2.03551300	-2.17267600
H	-5.26576300	-0.52353400	0.69985500
H	-5.41748700	0.96387900	-1.28150300
C	-0.60361200	-0.88758800	2.23692900
H	0.41493200	-0.99998200	2.61781600
H	-1.22409900	-0.50009200	3.04868400
H	-0.97868500	-1.87764900	1.95679500
C	0.94903700	-2.74516600	-0.66657000
C	2.37657600	-2.27629300	-0.93813600
H	0.64078600	-3.52154300	-1.37376800
H	0.89001500	-3.17782600	0.34128900
H	3.06698000	-3.12384600	-0.95315500
H	2.43510000	-1.80333300	-1.92694300
N	3.30539500	1.80261300	-1.00543600
N	3.28015100	2.24267100	0.10290700
N	3.16429600	2.61450000	1.19998500

TS-N₃-2 Imaginary frequency: -550.55

C	1.261161	-0.332897	1.545619
C	-1.461264	-1.528384	1.394328
H	2.317396	-0.491764	1.313835
H	1.173389	0.661656	2.000588
H	-2.532633	-1.305211	1.438542
H	-1.353579	-2.595454	1.164349
C	-0.895657	-0.736313	0.234662
C	-0.916645	0.728278	0.221738
H	-1.139160	-1.184809	-0.728577
H	-0.780030	1.285055	1.139650
H	-0.839437	1.237814	-0.732219
C	1.294300	-0.630590	-0.971463
H	0.611040	-0.407323	-1.801078
N	0.531521	-0.326812	0.257232
C	2.500613	0.290946	-1.091398
C	2.374242	1.651331	-0.779866
C	3.738625	-0.176076	-1.537600
C	3.454066	2.517991	-0.913042
H	1.424955	2.033706	-0.415771
C	4.822878	0.692274	-1.674871
H	3.870573	-1.224084	-1.784285
C	4.685292	2.041076	-1.363602
H	3.334712	3.567198	-0.661474
H	5.776224	0.307633	-2.023819
H	5.528975	2.716160	-1.466292
C	1.613436	-2.122221	-1.032930
H	0.693495	-2.696918	-0.897196
H	2.013553	-2.392602	-2.012951
H	2.336145	-2.407328	-0.260282
C	0.745479	-1.378845	2.528750
C	-0.762660	-1.227322	2.718229
H	1.278741	-1.245614	3.475241
H	0.974119	-2.387308	2.157510
H	-1.128215	-1.910654	3.490308
H	-0.989380	-0.207107	3.052726
N	-2.951745	1.260135	0.338309
N	-3.409166	0.534939	-0.492796
H	-3.923158	2.817078	3.716607
C	-3.324196	3.156397	2.869608
C	-1.933288	2.752914	3.059729
H	-3.681353	2.690779	1.945630
N	-0.831766	2.425054	3.195908
H	-3.384876	4.243566	2.795386
H	-3.798947	-0.676505	-3.971138
C	-3.523658	-1.724880	-3.850633
C	-2.145109	-1.804288	-3.373870
H	-4.186946	-2.153872	-3.098813
N	-1.047384	-1.880679	-3.016841
H	-3.615411	-2.259673	-4.797642
N	-3.799258	-0.196442	-1.304035

TS-NH₂-1 Imaginary frequency: -494.51

C	-0.56232900	-0.62302300	1.18209900
C	-3.22486300	-0.62211300	-0.25919100
H	0.35096400	-1.21644800	1.26492800
H	-0.43885500	0.26256200	1.81248600
H	-4.02842100	0.07632100	-0.51646400
H	-3.42632600	-1.61646900	-0.67684400
C	-1.99958700	-0.04452600	-0.91513500
C	-1.39942000	1.19516800	-0.45201600
H	-1.89497500	-0.25437600	-1.97818000
H	-1.78052600	1.62720700	0.46486700
H	-0.93204900	1.85928100	-1.16781100
C	0.50587100	-0.49346600	-1.11244900
H	0.34639800	0.09443500	-2.02506000
N	-0.64469300	-0.13833200	-0.23105300
C	1.81352400	-0.04293200	-0.47773600
C	1.98351700	1.30619200	-0.14185000
C	2.85693800	-0.93386800	-0.22035700
C	3.16461600	1.75025200	0.44303600
H	1.18672100	2.01881900	-0.33438800
C	4.04484900	-0.48893900	0.36196100
H	2.75825600	-1.98441400	-0.47347000
C	4.20153700	0.85200700	0.69662500
H	3.27679400	2.79949000	0.69682400
H	4.84574800	-1.19654900	0.55168900
H	5.12525900	1.19840600	1.14899500
C	0.42781200	-1.97447300	-1.46229800
H	-0.54216200	-2.20118600	-1.91212200
H	1.20753200	-2.23952700	-2.18015800
H	0.54801900	-2.60452700	-0.57533300
C	-1.78524500	-1.42348500	1.61304300
C	-3.08460700	-0.70382400	1.25672000
H	-1.70047200	-1.59114700	2.69146600
H	-1.76584300	-2.41020600	1.12942700
H	-3.94153800	-1.24196700	1.67099800
H	-3.11676800	0.31496000	1.66289900
N	-3.60510100	2.41538400	-0.27805000
H	-4.49310900	2.45851800	-0.78962300
H	-3.49176300	3.38962800	0.02388200

TS-NH₂-2 Imaginary frequency: -364.59

C	0.53828700	-1.33382400	-0.76143500
C	3.30597600	-0.29546100	0.04548000
H	-0.31568300	-1.89725100	-0.37968100
H	0.29757100	-1.04058700	-1.78906600
H	4.07100400	0.42598700	-0.25520100
H	3.63783300	-0.80220400	0.95899100
C	2.11921100	0.56763700	0.37539400
C	1.23694200	1.11547000	-0.62875500
H	2.07977300	1.02914400	1.35274200
H	1.47658700	0.95768400	-1.67561700
H	0.73912900	2.05285500	-0.40785600
C	-0.38445300	0.13929900	1.08496200
H	-0.15846100	1.13416100	1.48479400
N	0.66118600	-0.09387500	0.04730200
C	-1.76655000	0.19172900	0.45671200
C	-2.18667600	1.37170600	-0.16759500
C	-2.63347100	-0.90478800	0.46679500
C	-3.43085800	1.44784400	-0.78750700
H	-1.54157500	2.24614800	-0.15680100
C	-3.88131400	-0.83128300	-0.15058200
H	-2.34757700	-1.82472700	0.96898100
C	-4.28090000	0.34307200	-0.78358400
H	-3.74010400	2.37303800	-1.26333800
H	-4.54218200	-1.69205200	-0.13060200
H	-5.25378900	0.40220600	-1.26105400
C	-0.21235700	-0.87895200	2.20555700
H	0.77886900	-0.76940000	2.65291000
H	-0.96731500	-0.71821200	2.97875100
H	-0.30794400	-1.90769700	1.84547900
C	1.80886600	-2.17382700	-0.72152800
C	3.04301300	-1.33460200	-1.04555600
H	1.68888400	-2.99756800	-1.43282400
H	1.92127600	-2.61706100	0.27694800
H	3.92225400	-1.97876700	-1.13579700
H	2.91796300	-0.84683400	-2.02107200
N	3.41952900	2.60770900	0.14031000
H	4.40509700	2.77880400	0.36437800
H	3.01909200	3.55138300	0.18150200

6. Transition states for the ring-expansion of 1-azoniabicyclo[4.1.0]heptane 5 with different nucleophiles (M062X/6-31+G(d,p) level of theory, 298 K and 1 atm, IEFPCM in acetonitrile, ($\epsilon = 35.688$))

TS-CN-1 Imaginary frequency: -600.73

C	0.28245800	-1.05268900	-1.12499400
C	2.94569100	-1.08001900	0.20793300
H	-0.72865800	-1.46367600	-1.08329100
H	0.31088700	-0.35968200	-1.97436600
H	3.89836100	-0.55092900	0.31162000
H	2.96924500	-1.93797400	0.88898600
C	1.85776300	-0.13488500	0.67607100
C	1.58938400	1.13276800	-0.00225200
H	1.81815500	-0.05806300	1.76281900
H	1.70527000	1.21386800	-1.07482000
H	1.07292200	1.91877700	0.52984700
C	-0.61115400	-0.28898900	1.11418100
H	-0.34065500	0.47311300	1.85685000
N	0.48686900	-0.27018000	0.11894200
C	-1.91799600	0.14632900	0.46320500
C	-1.94592600	1.31612900	-0.30815100
C	-3.10300500	-0.57363700	0.62719200
C	-3.12698400	1.75526200	-0.89806300
H	-1.03361900	1.88616500	-0.45720700
C	-4.29089700	-0.13390800	0.03752200
H	-3.11574200	-1.48449900	1.21618100
C	-4.30758400	1.03013400	-0.72553300
H	-3.12619900	2.66318300	-1.49299900
H	-5.20215800	-0.70709400	0.17749700
H	-5.23063100	1.37104200	-1.18383000
C	-0.65976500	-1.64681600	1.80999200
H	0.32416500	-1.88805800	2.22141700
H	-1.37446100	-1.63420900	2.63610100
H	-0.94762600	-2.44100500	1.11365600
C	1.31536200	-2.15397400	-1.32600500
C	2.72727200	-1.58512900	-1.21614600
H	1.14265100	-2.60368200	-2.30799400
H	1.17561800	-2.93985900	-0.57263600
H	3.47453100	-2.34840300	-1.44815700
H	2.86144000	-0.77452900	-1.94426100
C	3.46710600	2.28474000	0.21823300
N	4.51543900	2.78069600	0.38183900

TS-CN-2 Imaginary frequency: -575.95

C	0.28026500	-1.57726000	-0.75206500
C	3.15972800	-0.72971000	0.11577000
H	-0.60076700	-2.10238200	-0.37996800
H	0.06827000	-1.28309100	-1.78691700
H	4.11915600	-0.26532000	-0.11257200
H	3.28185700	-1.26898600	1.06159400
C	2.15487300	0.38090700	0.35124500
C	1.12370300	0.77489400	-0.60937600
H	2.00562100	0.72714700	1.36613000
H	1.33234800	0.59198300	-1.66196200
H	0.64882600	1.74101800	-0.44832800
C	-0.54960200	-0.02757300	1.08474400
H	-0.21099300	0.91647600	1.52609000
N	0.46749000	-0.35524800	0.05352400
C	-1.90958000	0.23112800	0.45359800
C	-2.23071100	1.52617000	0.02968700
C	-2.85140800	-0.78697400	0.26555000
C	-3.44870500	1.79574500	-0.59191900
H	-1.53052900	2.33917400	0.20419500
C	-4.07131700	-0.52089900	-0.35528200
H	-2.64847000	-1.79502100	0.61525900
C	-4.37112200	0.76920100	-0.79140000
H	-3.67947600	2.80772200	-0.90970000
H	-4.79089200	-1.32208000	-0.49153300
H	-5.32265800	0.97494500	-1.27143300
C	-0.53770200	-1.08953500	2.17813600
H	0.45758000	-1.14243600	2.62772200
H	-1.26356600	-0.83237400	2.95322600
H	-0.78901300	-2.08319100	1.79718800
C	3.51951700	2.18259400	0.14320700
C	1.50267100	-2.48446400	-0.68930100
C	2.79575400	-1.72970100	-0.98666800
H	1.36065300	-3.29798500	-1.40735300
H	1.56850500	-2.93414800	0.30962900
H	3.62284600	-2.44094900	-1.06556500
H	2.72758900	-1.22721700	-1.96007400
N	4.13892800	3.15661800	-0.05940800

