Electronic Supplementary Information

Probing the anomeric effect and mechanism of isomerization of oxazinane rings by DFT methods

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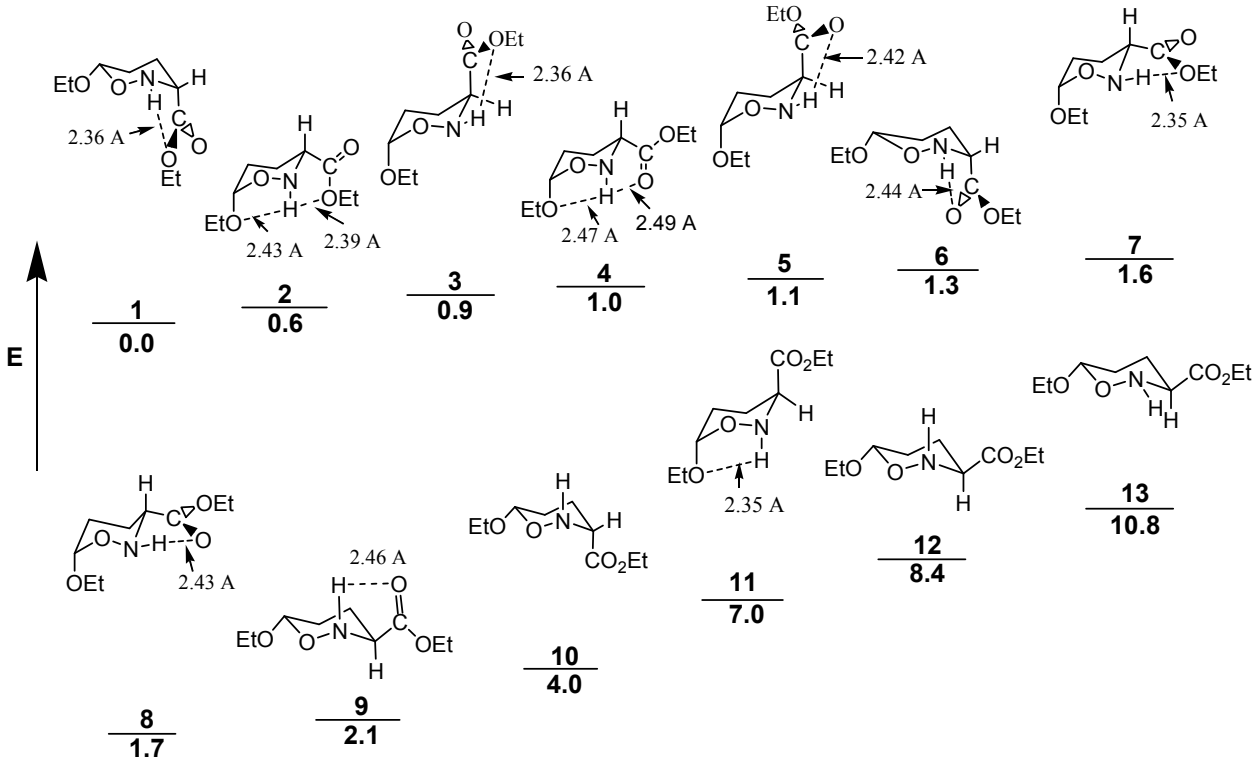


Figure S1. Gas-phase ωB97XD/Def2-TZVP structures of **1** to **13** oxazinane ring conformers studied. The energy classification of the conformers was based on their sum of electronic and zero-point energy differences.

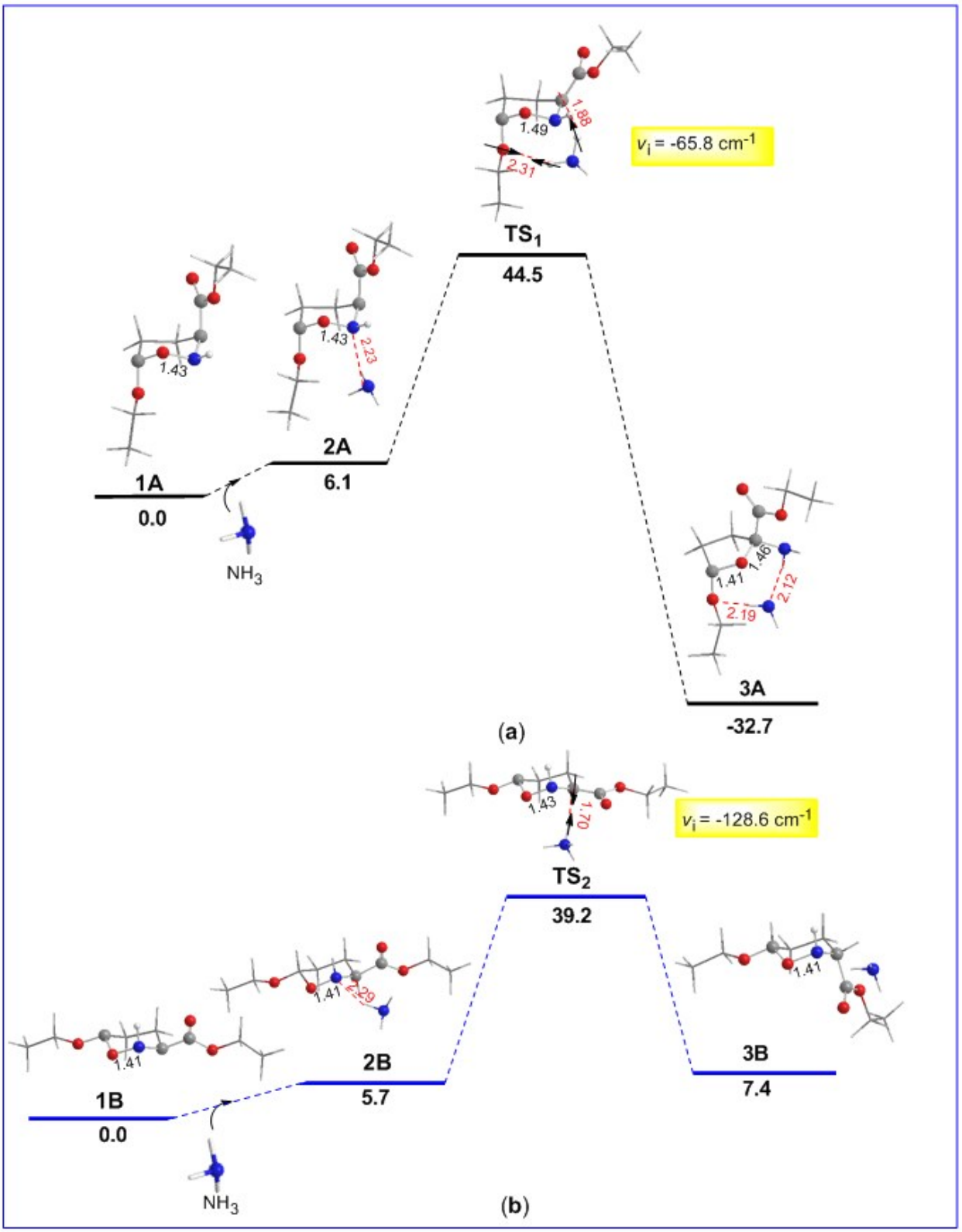
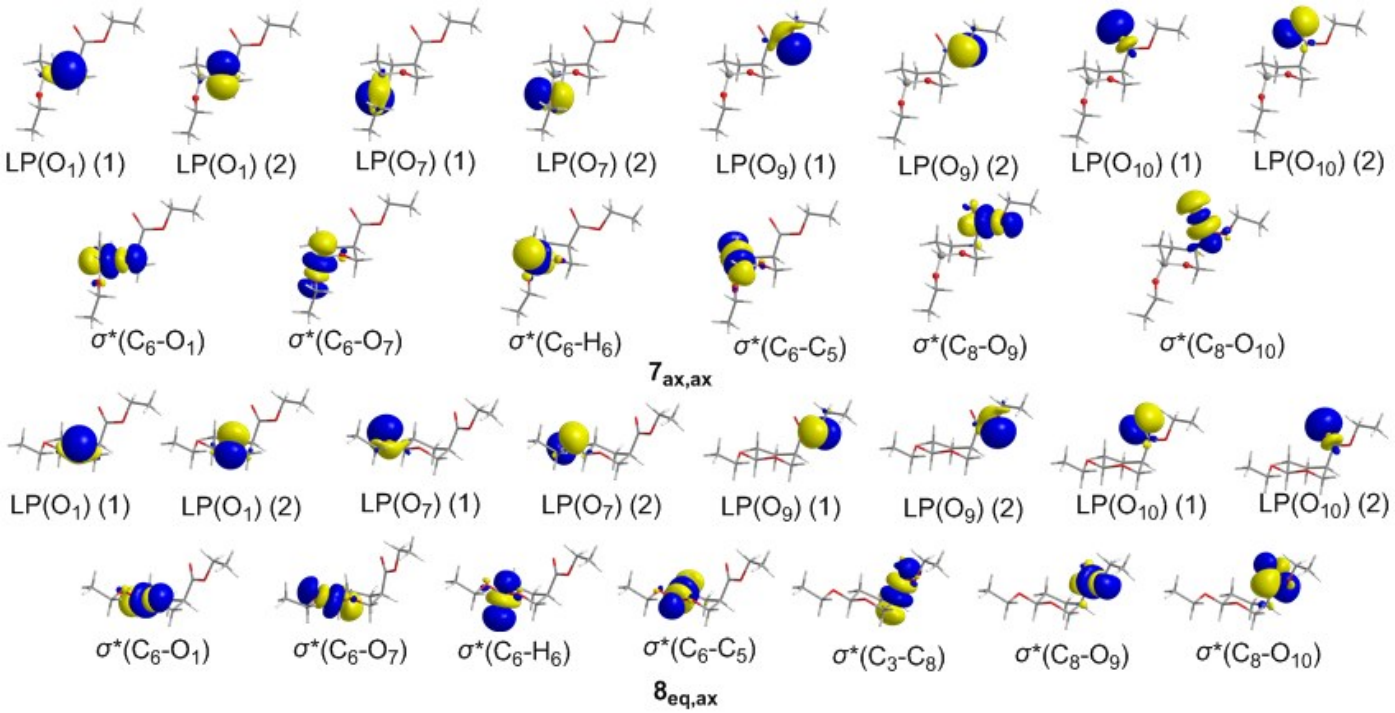


Figure S2 SMD Liq-phase geometric and free energy, Δ*G* (in kcal/mol) reaction profiles of the thermal amine-promoted transformations of oxazinane rings of **1A** (**a**) and **1B** (**b**) conformers calculated by the ωB97XD/Def2-TZVP computational protocol in chloroform solution.



Scheme S1. 3D plots of the relevant NBOs involved in hyperconjucative interactions in **7ax,ax** and **8eq,ax** conformers.

Table S1. Free energies (G, a.u.) of all stationary points found in the Potential Energy Surface of the reactions **1A**+$\mathbf{NH_3}$ and **1B**+$\mathbf{NH_3}$ studied at the ωB97XD/Def2-TZVP level of theory in the gas-, SMD liq-and the temperature corrected liq-phase (334.35 K).

Compound	Gas-Phase	Liq-Phase (298 K)	Liq-Phase (334.35 K)
1A	-708.6315420	-708.6472350	-708.6524860
$\mathbf{NH_3}$	-56.5488420	-56.5532430	-56.5560510
2A	-765.1737780	-765.1907080	-765.1996960
TS1	-765.0943550	-765.1295600	-765.1368890
3A	-765.2356050	-765.2526180	-765.2585870
1B	-708.6302250	-765.6469650	-708.6553940
2B	-765.1724610	-765.1911960	-765.1995440
3B	-765.1884580	-765.1884580	-765.1954150
TS2	-765.1682270	-765.1378080	-765.1448520

Table S2. Gas-phase Cartesian coordinates of all stationary points found in the Potential Energy Surface of the reactions **1A** + **NH_3** and **1B** + **NH_3** studied at the ωB97XD/Def2-TZVP level of theory.

1A

N	0.25431000	-0.52768500	0.88328700
O	0.56783800	-0.71381500	-0.50205900
O	-2.44063200	-0.41778900	0.34289900
C	-3.69645600	-0.52275200	-0.34017900
C	1.54872500	0.22273700	-0.90813200
C	-4.21193900	-1.92658100	-0.14315100
O	-2.24402600	1.70569100	-0.33348300
O	2.73609800	0.11963000	-0.20134700
C	1.02091900	1.64084500	-0.76307000
C	0.44429600	1.86880500	0.63169200
C	-0.48123400	0.72058800	1.01976300
C	-1.80317200	0.75217100	0.24746100
C	3.34213300	-1.15692200	-0.24223500
C	4.69703400	-1.06006100	0.41839700
H	-0.36970200	-1.30698300	1.05257300
H	-3.53987600	-0.29183800	-1.39494000
H	-4.38124300	0.22381500	0.06585100
H	1.70126900	-0.04580800	-1.96192400
H	-4.35972200	-2.14341400	0.91532900
H	-3.51494000	-2.65736400	-0.55436900
H	-5.16934100	-2.03970800	-0.65335900
H	1.82656000	2.34509300	-0.96952200
H	0.24194700	1.79025000	-1.51240300
H	-0.09831400	2.81212100	0.66627700
H	1.25037500	1.90521000	1.36478900
H	-0.74659400	0.80079400	2.07889400
H	3.43987900	-1.48359500	-1.28704500
H	2.70961000	-1.88377400	0.27528100
H	5.18996200	-2.03349900	0.40952300
H	4.59112700	-0.73631200	1.45438000
H	5.33276600	-0.34390600	-0.10369100

NH_3

N	-0.00000800	-0.00000600	-0.11045500
H	-0.50288000	-0.79629200	0.25774600
H	-0.43816700	0.83368100	0.25772700
H	0.94110200	-0.03734800	0.25771500

2A

N	0.10369700	-0.44733100	0.66996400
O	0.29350700	-0.84914600	-0.69002700
O	-2.62602400	-0.35536300	0.40618600
C	-3.94720900	-0.53860900	-0.11917400
C	1.24937900	-0.00847800	-1.31032400
C	-4.45403900	-1.87447000	0.36434000
O	-2.48122500	1.62065400	-0.63319500
O	2.48797200	-0.03836000	-0.68510700
C	0.75020400	1.42596100	-1.34533200
C	0.28877200	1.88498500	0.03519600
C	-0.59942400	0.82979600	0.68483400
C	-1.99194700	0.76716300	0.05407100
C	3.07682900	-1.32230400	-0.60476200

C	4.47583900	-1.17325700	-0.05572400
H	-0.51244300	-1.17449900	1.01200700
H	-3.89892000	-0.49217500	-1.20816600
H	-4.57792500	0.28430800	0.22142900
H	1.31697900	-0.43777100	-2.31826600
H	-4.49271400	-1.90640700	1.45368500
H	-3.81197900	-2.68347500	0.01458000
H	-5.46066700	-2.04448100	-0.01972700
H	1.54257200	2.07139600	-1.72397500
H	-0.08456800	1.47118100	-2.04695200
H	-0.25778400	2.82305400	-0.04532100
H	1.14291100	2.04307500	0.69277800
H	-0.74357600	1.07779100	1.74113600
H	3.09572900	-1.77888400	-1.60385500
H	2.47417700	-1.96665600	0.04233500
H	4.96244900	-2.14816300	0.00096200
H	4.44442800	-0.74675900	0.94769200
H	5.07534400	-0.52212000	-0.69292900
N	2.39576900	0.71241500	2.58251400
H	2.75419600	0.15898300	3.34916100
H	3.18767000	1.04575900	2.04863200
H	1.86361000	0.10325400	1.96584500

TS1

N	0.02506200	-0.57934100	0.36488600
O	0.62291600	-0.83626500	-1.18588900
O	-2.64890500	-0.48168900	0.18228000
C	-4.05481300	-0.47123600	-0.02128400
C	1.52913600	0.15752700	-1.35058300
C	-4.52531200	-1.90647300	-0.06261500
O	-2.67751300	1.76644400	0.11058000
O	2.61798300	0.08786200	-0.36739700
C	0.94353800	1.56626600	-1.26218800
C	0.21879200	1.83740600	0.05869200
C	-0.61412600	0.63569100	0.45643100
C	-2.03498400	0.73890400	0.21484400
C	3.32595300	-1.13771000	-0.43123200
C	4.56535000	-1.04189000	0.43169100
H	-0.67275000	-1.31560000	0.33521400
H	-4.28438300	0.05007900	-0.95319200
H	-4.53603400	0.08439900	0.78701500
H	2.01032900	0.00994700	-2.32801100
H	-4.30162400	-2.41697200	0.87549000
H	-4.04015400	-2.44973300	-0.87476400
H	-5.60437400	-1.93950200	-0.22244500
H	1.73541000	2.29735100	-1.44037500
H	0.22819700	1.64163700	-2.08357400
H	-0.45423800	2.68526200	-0.05433300
H	0.95703800	2.15356500	0.80760600
H	0.66555500	0.47698600	2.02944800
H	3.60571200	-1.33508700	-1.47207400
H	2.67525800	-1.95758700	-0.11120800
H	5.13921200	-1.96738100	0.36799800
H	4.31433100	-0.88406700	1.48404000
H	5.20027900	-0.21670500	0.10755000
N	1.68209700	0.28332500	2.20485000
H	2.12295700	0.98975200	2.78317600
H	1.75488100	-0.63487700	2.62855500
H	2.09723100	0.23890700	1.22659000

3A

N	-0.48482800	-0.30275300	1.77748600
O	0.22290700	-0.25350200	-0.52815800
O	-2.57519300	-0.51096600	0.09022800
C	-3.90562800	-0.47451100	-0.43864700
C	1.20808100	0.55441600	-1.11113000
C	-4.49741000	-1.85397900	-0.28818800
O	-2.31717900	1.65511300	-0.40089700
O	2.49908300	0.19107200	-0.68822700
C	0.91686900	1.97489800	-0.65780400
C	0.28571900	1.76139300	0.71049300
C	-0.45390100	0.43252400	0.57136200
C	-1.88369500	0.62595200	0.04229300
C	2.89643600	-1.10035100	-1.11296600
C	4.36959500	-1.27616400	-0.82406500
H	-0.97034300	-1.18083300	1.66883400
H	-3.85904300	-0.16394100	-1.48393800
H	-4.48062100	0.27634600	0.10592000
H	1.14821500	0.41183600	-2.19652800
H	-4.53654000	-2.14805800	0.76115500
H	-3.90778900	-2.59116000	-0.83394600
H	-5.51329200	-1.86231200	-0.68553200
H	1.82130300	2.57908500	-0.64001500
H	0.19756700	2.42982800	-1.33845100
H	-0.39281700	2.55937500	0.99901300
H	1.04394300	1.65050000	1.48528100
H	0.45159500	-0.44710600	2.15036400
H	2.70211100	-1.20399300	-2.18846000
H	2.29934900	-1.85999300	-0.59756800
H	4.69852000	-2.26567100	-1.14510300
H	4.57187700	-1.17868800	0.24381200
H	4.95808800	-0.52571900	-1.35280600
N	2.58521000	-0.48763900	2.37290400
H	3.10957300	0.09153800	3.01455300
H	2.96952600	-1.42198500	2.41796100
H	2.73276300	-0.13511500	1.43107600

1B

N	-0.17140300	-1.09786400	-0.37048700
O	-1.46589400	-0.65601700	-0.68326900
O	3.09720400	0.16200100	-0.35269000
C	4.41117900	-0.21447800	0.08723200
C	-2.00373900	0.22845200	0.30133800
C	5.40522900	0.66116100	-0.63385000
O	2.19914400	-1.38872800	0.99307800
O	-3.28821800	0.53751700	-0.06884900
C	-1.17636200	1.49185400	0.37539700
C	0.27320800	1.13230600	0.67683500
C	0.74637100	0.03133900	-0.28411100
C	2.07894300	-0.50399900	0.18798000
C	-4.20837800	-0.54174200	0.00671700
C	-5.58477100	-0.01232200	-0.31657900
H	-0.20594100	-1.57989300	0.52632100
H	4.56397600	-1.27178600	-0.13406500
H	4.46803500	-0.08983900	1.16997600
H	-1.99020900	-0.30657800	1.27071400
H	5.23719200	1.71366400	-0.40371900
H	5.33182700	0.52586200	-1.71317300
H	6.41683700	0.39819700	-0.32206800
H	-1.26179200	1.99940700	-0.58805300

H	-1.58421400	2.15064500	1.14312300
H	0.35733800	0.75906900	1.70260000
H	0.91892500	2.00792000	0.59156600
H	0.85688400	0.44332400	-1.28813800
H	-4.18262600	-0.96617900	1.01940200
H	-3.91664000	-1.32719000	-0.69479100
H	-6.31705000	-0.81930100	-0.26365900
H	-5.60538900	0.40669500	-1.32299700
H	-5.87529300	0.76740900	0.38846100

2B

N	0.29654100	0.89379700	0.25023000
O	1.59714100	0.73106800	-0.24885500
O	-2.89555700	-0.51293200	-0.24908200
C	-4.22189000	-0.32653100	0.26190900
C	2.21109600	-0.48291700	0.19140700
C	-5.18420100	-0.92874400	-0.73098500
O	-2.04190900	0.47821400	1.57256000
O	3.49256600	-0.50425500	-0.29723700
C	1.44298300	-1.67533800	-0.33143100
C	-0.00863200	-1.58380400	0.12255300
C	-0.56958400	-0.19257200	-0.19806500
C	-1.90934600	-0.00902700	0.47964600
C	4.36752100	0.45753900	0.27406600
C	5.75237400	0.22418200	-0.27997800
H	0.33957500	0.89748900	1.26817900
H	-4.38590400	0.74485100	0.38695200
H	-4.29614200	-0.80014000	1.24244800
H	2.21068200	-0.47078100	1.29860900
H	-5.00007100	-1.99634500	-0.85671400
H	-5.08991500	-0.44204500	-1.70182600
H	-6.20702600	-0.79618500	-0.37566400
H	1.51337900	-1.66181800	-1.42137000
H	1.90900800	-2.59400200	0.02720200
H	-0.06995900	-1.74538100	1.20388400
H	-0.61794100	-2.35053700	-0.35778200
H	-0.70152500	-0.08215800	-1.27505000
H	4.36143400	0.34541800	1.36663300
H	4.01636800	1.46498400	0.03721400
H	6.45069500	0.94768600	0.14325100
H	5.75325400	0.33746200	-1.36442600
H	6.10234500	-0.77977400	-0.03711000
N	-2.14264000	2.74000600	-0.66276500
H	-2.17798400	3.46650200	-1.36502700
H	-1.16614500	2.52411400	-0.48027000
H	-2.52128400	3.12055800	0.19478600

3B

N	0.14061400	1.63536800	0.02819400
O	1.13210900	0.75371000	-0.43633500
O	-2.09777800	-1.05095500	0.11899400
C	-2.94508700	-1.79354600	-0.76657300
C	1.80598900	0.07487300	0.62682500
C	-3.16465000	-3.15565300	-0.15626100
O	-2.14671700	0.67475100	-1.29850900
O	2.79239800	-0.69965400	0.07043100
C	0.83804900	-0.79812300	1.39201900
C	-0.33398700	0.04597200	1.88150200
C	-0.89524600	0.90940200	0.75191500
C	-1.76387100	0.18100500	-0.27586700

C	3.86206700	0.02468500	-0.51892700
C	4.90683500	-0.96455400	-0.97638900
H	0.58890300	2.29773600	0.65806800
H	-2.46141500	-1.85749900	-1.74243400
H	-3.88211600	-1.24917000	-0.89633400
H	2.24184800	0.85099200	1.28694300
H	-3.64579600	-3.07371700	0.81894900
H	-2.21849500	-3.68367800	-0.03327000
H	-3.80718500	-3.74961100	-0.80752900
H	0.49432300	-1.58474100	0.71815300
H	1.35805600	-1.27036300	2.22665200
H	0.00799800	0.72250000	2.67107200
H	-1.11071300	-0.58286200	2.31314700
H	-1.54788900	1.68944100	1.15770400
H	4.28074100	0.71681800	0.22429000
H	3.49042500	0.61708200	-1.35865000
H	5.74606900	-0.43740800	-1.43255300
H	4.48674000	-1.64822700	-1.71462000
H	5.27986000	-1.55051500	-0.13557900
N	-2.15184600	3.75786900	-0.24338800
H	-1.95721200	4.72990600	-0.44414400
H	-1.49632000	3.19193100	-0.77423100
H	-3.06989100	3.55154900	-0.61539300

TS2

N	-0.26105300	0.74322000	-0.99551200
O	-1.53646600	0.70545200	-0.35015500
O	2.95885400	-0.51999300	-0.07216200
C	4.30900600	-0.09060800	0.04320300
C	-2.02561100	-0.63208300	-0.23429200
C	5.15189400	-1.30935400	0.33850000
O	2.40357400	1.60470000	-0.56918800
O	-3.25872200	-0.57349100	0.37725700
C	-1.08800100	-1.49987300	0.57722600
C	0.32501700	-1.45320300	-0.00979100
C	0.69989900	-0.01569200	-0.24050200
C	2.03614700	0.44041500	-0.35047600
C	-4.29096100	-0.01149500	-0.41520300
C	-5.58705100	-0.11051100	0.35369000
H	-0.42663900	0.35037800	-1.92134500
H	4.39331200	0.65217300	0.84130700
H	4.62068700	0.39530300	-0.88339100
H	-2.12203400	-1.03088800	-1.26239800
H	5.06567100	-2.04234300	-0.46458300
H	4.83925300	-1.78321000	1.27009000
H	6.20065700	-1.02250200	0.43222200
H	-1.08608900	-1.11853200	1.60156200
H	-1.48568600	-2.51659100	0.59615700
H	0.34158400	-2.02957800	-0.94814100
H	1.02779300	-1.93960600	0.66514900
H	0.50335900	1.19498400	0.95314600
H	-4.36016400	-0.56218400	-1.36300400
H	-4.05644600	1.03024300	-0.65171700
H	-6.40491100	0.30917200	-0.23408000
H	-5.51815300	0.44067000	1.29221100
H	-5.82142700	-1.15080100	0.58222000
N	0.43872800	2.31175700	1.10706500
H	-0.49691800	2.58568400	0.83094600
H	1.14177000	2.57428500	0.39094600
H	0.68069800	2.63959600	2.03170100

Table S3. SMD Liq-phase Cartesian coordinates of all stationary points found in the Potential Energy Surface of the reactions **1A**+$\mathbf{NH_3}$ and **1B**+ $\mathbf{NH_3}$ studied at the ωB97XD/Def2-TZVP level of theory.

1A

N	0.24258800	-0.46775500	0.94615000
O	0.56059800	-0.73517400	-0.42539000
O	-2.41584700	-0.42015600	0.31598400
C	-3.68456500	-0.56508600	-0.34559500
C	1.53490100	0.18215700	-0.89146100
C	-4.14708900	-1.98499500	-0.14678700
O	-2.30517100	1.72187900	-0.31173100
O	2.73146000	0.11162700	-0.19246000
C	1.00331800	1.60410600	-0.81777300
C	0.42278400	1.90894300	0.56025300
C	-0.49996900	0.78143400	1.01143100
C	-1.82426000	0.76724500	0.24368100
C	3.36040400	-1.15804700	-0.22253900
C	4.73219500	-1.02762200	0.39236800
H	-0.36931800	-1.24365600	1.16994100
H	-3.55402900	-0.32791600	-1.40254300
H	-4.38687900	0.15271800	0.08142700
H	1.67911800	-0.13783900	-1.93112900
H	-4.27719200	-2.21087700	0.91283400
H	-3.43307200	-2.69210100	-0.57189100
H	-5.10702700	-2.12484800	-0.64655300
H	1.80436100	2.30039400	-1.06632700
H	0.22660800	1.70642000	-1.57819400
H	-0.11921000	2.85305700	0.54272100
H	1.22460900	1.99316700	1.29446100
H	-0.77037800	0.92145000	2.06282400
H	3.43113800	-1.50666600	-1.26170400
H	2.75833800	-1.88466100	0.33155500
H	5.23671900	-1.99572100	0.38569700
H	4.65944700	-0.68649400	1.42675900
H	5.34401500	-0.31634700	-0.16562400

NH_3

N	-0.00002000	-0.00002600	-0.11356400
H	0.64045800	-0.68741900	0.26500200
H	-0.91562100	-0.21073100	0.26496200
H	0.27530300	0.89833300	0.26498300

2A

N	0.10026000	-0.37822000	0.73237900
O	0.27669200	-0.85369900	-0.60573300
O	-2.60695600	-0.36124400	0.38945700
C	-3.94290000	-0.57067400	-0.10096200
C	1.20950500	-0.03729800	-1.29271600
C	-4.36849100	-1.95815600	0.30158800
O	-2.55203200	1.66531300	-0.55203500
O	2.46513700	-0.02852800	-0.70024100
C	0.69781000	1.39029600	-1.38516000
C	0.25745800	1.91297500	-0.02063500
C	-0.61914500	0.88668200	0.69001300

C	-2.02014700	0.79056500	0.08234400
C	3.06197400	-1.30624400	-0.55649400
C	4.51590800	-1.12170700	-0.19705100
H	-0.48816400	-1.09794700	1.13485000
H	-3.93875600	-0.44916000	-1.18512500
H	-4.59531300	0.19280300	0.32631400
H	1.25475500	-0.51295800	-2.28014900
H	-4.36645100	-2.07095200	1.38692700
H	-3.70731100	-2.71053700	-0.13124500
H	-5.38140200	-2.14271700	-0.05994800
H	1.47507200	2.02396000	-1.81262900
H	-0.14866700	1.39313100	-2.07484100
H	-0.28383900	2.85097000	-0.13157700
H	1.12556300	2.10015200	0.61203300
H	-0.76411200	1.18674500	1.73279900
H	2.96277900	-1.86465600	-1.49661000
H	2.54206600	-1.87300800	0.22238300
H	4.99510400	-2.09517200	-0.07607800
H	4.61339100	-0.57423700	0.74229500
H	5.04439100	-0.57132000	-0.97756000
N	2.50072000	0.63867600	2.61346500
H	2.85846100	-0.07261600	3.23971500
H	3.29091500	0.99404500	2.08913000
H	1.89009300	0.17691100	1.94125900