TS-N3-1 Imaginary frequency: -613.57

C	0.08852000	1.41349400	-0.95021700
C	-2.68204300	1.26648900	0.12192000
H	1.10671900	1.73345000	-0.71769000
H	0.11627200	0.97156400	-1.95400700
H	-3.66865500	0.80395800	0.01263000
H	-2.71689300	1.91118900	1.00732300
C	-1.68615900	0.15413800	0.38958700
C	-1.43797200	-0.90591300	-0.59373000
H	-1.75920500	-0.21563400	1.41282700
H	-1.42663100	-0.66842600	-1.64956200
H	-0.98663900	-1.83171800	-0.25892100
C	0.72199700	0.03641000	1.07602600
H	0.35239300	-0.88197900	1.55161000
N	-0.26511500	0.35143600	0.02014300
C	2.07515300	-0.28415500	0.45323900
C	2.14196700	-1.17688800	-0.62480600
C	3.26223400	0.27121000	0.93545500
C	3.36307400	-1.50712900	-1.20418800
H	1.22842500	-1.61007400	-1.02194500
C	4.48992100	-0.06025000	0.35684900
H	3.24545000	0.96825400	1.76650600
C	4.54515200	-0.94848800	-0.71332100
H	3.39268800	-2.19872300	-2.04042600
H	5.40179000	0.38202400	0.74592900
H	5.49889600	-1.20355500	-1.16456000
C	0.74352200	1.14819200	2.12280200
H	-0.26982100	1.33157100	2.49098300
H	1.36287400	0.86677200	2.97760000
H	1.13304800	2.08126000	1.70308600
C	-0.87319300	2.59539500	-0.93733000
C	-2.31270300	2.11326600	-1.09317300
H	-0.58930200	3.27108000	-1.74936000
H	-0.77116400	3.14790100	0.00554000
H	-3.00081000	2.95919900	-1.16936500
H	-2.41552900	1.53323500	-2.01985600
N	-3.24830800	-1.87306800	-0.89940800
N	-3.72728100	-1.93771500	0.19152100
N	-4.16940100	-1.97579200	1.26445600

TS-N3-2 Imaginary frequency: -573.23

C	0.23788400	-1.97320200	-0.50086200
C	3.15577700	-0.87971500	-0.04503900
H	-0.58449500	-2.46250800	0.02275200
H	-0.05659200	-1.88203000	-1.55383000
H	4.03901300	-0.40642300	-0.48044700
H	3.43861500	-1.23099800	0.95271400
C	2.11637400	0.20300100	0.11680800
C	1.00354900	0.38479000	-0.82022500
H	1.99149200	0.65989000	1.09430600
H	1.16136900	0.02743500	-1.83623700
H	0.49231500	1.34741400	-0.80559700
C	-0.56514500	-0.11649100	1.05171400
H	-0.17941600	0.86835200	1.34586700
N	0.41177900	-0.62483900	0.06246300
C	-1.92735500	0.11060800	0.41424700
C	-2.23966000	1.37464900	-0.09893900
C	-2.87674800	-0.91201100	0.30187300
C	-3.46029900	1.61025700	-0.73035400
H	-1.52770700	2.18971600	0.01202800
C	-4.09805700	-0.67996500	-0.32921300
H	-2.67923400	-1.89527300	0.71885400
C	-4.39157200	0.57978800	-0.85127700
H	-3.68457700	2.59882000	-1.11887500
H	-4.82400400	-1.48337200	-0.40704700
H	-5.34470800	0.75900600	-1.33874000
C	-0.57428600	-0.99938100	2.29445700
H	0.43463600	-1.05443800	2.71250700
H	-1.24529800	-0.57168400	3.04302100
H	-0.91191400	-2.01776300	2.08610000
C	1.50976400	-2.80487500	-0.36567900
C	2.74093900	-2.07972100	-0.90567700
H	1.35925200	-3.74809900	-0.90004900
H	1.66722400	-3.04744300	0.69309800
H	3.58971400	-2.76917900	-0.92679700
H	2.57044800	-1.76991000	-1.94453700
N	1.79493400	3.52633900	0.45395500
N	2.56418000	2.75718100	0.04414100
N	3.30151900	1.91019100	-0.35485900

TS-NH2-1 Imaginary frequency: -554.87

C	0.56568100	-0.83500400	-1.13328200
C	3.22554700	-0.64107300	0.22494000
H	-0.37815000	-1.38293300	-1.10908300
H	0.48588700	-0.08622300	-1.92864800
H	4.10014000	-0.00017100	0.37678000
H	3.36308900	-1.54346700	0.83123200
C	2.03570600	0.12120600	0.75990800
C	1.51796000	1.32917200	0.12766700
H	1.97369800	0.12028400	1.84711400
H	1.70995600	1.53759700	-0.91452800
H	0.97932200	2.05707200	0.71496800
C	-0.42806400	-0.29578200	1.13382700
H	-0.25049700	0.45394000	1.91485500
N	0.68281600	-0.10468800	0.16042000
C	-1.76225500	0.02347300	0.47343000
C	-1.93715900	1.26432100	-0.15385800
C	-2.82776600	-0.87904100	0.48051500
C	-3.14522600	1.59298000	-0.76091000
H	-1.12164700	1.98135000	-0.17275800
C	-4.04261000	-0.55000100	-0.12544300
H	-2.72490600	-1.84830700	0.95704100
C	-4.20496300	0.68417100	-0.74861200
H	-3.26073800	2.55969700	-1.24090100
H	-4.85963600	-1.26455800	-0.10888400
H	-5.14874800	0.93893800	-1.22035900
C	-0.32806100	-1.68450900	1.75465100
H	0.66191200	-1.82601600	2.19572600
H	-1.07010300	-1.80329700	2.54731400
H	-0.48856900	-2.47007900	1.00976000
C	1.73421600	-1.77165600	-1.40727600
C	3.06490400	-1.04397300	-1.23879200
H	1.61736800	-2.16016500	-2.42289600
H	1.69433800	-2.62787900	-0.72159700
H	3.89803400	-1.68760600	-1.53202700
H	3.09572700	-0.16207000	-1.89162900
N	3.22523200	2.94358100	0.32860400
H	3.54233100	2.92142800	1.30414400
H	4.01740500	2.53450000	-0.17938100

TS-NH2-2 Imaginary frequency: -605.05

C	0.54216500	-1.38305200	-0.71776800
C	3.31893700	-0.25717200	0.02474100
H	-0.30062900	-1.94265600	-0.30952400
H	0.30415300	-1.15224000	-1.76169000
H	4.15249900	0.36522900	-0.30479900
H	3.60028800	-0.71831800	0.97838200
C	2.16936500	0.68594100	0.28565400
C	1.17456800	1.06326400	-0.70721800
H	2.05366000	1.10613300	1.27362600
H	1.38745400	0.85338100	-1.75263200
H	0.62596400	1.98845500	-0.55501200
C	-0.38835100	0.16150200	1.06659900
H	-0.16109700	1.16614200	1.43941600
N	0.64564600	-0.10568600	0.02671800
C	-1.77814800	0.20382100	0.45140700
C	-2.23497400	1.39433500	-0.12692600
C	-2.61686800	-0.91595900	0.42919700
C	-3.48570300	1.45871500	-0.73794500
H	-1.61681700	2.28741200	-0.08599100
C	-3.86985100	-0.85459700	-0.17997400
H	-2.30549600	-1.84498300	0.89799700
C	-4.30530500	0.33065800	-0.77057700
H	-3.82329700	2.39175600	-1.17811200
H	-4.50638600	-1.73372800	-0.18689600
H	-5.28168500	0.37932100	-1.24234800
C	-0.21648500	-0.82570400	2.21457100
H	0.77938600	-0.71285700	2.65080400
H	-0.96421800	-0.63196700	2.98704200
H	-0.32658600	-1.86380900	1.88876100
C	1.82484000	-2.19742700	-0.62330700
C	3.04293700	-1.36081800	-1.00077500
H	1.72606100	-3.06392000	-1.28416300
H	1.94263800	-2.57467100	0.40065000
H	3.93099200	-1.99682300	-1.05509200
H	2.90638800	-0.93263800	-2.00230300
N	3.54823500	2.62210600	0.04433400
H	4.35739200	2.51678800	0.66751500
H	3.09939700	3.47800400	0.39092800

7. Transition states for the ring-expansion of 1-azoniabicyclo[4.1.0]heptane 5 with different nucleophiles (M062X/6-31+G(d,p) level of theory, 298 K and 1 atm, CPCM in acetonitrile, ($\epsilon = 35.688$))

TS-CN-1 Imaginary frequency: -601.26

C	0.28281000	-1.05211700	-1.12520400
C	2.94578900	-1.07873300	0.20810000
H	-0.72798600	-1.46391900	-1.08366400
H	0.31092400	-0.35886200	-1.97438300
H	3.89827000	-0.54936500	0.31239800
H	2.96940200	-1.93691400	0.88882000
C	1.85743200	-0.13400200	0.67609500
C	1.58939500	1.13380800	-0.00220200
H	1.81769700	-0.05725700	1.76283700
H	1.70462100	1.21476500	-1.07485600
H	1.07257100	1.91955300	0.52993100
C	-0.61135800	-0.28903200	1.11412300
H	-0.34121900	0.47324000	1.85675200
N	0.48669000	-0.26984200	0.11894600
C	-1.91833900	0.14599800	0.46316500
C	-1.94674800	1.31637500	-0.30732800
C	-3.10305000	-0.57466300	0.62644500
C	-3.12795300	1.75537800	-0.89711000
H	-1.03471300	1.88695400	-0.45585500
C	-4.29109200	-0.13508600	0.03689500
H	-3.11544200	-1.48601300	1.21467700
C	-4.30825900	1.02955200	-0.72529100
H	-3.12748500	2.66369300	-1.49144900
H	-5.20206800	-0.70888900	0.17621700
H	-5.23139700	1.37031200	-1.18352300
C	-0.65968200	-1.64687300	1.80992900
H	0.32408700	-1.88751800	2.22207200
H	-1.37501300	-1.63462100	2.63550300
H	-0.94659200	-2.44122600	1.11339300
C	1.31632600	-2.15280600	-1.32649400
C	2.72797200	-1.58335000	-1.21625100
H	1.14395200	-2.60219900	-2.30867900
H	1.17689000	-2.93899200	-0.57341000
H	3.47557700	-2.34625600	-1.44839100
H	2.86177200	-0.77242000	-1.94409800
C	3.46690300	2.28408600	0.21796700
N	4.51692200	2.77623100	0.38229300

TS-CN-2 Imaginary frequency: -576.54

C	0.28026200	-1.57633100	-0.75256300
C	3.15983900	-0.72995600	0.11616300
H	-0.60067100	-2.10185600	-0.38083200
H	0.06840500	-1.28140400	-1.78724100
H	4.11968000	-0.26596800	-0.11132500
H	3.28115600	-1.27019600	1.06152100
C	2.15546100	0.38101600	0.35228100
C	1.12402900	0.77558000	-0.60788100
H	2.00606500	0.72629600	1.36746500
H	1.33250200	0.59361100	-1.66067400
H	0.64942300	1.74170500	-0.44586500
C	-0.54978500	-0.02781000	1.08515400
H	-0.21131300	0.91599700	1.52713200
N	0.46743000	-0.35491300	0.05394400
C	-1.90969700	0.23101000	0.45372700
C	-2.23088000	1.52613000	0.03001000
C	-2.85139200	-0.78717200	0.26514800
C	-3.44882900	1.79576700	-0.59172200
H	-1.53073400	2.33911900	0.20462500
C	-4.07126000	-0.52101900	-0.35582600
H	-2.64837300	-1.79542700	0.61423300
C	-4.37118300	0.76919400	-0.79158200
H	-3.67959500	2.80779400	-0.90936600
H	-4.79064400	-1.32229400	-0.49258000
H	-5.32263900	0.97498600	-1.27176200
C	-0.53827100	-1.09041600	2.17793900
H	0.45688200	-1.14366100	2.62775100
H	-1.26438400	-0.83364300	2.95294300
H	-0.78952600	-2.08378100	1.79625800
C	3.51993700	2.18155300	0.14418600
C	1.50265800	-2.48359300	-0.69043000
C	2.79577800	-1.72873100	-0.98732200
H	1.36055000	-3.29672700	-1.40890000
H	1.56859800	-2.93365400	0.30830400
H	3.62274900	-2.44006300	-1.06682700
H	2.72763400	-1.22534400	-1.96027300
N	4.13888900	3.15536600	-0.06084000