TS1

N	0.10419400	-0.62767500	0.13974800
O	0.62795100	-0.70066600	-1.24829900
O	-2.57786700	-0.48370100	0.05512000
C	-3.99428600	-0.47268700	-0.04603200
C	1.62239300	0.27278200	-1.37406300
C	-4.45780100	-1.89918300	-0.22237700
O	-2.62811000	1.76500900	0.24195500
O	2.65422900	0.12125700	-0.42168000
C	1.04263600	1.67022200	-1.22795000
C	0.31130300	1.82483700	0.10854400
C	-0.55352100	0.61855000	0.40012900
C	-1.95429100	0.73503600	0.20913800
C	3.34437000	-1.11258700	-0.51166800
C	4.42275300	-1.14204300	0.54442600
H	-0.59695200	-1.35774700	0.10849500
H	-4.30077100	0.14447300	-0.89415500
H	-4.42689400	-0.02945800	0.85495100
H	2.03304100	0.11396500	-2.37923300
H	-4.16755600	-2.51559700	0.63109100
H	-4.03335400	-2.33872700	-1.12714800
H	-5.54603800	-1.92596200	-0.30748200
H	1.84069600	2.40780900	-1.34033800
H	0.33820600	1.80730800	-2.05154000
H	-0.32563900	2.70815200	0.08317000
H	1.06352300	2.01745300	0.88378700
H	0.31178500	0.36986200	2.05241800
H	3.78255200	-1.21430000	-1.51291400
H	2.64431600	-1.94136000	-0.37005300
H	4.97936200	-2.07891000	0.48331300
H	3.99133200	-1.07362800	1.54652900
H	5.12391000	-0.31590000	0.41331600
N	1.23751700	0.12955100	2.52896500
H	1.52225200	0.84453400	3.19207100
H	1.15472100	-0.76900400	2.99575200
H	1.90857900	0.04915500	1.75933700

3A

N	-0.44756600	-0.22510500	1.76905200
O	0.19490600	-0.25867100	-0.55384300
O	-2.56092100	-0.50461300	0.10747300
C	-3.91539600	-0.50661800	-0.37568100
C	1.20534000	0.50939600	-1.16188500
C	-4.45178200	-1.90686500	-0.23171700
O	-2.35847300	1.66532600	-0.38802600
O	2.48144600	0.15548000	-0.69995700
C	0.91792000	1.94935000	-0.77706200
C	0.29848600	1.80019100	0.60544900
C	-0.44791300	0.46997700	0.53225500
C	-1.89473800	0.64008600	0.04119700
C	2.86975800	-1.17028400	-1.02875700
C	4.35154500	-1.32026100	-0.78166200
H	-0.91494500	-1.11849500	1.69362500
H	-3.91493000	-0.17953200	-1.41672200
H	-4.49574100	0.20977400	0.20818900
H	1.15418200	0.31366000	-2.23852700
H	-4.44605200	-2.22342500	0.81245100
H	-3.86130400	-2.61381300	-0.81655000
H	-5.48099100	-1.93768900	-0.59333100
H	1.82045400	2.55664100	-0.79241600
H	0.19763100	2.37051100	-1.47867900
H	-0.36970700	2.61560800	0.86965300
H	1.06778400	1.72105600	1.37367000
H	0.50372900	-0.35617800	2.11431900
H	2.63499100	-1.36652200	-2.08255800
H	2.29910800	-1.88349300	-0.42489200
H	4.66421000	-2.34001600	-1.01404600
H	4.59727600	-1.11859000	0.26294100
H	4.92191000	-0.63299600	-1.40892700
N	2.60213600	-0.37697500	2.41258300
H	3.06602400	0.27348300	3.03461100
H	3.06859700	-1.27073700	2.50744000
H	2.75080300	-0.05468500	1.46030900

1B

N	-0.19496700	-1.15009400	-0.36892800
O	-1.48338800	-0.67979300	-0.68183300
O	3.08309900	0.17831800	-0.32797100
C	4.41403200	-0.18024400	0.09018300
C	-1.99578700	0.22764200	0.30360800
C	5.36720000	0.82440700	-0.50207500
O	2.23106600	-1.54535800	0.82077500
O	-3.27475700	0.55994500	-0.07248300
C	-1.13620600	1.46890000	0.36213000
C	0.30892100	1.07894700	0.64661200
C	0.74563900	-0.03448200	-0.31605900
C	2.08752600	-0.57670900	0.11744000
C	-4.24129900	-0.46953600	0.11270600
C	-5.58772700	0.06037900	-0.31245700
H	-0.24455600	-1.59743600	0.54542700
H	4.62699500	-1.19261600	-0.25614400
H	4.45019300	-0.17698100	1.18078600
H	-1.99246700	-0.30097700	1.27302800
H	5.14389600	1.83249700	-0.14941300
H	5.31934100	0.81543300	-1.59208100
H	6.38614400	0.57384100	-0.20235600
H	-1.21753800	1.98063500	-0.60014300

H	-1.51569600	2.13645700	1.13717400
H	0.39774100	0.71060900	1.67383700
H	0.96971600	1.94080600	0.54650700
H	0.83423500	0.36968000	-1.32575700
H	-4.25428400	-0.76229700	1.17010600
H	-3.96758300	-1.34748100	-0.47869300
H	-6.34909100	-0.70927700	-0.17288500
H	-5.57608800	0.34329100	-1.36647400
H	-5.86814100	0.93375200	0.27913800

2B

N	0.29752200	0.90447400	0.31497900
O	1.58927900	0.74827700	-0.21609400
O	-2.90261200	-0.49358700	-0.24627300
C	-4.23793700	-0.39892800	0.28107600
C	2.19710700	-0.49048200	0.17762000
C	-5.17497800	-1.00073700	-0.73326200
O	-2.08206500	0.52021400	1.57489800
O	3.47231100	-0.50361400	-0.33142300
C	1.40741000	-1.65389800	-0.37540000
C	-0.03983300	-1.56069600	0.09279200
C	-0.58284000	-0.15251100	-0.17889300
C	-1.92853400	0.02123400	0.48708400
C	4.38188700	0.39424500	0.29717000
C	5.76097400	0.13715100	-0.25647300
H	0.37044300	0.84278200	1.32977600
H	-4.46237900	0.65333300	0.46179500
H	-4.27887000	-0.92895200	1.23423900
H	2.21128700	-0.51213100	1.28169600
H	-4.93727800	-2.05015000	-0.91493100
H	-5.12362000	-0.45994400	-1.67928900
H	-6.19815100	-0.94110700	-0.35842800
H	1.46502500	-1.61282400	-1.46590000
H	1.86083100	-2.58902100	-0.04411200
H	-0.09520600	-1.75921300	1.16806000
H	-0.65840300	-2.30329900	-0.41238600
H	-0.70237800	-0.00159500	-1.25282700
H	4.36025400	0.22589800	1.38121100
H	4.07549900	1.42676300	0.10883100
H	6.47848700	0.81589500	0.20813100
H	5.78145000	0.30387700	-1.33484200
H	6.07621800	-0.88843400	-0.05648300
N	-2.01777300	2.87034000	-0.74288100
H	-1.87755000	3.69648700	-1.31174600
H	-1.10164000	2.55270100	-0.43514000
H	-2.51710600	3.16264000	0.08851100

3B

N	0.28761300	1.49621500	0.50045900
O	1.27391500	0.76578500	-0.19033600
O	-2.47135500	-0.77764200	0.09391200
C	-3.39121900	-1.22550800	-0.91588900
C	1.89463500	-0.23531500	0.62771900
C	-4.19083400	-2.36224200	-0.33438400
O	-1.63461000	0.73695700	-1.31857100
O	2.86767100	-0.83814200	-0.13187700
C	0.87107600	-1.25811300	1.06372600
C	-0.26999100	-0.55454300	1.78850900
C	-0.78393800	0.62187300	0.95481400
C	-1.64708200	0.21385400	-0.23733500

C	4.01741800	-0.03677900	-0.38360000
C	5.00738200	-0.85944300	-1.16941200
H	0.73826700	1.91131700	1.31407600
H	-2.82385100	-1.53943100	-1.79338900
H	-4.02978600	-0.38870500	-1.20398500
H	2.33601200	0.27725700	1.50182000
H	-4.75083200	-2.03913900	0.54469700
H	-3.54188100	-3.19280100	-0.05178200
H	-4.90177800	-2.72279400	-1.07970900
H	0.50794500	-1.77432800	0.17081100
H	1.34741600	-1.99515500	1.71163500
H	0.09251500	-0.15296700	2.73881800
H	-1.07641500	-1.24834600	2.01719400
H	-1.43461600	1.24983800	1.57173300
H	4.44875300	0.28174200	0.57385000
H	3.73161400	0.85884800	-0.94150200
H	5.90345700	-0.26873700	-1.36825800
H	4.58041800	-1.16712800	-2.12544800
H	5.29950000	-1.75307500	-0.61484300
N	-1.82992300	3.81725900	-0.14528400
H	-1.47072800	4.75422400	-0.28410000
H	-1.04462700	3.17580100	-0.23191700
H	-2.44487500	3.62088300	-0.92583100

TS2

N	-0.26850900	0.74571800	-1.07107700
O	-1.52710400	0.72753700	-0.38632000
O	2.95611500	-0.49911800	-0.06067600
C	4.31341300	-0.08645800	0.01939000
C	-2.02074700	-0.60525800	-0.24325500
C	5.12810400	-1.27286100	0.47695000
O	2.43622000	1.56006700	-0.82405800
O	-3.24605600	-0.52979300	0.38763000
C	-1.07400600	-1.45597700	0.57446000
C	0.32969700	-1.42491000	-0.03560000
C	0.71070600	0.00357000	-0.32368600
C	2.04527300	0.44400800	-0.46836900
C	-4.29903400	-0.00032900	-0.40749300
C	-5.59248600	-0.14246500	0.35626000
H	-0.46758600	0.31311700	-1.97327500
H	4.40916700	0.74678100	0.72178200
H	4.65378100	0.26798900	-0.95641900
H	-2.13480800	-1.02405400	-1.25963900
H	5.04049500	-2.10024400	-0.22984200
H	4.79898500	-1.62076900	1.45822200
H	6.18128500	-0.99339900	0.54748100
H	-1.05510900	-1.05325300	1.59124600
H	-1.46907500	-2.47334200	0.62005000
H	0.32715400	-2.03245000	-0.95442300
H	1.03846400	-1.89408700	0.64580700
H	0.57494100	1.17079300	0.90453400
H	-4.34705800	-0.55109900	-1.35536100
H	-4.10074500	1.04983100	-0.64049200
H	-6.41797800	0.26064800	-0.23334000
H	-5.54765800	0.40445700	1.29983300
H	-5.80378500	-1.19115300	0.57332200
N	0.41481400	2.17658900	1.37639600
H	-0.58464300	2.34548900	1.43876000
H	0.83893900	2.85212200	0.74554900
H	0.84220000	2.24101700	2.29442400

Table S4. Gas-phase Cartesian coordinates and energies of the **1** to **13** oxazinane ring conformers studied at the ωB97XD/Def2-TZVP level of theory.

1

N	0.25431000	-0.52768500	0.88328700
O	0.56783800	-0.71381500	-0.50205900
O	-2.44063200	-0.41778900	0.34289900
C	-3.69645600	-0.52275200	-0.34017900
C	1.54872500	0.22273700	-0.90813200
C	-4.21193900	-1.92658100	-0.14315100
O	-2.24402600	1.70569100	-0.33348300
O	2.73609800	0.11963000	-0.20134700
C	1.02091900	1.64084500	-0.76307000
C	0.44429600	1.86880500	0.63169200
C	-0.48123400	0.72058800	1.01976300
C	-1.80317200	0.75217100	0.24746100
C	3.34213300	-1.15692200	-0.24223500
C	4.69703400	-1.06006100	0.41839700
H	-0.36970200	-1.30698300	1.05257300
H	-3.53987600	-0.29183800	-1.39494000
H	-4.38124300	0.22381500	0.06585100
H	1.70126900	-0.04580800	-1.96192400
H	-4.35972200	-2.14341400	0.91532900
H	-3.51494000	-2.65736400	-0.55436900
H	-5.16934100	-2.03970800	-0.65335900
H	1.82656000	2.34509300	-0.96952200
H	0.24194700	1.79025000	-1.51240300
H	-0.09831400	2.81212100	0.66627700
H	1.25037500	1.90521000	1.36478900
H	-0.74659400	0.80079400	2.07889400
H	3.43987900	-1.48359500	-1.28704500
H	2.70961000	-1.88377400	0.27528100
H	5.18996200	-2.03349900	0.40952300
H	4.59112700	-0.73631200	1.45438000
H	5.33276600	-0.34390600	-0.10369100

Sum of electronic and zero-point Energies=	-708.588117
Sum of electronic and thermal Energies=	-708.573335
Sum of electronic and thermal Enthalpies=	-708.572390
Sum of electronic and thermal Free Energies=	-708.631542

2

N	-0.71060000	1.27078500	0.47992700
O	-0.96805200	0.76605200	-0.83820300
O	2.57093500	-0.17283100	0.25889900
C	3.82358400	0.04900900	-0.40544600
C	-1.47307400	-0.55034200	-0.77545400
C	4.62869900	-1.22244700	-0.30364600
O	1.92886300	1.90479500	-0.26396100
O	-2.65155400	-0.66240600	-0.05363400
C	-0.44356400	-1.48213400	-0.15619800
C	0.04678000	-0.92298100	1.17478900
C	0.42393400	0.54959700	1.03389500
C	1.70821200	0.84280600	0.25242700
C	-3.70197400	0.17171100	-0.50217800
C	-4.95095700	-0.18307800	0.26952400
H	-0.41372900	2.21700400	0.26577700
H	4.32883000	0.89101800	0.07065700
H	3.62515400	0.32463400	-1.44225500

H	-1.64472500	-0.78348300	-1.83478500
H	4.10844000	-2.05229600	-0.78298700
H	4.81402100	-1.48469200	0.73841700
H	5.59039000	-1.08716400	-0.80023500
H	-0.88318600	-2.47075900	-0.02518900
H	0.39072100	-1.57408400	-0.85489100
H	0.89446500	-1.49702100	1.54449100
H	-0.75391000	-0.98471000	1.91239800
H	0.59277800	0.97380300	2.02941500
H	-3.85371900	0.02274800	-1.58035000
H	-3.43351900	1.22006700	-0.34563200
H	-5.78153500	0.44862000	-0.04937800
H	-4.79243700	-0.03080900	1.33772000
H	-5.22520500	-1.22609300	0.10625800

Sum of electronic and zero-point Energies= -708.587640
Sum of electronic and thermal Energies= -708.572886
Sum of electronic and thermal Enthalpies= -708.571941
Sum of electronic and thermal Free Energies= -708.631024