TS-N₃-1

Imaginary frequency: -613.92

C	0.08731000	1.41313000	-0.95180300
C	-2.68208300	1.26537100	0.12291200
H	1.10534000	1.73423000	-0.72005700
H	0.11483500	0.97029800	-1.95519900
H	-3.66884600	0.80268600	0.01552500
H	-2.71562900	1.91080500	1.00784100
C	-1.68549700	0.15350500	0.39009700
C	-1.43788900	-0.90710600	-0.59284800
H	-1.75752700	-0.21582200	1.41359800
H	-1.42658100	-0.66997500	-1.64877900
H	-0.98568100	-1.83242600	-0.25785600
C	0.72292900	0.03872000	1.07551200
H	0.35376000	-0.87881100	1.55304300
N	-0.26487600	0.35173200	0.01979000
C	2.07588300	-0.28291700	0.45277100
C	2.14239300	-1.17537200	-0.62555700
C	3.26335400	0.27086200	0.93598100
C	3.36357600	-1.50692300	-1.20413300
H	1.22866900	-1.60733600	-1.02356200
C	4.49108800	-0.06193400	0.35821100
H	3.24679800	0.96768300	1.76720300
C	4.54603300	-0.94996700	-0.71218700
H	3.39294100	-2.19819300	-2.04065000
H	5.40318800	0.37917800	0.74807400
H	5.49978700	-1.20608700	-1.16281300
C	0.74499600	1.15243400	2.12029000
H	-0.26843200	1.33738300	2.48739500
H	1.36354300	0.87196100	2.97598400
H	1.13565500	2.08438300	1.69915000
C	-0.87525800	2.59438600	-0.93955900
C	-2.31461900	2.11115300	-1.09344300
H	-0.59256900	3.26913600	-1.75277400
H	-0.77287400	3.14819600	0.00248500
H	-3.00329100	2.95662300	-1.16974300
H	-2.41796900	1.53011300	-2.01944900
N	-3.24754600	-1.87446900	-0.89738800
N	-3.72812200	-1.93774700	0.19294200
N	-4.17208700	-1.97467000	1.26510200

TS-N₃-2

Imaginary frequency: -573.91

C	0.56566800	-0.83617100	-1.13248800
C	3.22534600	-0.64001100	0.22521200
H	-0.37800700	-1.38433400	-1.10747200
H	0.48568000	-0.08852200	-1.92890900
H	4.10018200	0.00071500	0.37641300
H	3.36237900	-1.54154100	0.83286000
C	2.03553600	0.12328000	0.75891900
C	1.51837000	1.33073300	0.12513200
H	1.97395300	0.12424400	1.84615000
H	1.70905000	1.53689500	-0.91776400
H	0.97883400	2.05888300	0.71136700
C	-0.42786000	-0.29452300	1.13407600
H	-0.25042800	0.45611300	1.91422800
N	0.68268100	-0.10414200	0.16019800
C	-1.76228200	0.02374500	0.47362600
C	-1.93847300	1.26516200	-0.15221900
C	-2.82672200	-0.88007700	0.47908300
C	-3.14666100	1.59313300	-0.75945900
H	-1.12378700	1.98317700	-0.16970700
C	-4.04172100	-0.55174900	-0.12701900
H	-2.72290600	-1.84987300	0.95430300
C	-4.20533200	0.68301600	-0.74875000
H	-3.26315600	2.56029200	-1.23833400
H	-4.85785300	-1.26736100	-0.11176300
H	-5.14921500	0.93720000	-1.22061600
C	-0.32736600	-1.68258100	1.75637300
H	0.66244800	-1.82280500	2.19819700
H	-1.06987000	-1.80112300	2.54867100
H	-0.48670800	-2.46899100	1.01213700
C	1.73431700	-1.77300900	-1.40548400
C	3.06491200	-1.04494500	-1.23797800
H	1.61740400	-2.16265400	-2.42066000
H	1.69466900	-2.62842300	-0.71881000
H	3.89809800	-1.68898200	-1.53018700
H	3.09568500	-0.16398900	-1.89215200
N	3.22591300	2.94250900	0.32630300
H	3.53915200	2.91486700	1.30293000
H	4.01784100	2.53160800	-0.18051800

TS-NH₂-1 Imaginary frequency: -559.61

C	0.56566800	-0.83617100	-1.13248800
C	3.22534600	-0.64001100	0.22521200
H	-0.37800700	-1.38433400	-1.10747200
H	0.48568000	-0.08852200	-1.92890900
H	4.10018200	0.00071500	0.37641300
H	3.36237900	-1.54154100	0.83286000
C	2.03553600	0.12328000	0.75891900
C	1.51837000	1.33073300	0.12513200
H	1.97395300	0.12424400	1.84615000
H	1.70905000	1.53689500	-0.91776400
H	0.97883400	2.05888300	0.71136700
C	-0.42786000	-0.29452300	1.13407600
H	-0.25042800	0.45611300	1.91422800
N	0.68268100	-0.10414200	0.16019800
C	-1.76228200	0.02374500	0.47362600
C	-1.93847300	1.26516200	-0.15221900
C	-2.82672200	-0.88007700	0.47908300
C	-3.14666100	1.59313300	-0.75945900
H	-1.12378700	1.98317700	-0.16970700
C	-4.04172100	-0.55174900	-0.12701900
H	-2.72290600	-1.84987300	0.95430300
C	-4.20533200	0.68301600	-0.74875000
H	-3.26315600	2.56029200	-1.23833400
H	-4.85785300	-1.26736100	-0.11176300
H	-5.14921500	0.93720000	-1.22061600
C	-0.32736600	-1.68258100	1.75637300
H	0.66244800	-1.82280500	2.19819700
H	-1.06987000	-1.80112300	2.54867100
H	-0.48670800	-2.46899100	1.01213700
C	1.73431700	-1.77300900	-1.40548400
C	3.06491200	-1.04494500	-1.23797800
H	1.61740400	-2.16265400	-2.42066000
H	1.69466900	-2.62842300	-0.71881000
H	3.89809800	-1.68898200	-1.53018700
H	3.09568500	-0.16398900	-1.89215200
N	3.22591300	2.94250900	0.32630300
H	3.53915200	2.91486700	1.30293000
H	4.01784100	2.53160800	-0.18051800

TS-NH₂-2 Imaginary frequency: -605.94

C	0.54302900	-1.38262900	-0.71855200
C	3.31879400	-0.25691100	0.02695000
H	-0.29950800	-1.94312800	-0.31107500
H	0.30511400	-1.15084700	-1.76226300
H	4.15423400	0.36458100	-0.29945500
H	3.59694400	-0.71955300	0.98080700
C	2.16957100	0.68713900	0.28620700
C	1.17413500	1.06342300	-0.70645800
H	2.05323500	1.10743200	1.27412000
H	1.38673600	0.85371800	-1.75200800
H	0.62512800	1.98839100	-0.55401400
C	-0.38842300	0.16012300	1.06705900
H	-0.16127900	1.16431100	1.44110400
N	0.64576600	-0.10586200	0.02713400
C	-1.77811100	0.20308500	0.45160200
C	-2.23535300	1.39450300	-0.12460600
C	-2.61632800	-0.91705400	0.42711000
C	-3.48602800	1.45944600	-0.73576700
H	-1.61756300	2.28775200	-0.08192000
C	-3.86922600	-0.85513900	-0.18224700
H	-2.30458300	-1.84681800	0.89417200
C	-4.30512600	0.33106000	-0.77070200
H	-3.82396800	2.39315400	-1.17425600
H	-4.50531500	-1.73457400	-0.19097000
H	-5.28142400	0.38016500	-1.24260300
C	-0.21689200	-0.82840800	2.21398400
H	0.77918500	-0.71669000	2.65001700
H	-0.96430600	-0.63476800	2.98680100
H	-0.32786300	-1.86615500	1.88737000
C	1.82600800	-2.19660300	-0.62486500
C	3.04409700	-1.35908500	-1.00045000
H	1.72773800	-3.06207000	-1.28712200
H	1.94354400	-2.57536700	0.39853600
H	3.93235000	-1.99482300	-1.05475700
H	2.90823000	-0.92965700	-2.00159100
N	3.54645600	2.62329100	0.04224900
H	4.35363000	2.51874700	0.66807000
H	3.09330600	3.47650000	0.38975800

8. Reactants and products for the ring-expansion of 1-azoniabicyclo[n.1.0]alkanes 1 and 5 with different nucleophiles (M062X/6-31+G(d,p), 298 K and 1 atm, IEF-PCM in acetonitrile, ($\epsilon = 35.688$)).

Bicyclic aziridinium 1

C	2.83326900	-0.87377800	-1.27666100
C	1.41591100	-1.02539800	-0.71391700
C	3.56054700	0.03323000	-0.26949400
H	3.31288200	-1.84778400	-1.37503200
H	2.80942800	-0.41768200	-2.26820100
H	1.35816500	-1.84430700	0.00453900
H	0.63912300	-1.13942100	-1.47087400
H	4.36476700	0.61032200	-0.72925300
H	3.97848100	-0.54646600	0.55795500
C	2.47173800	0.93264900	0.26839400
C	1.46752900	1.49002300	-0.67193200
H	2.57827700	1.40453200	1.23991500
H	1.59596300	1.38087600	-1.74254600
H	0.86922900	2.33418400	-0.34982000
C	0.10449000	0.26267100	1.11896400
H	0.17368900	1.27154300	1.53626100
N	1.17030600	0.23705200	0.05397100
C	-1.25464600	0.10594500	0.46926200
C	-2.01169700	1.24759600	0.19003600
C	-1.76518600	-1.15046300	0.12574500
C	-3.25574200	1.14002800	-0.43025500
H	-1.63509300	2.22811900	0.47062700
C	-3.00667500	-1.25914000	-0.49741100
H	-1.20198800	-2.05355000	0.34248400
C	-3.75364500	-0.11457900	-0.77706300
H	-3.83432200	2.03439500	-0.63742700
H	-3.39204800	-2.23915400	-0.75967500
H	-4.72286900	-0.20280600	-1.25747600
C	0.42913000	-0.73828100	2.21892700
H	1.44722900	-0.58822000	2.58837100
H	-0.26431000	-0.57115600	3.04553500
H	0.32111100	-1.77580300	1.89924600

3-CI

C	2.123247	-1.642561	-1.064957
C	0.644795	-1.461625	-0.729759
H	2.231363	-1.911810	-2.120026
H	0.111846	-2.400672	-0.899927
H	0.208301	-0.702398	-1.405737
C	2.631695	0.071071	0.654700
C	1.136037	0.215249	0.912039
H	3.063041	-0.635975	1.366656
H	0.737671	1.014731	0.258567
H	0.965563	0.513216	1.951451
C	-0.886984	-1.118883	1.197254
H	-0.810087	-0.731761	2.220550
N	0.492827	-1.070984	0.672180
C	-1.854947	-0.205501	0.450931
C	-2.100333	1.085872	0.930715
C	-2.484717	-0.602496	-0.734990
C	-2.944572	1.961208	0.246877
H	-1.627226	1.409412	1.855740
C	-3.328497	0.267970	-1.423919
H	-2.319781	-1.600916	-1.130699
C	-3.560570	1.554062	-0.935634
H	-3.122729	2.957714	0.639714
H	-3.806879	-0.060581	-2.341768
H	-4.219304	2.230877	-1.470950
C	-1.381546	-2.560324	1.302663
H	-1.516089	-3.037675	0.328910
H	-0.663564	-3.151773	1.876301
H	-2.347185	-2.581923	1.815184
Cl	3.443506	1.658425	1.004366
H	2.526960	-2.468274	-0.467551
C	2.907810	-0.358491	-0.775975
H	3.980356	-0.505735	-0.931298
H	2.575496	0.439010	-1.452777

4-Cl

C	1.255145	-1.627746	1.987780
C	-0.092769	-1.022508	1.610929
C	2.153196	-0.384326	2.024425
H	1.229912	-2.163441	2.939086
H	1.584925	-2.322589	1.207728
H	-0.555566	-0.564752	2.501106
H	-0.799897	-1.747921	1.195052
H	3.219071	-0.606917	1.924023
H	2.007956	0.144610	2.971892
C	1.623477	0.478158	0.865865
C	2.422079	0.314731	-0.424165
H	1.617644	1.543290	1.137809
H	2.613972	-0.738627	-0.635703
H	1.904943	0.771238	-1.269266
C	-0.735369	0.967563	0.242950
H	-0.248683	1.631742	-0.486013
N	0.273029	-0.032162	0.597094
C	-1.882811	0.285549	-0.496921
C	-1.578088	-0.544108	-1.584924
C	-3.223996	0.462920	-0.152437
C	-2.583634	-1.177955	-2.307639
H	-0.535081	-0.693018	-1.852292
C	-4.238328	-0.174580	-0.874301
H	-3.496592	1.099013	0.683272
C	-3.923233	-0.996379	-1.952212
H	-2.325329	-1.814180	-3.149018
H	-5.274909	-0.025408	-0.587087
H	-4.710165	-1.491074	-2.513232
C	-1.186936	1.838795	1.420995
H	-0.314750	2.253189	1.934968
H	-1.798401	2.675630	1.072198
H	-1.771721	1.271860	2.150754
Cl	4.035480	1.130604	-0.310030