3

N	0.42984800	0.06384000	1.23284900
O	1.53278000	-0.80582600	1.37925300
O	-2.88858600	-0.11199800	0.09458200
C	-3.99649300	0.75746400	-0.18163600
C	2.15117600	-1.15042600	0.15097900
C	-5.23633200	-0.09581200	-0.28131800
O	-1.50552200	1.65165400	0.10481200
O	2.65912500	-0.03531200	-0.50826000
C	1.17545700	-1.85361000	-0.77419300
C	-0.07448500	-1.00592000	-0.96952400
C	-0.59664600	-0.55131900	0.40158800
C	-1.69390200	0.46913600	0.20427600
C	3.72716300	0.61156900	0.16456100
C	4.16439600	1.79520000	-0.66468800
H	0.76925900	0.90388600	0.76983300
H	-3.79726400	1.29673100	-1.10935800
H	-4.07235600	1.49338100	0.62027100
H	2.96217200	-1.81809900	0.46561100
H	-5.41849700	-0.62813100	0.65258900
H	-5.14309300	-0.82691400	-1.08495700
H	-6.09964100	0.53712700	-0.49070500
H	1.66410600	-2.05807300	-1.72701600
H	0.91419600	-2.81009400	-0.31578500
H	-0.84656700	-1.56881700	-1.49675800
H	0.16630500	-0.12287100	-1.56597600
H	-0.99612000	-1.40800600	0.94724300
H	4.55358900	-0.09910500	0.29672900
H	3.40353900	0.93021300	1.16016900
H	4.99191700	2.31020900	-0.17472400
H	3.34289200	2.50216200	-0.78665000
H	4.49225300	1.47368300	-1.65382700

Sum of electronic and zero-point Energies= -708.589640
Sum of electronic and thermal Energies= -708.574765
Sum of electronic and thermal Enthalpies= -708.573821
Sum of electronic and thermal Free Energies= -708.633413

4

N	-0.14778500	-0.50514500	1.55639600
O	0.67486200	0.27266000	0.69091800

O	-2.38697700	0.40685200	0.26048700
C	-3.24488200	1.18418400	-0.58518300
C	1.73033300	-0.57203400	0.23537200
C	-3.69972700	2.38761600	0.20219800
O	-2.06086200	-1.05415600	-1.40271100
O	2.61437800	0.20258800	-0.47605200
C	1.15183100	-1.64243400	-0.66764700
C	0.01676100	-2.38190900	0.04103300
C	-0.93482700	-1.40167500	0.71992300
C	-1.83503900	-0.67928900	-0.28530000
C	3.38531800	1.09844700	0.30828200
C	4.36280600	1.80317500	-0.60167000
H	-0.75155300	0.19568300	1.96839100
H	-4.08438600	0.56251000	-0.90132600
H	-2.68677800	1.46987800	-1.47792200
H	2.20329900	-1.00988500	1.12937100
H	-2.84765300	2.99488500	0.50894700
H	-4.25178400	2.08615100	1.09307500
H	-4.35532500	3.00245700	-0.41575800
H	0.78162500	-1.14869800	-1.56806600
H	1.93867200	-2.33740000	-0.96341900
H	0.42453600	-3.03267700	0.81732600
H	-0.53063700	-3.00177700	-0.66690500
H	-1.60361000	-1.94477900	1.39547100
H	3.91563200	0.53385500	1.08652600
H	2.72814800	1.81742100	0.80537800
H	4.97520900	2.49913100	-0.02629000
H	3.83163100	2.36450100	-1.37093300
H	5.02081100	1.08471200	-1.09181700

Sum of electronic and zero-point Energies=	-708.588265
Sum of electronic and thermal Energies=	-708.573463
Sum of electronic and thermal Enthalpies=	-708.572519
Sum of electronic and thermal Free Energies=	-708.631842

5

N	0.14012000	-0.44761300	1.17698200
O	1.46829600	-0.91013000	1.32644300
O	-2.08795300	0.48304400	0.07216300
C	-3.38933300	1.05376700	-0.12073500
C	2.19306900	-0.93388300	0.10809000
C	-3.23836800	2.55452000	-0.10871500
O	-2.96229200	-1.57706800	-0.03205200
O	2.30818700	0.33690500	-0.45031900
C	1.53400700	-1.84947100	-0.90713800
C	0.07073100	-1.47191200	-1.09885300
C	-0.59413600	-1.33276700	0.27747600
C	-2.01820800	-0.85010300	0.10941100
C	3.09279900	1.24331100	0.30766300
C	3.11107500	2.57212500	-0.40921500
H	0.20382900	0.47628600	0.75647900
H	-4.04611100	0.70424300	0.67724200
H	-3.79412200	0.69190000	-1.06737500
H	3.17533200	-1.31234600	0.41466400
H	-2.57708700	2.88631100	-0.90989900
H	-2.83072900	2.89629800	0.84305000
H	-4.21354500	3.02137700	-0.25290000
H	2.08110900	-1.79710000	-1.84859100
H	1.60963300	-2.87146300	-0.52911300
H	-0.45101600	-2.22577500	-1.69025800
H	-0.00126800	-0.51905500	-1.62882500

H	-0.64999100	-2.31035600	0.75832900
H	4.10952400	0.84219100	0.41036900
H	2.67585300	1.34767000	1.31409100
H	3.71667500	3.28933900	0.14656300
H	2.10068900	2.97303500	-0.50041600
H	3.53066400	2.46520100	-1.41005300

Sum of electronic and zero-point Energies= -708.588636
Sum of electronic and thermal Energies= -708.573782
Sum of electronic and thermal Enthalpies= -708.572838
Sum of electronic and thermal Free Energies= -708.632315

6

N	-0.32455200	-1.94369600	-0.36923500
O	-1.05817200	-0.75205300	-0.64763100
O	2.42630500	0.26617600	0.14927700
C	3.31399600	1.10176800	-0.60851100
C	-1.66463900	-0.32451000	0.56663500
C	3.90280200	2.12022200	0.33542800
O	1.91884200	-0.87539400	-1.70609000
O	-2.50098000	0.72683600	0.27668300
C	-0.58185800	0.13894800	1.52029500
C	0.46703000	-0.95791200	1.69449200
C	0.87984300	-1.55214100	0.35006200
C	1.78123700	-0.68074400	-0.52865500
C	-3.67156200	0.37345900	-0.44332100
C	-4.52283600	1.61083100	-0.59895900
H	-0.06177100	-2.25012100	-1.29998600
H	2.74734100	1.57130000	-1.41378500
H	4.08236500	0.47480200	-1.06396000
H	-2.22054200	-1.18385800	0.97620700
H	4.46153400	1.63397300	1.13573000
H	3.12040400	2.73480300	0.78162800
H	4.58373800	2.77413500	-0.21087800
H	-0.13335800	1.03822400	1.09289500
H	-1.02446300	0.40636300	2.48066200
H	0.04796200	-1.77267400	2.28928900
H	1.33740200	-0.57568100	2.22463400
H	1.44628200	-2.47324700	0.52184000
H	-4.21405500	-0.40546600	0.10862300
H	-3.39750300	-0.03636000	-1.41915000
H	-5.43509700	1.37084300	-1.14720400
H	-3.98100000	2.37992800	-1.15026000
H	-4.79941100	2.01485400	0.37564500

Sum of electronic and zero-point Energies= -708.587874
Sum of electronic and thermal Energies= -708.573093
Sum of electronic and thermal Enthalpies= -708.572149
Sum of electronic and thermal Free Energies= -708.631488

7

N	-0.08574900	0.30195700	-0.64214900
O	-1.20281300	0.01809600	-1.48651800
O	2.54529800	0.31378100	-0.20739300
C	3.81849700	0.66237000	0.35452200
C	-2.21289400	-0.64382100	-0.75003700
C	4.35811100	1.83720700	-0.42240700
O	2.31506700	-1.32065700	1.30571000
O	-2.69874900	0.09798500	0.31407800

C	-1.69851600	-1.97094900	-0.21391800
C	-0.38181200	-1.78574000	0.53406100
C	0.56942300	-0.96255600	-0.32124200
C	1.88884200	-0.69321500	0.37753800
C	-3.20571700	1.37182900	-0.03184500
C	-3.84148300	1.97808100	1.19682400
H	0.50815800	0.85099400	-1.25018100
H	4.47791800	-0.20489200	0.29240900
H	3.68094300	0.90092000	1.41018700
H	-2.99282200	-0.78990800	-1.50921600
H	3.68651800	2.69317000	-0.34984400
H	4.48636600	1.58346600	-1.47514900
H	5.32890600	2.12726600	-0.01857100
H	-2.45635700	-2.41356100	0.43218700
H	-1.55198900	-2.63869400	-1.06654200
H	0.06927200	-2.74822700	0.77220300
H	-0.55177300	-1.25672500	1.47240900
H	0.81437300	-1.52224200	-1.23934100
H	-3.94193800	1.26655700	-0.84104800
H	-2.39420700	2.00518900	-0.40102200
H	-4.23779500	2.96795800	0.96510400
H	-3.10415100	2.07919800	1.99389300
H	-4.65830400	1.35295600	1.55956600

Sum of electronic and zero-point Energies=	-708.586903
Sum of electronic and thermal Energies=	-708.572063
Sum of electronic and thermal Enthalpies=	-708.571119
Sum of electronic and thermal Free Energies=	-708.630593

8

N	0.54081300	-0.60566700	-0.97838100
O	1.63484300	0.14562500	-1.50028900
O	-2.72563400	0.11926400	0.19489100
C	-3.96841400	-0.56614000	0.40829600
C	2.17016600	0.97234400	-0.48568100
C	-4.84282500	0.32334300	1.25633700
O	-1.97274900	-1.61776000	-0.99936500
O	2.65453300	0.26991400	0.60574100
C	1.12153600	1.95795700	0.00905100
C	-0.17862000	1.24714300	0.37907200
C	-0.56829500	0.31028100	-0.75867900
C	-1.81340300	-0.52193000	-0.53182300
C	3.63122900	-0.70570400	0.29808300
C	4.17404400	-1.25748800	1.59504200
H	0.31717400	-1.24623700	-1.72960800
H	-3.76262800	-1.52001000	0.89613700
H	-4.42215900	-0.77986600	-0.56098000
H	2.98741100	1.48462000	-1.01073500
H	-5.03605500	1.27247000	0.75556700
H	-4.37267300	0.52779000	2.21860400
H	-5.79834000	-0.17024700	1.43820800
H	1.52223000	2.50802100	0.86034300
H	0.93383200	2.67360300	-0.79530200
H	-0.97023900	1.97203300	0.56372300
H	-0.03881600	0.65723800	1.28621100
H	-0.77252700	0.91183300	-1.66100800
H	4.43300600	-0.24699100	-0.29738500
H	3.18272200	-1.50073500	-0.30383200
H	4.92765600	-2.02007300	1.39236600
H	3.37219500	-1.71158200	2.17818200
H	4.63107200	-0.46736800	2.19215900

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Sum of electronic and zero-point Energies=           -708.587137
Sum of electronic and thermal Energies=              -708.572308
Sum of electronic and thermal Enthalpies=            -708.571363
Sum of electronic and thermal Free Energies=         -708.630824
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9

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N                 -0.17140300   -1.09786400   -0.37048700
O                 -1.46589400   -0.65601700   -0.68326900
O                  3.09720400    0.16200100   -0.35269000
C                  4.41117900   -0.21447800    0.08723200
C                 -2.00373900    0.22845200    0.30133800
C                  5.40522900    0.66116100   -0.63385000
O                  2.19914400   -1.38872800    0.99307800
O                 -3.28821800    0.53751700   -0.06884900
C                 -1.17636200    1.49185400    0.37539700
C                  0.27320800    1.13230600    0.67683500
C                  0.74637100    0.03133900   -0.28411100
C                  2.07894300   -0.50399900    0.18798000
C                 -4.20837800   -0.54174200    0.00671700
C                 -5.58477100   -0.01232200   -0.31657900
H                 -0.20594100   -1.57989300    0.52632100
H                  4.56397600   -1.27178600   -0.13406500
H                  4.46803500   -0.08983900    1.16997600
H                 -1.99020900   -0.30657800    1.27071400
H                  5.23719200    1.71366400   -0.40371900
H                  5.33182700    0.52586200   -1.71317300
H                  6.41683700    0.39819700   -0.32206800
H                 -1.26179200    1.99940700   -0.58805300
H                 -1.58421400    2.15064500    1.14312300
H                  0.35733800    0.75906900    1.70260000
H                  0.91892500    2.00792000    0.59156600
H                  0.85688400    0.44332400   -1.28813800
H                 -4.18262600   -0.96617900    1.01940200
H                 -3.91664000   -1.32719000   -0.69479100
H                 -6.31705000   -0.81930100   -0.26365900
H                 -5.60538900    0.40669500   -1.32299700
H                 -5.87529300    0.76740900    0.38846100

Sum of electronic and zero-point Energies=           -708.586337
Sum of electronic and thermal Energies=              -708.571362
Sum of electronic and thermal Enthalpies=            -708.570417
Sum of electronic and thermal Free Energies=         -708.630225
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10

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N                 -0.18795100   -0.31366900    1.52030800
O                  0.75893300    0.34496000    0.71541400
O                 -2.48661300    0.38287400    0.26818700
C                 -3.39245300    1.08159800   -0.59463700
C                  1.76413500   -0.54386400    0.21483800
C                 -3.97726200    2.22895900    0.19094600
O                 -2.00234400   -1.03405900   -1.39029700
O                  2.67164900    0.20479000   -0.48988800
C                  1.14589800   -1.58674200   -0.68765500
C                  0.03061700   -2.31705700    0.05430000
C                 -0.89889600   -1.31625400    0.73784700
C                 -1.83770700   -0.64260500   -0.26516200
C                  3.45660600    1.09082400    0.29385200
C                  4.47481400    1.74421700   -0.60939200
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H	0.32614400	-0.77365600	2.26941100
H	-4.16211000	0.38743800	-0.93772800
H	-2.84330500	1.42806200	-1.47165600
H	2.24513500	-1.01759700	1.09400800
H	-3.19182300	2.90447500	0.53004800
H	-4.52193500	1.86634600	1.06317900
H	-4.66911200	2.78944000	-0.43939900
H	0.74956200	-1.07788800	-1.56760300
H	1.91789700	-2.28303000	-1.01781900
H	0.45901100	-2.96158000	0.82814200
H	-0.53167200	-2.95129000	-0.62922500
H	-1.54980000	-1.83392700	1.44997300
H	3.95288900	0.52232100	1.09217000
H	2.81365700	1.83927500	0.76382600
H	5.09740200	2.43171200	-0.03488600
H	3.97732700	2.30712700	-1.39961100
H	5.11887800	0.99547600	-1.07193000

Sum of electronic and zero-point Energies= -708.583241
Sum of electronic and thermal Energies= -708.568421
Sum of electronic and thermal Enthalpies= -708.567477
Sum of electronic and thermal Free Energies= -708.627101

11

N	-0.04423900	-0.72221900	0.16935000
O	0.63148200	-0.31408600	-1.00073100
O	-2.88795900	0.05265200	-0.27331500
C	-3.01896600	-1.21711300	0.37626100
C	1.67807200	0.61213800	-0.73323600
C	-4.27856200	-1.85968000	-0.15202200
O	-1.92726800	1.99952200	-0.51027900
O	2.64572900	0.05019700	0.09819700
C	1.14311000	1.87548600	-0.08955000
C	0.28265400	1.54855600	1.12725800
C	-0.69680900	0.41900700	0.81226000
C	-1.87556400	0.89487700	-0.04828400
C	3.39971800	-0.99302400	-0.49826500
C	4.39796900	-1.50048200	0.51469500
H	0.67559000	-1.07205000	0.79741100
H	-3.09514200	-1.06127300	1.45696300
H	-2.13982600	-1.82485300	0.16840900
H	2.09056400	0.80865100	-1.72900600
H	-4.20521800	-2.01456000	-1.22846900
H	-5.14907400	-1.23522900	0.04978300
H	-4.42534900	-2.82845700	0.32800300
H	1.98121400	2.51465900	0.18869300
H	0.54094300	2.40021500	-0.83010800
H	-0.25592700	2.43624300	1.45654600
H	0.91959800	1.21780400	1.95115700
H	-1.11055100	0.02343600	1.74496200
H	3.91234500	-0.60403100	-1.38731200
H	2.73271400	-1.79640700	-0.82686400
H	5.00259100	-2.29676900	0.07841600
H	3.88797600	-1.89901600	1.39288000
H	5.06161300	-0.69770500	0.83740200