3-CN

C	2.307624	-1.244153	-1.279065
C	0.826530	-1.206158	-0.911200
C	2.997924	0.065052	-0.899588
H	2.413275	-1.421081	-2.353668
H	0.363258	-2.165216	-1.156583
H	0.321528	-0.427582	-1.513281
H	4.075009	0.011904	-1.080380
C	2.722621	0.367843	0.583720
C	1.209987	0.353819	0.867511
H	3.198134	-0.398242	1.207828
H	0.734371	1.171705	0.293655
H	1.032020	0.543660	1.930611
C	-0.695476	-1.149664	1.052548
H	-0.627001	-0.865296	2.109722
N	0.669001	-0.951471	0.520946
C	-1.737981	-0.235118	0.416147
C	-2.075274	0.971919	1.038529
C	-2.348266	-0.544308	-0.805565
C	-2.990493	1.851175	0.458988
H	-1.617822	1.225353	1.992836
C	-3.262566	0.330842	-1.390753
H	-2.112284	-1.476869	-1.310826
C	-3.585941	1.532850	-0.760695
H	-3.239179	2.781185	0.961353
H	-3.724288	0.071510	-2.338777
H	-4.299405	2.213086	-1.215451
C	-1.088645	-2.625149	1.014399
H	-1.221295	-3.006183	-0.001179
H	-0.316282	-3.222412	1.505542
H	-2.034725	-2.766186	1.543988
N	3.737342	2.692528	1.260882
C	3.295101	1.663478	0.969204
H	2.784848	-2.080530	-0.754997
H	2.597767	0.886940	-1.506295

4-CN

C	-2.552200	0.321406	0.544965
N	-0.415682	-0.101938	-0.549782
C	-0.066926	-1.148923	-1.510731
C	-1.408447	-1.829998	-1.757652
C	-2.354217	-0.624872	-1.838306
C	-1.785778	0.355359	-0.795010
C	0.579163	0.943548	-0.307804
C	0.980011	1.721485	-1.566787
C	1.761091	0.349535	0.454396
C	1.502939	-0.440180	1.583400
C	2.542176	-0.988019	2.328714
C	3.869385	-0.758235	1.955856
C	4.138338	0.024914	0.837317
C	3.090521	0.575633	0.092445
C	-3.899672	0.885543	0.421312
N	-4.958126	1.334661	0.289889
H	-1.417826	-2.438795	-2.664123
H	-1.664893	-2.469892	-0.906499
H	0.324428	-0.743419	-2.458655
H	0.692078	-1.814120	-1.085608
H	-3.402620	-0.876504	-1.653072
H	-2.290010	-0.174532	-2.833835
H	-1.813565	1.386219	-1.176111
H	-2.634571	-0.712284	0.896119
H	-2.009904	0.891833	1.305844
H	0.097138	1.656500	0.377063
H	0.469806	-0.627652	1.863939
H	3.327859	1.182573	-0.775039
H	2.319338	-1.595499	3.200941
H	5.164953	0.210549	0.535894
H	4.682368	-1.186344	2.534196
H	0.085104	2.055440	-2.100158
H	1.564184	2.608440	-1.306689
H	1.575002	1.111114	-2.252093

3-N₃

C	-2.026319	1.491686	-1.351957
C	-0.543728	1.323432	-1.030218
C	-2.846642	0.360167	-0.730779
H	-2.166752	1.504146	-2.437128
H	0.020895	2.159438	-1.450881
H	-0.171879	0.395914	-1.505310
H	-2.571507	-0.589063	-1.212927
H	-3.919018	0.512344	-0.887205
C	-2.542184	0.267158	0.760933
C	-1.035724	0.148903	1.002748
H	-2.909140	1.161697	1.270268
H	-0.679448	-0.810851	0.576300
H	-0.843024	0.125135	2.080605
C	1.059961	1.383630	0.867041
H	1.008822	1.296430	1.959476
N	-0.344580	1.291392	0.419018
C	1.936933	0.235708	0.375342
C	2.152773	-0.874878	1.198841
C	2.510551	0.234741	-0.902429
C	2.914391	-1.959592	0.763092
H	1.722298	-0.887676	2.198104
C	3.270264	-0.847500	-1.345040
H	2.369130	1.085282	-1.563903
C	3.474119	-1.949367	-0.513914
H	3.072206	-2.809065	1.420864
H	3.705646	-0.828465	-2.339598
H	4.067972	-2.790635	-0.857798
C	1.648110	2.759219	0.558031
H	1.786042	2.934653	-0.511655
H	0.987099	3.536761	0.949661
H	2.627236	2.854948	1.035281
N	-3.073448	-1.958813	0.927297
N	-3.266803	-0.848916	1.425096
N	-2.970778	-3.019359	0.544147
H	-2.368755	2.457271	-0.961750

4-N₃

C	-1.311828	0.529000	2.276113
C	0.027973	-0.047841	1.829940
C	-2.300077	-0.370040	1.523048
H	-1.448243	0.502536	3.359271
H	-1.400473	1.568359	1.941348
H	0.243640	-0.967609	2.398769
H	0.868689	0.640561	1.966978
H	-3.298047	0.067404	1.420491
H	-2.409858	-1.321011	2.054567
C	-1.608694	-0.609536	0.168979
C	-2.115870	0.315796	-0.940815
H	-1.758271	-1.646517	-0.165096
H	-2.118895	1.355012	-0.589993
H	-1.453224	0.246968	-1.807479
C	0.774082	-1.164071	-0.275646
H	0.399305	-1.269786	-1.304224
N	-0.192082	-0.303797	0.406326
C	2.114668	-0.440660	-0.379071
C	2.130274	0.889516	-0.820820
C	3.332389	-1.053826	-0.076395
C	3.326864	1.586164	-0.958007
H	1.183332	1.373885	-1.044396
C	4.537063	-0.356710	-0.210436
H	3.358825	-2.082230	0.268738
C	4.539981	0.963469	-0.650785
H	3.315309	2.615968	-1.303005
H	5.472734	-0.851435	0.032574
H	5.475439	1.504844	-0.753855
C	0.876865	-2.574758	0.317517
H	-0.122229	-3.006665	0.428457
H	1.452794	-3.233064	-0.338715
H	1.356351	-2.571540	1.300594
N	-3.462713	-0.091176	-1.410861
N	-4.393538	0.580857	-0.975168
N	-5.313744	1.148444	-0.636989

Bicyclic aziridinium 5

C	1.08573300	-0.92363800	-0.79082500
C	3.54280100	0.56948500	0.15636600
H	0.36331000	-1.65402600	-0.43382200
H	0.78641600	-0.63041400	-1.79863200
H	4.19385900	1.42853300	-0.04075700
H	3.91893500	0.08357100	1.06323100
C	2.16454800	1.11721900	0.45880100
C	1.22715400	1.62469700	-0.56644000
H	2.04898600	1.54733100	1.44953300
H	1.48261500	1.54740000	-1.61732900
H	0.54168200	2.42427700	-0.31326000
C	-0.19694100	0.27809900	1.12071500
H	-0.16248200	1.27660800	1.56380300
N	0.93104700	0.30823700	0.08154200
C	-1.55149400	0.11335900	0.44768500
C	-2.23353300	1.25622100	-0.00191500
C	-2.16032700	-1.14002800	0.27839400
C	-3.47584100	1.14970100	-0.63092400
H	-1.80263100	2.24136500	0.15328400
C	-3.40443200	-1.24897000	-0.34890500
H	-1.68104100	-2.04183100	0.64471700
C	-4.06280400	-0.10612300	-0.81102800
H	-3.98640000	2.04615400	-0.96921700
H	-3.85915900	-2.22743300	-0.47009100
H	-5.03040600	-0.19225400	-1.29608000
C	0.14027600	-0.74172600	2.20657800
H	1.09455700	-0.49841900	2.68070600
H	-0.63855400	-0.70942600	2.97243500
H	0.19754700	-1.76512700	1.82893800
C	2.49829200	-1.50484400	-0.77757700
C	3.56626700	-0.43236300	-1.00460500
H	2.53415700	-2.26879800	-1.56055900
H	2.68333000	-2.01278800	0.17637400
H	4.55740300	-0.89140100	-1.05724200
H	3.40234700	0.07249600	-1.96474800

7-CN

C	0.415137	-1.763317	-0.276124
C	3.368830	-0.527085	-0.004177
H	-0.230661	-2.508662	0.194353
H	-0.059004	-1.486935	-1.235318
H	4.413430	-0.253888	-0.180779
H	3.328597	-1.005204	0.979077
C	2.535953	0.768915	0.082007
C	1.013889	0.569578	-0.113159
H	2.706727	1.227296	1.062384
H	0.791653	0.493422	-1.189286
H	0.513701	1.475761	0.239711
C	-0.713845	-0.290077	1.381869
H	-0.446886	0.588578	1.981175
N	0.508498	-0.594330	0.604622
C	-1.911403	0.110224	0.523722
C	-2.263489	1.460040	0.414096
C	-2.670033	-0.830843	-0.186498
C	-3.330724	1.867441	-0.386928
H	-1.699668	2.204518	0.971966
C	-3.735092	-0.429394	-0.991752
H	-2.438328	-1.889424	-0.110178
C	-4.068404	0.921680	-1.096822
H	-3.585592	2.920819	-0.452556
H	-4.309890	-1.174220	-1.533946
H	-4.900568	1.232511	-1.720832
C	-1.044075	-1.407727	2.368890
H	-0.149937	-1.672567	2.939962
H	-1.816529	-1.062624	3.061584
H	-1.423376	-2.309904	1.882578
C	2.998875	1.743620	-0.918798
C	1.762254	-2.433254	-0.545212
C	2.883404	-1.525124	-1.061193
H	1.587340	-3.239181	-1.267667
H	2.107747	-2.906527	0.382954
H	3.727168	-2.160108	-1.349686
H	2.569958	-1.000861	-1.975127
N	3.350760	2.498180	-1.723324

8-CN

C	0.375182	-0.951203	-1.216091
C	2.741067	-0.948414	0.469336
H	-0.659165	-1.273364	-1.375404
H	0.635789	-0.321125	-2.080368
H	3.741800	-0.577118	0.717527
H	2.458054	-1.647146	1.264822
C	1.738191	0.219453	0.471054
C	2.240112	1.416055	-0.381336
H	1.633352	0.586433	1.498041
H	2.319858	1.141303	-1.437615
H	1.517935	2.233230	-0.305635
C	-0.619105	-0.402558	1.002240
H	-0.411311	0.297773	1.822466
N	0.405393	-0.126256	-0.007538
C	-1.989458	-0.006082	0.449787
C	-2.140775	1.273094	-0.102983
C	-3.103684	-0.846718	0.489846
C	-3.368360	1.702365	-0.596911
H	-1.273329	1.926407	-0.148045
C	-4.339223	-0.422156	-0.010398
H	-3.023955	-1.844648	0.908610
C	-4.476828	0.851666	-0.553254
H	-3.464126	2.699367	-1.016716
H	-5.192035	-1.093292	0.026706
H	-5.435921	1.182328	-0.939852
C	-0.591422	-1.815921	1.595204
H	0.402363	-2.034003	1.993536
H	-1.309700	-1.908814	2.415365
H	-0.833370	-2.573195	0.842101
C	1.326802	-2.152989	-1.199786
C	2.746384	-1.694051	-0.866066
H	1.295818	-2.646474	-2.177557
H	0.999553	-2.885485	-0.452268
H	3.429676	-2.547440	-0.815371
H	3.120442	-1.040860	-1.666721
C	3.546353	1.913007	0.056047
N	4.575005	2.295325	0.423890