Sum of electronic and zero-point Energies= -708.578504
Sum of electronic and thermal Energies= -708.563706
Sum of electronic and thermal Enthalpies= -708.562762
Sum of electronic and thermal Free Energies= -708.621862

12

N	-0.28781600	-0.35985300	-0.64123000
O	0.98455100	-0.70242800	-0.15754800
O	-3.28412600	-0.01579700	-0.18608900
C	-3.09263300	-1.25242900	0.51564300
C	1.85407200	0.43415700	-0.06290500
C	-4.29710300	-2.11780600	0.23644400
O	-2.52207000	1.89254600	-0.94118600
O	3.07612000	-0.01288500	0.36700100
C	1.30138000	1.44410900	0.91777000
C	-0.11743100	1.83680600	0.51768500
C	-0.93882100	0.57845500	0.27773400
C	-2.31035800	0.88490000	-0.32729200
C	3.79155000	-0.80386300	-0.57179900
C	5.15160700	-1.10950400	0.00757200
H	-0.15521800	0.09454200	-1.54480200
H	-3.00938000	-1.04487200	1.58608700
H	-2.17438000	-1.72850600	0.17031400
H	1.92772300	0.87287800	-1.07670500
H	-4.37825900	-2.32957000	-0.82968000
H	-5.21333200	-1.62601700	0.56354100
H	-4.19951300	-3.06355100	0.77134900
H	1.31794900	0.98366900	1.90857400
H	1.95677500	2.31544900	0.94255400
H	-0.11162100	2.43132000	-0.39844600
H	-0.58221600	2.45229900	1.28949500
H	-1.06158100	0.03929500	1.21978400
H	3.88577800	-0.24656400	-1.51333000
H	3.23894300	-1.72383500	-0.77853400
H	5.72835100	-1.71469100	-0.69334800
H	5.05281800	-1.66344400	0.94149800
H	5.70248600	-0.18986600	0.20772500

Sum of electronic and zero-point Energies=	-708.576196
Sum of electronic and thermal Energies=	-708.561345
Sum of electronic and thermal Enthalpies=	-708.560400
Sum of electronic and thermal Free Energies=	-708.619292

13

N	-0.20280800	-0.19854200	-0.78829800
O	0.99351000	-0.67310600	-0.19049700
O	-3.26065000	-0.06691600	-0.26431300
C	-3.12474300	-1.24619100	0.53082900
C	1.88154200	0.44250900	-0.08564900
C	-4.34296200	-2.10185500	0.28031500
O	-2.57965000	1.93200700	-0.84373500
O	3.08806800	-0.02328500	0.37423600
C	1.31016400	1.43910300	0.90340300
C	-0.12103400	1.81650200	0.52365800
C	-0.93187100	0.56131000	0.23453500
C	-2.31485900	0.88957200	-0.32514400
C	3.83521900	-0.77662300	-0.56889000
C	5.16380300	-1.13120500	0.05453900
H	-0.68835700	-1.05304100	-1.03185500
H	-3.05920100	-0.96746700	1.58565400
H	-2.21588900	-1.79270800	0.26579500
H	1.96925100	0.88084800	-1.09194200
H	-4.40596400	-2.38289900	-0.77095400

H	-5.25101800	-1.56270200	0.54901400
H	-4.28518300	-3.01039400	0.88119200
H	1.34106900	0.96909900	1.88966700
H	1.94647800	2.32425400	0.93486500
H	-0.13268300	2.43957500	-0.37103200
H	-0.59120700	2.38883600	1.32424600
H	-1.02716500	-0.02816900	1.15506900
H	3.97877000	-0.17732600	-1.47725200
H	3.28190100	-1.67834600	-0.84577000
H	5.76494500	-1.70864700	-0.64936100
H	5.01634700	-1.72899500	0.95450000
H	5.71579000	-0.23044100	0.32513700

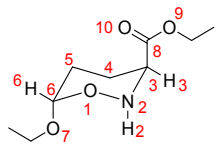
Sum of electronic and zero-point Energies= -708.572462
Sum of electronic and thermal Energies= -708.557532
Sum of electronic and thermal Enthalpies= -708.556587
Sum of electronic and thermal Free Energies= -708.615845

Table S5 Total energies, E_{tot}, Lewis energies, E_{Lewis} (in Hartrees) and electronic delocalization contribution to the AE for selected conformer pairs ($\Delta\Delta E_{deloc}$ in kcal/mol) of substituted oxazinane ring conformers bearing OEt and esteric CO_2Et substituents calculated at the ωB97XD/Def2-TZVP level of theory.

Conformer	E_{tot}	E_{Lewis}	Conformer pairs	ΔE_{total}[a]	ΔE_{Lewis}[b]	$\Delta\Delta E_{deloc}$
$\mathbf{9_{ax,ax}}$	-441.641791	-440.893193				
$\mathbf{9_{eq,eq}}$	-441.639565	-440.914015	$\mathbf{9_{eq,eq}}$ - $\mathbf{9_{ax,ax}}$	1.40	-13.07	14.47
$\mathbf{9_{ax,eq}}$	-441.639386	-440.903350	$\mathbf{9_{ax,eq}}$ - $\mathbf{9_{ax,ax}}$	1.51	-6.37	7.88
$\mathbf{9_{eq,ax}}$	-441.637843	-440.882866	$\mathbf{9_{eq,ax}}$ - $\mathbf{9_{ax,ax}}$	2.48	6.48	-4.00
$\mathbf{1_{ax,ax,eq}}$	-708.858604	-707.461685	$\mathbf{1_{eq,ax,eq}(A)}$ - $\mathbf{1_{ax,ax,eq}}$	2.37	2.52	-0.15
$\mathbf{2_{ax,ax,eq}(A)}$	-708.858604	-707.461685	$\mathbf{2_{ax,eq,eq}}$ - $\mathbf{2_{ax,ax,eq}(A)}$	1.77	-10.44	12.21
$\mathbf{2_{eq,eq,ax}(A)}$	-708.857231	-707.483943	$\mathbf{1_{ax,eq,eq}}$ - $\mathbf{2_{eq,eq,ax}(A)}$	0.91	5.73	-4.82
$\mathbf{1_{ax,eq,ax}(A)}$	-708.857209	-707.473984	$\mathbf{2_{eq,eq,ax}(B)}$ - $\mathbf{1_{ax,eq,ax}(A)}$	0.21	-4.10	4.31
$\mathbf{2_{eq,eq,ax}(B)}$	-708.856877	-707.480512	$\mathbf{2_{eq,eq,ax}(B)}$ - $\mathbf{2_{eq,ax,ax}}$	-9.21	-29.03	19.82
$\mathbf{1_{ax,eq,ax}(B)}$	-708.856777	-707.470878	$\mathbf{1_{ax,eq,eq}}$ - $\mathbf{1_{ax,eq,ax}(B)}$	0.48	-2.46	2.94
$\mathbf{1_{ax,eq,eq}}$	-708.856020	-707.474806	$\mathbf{1_{eq,eq,eq}}$ - $\mathbf{1_{ax,eq,eq}}$	0.16	-11.04	11.20
$\mathbf{1_{eq,eq,eq}}$	-708.855769	-707.492398	$\mathbf{1_{eq,eq,eq}}$ - $\mathbf{1_{ax,ax,ax}}$	-5.24	-26.04	20.80
$\mathbf{2_{ax,eq,eq}}$	-708.855781	-707.478327	$\mathbf{2_{ax,eq,eq}}$ - $\mathbf{2_{ax,ax,eq}(A)}$	1.77	-10.44	12.21
$\mathbf{1_{eq,ax,eq}(A)}$	-708.854828	-707.457675	$\mathbf{1_{eq,eq,eq}}$ - $\mathbf{1_{eq,ax,eq}(A)}$	-0.59	-21.79	21.20
$\mathbf{1_{eq,ax,eq}(B)}$	-708.853421	-707.463525	$\mathbf{1_{eq,ax,eq}(A)}$ - $\mathbf{1_{eq,ax,eq}(B)}$	-0.88	3.67	-4.55
$\mathbf{2_{ax,ax,eq}(B)}$	-708.848773	-707.454249	$\mathbf{2_{ax,ax,eq}(B)}$ - $\mathbf{1_{ax,ax,ax}}$	-0.85	-2.10	1.25
$\mathbf{1_{ax,ax,ax}}$	-708.847411	-707.450900	$\mathbf{2_{ax,ax,eq}(C)}$ - $\mathbf{1_{ax,ax,ax}}$	0.25	18.82	-18.57
$\mathbf{2_{ax,ax,eq}(C)}$	-708.847012	-707.420909	$\mathbf{1_{eq,ax,eq}(C)}$ - $\mathbf{2_{ax,ax,eq}(C)}$	1.34	-15.71	17.05
$\mathbf{1_{eq,ax,eq}(C)}$	-708.844877	-707.445944	$\mathbf{1_{eq,ax,eq}(C)}$ - $\mathbf{1_{ax,eq,eq}}$	6.99	18.11	-11.12
$\mathbf{2_{eq,ax,ax}}$	-708.842197	-707.434244	$\mathbf{2_{ax,eq,eq}}$ - $\mathbf{2_{eq,ax,ax}}$	-8.52	-27.66	19.14

[a] $\Delta E_{total} = (E_{total})_{eq} - (E_{total})_{ax}$. [b] $\Delta E_{Lewis} = (E_{Lewis})_{eq} - (E_{Lewis})_{ax}$.

Table S6 Predominant hyperconjugative interactions (in kcal/mol) contributing to the AE in the substituted oxazinane ring conformers bearing the OEt^- and esteric C(O)OEt substituents respectively calculated at the ωB97XD/Def2-TZVP level of theory



Conformer	LP(O_1) → σ^*(C_6-O_7)	LP(O_1) → σ^*(C_6-C_5)	LP(O_1) → σ^*(C_6-H_6)	LP(O_1) → σ^*(N_2-H_2)	LP(O_1) → σ^*(C_3-N_2)	LP(O_7) → σ^*(C_6-O_1)	LP(O_7) → σ^*(C_6-H_6)	LP(N_2) → σ^*(C_3-C_4)	LP(N_2) → σ^*(C_6-O_1)	LP(N_2) → σ^*(C_3-C_8)	LP(O_{10}) → σ^*(C_3-C_8)	LP(O_{10}) → σ^*(C_8-O_9)	LP(O_9) → σ^*(C_8-O_{10})
$9_{ax,ax}$	16.84	9.13	2.39	5.63	6.26	19.36	9.59	9.05	7.29				
$9_{eq,eq}$	2.61	8.59	7.87	1.70	6.17	20.18	10.34						
$9_{ax,eq}$	16.49	9.23	2.11	1.45	5.82	19.51	11.54						
$9_{eq,ax}$	2.79	8.82	9.36	6.25	6.72	20.28	11.49	9.24	6.98				
$1_{ax,ax,eq}$	16.38	9.01	2.41	6.03	6.76	19.90	9.95	9.94	7.63	0.72	29.35	45.91	83.48
$2_{ax,ax,eq}$(A)	16.38	9.02	2.39	5.76	6.66	19.75	9.74	9.66	7.41	0.93	28.74	47.35	80.62
$2_{eq,eq,ax}$(A)	2.61	8.21	7.53	1.58	6.59	20.64	10.36			10.35	30.77	46.17	80.09
$1_{ax,eq,ax}$(A)	16.21	9.20	2.20	1.32	4.55	19.62	11.58	0.58		9.38	29.87	45.84	81.37
$2_{eq,eq,ax}$(B)	2.72	8.48	7.70	1.05	6.52	20.32	10.47			9.04	29.85	45.77	82.17
$1_{ax,eq,ax}$(B)	15.77	8.85	2.11	1.31	6.30	20.01	11.52			10.51	30.58	46.17	79.89
$1_{ax,eq,eq}$	16.11	9.08		1.37	2.13	19.88	11.67	1.46			29.41	45.35	83.05
$1_{eq,eq,eq}$	2.57	8.35	7.63	1.68	6.61	20.59	10.34	1.27		8.51	30.11	46.55	79.80
$2_{ax,eq,eq}$	15.97	8.99				20.01	11.60	1.22				46.57	79.65
$1_{eq,ax,eq}$(A)	2.79	8.72	8.99	7.45		20.58	11.39	10.10	7.28	3.30	29.16	45.62	84.61
$1_{eq,ax,eq}$(B)	8.71	8.71	9.05	6.31	7.20	20.64	11.50	9.85	7.10		28.84	47.57	80.15
$2_{ax,ax,eq}$(B)	15.75	8.68		5.78	7.00	20.38	9.76	8.57	7.11	1.05	30.91	43.60	72.25
$1_{ax,ax,ax}$	25.54	8.49	2.29	5.85	7.47	19.94	9.28	8.67	7.12	2.54	31.51	43.17	70.30
$2_{ax,ax,eq}$(C)	17.75	8.72		6.37	7.01	19.98	6.40	10.67	7.49	0.61	28.65	45.72	85.24
$1_{eq,ax,eq}$(C)	2.66	8.37	8.71	6.40	7.56	21.21	11.30	8.83	6.88	0.89	30.79	43.45	72.96
$2_{eq,ax,ax}$	2.61	8.15	8.46	6.49	7.95	21.31	11.48	8.84	6.88		31.90	43.30	70.17

Table S7. Gas-phase Cartesian coordinates and energies of the cyclohexane conformers calculated at the ωB97XD/Def2-TZVP level of theory.