7-N₃

C	0.245301	-2.031068	-0.155771
C	3.261245	-0.915140	-0.054484
H	-0.420960	-2.718583	0.371217
H	-0.239083	-1.789612	-1.119525
H	4.299924	-0.676155	-0.304416
H	3.269293	-1.345035	0.952623
C	2.494957	0.403944	-0.000616
C	0.970271	0.270124	-0.141151
H	2.728677	0.909893	0.945167
H	0.728333	0.146209	-1.209860
H	0.518218	1.219138	0.166446
C	-0.790679	-0.403293	1.412063
H	-0.475764	0.497261	1.952770
N	0.410203	-0.819568	0.653157
C	-1.970894	0.003175	0.533008
C	-2.248899	1.359674	0.329487
C	-2.786865	-0.941359	-0.104625
C	-3.297984	1.768195	-0.494418
H	-1.641425	2.109314	0.832012
C	-3.834263	-0.539350	-0.932210
H	-2.613927	-2.003093	0.046875
C	-4.092405	0.817363	-1.132649
H	-3.495386	2.826922	-0.632768
H	-4.453726	-1.287867	-1.417181
H	-4.911184	1.129034	-1.773733
C	-1.173974	-1.436829	2.469247
H	-0.292992	-1.708634	3.057151
H	-1.927425	-1.010633	3.137271
H	-1.597845	-2.348544	2.040910
C	1.553979	-2.775967	-0.418717
C	2.693597	-1.952830	-1.029108
H	1.319088	-3.618633	-1.080061
H	1.909027	-3.203252	0.528091
H	3.495988	-2.642634	-1.310952
H	2.366474	-1.466288	-1.958476
N	2.275466	3.499162	-1.180751
N	2.592364	2.413855	-1.110532
N	3.003920	1.254966	-1.120177

8-N₃

C	0.078243	1.343212	-1.095834
C	-2.415876	1.308009	0.394392
H	1.153174	1.550309	-1.109621
H	-0.172454	0.957289	-2.095610
H	-3.471891	1.031784	0.486213
H	-2.126844	1.782254	1.339379
C	-1.567477	0.038473	0.201401
C	-2.118851	-0.875587	-0.910418
H	-1.593335	-0.537286	1.136266
H	-2.041053	-0.395023	-1.886527
H	-1.523539	-1.795147	-0.935230
C	0.798466	0.184450	0.989640
H	0.455190	-0.667503	1.592528
N	-0.161993	0.287263	-0.110867
C	2.162777	-0.221758	0.430495
C	2.230361	-1.334340	-0.419784
C	3.347518	0.449658	0.738454
C	3.444443	-1.765115	-0.944758
H	1.309249	-1.853085	-0.672858
C	4.570500	0.023213	0.209805
H	3.333821	1.316260	1.391378
C	4.624257	-1.083558	-0.632100
H	3.473292	-2.631792	-1.598555
H	5.479097	0.562993	0.459459
H	5.573332	-1.415319	-1.041893
C	0.860311	1.401223	1.919840
H	-0.137404	1.623074	2.306336
H	1.515642	1.206803	2.774482
H	1.232213	2.289328	1.398084
C	-0.720900	2.631761	-0.871374
C	-2.209600	2.308711	-0.743393
H	-0.538603	3.315319	-1.708184
H	-0.381750	3.134680	0.042657
H	-2.790628	3.216917	-0.553827
H	-2.579094	1.890140	-1.689912
N	-3.556463	-1.201995	-0.760842
N	-3.831279	-1.825660	0.263681
N	-4.185329	-2.396949	1.175004

7-NH₂

C	0.726784	-1.506294	-0.135256
C	3.601573	-0.060117	-0.076137
H	0.153352	-2.277670	0.385445
H	0.197858	-1.300704	-1.084110
H	4.600751	0.295058	-0.357433
H	3.705775	-0.517344	0.914584
C	2.694379	1.170181	0.034621
C	1.196507	0.860518	-0.076021
H	2.865801	1.620952	1.025394
H	0.944742	0.738192	-1.143633
H	0.651586	1.748041	0.264856
C	-0.484844	-0.048038	1.454028
H	-0.309769	0.903453	1.969344
N	0.763313	-0.302061	0.699740
C	-1.714581	0.150511	0.569241
C	-2.149192	1.444584	0.258722
C	-2.424061	-0.929760	0.028233
C	-3.246175	1.658971	-0.576759
H	-1.629397	2.299074	0.686419
C	-3.519506	-0.722559	-0.809019
H	-2.129067	-1.948321	0.263279
C	-3.933325	0.573671	-1.117637
H	-3.565951	2.672666	-0.798848
H	-4.052951	-1.575848	-1.217226
H	-4.788506	0.734310	-1.766855
C	-0.704336	-1.099915	2.540129
H	0.195286	-1.186212	3.154992
H	-1.541202	-0.800538	3.177512
H	-0.938839	-2.088495	2.137266
C	2.104285	-2.091883	-0.441819
C	3.127037	-1.133693	-1.061130
H	1.948541	-2.943323	-1.115824
H	2.527595	-2.496162	0.487132
H	3.990462	-1.725249	-1.385007
H	2.718236	-0.663648	-1.965858
N	3.017606	2.111177	-1.048270
H	3.959832	2.471736	-0.920998
H	2.399130	2.918848	-1.008270

8-NH₂

C	0.730544	-0.667988	-1.186644
C	3.039946	-0.315553	0.535466
H	-0.233818	-1.156819	-1.362528
H	0.893644	0.006890	-2.040736
H	3.968577	0.194326	0.816003
H	2.857275	-1.068239	1.311549
C	1.874895	0.691345	0.528579
C	2.195119	1.969499	-0.277066
H	1.697173	1.011052	1.564706
H	2.309781	1.725682	-1.339210
H	1.319680	2.623314	-0.199659
C	-0.362763	-0.315045	1.019936
H	-0.297404	0.413714	1.839746
N	0.614143	0.136264	0.029442
C	-1.772768	-0.168821	0.443212
C	-2.128039	1.050617	-0.150489
C	-2.732080	-1.182127	0.497409
C	-3.402987	1.253782	-0.668758
H	-1.379009	1.835996	-0.209643
C	-4.013810	-0.984920	-0.027042
H	-2.493826	-2.140641	0.947085
C	-4.354726	0.231790	-0.609958
H	-3.656831	2.207803	-1.121598
H	-4.742540	-1.788729	0.021851
H	-5.349761	0.385973	-1.016091
C	-0.101430	-1.698737	1.627841
H	0.908606	-1.737422	2.042122
H	-0.804904	-1.908583	2.439566
H	-0.197327	-2.492077	0.879317
C	1.865324	-1.699922	-1.176968
C	3.187518	-1.025076	-0.811537
H	1.926940	-2.172369	-2.164049
H	1.652942	-2.492014	-0.448370
H	3.998598	-1.759320	-0.765623
H	3.460360	-0.303518	-1.594347
N	3.376807	2.723500	0.137256
H	3.353431	2.896821	1.139343
H	4.226528	2.199386	-0.048989

9)Reactants and products for the ring-expansion of 1-azoniabicyclo[n.1.0]alkanes 1 and 5 with different nucleophiles (M062X/6-31+G(d,p), 298 K and 1 atm, explicit solvation)

1-PRC-CN

C	0.015714	-3.105164	-0.947628
C	-1.116672	-2.306057	-0.284177
C	1.306346	-2.367732	-0.548706
H	0.004017	-4.144004	-0.613192
H	-0.102200	-3.112124	-2.033620
H	-1.300713	-2.654011	0.734799
H	-2.056397	-2.302153	-0.841143
H	2.107281	-2.457546	-1.284176
H	1.678988	-2.707210	0.423662
C	0.884036	-0.925469	-0.430497
C	-0.020529	-0.356941	-1.438411
H	1.454623	-0.234116	0.179316
H	-0.255646	-0.911348	-2.339320
H	-0.075037	0.723926	-1.506491
C	-1.178084	0.027629	0.831553
H	-0.584531	0.937787	0.710317
N	-0.598416	-0.915357	-0.180025
C	-2.609264	0.344158	0.453405
C	-2.859711	1.483401	-0.317605
C	-3.678028	-0.476373	0.826349
C	-4.158131	1.791117	-0.719683
H	-2.030273	2.134714	-0.585328
C	-4.975922	-0.169894	0.423262
H	-3.505205	-1.356374	1.440762
C	-5.217183	0.963035	-0.352643
H	-4.342582	2.680794	-1.313458
H	-5.799657	-0.811657	0.719815
H	-6.229329	1.203402	-0.662550
C	-0.954997	-0.502308	2.241776
H	-1.530093	-1.405054	2.462175
H	0.109115	-0.699042	2.405271
H	-1.268363	0.268105	2.950193
N	3.455686	-0.130355	-1.639623
C	2.772585	-0.054265	-2.596368
C	1.821615	2.683697	-0.219683
N	0.666665	2.614630	-0.195457
C	3.277624	2.770419	-0.255694
H	3.659494	2.831341	0.765871
H	3.651698	1.869587	-0.759570
H	3.575133	3.659557	-0.814763
C	5.083086	-0.284092	1.058850
H	5.716780	0.567478	1.315387
H	4.927093	-0.335550	-0.026498
H	5.547742	-1.201296	1.425533
C	3.767784	-0.119553	1.672022
N	2.716987	0.014103	2.139427

1-PRC-CI

C	0.313932	-1.676263	2.153296
C	-0.983008	-1.149856	1.522972
C	1.213408	-0.438240	2.318831
H	0.107429	-2.171303	3.104090
H	0.782958	-2.406141	1.490698
H	-1.706532	-0.824675	2.275934
H	-1.464646	-1.855583	0.842590
H	2.278831	-0.665465	2.231177
H	1.030418	0.069670	3.271637
C	0.809473	0.465359	1.181806
C	0.599160	-0.119527	-0.145454
H	0.985474	1.534873	1.219426
H	0.872756	-1.150517	-0.345773
H	0.615517	0.567814	-0.983679
C	-1.625001	1.087958	0.429151
H	-1.141403	1.757762	-0.287333
N	-0.579842	0.065403	0.759170
C	-2.784991	0.380754	-0.245614
C	-2.616290	-0.090227	-1.552401
C	-3.998111	0.148935	0.404601
C	-3.634504	-0.790366	-2.192161
H	-1.679373	0.095261	-2.072315
C	-5.023083	-0.546887	-0.237101
H	-4.157298	0.513850	1.415008
C	-4.842212	-1.021067	-1.533420
H	-3.487841	-1.151054	-3.205173
H	-5.963059	-0.716730	0.278421
H	-5.639700	-1.562703	-2.031945
C	-1.965524	1.901779	1.669129
H	-1.082390	2.451620	2.002755
H	-2.740612	2.630404	1.419929
H	-2.328521	1.286413	2.497332
Cl	3.652876	0.335173	-0.139297
C	1.825206	3.366637	-0.850618
N	0.715623	3.211586	-0.558689
C	3.226951	3.551641	-1.211679
H	3.757331	2.625071	-0.953074
H	3.305217	3.744726	-2.283093
H	3.638797	4.396441	-0.656590
C	4.225876	-2.907681	-1.087032
H	4.850417	-3.543631	-0.457093
H	4.430065	-1.849018	-0.879535
H	4.419412	-3.132097	-2.137505
C	2.818598	-3.151317	-0.785748
N	1.701160	-3.335950	-0.546079

1-PRC-N₃

C	-0.298370	-2.826830	-1.456716
C	0.888884	-1.856007	-1.521086
C	-1.506337	-1.935735	-1.122685
H	-0.417042	-3.352421	-2.405618
H	-0.146036	-3.580219	-0.679539
H	0.971609	-1.406332	-2.511867
H	1.846376	-2.291655	-1.225942
H	-2.296949	-2.475625	-0.599153
H	-1.927886	-1.463692	-2.015577
C	-0.919904	-0.849165	-0.258088
C	0.095950	-1.186599	0.762416
H	-1.422498	0.102673	-0.154229
H	0.309827	-2.218619	1.015231
H	0.280648	-0.447693	1.535894
C	1.221255	0.586894	-0.703402
H	0.589423	1.247562	-0.103411
N	0.540119	-0.751741	-0.581959
C	2.587416	0.505148	-0.055212
C	2.763696	1.023498	1.230986
C	3.675770	-0.088339	-0.702955
C	4.003558	0.943756	1.863171
H	1.923707	1.500785	1.732110
C	4.913393	-0.174555	-0.070469
H	3.564620	-0.478513	-1.711319
C	5.079062	0.340716	1.214868
H	4.128367	1.355515	2.859602
H	5.750433	-0.638127	-0.583055
H	6.045309	0.276998	1.705253
C	1.210351	1.083268	-2.142389
H	1.897374	0.527452	-2.785650
H	0.192757	1.049322	-2.544804
H	1.541487	2.124731	-2.136121
N	-2.923897	0.878888	-1.603462
N	-3.741365	0.498368	-0.846768
N	-2.060120	1.252789	-2.312426
C	-2.810474	3.339205	0.152589
H	-2.540391	3.288715	-0.907356
H	-2.789660	4.371118	0.506104
H	-3.803346	2.902244	0.274134
C	-1.846469	2.540520	0.904657
N	-1.070843	1.912835	1.492898
C	-3.547400	-0.646480	2.231452
H	-4.492979	-0.843186	2.740376
H	-3.738550	-0.338923	1.194265
H	-3.014444	0.157527	2.744342
C	-2.723124	-1.853036	2.242957
N	-2.054708	-2.797880	2.228256

5-PRC-CN

C	0.73534200	-2.08624900	-0.46610000
C	-1.72702800	-1.48035200	-2.12899000
H	1.81311300	-2.21560800	-0.55271000
H	0.46958300	-2.19009900	0.58816000
H	-2.76474900	-1.13580300	-2.03986000
H	-1.49611800	-1.60620100	-3.19461000
C	-0.88341900	-0.35066100	-1.58587000
C	-0.75260000	-0.02772100	-0.15944000
H	-0.75053000	0.49446900	-2.25639000
H	-1.20523900	-0.67036100	0.58350000
H	-0.61657100	1.00570000	0.12758000
C	1.61018000	0.24301200	-1.19769000
H	1.15098900	1.22119200	-1.36238000
N	0.43112100	-0.65890900	-0.85702000
C	2.56030000	0.37813300	-0.01597000
C	2.31658900	1.38303300	0.93419000
C	3.68226100	-0.44715600	0.15463000
C	3.15450800	1.53940400	2.03990000
H	1.47985800	2.06083200	0.79333000
C	4.52309000	-0.29057500	1.25913000
H	3.92185200	-1.21071500	-0.57914000
C	4.25744900	0.69883500	2.20864000
H	2.94936800	2.32335300	2.76274000
H	5.38706100	-0.93858400	1.37350000
H	4.91150900	0.82095600	3.06687000
C	2.24781000	-0.21981700	-2.50848000
H	1.51223000	-0.20697800	-3.31796000
H	3.05682000	0.46526400	-2.77531000
H	2.66854200	-1.22754700	-2.44842000
C	-0.01174600	-3.11977000	-1.31042000
C	-1.51016700	-2.81019100	-1.39744000
H	0.16263500	-4.09716000	-0.84704000
H	0.41758400	-3.16122900	-2.32085000
H	-2.03040600	-3.60619200	-1.93926000
H	-1.94467700	-2.77510200	-0.39197000
C	-3.89637000	0.56012600	-0.43914000
N	-3.50934100	1.11941600	0.52845000
H	-4.61296800	-1.45431500	3.17858000
C	-3.71462900	-0.83037400	3.17270000
C	-2.55544800	-1.62997300	2.79467000
H	-3.83642000	-0.02707400	2.43064000
N	-1.62476700	-2.24168200	2.45978000
H	-3.56687900	-0.40367400	4.16905000
H	-3.17438300	3.25515700	-0.07278000
C	-2.64221400	4.10350700	-0.52849000
C	-1.30678400	3.65186900	-0.89736000
H	-3.18473500	4.43235700	-1.41943000
N	-0.24922300	3.25584000	-1.17500000
H	-2.57473500	4.93421700	0.17991000

5-PRC-NH₂

C	-0.14824600	-2.16452800	-0.65670300
C	-3.00866500	-1.90138700	0.27776200
H	0.44982700	-2.06650900	-1.56208100
H	0.53263000	-2.39943300	0.16472600
H	-3.65672100	-1.79148600	1.15556200
H	-3.66681700	-1.89595500	-0.59989900
C	-2.12262500	-0.67277000	0.21577300
C	-0.94537800	-0.44809300	1.08132700
H	-2.61434700	0.22404200	-0.15457600
H	-0.62898900	-1.25125300	1.73843400
H	-0.62755400	0.57259200	1.38380400
C	-0.29551900	0.33283200	-1.30294100
H	-0.67766900	1.22937200	-0.80938200
N	-0.72522200	-0.79865300	-0.36848900
C	1.22189200	0.44570500	-1.36331300
C	1.89570300	1.04986300	-0.28870700
C	1.96267300	-0.00492500	-2.46649900
C	3.28588800	1.18383900	-0.32245500
H	1.33045700	1.41763300	0.57209000
C	3.35325900	0.13134200	-2.49492000
H	1.46389400	-0.45189600	-3.32113600
C	4.01907200	0.72482400	-1.42021000
H	3.79506300	1.65904000	0.51135700
H	3.91140800	-0.22047100	-3.35781900
H	5.09956900	0.83539100	-1.44252300
C	-1.00740400	0.17130600	-2.64549100
H	-2.09035000	0.23044800	-2.51368100
H	-0.71243400	0.98814900	-3.30931400
H	-0.76329500	-0.77184300	-3.14447500
C	-1.20921100	-3.25282500	-0.81776300
C	-2.23403800	-3.22491600	0.32051500
H	-0.68496700	-4.21412300	-0.85083900
H	-1.72757600	-3.13691700	-1.77897500
H	-2.93709000	-4.05815900	0.22164700
H	-1.72593800	-3.35301200	1.28432700
N	0.07132300	2.18611600	2.18935500
H	0.69449700	3.00217100	2.17967900
H	1.46054300	0.81389800	3.07304400
C	2.14881000	0.06512200	3.54922800
C	1.87376500	-1.25899700	3.01255800
H	3.18646200	0.34437100	3.34225500
N	1.60024700	-2.29039400	2.54669800
H	1.99128300	0.07067700	4.63218800
H	-1.39475800	3.34098700	1.30464700
C	-2.21032600	3.94607500	0.81285400
C	-2.89150700	3.09997300	-0.15158500
H	-2.91505600	4.29543400	1.57363200
N	-3.38233000	2.35595000	-0.90169100
H	-1.76941000	4.81275800	0.31073200
H	-0.39963400	2.26831500	3.09889300

5-PRC-N₃

C	-0.75138900	-1.62407900	1.35057300
C	1.85178500	-0.34252700	2.21816500
H	-1.80381500	-1.67218600	1.62491300
H	-0.60904200	-2.22265100	0.44864400
H	2.86546500	-0.08079100	1.89772900
H	1.72293200	0.05452000	3.23347100
C	0.91403200	0.40883300	1.30084100
C	0.59122300	0.01158200	-0.07979700
H	0.83031700	1.47339600	1.49903000
H	0.99593200	-0.90575500	-0.48794900
H	0.36484300	0.78999100	-0.79810200
C	-1.63247600	0.79008800	0.99551700
H	-1.19164700	1.72988800	0.65479300
N	-0.46221100	-0.18694900	0.97847300
C	-2.69927600	0.39651500	-0.01623200
C	-2.61380200	0.91597300	-1.31823700
C	-3.77892600	-0.44231600	0.30033600
C	-3.56332900	0.58124700	-2.28551600
H	-1.81350400	1.60683700	-1.56721200
C	-4.73047500	-0.77712900	-0.66573000
H	-3.89877200	-0.83137700	1.30686900
C	-4.62153100	-0.27161800	-1.96342600
H	-3.47989800	0.99482700	-3.28610100
H	-5.55833600	-1.42865100	-0.40191600
H	-5.36222200	-0.53153700	-2.71383600
C	-2.12187900	0.98103800	2.43173200
H	-1.30863400	1.33815900	3.07050000
H	-2.91438800	1.73396100	2.44021700
H	-2.52599000	0.06640700	2.87446200
C	0.13228900	-2.14717600	2.48353800
C	1.61557600	-1.85665600	2.23173400
H	-0.05026900	-3.22481500	2.55768900
H	-0.17513400	-1.70082800	3.43916900
H	2.22815700	-2.30787100	3.01870600
H	1.93211900	-2.30727900	1.28493800
N	3.76861300	1.62871000	0.13360500
N	3.60271000	0.66170200	-0.53454300
H	3.78016400	-3.96108200	-2.38643400
C	3.07850200	-3.14974400	-2.60067400
C	1.85216200	-3.33623000	-1.83394000
H	3.51850000	-2.18674800	-2.30927100
N	0.87988800	-3.45890700	-1.20813000
H	2.85320400	-3.14678200	-3.67105700
H	2.61447200	4.66167800	-1.86717100
C	2.46859500	4.37597200	-0.82147100
C	1.10482800	3.90670200	-0.61802900
H	3.15180200	3.54940500	-0.55824500
N	0.03249300	3.49138700	-0.44478400
H	2.66761200	5.24065400	-0.18177800
N	3.40574800	-0.31511800	-1.17867200

3-CN

C	0.266290	-2.695166	0.034443
C	-1.101218	-2.025419	0.162533
C	1.237713	-1.809886	-0.745705
H	0.159581	-3.663069	-0.466474
H	-1.762406	-2.659266	0.760080
H	-1.555788	-1.921237	-0.842349
H	2.243309	-2.242937	-0.750339
C	1.272292	-0.408558	-0.112301
C	-0.147295	0.166282	0.009681
H	1.708602	-0.467013	0.892698
H	-0.567438	0.306069	-1.005485
H	-0.096561	1.142170	0.499902
C	-2.195671	-0.096132	1.291716
H	-1.863565	0.843824	1.749871
N	-0.953891	-0.731933	0.819406
C	-3.157392	0.271645	0.165983
C	-3.139579	1.566348	-0.362413
C	-4.035127	-0.661338	-0.397744
C	-3.969916	1.924056	-1.423176
H	-2.466174	2.304717	0.067792
C	-4.867508	-0.310271	-1.459008
H	-4.075830	-1.673980	-0.005198
C	-4.837055	0.984151	-1.975903
H	-3.941218	2.936481	-1.814287
H	-5.544018	-1.047768	-1.880452
H	-5.487836	1.258385	-2.800346
C	-2.850565	-0.919686	2.398823
H	-3.275096	-1.860193	2.038343
H	-2.108180	-1.149212	3.167368
H	-3.665876	-0.346493	2.848302
N	2.801389	1.183108	-1.534053
C	2.122798	0.492511	-0.898413
C	2.729163	2.223546	1.757195
N	1.608888	2.135734	2.030374
C	4.142908	2.332246	1.403078
H	4.671572	1.444757	1.756092
H	4.228931	2.389556	0.315094
H	4.569877	3.227896	1.857751
C	5.270836	-0.815693	-1.646272
H	6.287330	-1.198063	-1.752767
H	5.223417	0.231719	-1.949782
H	4.595345	-1.387569	-2.285990
C	4.836776	-0.930800	-0.255129
N	4.483410	-1.013844	0.843133
H	0.663707	-2.878361	1.039262
H	0.903543	-1.718474	-1.787789