5_{ax}

C	-1.311486000	1.374841000	-0.453818000
C	-0.608766000	1.139558000	0.880062000
H	-2.819786000	0.448631000	-1.697998000
H	-0.567996000	1.369066000	-1.256409000
C	0.029815000	-0.249957000	0.943737000
H	-1.779433000	2.361767000	-0.460342000
H	-1.333980000	1.209419000	1.697439000
O	1.056775000	-0.423592000	-0.015982000
C	-1.010435000	-1.328983000	0.671067000
C	-1.730883000	-1.102857000	-0.656655000
C	-2.352393000	0.290325000	-0.723460000
H	0.139124000	1.912839000	1.067693000
C	2.211035000	0.351863000	0.185968000
C	3.293718000	-0.147649000	-0.743783000
H	0.459092000	-0.400979000	1.945231000
H	-0.520540000	-2.304364000	0.682257000
H	-1.735657000	-1.318521000	1.491029000
H	-2.498718000	-1.867285000	-0.795310000
H	-1.013526000	-1.219017000	-1.473055000
H	-3.150413000	0.366736000	0.024497000
H	2.536740000	0.272238000	1.233628000
H	2.009896000	1.412796000	-0.012237000
H	4.202941000	0.442696000	-0.618661000
H	2.969725000	-0.067117000	-1.782164000
H	3.524700000	-1.193015000	-0.536458000

Sum of electronic and zero-point Energies= -389.512112

Sum of electronic and thermal Energies= -389.502648
Sum of electronic and thermal Enthalpies= -389.501704
Sum of electronic and thermal Free Energies= -389.546976

5_{eq}

C	1.918434000	1.344101000	0.170458000
C	0.469961000	1.158730000	-0.277790000
H	1.948455000	1.446289000	1.261128000
H	2.317866000	2.274137000	-0.239520000
C	-0.108223000	-0.154683000	0.245812000
H	0.415208000	1.139642000	-1.371406000
H	-0.133514000	2.003421000	0.060827000
O	-1.412793000	-0.407881000	-0.230455000
C	0.758147000	-1.332653000	-0.170583000
C	2.206893000	-1.151700000	0.273842000
C	2.787724000	0.160909000	-0.244385000
H	3.808599000	0.294655000	0.120506000
C	-2.421046000	0.410890000	0.309169000
C	-3.763660000	-0.128723000	-0.129001000
H	-0.134477000	-0.108528000	1.347779000
H	0.334183000	-2.250098000	0.241718000
H	0.710675000	-1.419189000	-1.260976000
H	2.808159000	-1.996536000	-0.068348000
H	2.254424000	-1.157766000	1.368546000
H	2.844713000	0.122482000	-1.337742000
H	-2.307225000	1.448545000	-0.029766000
H	-2.349255000	0.416247000	1.406805000
H	-4.569037000	0.490075000	0.270148000
H	-3.899985000	-1.150769000	0.226031000
H	-3.835830000	-0.130787000	-1.217228000

Sum of electronic and zero-point Energies= -389.512560

Sum of electronic and thermal Energies= -389.503005
Sum of electronic and thermal Enthalpies= -389.502060
Sum of electronic and thermal Free Energies= -389.547553

6_{ax}

C	1.115345000	1.414647000	0.170867000
O	0.502102000	0.907571000	-1.004752000
H	2.700216000	0.952682000	1.541915000
H	0.372943000	1.486597000	0.975205000
C	0.017508000	-0.406029000	-0.877139000
H	1.441553000	2.423251000	-0.081936000
O	-1.020741000	-0.497420000	0.055490000
C	1.109460000	-1.376298000	-0.453006000
C	1.815200000	-0.892054000	0.810106000
C	2.280776000	0.548356000	0.617770000
C	-2.178985000	0.237538000	-0.286159000
C	-3.225047000	0.002190000	0.777952000
H	-0.361008000	-0.649490000	-1.877488000
H	0.667751000	-2.363070000	-0.309988000
H	1.826250000	-1.445816000	-1.275247000
H	2.658831000	-1.543963000	1.043865000
H	1.123050000	-0.943621000	1.654337000
H	3.065655000	0.586783000	-0.143657000
H	-2.543777000	-0.091574000	-1.268958000
H	-1.938758000	1.302580000	-0.366573000
H	-4.135254000	0.554748000	0.539802000
H	-2.862979000	0.337513000	1.750757000
H	-3.470903000	-1.057920000	0.849726000

Sum of electronic and zero-point Energies= -425.444476
Sum of electronic and thermal Energies= -425.435301
Sum of electronic and thermal Enthalpies= -425.434357

Sum of electronic and thermal Free Energies= -425.478968

6_{eq}

C	2.284212000	1.037944000	0.243030000
C	0.842209000	1.357044000	-0.145392000
H	2.376484000	1.046931000	1.334707000
H	2.958198000	1.808352000	-0.134864000
C	-0.074642000	0.221545000	0.266488000
H	0.751801000	1.475583000	-1.227967000
H	0.499665000	2.280650000	0.323580000
O	-1.352329000	0.488218000	-0.174983000
O	0.352691000	-1.003869000	-0.292852000
C	1.646762000	-1.371716000	0.133340000
C	2.682348000	-0.338306000	-0.282848000
H	3.665496000	-0.631399000	0.092706000
C	-2.340369000	-0.413177000	0.291168000
C	-3.690450000	0.082354000	-0.170322000
H	-0.068051000	0.108711000	1.369610000
H	1.849839000	-2.345016000	-0.312999000
H	1.659121000	-1.492485000	1.228015000
H	2.738741000	-0.316917000	-1.374638000
H	-2.299040000	-0.461507000	1.388309000
H	-2.140561000	-1.416470000	-0.094732000
H	-4.475535000	-0.592517000	0.174330000
H	-3.727747000	0.127656000	-1.259229000
H	-3.891728000	1.079505000	0.223071000

Sum of electronic and zero-point Energies= -425.442951
Sum of electronic and thermal Energies= -425.433739
Sum of electronic and thermal Enthalpies= -425.432795
Sum of electronic and thermal Free Energies= -425.477433

Table S8. Gas-phase Cartesian coordinates and energies of the tetrahydro-*2H*-pyran conformers calculated at the ωB97XD/Def2-TZVP level of theory.

$7_{ax,ax}$

O	0.714498000	-0.740956000	-0.666426000
O	-2.596022000	-0.408977000	0.346830000
C	-3.850794000	-0.380808000	-0.343232000
C	1.644086000	0.297004000	-0.888710000
C	-4.535242000	-1.704413000	-0.106838000
O	-2.151016000	1.650452000	-0.397007000
O	2.790116000	0.147298000	-0.103827000
C	1.041977000	1.660148000	-0.595099000
C	0.412073000	1.707580000	0.794847000
C	-0.528681000	0.521589000	1.004216000
C	-1.824087000	0.676376000	0.226218000
C	3.549390000	-1.010847000	-0.390640000
C	4.780021000	-1.004133000	0.485220000
H	1.013682000	-0.926509000	1.369495000
H	-3.664797000	-0.203959000	-1.403817000
H	-4.442603000	0.455634000	0.033063000
H	1.903119000	0.198078000	-1.949407000
H	-4.711495000	-1.867970000	0.956811000
H	-3.931315000	-2.527892000	-0.489163000
H	-5.497474000	-1.716203000	-0.620541000
H	1.820905000	2.416642000	-0.692914000
H	0.279683000	1.862323000	-1.348295000
H	-0.125388000	2.645885000	0.927362000
H	1.195832000	1.660574000	1.553658000
H	-0.821419000	0.455625000	2.056950000
H	3.828503000	-1.009938000	-1.453116000

H	2.948984000	-1.908630000	-0.210961000
H	5.390282000	-1.885753000	0.283357000
H	4.499757000	-1.013282000	1.539399000
H	5.382076000	-0.114408000	0.297554000
C	0.201095000	-0.774498000	0.650780000
H	-0.467960000	-1.630744000	0.693424000

Sum of electronic and zero-point Energies= -692.589888
Sum of electronic and thermal Energies= -692.575072
Sum of electronic and thermal Enthalpies= -692.574128
Sum of electronic and thermal Free Energies= -692.633398

$7_{eq,eq}$

O	-1.581359000	0.987827000	-0.474627000
O	2.963088000	-0.389757000	-0.307378000
C	4.359717000	-0.120065000	-0.127634000
C	-2.055271000	0.291402000	0.659772000
C	5.119493000	-1.375010000	-0.479508000
O	2.482934000	1.700120000	0.335361000
O	-3.418846000	0.109908000	0.531007000
C	-1.252934000	-0.990090000	0.860028000
C	0.230560000	-0.663021000	0.996294000
C	0.685938000	0.185083000	-0.200146000
C	2.122153000	0.612275000	-0.028483000
C	-3.860066000	-0.729113000	-0.525081000
C	-5.336255000	-0.479172000	-0.728316000
H	-0.115135000	2.053226000	0.520166000
H	4.530513000	0.181668000	0.907263000
H	4.641801000	0.718263000	-0.766833000
H	-1.936595000	0.935253000	1.543430000
H	4.937355000	-1.663203000	-1.515220000

H	4.826101000	-2.202546000	0.167172000
H	6.189197000	-1.202824000	-0.353422000
H	-1.620792000	-1.507020000	1.748123000
H	-1.403894000	-1.646331000	-0.000228000
H	0.823866000	-1.575456000	1.062983000
H	0.401250000	-0.095152000	1.917152000
H	0.618964000	-0.427956000	-1.102652000
H	-3.688282000	-1.780783000	-0.266691000
H	-3.302552000	-0.505034000	-1.438484000
H	-5.722114000	-1.127862000	-1.516502000
H	-5.511325000	0.558520000	-1.013007000
H	-5.889591000	-0.683131000	0.189268000
C	-0.238013000	1.391156000	-0.346427000
H	0.002756000	1.964907000	-1.240416000

Sum of electronic and zero-point Energies= -692.584488
Sum of electronic and thermal Energies= -692.569430
Sum of electronic and thermal Enthalpies= -692.568486
Sum of electronic and thermal Free Energies= -692.628815

$8_{eq,ax}$

O	0.824166000	-0.374188000	0.741307000
O	-2.565513000	-0.336786000	0.252915000
C	-3.462138000	-1.031678000	-0.622312000
C	1.798879000	0.523796000	0.237244000
C	-4.145663000	-2.109886000	0.181606000
O	-1.926600000	0.964004000	-1.448072000
O	2.724713000	-0.190514000	-0.487543000
C	1.157798000	1.565638000	-0.656194000
C	0.034551000	2.290947000	0.083060000
C	-0.929695000	1.298381000	0.731763000
C	-1.835534000	0.639473000	-0.295123000

C	3.518010000	-1.081783000	0.276110000
C	4.555818000	-1.692606000	-0.635350000
H	0.353833000	0.788151000	2.380018000
H	-2.889662000	-1.446201000	-1.453522000
H	-4.176847000	-0.317527000	-1.035328000
H	2.284609000	1.007338000	1.108747000
H	-4.710217000	-1.680570000	1.009982000
H	-3.417431000	-2.813861000	0.585447000
H	-4.837760000	-2.659902000	-0.457430000
H	1.921203000	2.271267000	-0.986418000
H	0.765431000	1.056565000	-1.537646000
H	-0.500485000	2.947872000	-0.601161000
H	0.459102000	2.916921000	0.873819000
H	-1.597302000	1.822769000	1.423236000
H	2.885518000	-1.855378000	0.720078000
H	3.998020000	-0.529182000	1.095798000
H	5.185202000	-2.385941000	-0.075249000
H	5.191028000	-0.920196000	-1.070497000
H	4.075102000	-2.240445000	-1.446411000
C	-0.135499000	0.271337000	1.541202000
H	-0.782639000	-0.503511000	1.945649000

Sum of electronic and zero-point Energies= -692.588074
Sum of electronic and thermal Energies= -692.573195
Sum of electronic and thermal Enthalpies= -692.572251
Sum of electronic and thermal Free Energies= -692.631815

$8_{ax,eq}$

O	-1.632146000	0.558420000	1.459122000
O	2.881595000	0.128751000	-0.004490000
C	4.043679000	-0.659031000	-0.291490000
C	-2.152790000	1.118577000	0.279033000

C	5.158260000	0.285684000	-0.667697000
O	1.729453000	-1.740585000	0.428480000
O	-2.689427000	0.153305000	-0.575047000
C	-1.088812000	1.880978000	-0.494150000
C	0.134463000	1.009545000	-0.754910000
C	0.616763000	0.395278000	0.567126000
C	1.775612000	-0.542522000	0.337133000
C	-3.793103000	-0.553510000	-0.041836000
C	-4.290038000	-1.521108000	-1.089624000
H	-0.849061000	-1.181679000	0.646587000
H	3.809091000	-1.352875000	-1.100680000
H	4.294531000	-1.252242000	0.589612000
H	-2.945417000	1.790738000	0.629443000
H	5.379551000	0.972305000	0.149964000
H	4.892387000	0.870509000	-1.548829000
H	6.061024000	-0.283817000	-0.892580000
H	-1.518521000	2.239305000	-1.429908000
H	-0.804376000	2.752138000	0.100926000
H	0.931981000	1.596100000	-1.211495000
H	-0.127727000	0.206612000	-1.448559000
H	0.967176000	1.204758000	1.214583000
H	-4.581721000	0.158919000	0.236490000
H	-3.494843000	-1.084626000	0.867494000
H	-5.145747000	-2.080600000	-0.708705000
H	-3.505809000	-2.230574000	-1.356593000
H	-4.595872000	-0.990067000	-1.991774000
C	-0.541950000	-0.321971000	1.248955000
H	-0.254959000	-0.685550000	2.234268000

Sum of electronic and zero-point Energies= -692.590130
Sum of electronic and thermal Energies= -692.575128
Sum of electronic and thermal Enthalpies= -692.574183

Sum of electronic and thermal Free Energies=   -692.634411

Table S9. Gas-phase Cartesian coordinates and energies of the oxazinane conformers calculated at the ωB97XD/Def2-TZVP level of theory.

$\mathbf{9_{ax,ax}}$

N	1.077801000	-1.447458000	-0.103451000
O	0.516923000	-0.859516000	1.059330000
C	0.038405000	0.455991000	0.844052000
O	-0.994843000	0.483437000	-0.093143000
C	1.143715000	1.383836000	0.369994000
C	1.849023000	0.799065000	-0.848744000
C	2.208724000	-0.656319000	-0.569095000
C	-2.182686000	-0.166773000	0.325954000
C	-3.205263000	-0.052612000	-0.779471000
H	0.340128000	-1.414994000	-0.804095000
H	-0.334839000	0.747887000	1.833112000
H	0.720530000	2.366157000	0.158028000
H	1.853854000	1.494076000	1.193194000
H	2.744959000	1.376258000	-1.086371000
H	1.188027000	0.850926000	-1.717664000
H	2.985218000	-0.720053000	0.197507000
H	-2.550070000	0.308457000	1.245092000
H	-1.973579000	-1.215585000	0.558720000
H	-4.136062000	-0.536906000	-0.480701000
H	-2.844006000	-0.534674000	-1.688924000
H	-3.414862000	0.993571000	-1.004945000
H	2.587943000	-1.153408000	-1.464431000

Sum of electronic and zero-point Energies= -441.444474
Sum of electronic and thermal Energies= -441.435394
Sum of electronic and thermal Enthalpies= -441.434450
Sum of electronic and thermal Free Energies= -441.478915

$\mathbf{9_{eq,eq}}$

N	1.637191000	-1.307736000	0.272890000
O	0.379242000	-0.985737000	-0.316055000
C	-0.071872000	0.223536000	0.283281000
O	-1.342967000	0.477252000	-0.176751000
C	0.847774000	1.359903000	-0.121736000
C	2.298345000	1.010006000	0.210891000
C	2.629247000	-0.392698000	-0.279970000
C	-2.340731000	-0.397650000	0.323312000
C	-3.680817000	0.067233000	-0.194747000
H	1.799487000	-2.247832000	-0.064936000
H	-0.060270000	0.072056000	1.375242000
H	0.724221000	1.507045000	-1.197577000
H	0.537980000	2.277023000	0.381423000
H	2.447297000	1.043760000	1.293467000
H	2.977208000	1.737845000	-0.236340000
H	3.606585000	-0.714331000	0.086113000
H	-2.320661000	-0.379942000	1.421109000
H	-2.132834000	-1.421870000	0.001497000
H	-4.472708000	-0.585096000	0.176596000
H	-3.697482000	0.044629000	-1.284865000
H	-3.888799000	1.086777000	0.132140000
H	2.637761000	-0.420005000	-1.377844000

Sum of electronic and zero-point Energies= -441.442394
Sum of electronic and thermal Energies= -441.433284
Sum of electronic and thermal Enthalpies= -441.432340
Sum of electronic and thermal Free Energies= -441.476865