4-CN

C	0.259563	-0.951525	2.166070
C	-1.101517	-0.404470	1.744310
C	1.214437	0.020882	1.466281
H	0.389359	-0.974074	3.250583
H	0.401747	-1.967124	1.781489
H	-1.363249	0.466714	2.367506
H	-1.912930	-1.134854	1.827743
H	2.230256	-0.370540	1.355967
H	1.270229	0.964988	2.019376
C	0.524668	0.275829	0.118016
C	1.053876	-0.642446	-1.006777
H	0.667361	1.317042	-0.194527
H	1.015764	-1.686638	-0.679698
H	0.431477	-0.536770	-1.901516
C	-1.843409	0.894850	-0.253942
H	-1.497736	1.047909	-1.288043
N	-0.889162	-0.039497	0.340675
C	-3.214850	0.232329	-0.354997
C	-3.294824	-1.104902	-0.764865
C	-4.402432	0.914822	-0.084930
C	-4.524758	-1.738363	-0.906779
H	-2.370467	-1.644529	-0.952952
C	-5.639268	0.281029	-0.224219
H	-4.377450	1.949918	0.239572
C	-5.706291	-1.045592	-0.636439
H	-4.563028	-2.776253	-1.224368
H	-6.550267	0.830134	-0.005596
H	-6.667782	-1.538264	-0.743432
C	-1.867354	2.272557	0.422998
H	-0.847956	2.649365	0.552609
H	-2.412766	2.997719	-0.187843
H	-2.345903	2.232743	1.406027
C	2.440484	-0.323823	-1.357697
N	3.541024	-0.056194	-1.599387
C	4.493656	3.020301	-0.633709
H	4.616939	3.803936	-1.383274
H	5.257482	3.137880	0.136940
H	4.594389	2.041005	-1.107576
C	3.166466	3.123578	-0.029688
N	2.115501	3.207565	0.445223
C	5.249059	-2.625329	-0.290757
H	5.257011	-1.722841	-0.905946
H	5.560752	-3.481625	-0.891204
H	5.935791	-2.506104	0.549030
C	3.892092	-2.841302	0.208036
N	2.815979	-3.004771	0.598296

3-Cl

C	0.783340	-2.624842	1.097935
C	-0.362268	-1.619997	1.195929
C	2.073020	-1.943340	0.630120
H	0.515165	-3.419727	0.394404
H	-1.254004	-2.114005	1.592672
H	-0.612290	-1.254317	0.181604
H	2.917169	-2.639117	0.649433
C	2.351048	-0.742993	1.517301
C	1.156022	0.202562	1.540610
H	2.592613	-1.053274	2.536788
H	0.981983	0.582192	0.516192
H	1.377056	1.060152	2.184323
C	-1.101920	0.372343	2.468824
H	-0.622454	1.204656	2.998750
N	0.007194	-0.516826	2.080053
C	-1.853351	0.986313	1.288830
C	-1.372565	2.161289	0.699388
C	-3.012271	0.407021	0.758446
C	-2.031348	2.750232	-0.378774
H	-0.468804	2.624989	1.088044
C	-3.679823	0.994944	-0.314986
H	-3.411681	-0.504663	1.194213
C	-3.193453	2.171120	-0.885039
H	-1.629296	3.655100	-0.823372
H	-4.584482	0.535397	-0.702814
H	-3.715986	2.631412	-1.718274
C	-2.015391	-0.323212	3.476615
H	-2.503784	-1.209982	3.064039
H	-1.423501	-0.638770	4.338482
H	-2.800159	0.361791	3.809927
Cl	3.807998	0.156252	0.926977
C	3.379439	0.591630	-2.550048
H	3.236290	-0.461222	-2.298341
H	4.291938	0.960359	-2.079641
H	3.452289	0.690688	-3.634784
C	2.233123	1.359623	-2.067608
N	1.320073	1.966549	-1.697940
C	-1.057838	-0.021412	-2.342025
H	-1.990195	-0.587115	-2.294245
H	-1.115565	0.725167	-3.136520
H	-0.898174	0.503454	-1.396104
C	0.063002	-0.924419	-2.591379
N	0.953139	-1.639803	-2.778553
H	0.937108	-3.083497	2.081897
H	1.949222	-1.598504	-0.404290

4-Cl

C	0.783340	-2.624842	1.097935
C	-0.362268	-1.619997	1.195929
C	2.073020	-1.943340	0.630120
H	0.515165	-3.419727	0.394404
H	-1.254004	-2.114005	1.592672
H	-0.612290	-1.254317	0.181604
H	2.917169	-2.639117	0.649433
C	2.351048	-0.742993	1.517301
C	1.156022	0.202562	1.540610
H	2.592613	-1.053274	2.536788
H	0.981983	0.582192	0.516192
H	1.377056	1.060152	2.184323
C	-1.101920	0.372343	2.468824
H	-0.622454	1.204656	2.998750
N	0.007194	-0.516826	2.080053
C	-1.853351	0.986313	1.288830
C	-1.372565	2.161289	0.699388
C	-3.012271	0.407021	0.758446
C	-2.031348	2.750232	-0.378774
H	-0.468804	2.624989	1.088044
C	-3.679823	0.994944	-0.314986
H	-3.411681	-0.504663	1.194213
C	-3.193453	2.171120	-0.885039
H	-1.629296	3.655100	-0.823372
H	-4.584482	0.535397	-0.702814
H	-3.715986	2.631412	-1.718274
C	-2.015391	-0.323212	3.476615
H	-2.503784	-1.209982	3.064039
H	-1.423501	-0.638770	4.338482
H	-2.800159	0.361791	3.809927
Cl	3.807998	0.156252	0.926977
C	3.379439	0.591630	-2.550048
H	3.236290	-0.461222	-2.298341
H	4.291938	0.960359	-2.079641
H	3.452289	0.690688	-3.634784
C	2.233123	1.359623	-2.067608
N	1.320073	1.966549	-1.697940
C	-1.057838	-0.021412	-2.342025
H	-1.990195	-0.587115	-2.294245
H	-1.115565	0.725167	-3.136520
H	-0.898174	0.503454	-1.396104
C	0.063002	-0.924419	-2.591379
N	0.953139	-1.639803	-2.778553
H	0.937108	-3.083497	2.081897
H	1.949222	-1.598504	-0.404290

3-N₃

C	0.583181	-2.987499	-1.041696
C	-0.682185	-2.247690	-0.609880
C	1.823917	-2.116237	-0.841170
H	0.497392	-3.280667	-2.093024
H	-1.547703	-2.908633	-0.711474
H	-0.844912	-1.380462	-1.280909
H	2.741203	-2.674674	-1.052925
C	1.855865	-1.588787	0.585139
C	0.541956	-0.884296	0.924630
H	1.996213	-2.422394	1.288481
H	0.435067	0.001281	0.270488
H	0.567909	-0.515980	1.958290
C	-1.798470	-1.352110	1.422388
H	-1.490817	-1.058883	2.433916
N	-0.560276	-1.825074	0.782068
C	-2.403323	-0.107634	0.776945
C	-2.101445	1.155184	1.296499
C	-3.248247	-0.181455	-0.338053
C	-2.640344	2.312451	0.736572
H	-1.430602	1.238961	2.148131
C	-3.784977	0.972893	-0.906510
H	-3.501590	-1.148748	-0.764077
C	-3.487042	2.224462	-0.366565
H	-2.388982	3.280218	1.160665
H	-4.444663	0.894145	-1.765552
H	-3.913821	3.122738	-0.802703
C	-2.804830	-2.490396	1.580892
H	-3.210127	-2.837012	0.626937
H	-2.319578	-3.337000	2.072883
H	-3.648137	-2.155644	2.191084
N	3.240862	-0.265681	1.837647
N	3.003351	-0.654551	0.693911
N	3.546679	0.160126	2.841972
C	3.604692	2.520095	0.279919
H	4.300588	2.543566	1.121430
H	3.759107	3.400247	-0.346680
H	3.762495	1.620728	-0.320451
C	2.231995	2.511389	0.783068
N	1.145570	2.497801	1.181335
C	-0.383520	1.944173	-1.761895
H	-0.805485	2.520442	-2.587439
H	-0.386461	2.540827	-0.847158
H	-0.997832	1.054782	-1.591923
C	0.991088	1.557491	-2.070396
N	2.085076	1.258211	-2.299355
H	0.668889	-3.904792	-0.446891
H	1.801661	-1.254808	-1.520262

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C	0.191319	-2.046525	2.070048
C	-1.089946	-1.257780	1.819932
C	1.266632	-0.970457	1.872116
H	0.226230	-2.505165	3.061129
H	0.306036	-2.835050	1.319714
H	-1.347311	-0.663200	2.714485
H	-1.952699	-1.884690	1.571687
H	2.247077	-1.389118	1.627135
H	1.366166	-0.371771	2.784641
C	0.699676	-0.096264	0.737349
C	1.313555	-0.402757	-0.628364
H	0.857836	0.972682	0.952316
H	1.243250	-1.474093	-0.828225
H	0.778077	0.145357	-1.411396
C	-1.624539	0.674685	0.323556
H	-1.141108	1.191101	-0.516547
N	-0.727927	-0.422951	0.676400
C	-2.943010	0.115002	-0.204359
C	-2.920224	-1.012354	-1.035906
C	-4.177041	0.704811	0.077462
C	-4.094493	-1.530386	-1.572293
H	-1.963079	-1.484760	-1.239266
C	-5.357902	0.187563	-0.459893
H	-4.232145	1.576653	0.721159
C	-5.321976	-0.930630	-1.286571
H	-4.054159	-2.407272	-2.211800
H	-6.306431	0.662228	-0.226527
H	-6.240160	-1.334861	-1.701638
C	-1.801262	1.712027	1.441120
H	-0.824282	1.991987	1.847407
H	-2.266718	2.623982	1.056443
H	-2.418547	1.330844	2.260581
N	2.761174	-0.080903	-0.726318
N	3.151837	0.915461	-0.128992
N	3.635624	1.799994	0.392692
C	2.324944	4.828055	-0.318742
H	1.808150	5.464644	0.401336
H	3.233187	4.425054	0.134332
H	2.586898	5.417801	-1.198688
C	1.460921	3.715697	-0.707951
N	0.792049	2.822810	-1.010651
C	4.621802	-2.647918	-1.569562
H	4.380873	-1.620978	-1.851461
H	4.657420	-3.281709	-2.457284
H	5.592945	-2.671610	-1.071714
C	3.588013	-3.132001	-0.656230
N	2.764913	-3.511934	0.061428

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C	-2.66839300	0.09194500	-0.62363900
N	-3.54021200	0.61962800	-0.07246300
H	-4.66712300	-0.68350400	3.56334000
C	-3.92365100	0.00859600	3.16410600
C	-2.67363600	-0.70526100	2.91117000
H	-4.28185600	0.43348700	2.22385500
N	-1.68632300	-1.27221500	2.70944700
H	-3.75101500	0.80687500	3.88803800
H	-3.57511400	3.02896100	-0.61177800
C	-3.01720400	3.75361600	-1.20951900
C	-1.77102800	3.13612200	-1.66016500
H	-3.61399700	4.04856800	-2.07429400
N	-0.78562200	2.64435100	-2.01340200
H	-2.79231900	4.63652400	-0.60876600
H	-1.27889300	-2.32182600	-2.49118300
H	-2.88950300	-2.17100700	-1.79997100
C	-1.82350100	-2.04936300	-1.58166100
H	2.58035400	-1.49119000	-2.97059900
H	-1.98380400	-3.91641200	-0.53940300
H	-1.43572200	-0.02996200	-2.27201500
C	3.06980500	-0.98746800	-2.13232100
C	-1.39813900	-2.99463800	-0.44989200
C	-1.54159500	-0.55376700	-1.31405600
H	3.81234400	-0.28526300	-2.52093800
H	3.60939600	-1.73595800	-1.54561000
H	2.09031100	-2.65811800	-0.43255000
H	-1.64505400	-2.56663400	0.53003100
C	1.09347100	-2.26969500	-0.20615100
C	0.08639600	-3.38140700	-0.50911300
N	0.85664000	-1.07073100	-1.00994400
H	0.29724200	-3.77348100	-1.51316400
C	2.02933300	-0.22751400	-1.31203100
H	1.63510700	0.56816000	-1.95662800
C	-0.26346800	-0.29951900	-0.48733900
H	1.07204900	-2.03114800	0.87156300
H	0.26999200	-4.19781700	0.19992800
H	-0.04637300	0.77081000	-0.52986700
H	-0.45638400	-0.54394600	0.56655800
H	3.61749300	-1.29631500	0.69661100
C	2.63266600	0.45697000	-0.08969000
C	3.40268200	-0.24203300	0.84770700
C	2.39032600	1.81647900	0.13231900
H	1.79740500	2.37397500	-0.59066400
C	3.90538600	0.39682000	1.97867000
H	4.49736800	-0.16402600	2.69575200
C	2.89669200	2.46177100	1.26010700
C	3.65364700	1.75217700	2.18906800
H	2.69940300	3.51890700	1.41157100
H	4.04858100	2.25011000	3.06931500

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C	-0.85833900	-1.94723200	-0.47843500
C	1.41708200	-1.43426900	1.25725500
H	-1.92739500	-2.14497400	-0.60886800
H	-0.43267300	-1.87970000	-1.49227500
H	2.46778600	-1.13860200	1.37365900
H	1.01303700	-1.57567800	2.26746400
C	0.63359200	-0.29684800	0.57490800
C	1.38660700	0.23387000	-0.67616200
H	0.55234300	0.54722200	1.26776400
H	1.66348100	-0.57523900	-1.36054500
H	0.73105500	0.93613000	-1.19829100
C	-1.81791900	-0.19841900	1.02581000
H	-1.50324300	0.78426400	1.40040200
N	-0.71756400	-0.65052300	0.17421700
C	-3.04595100	0.06376900	0.15678100
C	-2.92437200	1.00492000	-0.87356400
C	-4.27232500	-0.57579700	0.33556800
C	-3.99950900	1.29677700	-1.70406600
H	-1.96860400	1.50596300	-1.00641700
C	-5.35473600	-0.28965700	-0.50203600
H	-4.40074200	-1.30572700	1.12898900
C	-5.22215600	0.64514700	-1.52264500
H	-3.88803100	2.03492300	-2.49275600
H	-6.30108800	-0.80047400	-0.35091400
H	-6.06336700	0.86968000	-2.17136200
C	-2.10748200	-1.08857100	2.24018400
H	-1.20452900	-1.19375800	2.84808700
H	-2.89097600	-0.65074600	2.86705000
H	-2.43132100	-2.09033200	1.93935800
C	-0.16214500	-3.10073100	0.25383700
C	1.30823600	-2.75213200	0.48663300
H	-0.25170100	-4.01633100	-0.34203400
H	-0.65264800	-3.28761100	1.21747700
H	1.81499900	-3.54915100	1.04101700
H	1.82614000	-2.66915800	-0.47729200
C	2.60868000	0.94490000	-0.30161800
N	3.55348500	1.52441000	0.03619000
H	6.43394400	-1.19130700	0.24971100
C	6.03483000	-0.57043500	-0.55425900
C	4.87649400	-1.22751400	-1.15671900
H	5.71843500	0.39484900	-0.15227900
N	3.95622300	-1.73986200	-1.63371200
H	6.80702300	-0.42069200	-1.31071600
H	3.03602300	3.82106400	0.80823400
C	2.14736400	4.45581600	0.84165900
C	0.96974200	3.62840800	0.58615000
H	2.06137600	4.92543200	1.82296700
N	0.04497800	2.96417100	0.38316500
H	2.22467100	5.23055100	0.07687000

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C	0.89607100	-2.50818900	-0.36465200
C	-2.32291800	-2.66334700	-0.38935800
H	1.76049800	-2.79224400	-0.97043100
H	1.27227700	-2.22528500	0.63302600
H	-3.36226100	-2.89336900	-0.13366900
H	-2.18490600	-2.91938900	-1.44499200
C	-2.14512100	-1.15312500	-0.24888100
C	-0.68770900	-0.70662700	-0.08682600
H	-2.57752600	-0.65485200	-1.12615400
H	-0.38395200	-0.89384300	0.95685400
H	-0.64104700	0.37691500	-0.24843800
C	1.00113400	-0.44859000	-1.82313900
H	0.25131500	0.15966200	-2.34525900
N	0.21140000	-1.38434400	-1.00752100
C	1.86912900	0.52573800	-1.03171200
C	1.62864400	1.90117100	-1.12832000
C	2.91109700	0.08807300	-0.20504100
C	2.41332500	2.81919600	-0.42951400
H	0.81019800	2.24935700	-1.75482700
C	3.68843100	1.00076000	0.50583300
H	3.11671000	-0.97362900	-0.10242400
C	3.44582700	2.36997300	0.39199000
H	2.21451900	3.88278400	-0.52398700
H	4.48218100	0.63919800	1.15261800
H	4.05736200	3.07970100	0.94103000
C	1.81786600	-1.17261000	-2.89307200
H	1.19348200	-1.91235500	-3.40289700
H	2.18087200	-0.44689700	-3.62569000
H	2.69455000	-1.67664000	-2.47636200
C	-0.00349300	-3.73856600	-0.22957100
C	-1.35928900	-3.51007800	0.45288300
H	0.55772100	-4.49772800	0.32885000
H	-0.18896200	-4.14724100	-1.23184800
H	-1.81811100	-4.48979300	0.62427800
H	-1.22329900	-3.06065600	1.44630100
N	-2.70518100	1.48839800	1.72729200
N	-2.77523600	0.43396800	1.30745400
N	-2.93186500	-0.72567300	0.94955400
H	0.91758000	1.39832200	1.47187200
N	1.89039300	-1.16856100	3.01848300
C	1.43340700	-0.12573000	2.81465600
C	0.84770900	1.18561700	2.54280500
H	-0.20265800	1.19668700	2.84376300
H	1.39238600	1.95552800	3.09255300
H	-3.20771600	4.75480100	-0.76347700
N	-1.95455300	1.98639900	-1.62872500
C	-2.67750700	2.76603100	-1.17414500
C	-3.59119100	3.74749500	-0.59266400
H	-4.57541700	3.65308000	-1.05455700
H	-3.67297000	3.56343100	0.48047500

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C	1.577628	-0.219289	1.556378
C	-0.936996	-1.680874	1.519315
H	2.666200	-0.209144	1.440355
H	1.281372	0.820130	1.768046
H	-2.032570	-1.664759	1.534388
H	-0.629218	-2.727648	1.403632
C	-0.442177	-0.881493	0.299535
C	-1.168448	0.461113	0.171818
H	-0.681673	-1.443809	-0.611013
H	-1.093406	1.052002	1.091630
H	-0.727796	1.013451	-0.664483
C	1.805915	-1.455626	-0.603812
H	1.206604	-1.571190	-1.516766
N	0.992664	-0.619685	0.279802
C	3.052274	-0.681057	-1.023898
C	2.874059	0.560466	-1.648129
C	4.352237	-1.144109	-0.821189
C	3.965925	1.317793	-2.055228
H	1.860140	0.918881	-1.807008
C	5.453358	-0.383178	-1.224409
H	4.524237	-2.104399	-0.345166
C	5.264557	0.848761	-1.840799
H	3.807539	2.275726	-2.541815
H	6.457623	-0.759678	-1.053542
H	6.119484	1.440121	-2.154398
C	2.110494	-2.860057	-0.067384
H	1.176396	-3.377273	0.169062
H	2.648379	-3.456259	-0.811688
H	2.716066	-2.822627	0.844392
C	1.155922	-1.081995	2.751103
C	-0.369217	-1.138890	2.832678
H	1.580137	-0.659023	3.669330
H	1.555608	-2.098607	2.643708
H	-0.692805	-1.771343	3.666374
H	-0.769788	-0.135882	3.029255
N	-2.600860	0.183081	-0.113291
N	-3.315700	1.168274	-0.222854
H	-5.951649	2.465388	2.970199
C	-5.071037	3.044529	2.687176
C	-3.880835	2.199002	2.761621
H	-5.190561	3.401606	1.662520
N	-2.939085	1.530691	2.814378
H	-4.965219	3.893603	3.364332
H	-3.716123	0.664058	-2.992551
C	-3.284244	-0.321787	-3.181212
C	-1.826641	-0.246120	-3.091203
H	-3.653773	-1.020684	-2.428587
N	-0.674275	-0.187800	-3.015663
H	-3.577865	-0.657177	-4.177447
N	-4.060212	2.015655	-0.360362

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C	0.76830800	-1.46225600	0.94441700
C	-0.86082200	-2.17728200	-1.70943600
H	1.79433600	-1.37870700	1.31254000
H	0.10425500	-1.40544700	1.82723500
H	-1.49229000	-2.67250100	-2.45819000
H	0.12487600	-2.04194200	-2.17058400
C	-1.47339600	-0.79508000	-1.43073100
C	-0.93978400	-0.16116300	-0.13993700
H	-1.21110000	-0.13615800	-2.27149300
H	-1.48105200	-0.61399700	0.70786400
H	-1.21647300	0.89593800	-0.13425000
C	1.24829300	0.86907900	0.41564700
H	1.02981300	1.16288200	1.46125600
N	0.49869500	-0.33671000	0.04076300
C	2.74243900	0.59954900	0.31440800
C	3.61863700	1.10394400	1.27622100
C	3.26522300	-0.10640100	-0.77322900
C	4.99503700	0.91159900	1.15700700
H	3.21906000	1.64660800	2.13034800
C	4.63876800	-0.30225900	-0.89382700
H	2.57749800	-0.51305600	-1.51009900
C	5.50893300	0.20703900	0.07097700
H	5.66391500	1.30582500	1.91607100
H	5.03263400	-0.85593000	-1.74118700
H	6.57922200	0.05090200	-0.02211100
C	0.91852200	2.06200000	-0.49295600
H	-0.05602600	2.50359900	-0.27212000
H	1.66904800	2.84327000	-0.35032700
H	0.95038400	1.74412700	-1.54185800
C	0.61727700	-2.82527400	0.27155800
C	-0.70222100	-3.07112700	-0.47084500
H	0.74872400	-3.59304200	1.04337300
H	1.44165400	-2.94709800	-0.44379400
H	-0.71924900	-4.12005700	-0.78570300
H	-1.55471700	-2.94936700	0.21373900
N	-2.94087600	-0.79165800	-1.32694300
H	-3.23116400	-1.42809600	-0.58382600
H	-3.35038000	-1.15489500	-2.18436800
H	-3.07497500	1.49953600	-1.77795100
H	-3.48689200	3.12802100	-2.41283300
C	-2.71592300	3.07909800	-0.45788900
C	-2.77223200	2.55348000	-1.82067500
N	-2.66444100	3.45820400	0.63371600
H	-1.78269000	2.62796800	-2.27929600
H	-4.91275100	0.92675100	2.23449600
H	-3.14287100	1.09449200	2.11922400
C	-3.87332200	-0.85992000	1.82689900
C	-4.01891600	0.58943100	1.70720000
N	-3.73854600	-2.00800600	1.87511700
H	-4.09553900	0.84081800	0.64642200

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C	1.704435	-1.156786	1.286514
C	0.128571	-3.195546	-0.057104
H	2.577345	-0.495538	1.278800
H	1.165036	-0.939262	2.221825
H	-0.775370	-3.808524	-0.151279
H	0.757547	-3.436914	-0.923213
C	-0.255089	-1.705874	-0.119855
C	-1.411112	-1.351287	0.827412
H	-0.611683	-1.490394	-1.134949
H	-1.072015	-1.416331	1.872903
H	-1.650926	-0.300881	0.636715
C	1.503654	-0.141417	-0.977387
H	0.697121	0.058200	-1.695663
N	0.856334	-0.797935	0.155100
C	2.010479	1.231685	-0.537060
C	1.120689	2.069538	0.147177
C	3.299724	1.699697	-0.789844
C	1.505057	3.337681	0.563666
H	0.121437	1.692375	0.345677
C	3.693636	2.973150	-0.367643
H	4.016208	1.077326	-1.316770
C	2.800435	3.795681	0.309252
H	0.797829	3.974478	1.088625
H	4.703556	3.317058	-0.570354
H	3.106988	4.784475	0.636401
C	2.567968	-0.983995	-1.691309
H	2.138931	-1.943880	-1.991214
H	2.931631	-0.481435	-2.593328
H	3.426427	-1.182415	-1.039938
C	2.133655	-2.628860	1.319822
C	0.903965	-3.532272	1.218039
H	2.688364	-2.824643	2.244935
H	2.808017	-2.843533	0.480824
H	1.194048	-4.588391	1.218434
H	0.266739	-3.380858	2.101449
N	-2.610764	-2.148059	0.559574
H	-3.430882	-1.673454	0.930652
H	-2.146052	2.607056	0.076127
C	-2.706940	2.514405	1.010390
C	-3.657056	1.410890	0.881376
H	-2.015673	2.304911	1.829947
N	-4.396959	0.528508	0.771585
H	-3.243577	3.442012	1.217575
H	-3.341081	-1.568290	-1.600927
C	-3.587270	-0.701075	-2.224102
C	-2.568909	0.323102	-2.004567
H	-3.614351	-0.975519	-3.280196
N	-1.752611	1.121109	-1.812905
H	-4.558754	-0.311484	-1.913290
H	-2.558310	-3.055779	1.012050