$\mathbf{9}_{\mathbf{ax,eq}}$

N	1.022776000	-1.349912000	-0.263188000
O	0.519164000	-0.883416000	0.995743000
C	0.014575000	0.428085000	0.860573000

O	-1.035473000	0.529903000	-0.040533000
C	1.112287000	1.386933000	0.421787000
C	1.837000000	0.852426000	-0.810468000
C	2.230492000	-0.599454000	-0.579129000
C	-2.131234000	-0.321197000	0.228444000
C	-3.247965000	0.027230000	-0.727317000
H	1.259776000	-2.307774000	-0.038102000
H	-0.330494000	0.650494000	1.879398000
H	0.675068000	2.367503000	0.232912000
H	1.815940000	1.485752000	1.252170000
H	2.722116000	1.454975000	-1.021632000
H	1.177950000	0.905514000	-1.678630000
H	2.977129000	-0.666284000	0.225390000
H	-2.453892000	-0.187158000	1.270630000
H	-1.827941000	-1.364821000	0.106461000
H	-4.109501000	-0.618690000	-0.550445000
H	-2.920218000	-0.109306000	-1.758485000
H	-3.559343000	1.064658000	-0.598746000
H	2.653515000	-1.041511000	-1.483630000

Sum of electronic and zero-point Energies= -441.442065
Sum of electronic and thermal Energies= -441.433002
Sum of electronic and thermal Enthalpies= -441.432058
Sum of electronic and thermal Free Energies= -441.476445

$\mathbf{9}_{\mathbf{eq,ax}}$

N	1.641979000	-1.400337000	0.096677000
O	0.359338000	-1.004024000	-0.331583000
C	-0.062145000	0.223418000	0.263923000
O	-1.336966000	0.487513000	-0.172858000
C	0.858387000	1.356487000	-0.134269000
C	2.294520000	1.002079000	0.238872000

C	2.628416000	-0.394425000	-0.274125000
C	-2.329329000	-0.410637000	0.299605000
C	-3.676932000	0.086792000	-0.165496000
H	1.595718000	-1.481974000	1.111701000
H	-0.047990000	0.078811000	1.362932000
H	0.761398000	1.493807000	-1.213824000
H	0.531778000	2.276008000	0.353697000
H	2.408812000	1.023368000	1.328195000
H	2.992005000	1.736685000	-0.168396000
H	3.589115000	-0.742260000	0.111202000
H	-2.286943000	-0.449849000	1.396696000
H	-2.131243000	-1.415967000	-0.080276000
H	-4.463797000	-0.583049000	0.184529000
H	-3.714379000	0.123440000	-1.254608000
H	-3.874784000	1.087391000	0.220710000
H	2.689980000	-0.394242000	-1.364844000

Sum of electronic and zero-point Energies= -441.441014
Sum of electronic and thermal Energies= -441.431879
Sum of electronic and thermal Enthalpies= -441.430935
Sum of electronic and thermal Free Energies= -441.475479

$\mathbf{1}_{\mathbf{ax,ax,ax}}$

N	-0.044239000	-0.722219000	0.169350000
O	0.631482000	-0.314086000	-1.000731000
O	-2.887959000	0.052652000	-0.273315000
C	-3.018966000	-1.217113000	0.376261000
C	1.678073000	0.612138000	-0.733236000
C	-4.278562000	-1.859680000	-0.152022000
O	-1.927267000	1.999522000	-0.510279000
O	2.645729000	0.050197000	0.098197000
C	1.143110000	1.875486000	-0.089550000

C	0.282654000	1.548556000	1.127258000
C	-0.696809000	0.419007000	0.812260000
C	-1.875564000	0.894877000	-0.048284000
C	3.399718000	-0.993024000	-0.498265000
C	4.397969000	-1.500482000	0.514695000
H	0.675590000	-1.072050000	0.797411000
H	-3.095142000	-1.061273000	1.456963000
H	-2.139826000	-1.824853000	0.168409000
H	2.090564000	0.808651000	-1.729006000
H	-4.205218000	-2.014560000	-1.228469000
H	-5.149074000	-1.235229000	0.049783000
H	-4.425349000	-2.828457000	0.328003000
H	1.981214000	2.514659000	0.188693000
H	0.540943000	2.400215000	-0.830108000
H	-0.255927000	2.436243000	1.456546000
H	0.919598000	1.217804000	1.951157000
H	-1.110551000	0.023436000	1.744962000
H	3.912345000	-0.604031000	-1.387312000
H	2.732714000	-1.796407000	-0.826864000
H	5.002591000	-2.296769000	0.078416000
H	3.887976000	-1.899016000	1.392880000
H	5.061613000	-0.697705000	0.837402000

Sum of electronic and zero-point Energies= -708.578504
Sum of electronic and thermal Energies= -708.563706
Sum of electronic and thermal Enthalpies= -708.562762
Sum of electronic and thermal Free Energies= -708.621862

$\mathbf{1_{ax,eq,ax}(A)}$

N	-0.710600000	1.270767000	0.479957000
O	-0.968065000	0.766076000	-0.838186000

O	2.570933000	-0.172848000	0.258867000
C	3.823585000	0.049016000	-0.405464000
C	-1.473088000	-0.550319000	-0.775474000
C	4.628754000	-1.222400000	-0.303592000
O	1.928857000	1.904791000	-0.263938000
O	-2.651562000	-0.662405000	-0.053647000
C	-0.443574000	-1.482132000	-0.156256000
C	0.046781000	-0.923023000	1.174745000
C	0.423937000	0.549559000	1.033894000
C	1.708209000	0.842789000	0.252425000
C	-3.701985000	0.171727000	-0.502156000
C	-4.950960000	-0.183078000	0.269551000
H	-0.413730000	2.216992000	0.265835000
H	4.328786000	0.891071000	0.070608000
H	3.625162000	0.324583000	-1.442290000
H	-1.644749000	-0.783427000	-1.834810000
H	4.108535000	-2.052295000	-0.782897000
H	4.814075000	-1.484586000	0.738487000
H	5.590444000	-1.087100000	-0.800177000
H	-0.883197000	-2.470761000	-0.025276000
H	0.390705000	-1.574061000	-0.854959000
H	0.894468000	-1.497076000	1.544422000
H	-0.753903000	-0.984773000	1.912358000
H	0.592790000	0.973733000	2.029426000
H	-3.853743000	0.022793000	-1.580330000
H	-3.433525000	1.220079000	-0.345586000
H	-5.781540000	0.448629000	-0.049327000
H	-4.792428000	-0.030835000	1.337749000
H	-5.225211000	-1.226088000	0.106262000

Sum of electronic and zero-point Energies= -708.587640
Sum of electronic and thermal Energies= -708.572886

Sum of electronic and thermal Enthalpies= -708.571941
Sum of electronic and thermal Free Energies= -708.631024

$\mathbf{1_{ax,eq,ax}(B)}$

N	0.254020000	-0.528410000	0.882320000
O	0.568073000	-0.713341000	-0.503002000
O	-2.440705000	-0.417937000	0.342453000
C	-3.696291000	-0.522771000	-0.340944000
C	1.549120000	0.223302000	-0.908084000
C	-4.213030000	-1.925916000	-0.142167000
O	-2.243953000	1.705694000	-0.333782000
O	2.736424000	0.119622000	-0.201244000
C	1.021499000	1.641523000	-0.761980000
C	0.444345000	1.868401000	0.632848000
C	-0.481488000	0.720100000	1.019917000
C	-1.803241000	0.752128000	0.247193000
C	3.342142000	-1.157053000	-0.242286000
C	4.697086000	-1.060508000	0.418372000
H	-0.370171000	-1.307693000	1.051154000
H	-3.539121000	-0.293496000	-1.396039000
H	-4.380722000	0.224907000	0.063730000
H	1.701783000	-0.044193000	-1.962211000
H	-4.361237000	-2.141242000	0.916595000
H	-3.516683000	-2.657967000	-0.552327000
H	-5.170478000	-2.038856000	-0.652408000
H	1.827318000	2.345857000	-0.967582000
H	0.242799000	1.791675000	-1.511486000
H	-0.097993000	2.811939000	0.667991000
H	1.250208000	1.904343000	1.366257000
H	-0.746916000	0.799125000	2.079143000
H	3.439820000	-1.483749000	-1.287139000

H	2.709524000	-1.883902000	0.275214000
H	5.189755000	-2.034118000	0.409523000
H	4.591288000	-0.736757000	1.454405000
H	5.333123000	-0.344543000	-0.103667000

Sum of electronic and zero-point Energies= -708.588121
Sum of electronic and thermal Energies= -708.573346
Sum of electronic and thermal Enthalpies= -708.572402
Sum of electronic and thermal Free Energies= -708.631502

$\mathbf{1}_{\mathbf{eq,ax,eq}}$(A)

N	-1.03414300	1.93711300	0.17088700
O	-2.36871700	1.45593400	0.46075800
O	1.93678700	0.89651900	0.02065000
C	1.60195100	-0.08249800	1.02416800
C	-3.17408100	1.75269900	-0.69916200
C	2.81302100	-0.22299600	1.92928700
O	1.46770400	1.99702300	-1.83661600
O	-4.48643500	1.43264000	-0.39663000
C	-2.69707600	0.88770000	-1.86023500
C	-1.18563300	1.06285200	-2.08523200
C	-0.42491800	0.95362500	-0.75807000
C	1.05695800	1.31985300	-0.92723900
C	-5.12210800	2.31938100	0.53153900
C	-6.57408900	1.89440000	0.66316600
H	-0.59479000	1.87541800	1.08951600
H	1.36307300	-1.03676000	0.53959200
H	0.72483200	0.23663000	1.60011800
H	-3.05129100	2.82710700	-0.91610700
H	3.04712900	0.73110700	2.41123300
H	3.68707000	-0.54195800	1.35386400
H	2.61475000	-0.96824900	2.70721800

H	-2.93650000	-0.15205300	-1.60606100
H	-3.25497300	1.14482600	-2.76754100
H	-0.96672300	2.04499200	-2.51452400
H	-0.81309500	0.31174900	-2.79042500
H	-0.52514500	-0.06662200	-0.35898900
H	-5.04694200	3.35278400	0.15807400
H	-4.60817100	2.27580900	1.49939800
H	-7.09920000	2.55050900	1.36603100
H	-6.64165100	0.86603900	1.03246500
H	-7.08145000	1.94508200	-0.30570600

Sum of electronic and zero-point Energies= -708.586337
Sum of electronic and thermal Energies= -708.571362
Sum of electronic and thermal Enthalpies= -708.570417
Sum of electronic and thermal Free Energies= -708.630225

$\mathbf{1_{eq,ax,eq}(B)}$

N	0.119060000	0.304041000	-0.919931000
O	-1.277291000	0.149256000	-0.941091000
O	2.605323000	0.452022000	0.016608000
C	4.012325000	0.708549000	0.130501000
C	-1.822212000	-0.108027000	0.354960000
C	4.183856000	2.136810000	0.583946000
O	3.031103000	-1.644644000	-0.648733000
O	-3.186754000	-0.173482000	0.231610000
C	-1.295940000	-1.417958000	0.897574000
C	0.227659000	-1.390548000	0.915854000
C	0.747894000	-0.928272000	-0.451882000
C	2.251666000	-0.767452000	-0.400402000
C	-3.818855000	1.056801000	-0.090433000
C	-5.312658000	0.838775000	-0.073679000
H	0.334295000	1.067860000	-0.281827000

H	4.479003000	0.530499000	-0.839363000
H	4.441205000	0.000265000	0.841308000
H	-1.526014000	0.734589000	1.010401000
H	3.711046000	2.298439000	1.553322000
H	3.746812000	2.828725000	-0.136537000
H	5.246263000	2.364799000	0.678620000
H	-1.698245000	-1.584990000	1.897577000
H	-1.662236000	-2.215460000	0.247341000
H	0.634256000	-2.373773000	1.156890000
H	0.579071000	-0.692012000	1.682531000
H	0.540896000	-1.696822000	-1.197284000
H	-3.484551000	1.399174000	-1.072892000
H	-3.527910000	1.815109000	0.649148000
H	-5.828509000	1.769375000	-0.314800000
H	-5.643984000	0.502256000	0.909388000
H	-5.596272000	0.086392000	-0.810095000

Sum of electronic and zero-point Energies= -708.584889
Sum of electronic and thermal Energies= -708.569937
Sum of electronic and thermal Enthalpies= -708.568993
Sum of electronic and thermal Free Energies= -708.628580

$\mathbf{1}_{\mathbf{eq,ax,eq}}$(C)

N	-0.287816000	-0.359853000	-0.641230000
O	0.984551000	-0.702429000	-0.157548000
O	-3.284126000	-0.015797000	-0.186089000
C	-3.092633000	-1.252429000	0.515643000
C	1.854072000	0.434157000	-0.062905000
C	-4.297103000	-2.117806000	0.236444000
O	-2.522070000	1.892546000	-0.941186000
O	3.076120000	-0.012885000	0.367001000
C	1.301380000	1.444109000	0.917770000

C	-0.117431000	1.836806000	0.517685000
C	-0.938821000	0.578455000	0.277734000
C	-2.310358000	0.884900000	-0.327292000
C	3.791550000	-0.803863000	-0.571799000
C	5.151607000	-1.109504000	0.007572000
H	-0.155218000	0.094542000	-1.544802000
H	-3.009381000	-1.044872000	1.586087000
H	-2.174380000	-1.728506000	0.170315000
H	1.927723000	0.872878000	-1.076705000
H	-4.378259000	-2.329570000	-0.829680000
H	-5.213332000	-1.626017000	0.563541000
H	-4.199513000	-3.063551000	0.771349000
H	1.317949000	0.983669000	1.908574000
H	1.956775000	2.315449000	0.942554000
H	-0.111621000	2.431320000	-0.398446000
H	-0.582216000	2.452299000	1.289495000
H	-1.061581000	0.039295000	1.219784000
H	3.885778000	-0.246564000	-1.513330000
H	3.238943000	-1.723835000	-0.778534000
H	5.728351000	-1.714690000	-0.693348000
H	5.052818000	-1.663444000	0.941498000
H	5.702486000	-0.189866000	0.207725000

Sum of electronic and zero-point Energies= -708.576196
Sum of electronic and thermal Energies= -708.561345
Sum of electronic and thermal Enthalpies= -708.560400
Sum of electronic and thermal Free Energies= -708.619292

$\mathbf{1}_{\mathbf{eq,ax,eq}}\mathbf{(D)}$

N	-0.17140000	-1.09785900	-0.37048000
O	-1.46589100	-0.65601500	-0.68326600
O	3.09720500	0.16199900	-0.35269300

C	4.41118000	-0.21448100	0.08722700
C	-2.00374200	0.22845100	0.30133900
C	5.40523100	0.66114100	-0.63387400
O	2.19914500	-1.38870700	0.99310000
O	-3.28821900	0.53751400	-0.06885300
C	-1.17636700	1.49185600	0.37540200
C	0.27320300	1.13231100	0.67684400
C	0.74637100	0.03134700	-0.28410200
C	2.07894400	-0.50398900	0.18799100
C	-4.20837700	-0.54174700	0.00671000
C	-5.58477000	-0.01233100	-0.31659300
H	-0.20593900	-1.57988700	0.52632800
H	4.56397000	-1.27179300	-0.13405300
H	4.46804300	-0.08982400	1.16996900
H	-1.99021400	-0.30657900	1.27071500
H	5.23720200	1.71364900	-0.40376000
H	5.33182300	0.52582600	-1.71319400
H	6.41684000	0.39817600	-0.32209400
H	-1.26179600	1.99940900	-0.58804700
H	-1.58422300	2.15064400	1.14312800
H	0.35733100	0.75907300	1.70260800
H	0.91891800	2.00792700	0.59157800
H	0.85688400	0.44333200	-1.28812800
H	-4.18262900	-0.96618500	1.01939500
H	-3.91663400	-1.32719500	-0.69479700
H	-6.31704700	-0.81931200	-0.26367700
H	-5.60538400	0.40668500	-1.32301100
H	-5.87529700	0.76739900	0.38844500

Sum of electronic and zero-point Energies= -708.577684
Sum of electronic and thermal Energies= -708.562941
Sum of electronic and thermal Enthalpies= -708.561997
Sum of electronic and thermal Free Energies= -708.621017

$\mathbf{1}_{eq,eq,eq}(A)$

N	0.54081300	-0.60566700	-0.97838100

O	1.63484300	0.14562500	-1.50028900
O	-2.72563400	0.11926400	0.19489100
C	-3.96841400	-0.56614000	0.40829600
C	2.17016600	0.97234400	-0.48568100
C	-4.84282500	0.32334300	1.25633700
O	-1.97274900	-1.61776000	-0.99936500
O	2.65453300	0.26991400	0.60574100
C	1.12153600	1.95795700	0.00905100
C	-0.17862000	1.24714300	0.37907200
C	-0.56829500	0.31028100	-0.75867900
C	-1.81340300	-0.52193000	-0.53182300
C	3.63122900	-0.70570400	0.29808300
C	4.17404400	-1.25748800	1.59504200
H	0.31717400	-1.24623700	-1.72960800
H	-3.76262800	-1.52001000	0.89613700
H	-4.42215900	-0.77986600	-0.56098000
H	2.98741100	1.48462000	-1.01073500
H	-5.03605500	1.27247000	0.75556700
H	-4.37267300	0.52779000	2.21860400
H	-5.79834000	-0.17024700	1.43820800
H	1.52223000	2.50802100	0.86034300
H	0.93383200	2.67360300	-0.79530200
H	-0.97023900	1.97203300	0.56372300
H	-0.03881600	0.65723800	1.28621100
H	-0.77252700	0.91183300	-1.66100800
H	4.43300600	-0.24699100	-0.29738500
H	3.18272200	-1.50073500	-0.30383200
H	4.92765600	-2.02007300	1.39236600
H	3.37219500	-1.71158200	2.17818200
H	4.63107200	-0.46736800	2.19215900

Sum of electronic and zero-point Energies= -708.587137
Sum of electronic and thermal Energies= -708.572308
Sum of electronic and thermal Enthalpies= -708.571363
Sum of electronic and thermal Free Energies= -708.630824

$\mathbf{1}_{eq,eq,eq}$(B)

N	-0.145556000	-0.541873000	0.208046000
O	1.157299000	-0.678652000	-0.341021000
O	-2.798804000	-0.485387000	-0.161976000
C	-4.200798000	-0.557356000	0.135267000
C	1.980331000	0.318470000	0.260710000
C	-4.633629000	-1.992459000	-0.032229000
O	-2.808288000	1.709498000	0.281551000
O	3.271280000	0.112046000	-0.161666000
C	1.512176000	1.688579000	-0.189362000
C	0.021419000	1.865418000	0.092650000
C	-0.748645000	0.646652000	-0.394272000
C	-2.221272000	0.713708000	-0.036154000
C	3.900200000	-1.035464000	0.386807000
C	5.329072000	-1.070471000	-0.100063000
H	-0.621878000	-1.373810000	-0.116005000
H	-4.736221000	0.111450000	-0.540595000
H	-4.360909000	-0.199694000	1.153466000
H	1.886463000	0.202248000	1.352441000
H	-4.088529000	-2.645697000	0.649787000
H	-4.463173000	-2.334998000	-1.053329000
H	-5.698649000	-2.080371000	0.186032000
H	2.096040000	2.458313000	0.316711000
H	1.714762000	1.763127000	-1.260686000
H	-0.361150000	2.765439000	-0.386979000
H	-0.151301000	1.973276000	1.165782000
H	-0.695455000	0.592131000	-1.493000000
H	3.362023000	-1.936575000	0.079952000
H	3.863681000	-0.978551000	1.482661000
H	5.842714000	-1.941588000	0.309495000

H	5.865122000	-0.173104000	0.211079000
H	5.360342000	-1.130982000	-1.188359000

Sum of electronic and zero-point Energies= -708.587059
Sum of electronic and thermal Energies= -708.572133
Sum of electronic and thermal Enthalpies= -708.571189
Sum of electronic and thermal Free Energies= -708.630696

$2_{ax,ax,eq}$(A)

N	0.429745000	0.063154000	1.233103000
O	1.532880000	-0.806226000	1.379198000
O	-2.888488000	-0.112048000	0.094483000
C	-3.996157000	0.757713000	-0.181598000
C	2.151271000	-1.150463000	0.150762000
C	-5.236207000	-0.095270000	-0.281330000
O	-1.505068000	1.651363000	0.105112000
O	2.658971000	-0.035147000	-0.508373000
C	1.175657000	-1.853688000	-0.774468000
C	-0.074392000	-1.006138000	-0.969638000
C	-0.596638000	-0.551811000	0.401567000
C	-1.693693000	0.468824000	0.204305000
C	3.726605000	0.612105000	0.164668000
C	4.163655000	1.795838000	-0.664564000
H	0.768935000	0.903473000	0.770405000
H	-3.796810000	1.297038000	-1.109264000
H	-4.071791000	1.493568000	0.620392000
H	2.962428000	-1.817976000	0.465265000
H	-5.418475000	-0.627647000	0.652528000
H	-5.143178000	-0.826316000	-1.085048000
H	-6.099342000	0.537933000	-0.490622000
H	1.664333000	-2.057930000	-1.727333000
H	0.914557000	-2.810268000	-0.316178000

H	-0.846411000	-1.569053000	-1.496939000
H	0.166319000	-0.122974000	-1.565942000
H	-0.996352000	-1.408577000	0.946925000
H	4.553261000	-0.098266000	0.297122000
H	3.402643000	0.930711000	1.160179000
H	4.990858000	2.311154000	-0.174391000
H	3.341930000	2.502498000	-0.786813000
H	4.491899000	1.474358000	-1.653590000

Sum of electronic and zero-point Energies= -708.589639
Sum of electronic and thermal Energies= -708.574766
Sum of electronic and thermal Enthalpies= -708.573821
Sum of electronic and thermal Free Energies= -708.633404

$2_{ax,ax,eq}$(B)

N	0.140120000	-0.447613000	1.176982000
O	1.468297000	-0.910130000	1.326443000
O	-2.087953000	0.483044000	0.072163000
C	-3.389333000	1.053767000	-0.120735000
C	2.193069000	-0.933883000	0.108090000
C	-3.238368000	2.554520000	-0.108715000
O	-2.962292000	-1.577068000	-0.032052000
O	2.308187000	0.336905000	-0.450319000
C	1.534007000	-1.849471000	-0.907138000
C	0.070731000	-1.471912000	-1.098853000
C	-0.594136000	-1.332767000	0.277476000
C	-2.018208000	-0.850103000	0.109411000
C	3.092799000	1.243311000	0.307663000
C	3.111075000	2.572125000	-0.409215000
H	0.203829000	0.476285000	0.756479000
H	-4.046111000	0.704243000	0.677242000
H	-3.794122000	0.691900000	-1.067375000

H	3.175332000	-1.312346000	0.414664000
H	-2.577087000	2.886311000	-0.909899000
H	-2.830729000	2.896298000	0.843050000
H	-4.213545000	3.021377000	-0.252900000
H	2.081109000	-1.797100000	-1.848591000
H	1.609633000	-2.871463000	-0.529113000
H	-0.451016000	-2.225775000	-1.690258000
H	-0.001268000	-0.519055000	-1.628825000
H	-0.649991000	-2.310356000	0.758329000
H	4.109524000	0.842191000	0.410369000
H	2.675853000	1.347670000	1.314091000
H	3.716675000	3.289339000	0.146563000
H	2.100689000	2.973035000	-0.500416000
H	3.530664000	2.465201000	-1.410053000

Sum of electronic and zero-point Energies= -708.588636
Sum of electronic and thermal Energies= -708.573782
Sum of electronic and thermal Enthalpies= -708.572838
Sum of electronic and thermal Free Energies= -708.632315

$\mathbf{2_{ax,ax,eq}(C)}$

N	0.375556000	-0.597237000	-1.322629000
O	1.477852000	-1.463237000	-1.200576000
O	-2.804221000	-0.168841000	0.033300000
C	-3.889721000	0.771086000	0.001232000
C	2.281323000	-1.244270000	-0.057205000
C	-5.132195000	0.053703000	0.466279000
O	-1.405280000	1.417515000	-0.707049000
O	3.067376000	-0.094478000	-0.186691000
C	1.447846000	-1.376928000	1.215570000
C	0.144436000	-0.585137000	1.173755000
C	-0.530990000	-0.754876000	-0.196558000

C	-1.613264000	0.290357000	-0.342541000
C	2.739563000	1.126745000	0.448080000
C	3.879751000	2.086915000	0.198284000
H	0.724515000	0.354794000	-1.375179000
H	-3.994126000	1.148661000	-1.016928000
H	-3.641145000	1.616181000	0.645516000
H	2.989401000	-2.072253000	-0.115047000
H	-5.009965000	-0.319295000	1.483586000
H	-5.362794000	-0.788227000	-0.186833000
H	-5.978073000	0.742157000	0.451793000
H	1.216794000	-2.440251000	1.309740000
H	2.046107000	-1.104914000	2.086472000
H	0.327931000	0.476061000	1.346295000
H	-0.529272000	-0.928249000	1.961224000
H	-0.972995000	-1.749629000	-0.269665000
H	2.605182000	0.980109000	1.525711000
H	1.807875000	1.546548000	0.051907000
H	3.669525000	3.048959000	0.668205000
H	4.016881000	2.245012000	-0.871593000
H	4.808939000	1.691766000	0.609948000

Sum of electronic and zero-point Energies= -708.577684
Sum of electronic and thermal Energies= -708.562941
Sum of electronic and thermal Enthalpies= -708.561997
Sum of electronic and thermal Free Energies= -708.621017

$2_{ax,ax,eq}$(D)

N	0.37555600	-0.59723700	-1.32262900
O	1.47785200	-1.46323700	-1.20057600
O	-2.80422100	-0.16884100	0.03330000
C	-3.88972100	0.77108600	0.00123200
C	2.28132300	-1.24427000	-0.05720500

C	-5.13219500	0.05370300	0.46627900
O	-1.40528000	1.41751500	-0.70704900
O	3.06737600	-0.09447800	-0.18669100
C	1.44784600	-1.37692800	1.21557000
C	0.14443600	-0.58513700	1.17375500
C	-0.53099000	-0.75487600	-0.19655800
C	-1.61326400	0.29035700	-0.34254100
C	2.73956300	1.12674500	0.44808000
C	3.87975100	2.08691500	0.19828400
H	0.72451500	0.35479400	-1.37517900
H	-3.99412600	1.14866100	-1.01692800
H	-3.64114500	1.61618100	0.64551600
H	2.98940100	-2.07225300	-0.11504700
H	-5.00996500	-0.31929500	1.48358600
H	-5.36279400	-0.78822700	-0.18683300
H	-5.97807300	0.74215700	0.45179300
H	1.21679400	-2.44025100	1.30974000
H	2.04610700	-1.10491400	2.08647200
H	0.32793100	0.47606100	1.34629500
H	-0.52927200	-0.92824900	1.96122400
H	-0.97299500	-1.74962900	-0.26966500
H	2.60518200	0.98010900	1.52571100
H	1.80787500	1.54654800	0.05190700
H	3.66952500	3.04895900	0.66820500
H	4.01688100	2.24501200	-0.87159300
H	4.80893900	1.69176600	0.60994800

Sum of electronic and zero-point Energies= -708.577684
Sum of electronic and thermal Energies= -708.562941
Sum of electronic and thermal Enthalpies= -708.561997
Sum of electronic and thermal Free Energies= -708.621017

$\mathbf{2}_{\mathbf{ax,eq,eq}}$

N	-0.085749000	0.301957000	-0.642149000
O	-1.202813000	0.018096000	-1.486518000
O	2.545298000	0.313781000	-0.207393000

C	3.818497000	0.662370000	0.354522000
C	-2.212894000	-0.643821000	-0.750037000
C	4.358111000	1.837208000	-0.422406000
O	2.315067000	-1.320657000	1.305710000
O	-2.698749000	0.097986000	0.314078000
C	-1.698516000	-1.970949000	-0.213918000
C	-0.381812000	-1.785740000	0.534061000
C	0.569423000	-0.962556000	-0.321242000
C	1.888842000	-0.693215000	0.377538000
C	-3.205717000	1.371829000	-0.031845000
C	-3.841483000	1.978081000	1.196824000
H	0.508158000	0.850994000	-1.250181000
H	4.477918000	-0.204891000	0.292409000
H	3.680943000	0.900920000	1.410187000
H	-2.992822000	-0.789908000	-1.509216000
H	3.686518000	2.693170000	-0.349844000
H	4.486365000	1.583466000	-1.475149000
H	5.328906000	2.127266000	-0.018571000
H	-2.456357000	-2.413561000	0.432187000
H	-1.551989000	-2.638694000	-1.066542000
H	0.069272000	-2.748227000	0.772204000
H	-0.551773000	-1.256725000	1.472409000
H	0.814372000	-1.522242000	-1.239341000
H	-3.941938000	1.266557000	-0.841048000
H	-2.394207000	2.005189000	-0.401022000
H	-4.237795000	2.967958000	0.965104000
H	-3.104151000	2.079198000	1.993893000
H	-4.658304000	1.352956000	1.559566000

Sum of electronic and zero-point Energies= -708.586903
Sum of electronic and thermal Energies= -708.572063
Sum of electronic and thermal Enthalpies= -708.571119

Sum of electronic and thermal Free Energies= -708.630593

$2_{eq,eq,ax}$(A)

N	0.147779000	-0.505183000	1.556405000
O	-0.674824000	0.272622000	0.690951000
O	2.386798000	0.407000000	0.260469000
C	3.244826000	1.184247000	-0.585133000
C	-1.730273000	-0.572052000	0.235322000
C	3.699225000	2.387982000	0.202053000
O	2.061275000	-1.054408000	-1.402493000
O	-2.614287000	0.202603000	-0.476100000
C	-1.151724000	-1.642428000	-0.667711000
C	-0.016693000	-2.381930000	0.041004000
C	0.934847000	-1.401686000	0.719981000
C	1.835138000	-0.679324000	-0.285205000
C	-3.385184000	1.098507000	0.308207000
C	-4.362989000	1.802906000	-0.601666000
H	0.751512000	0.195620000	1.968495000
H	2.686976000	1.469609000	-1.478140000
H	4.084546000	0.562642000	-0.900848000
H	-2.203274000	-1.009942000	1.129285000
H	4.251067000	2.086861000	1.093183000
H	2.846947000	2.995180000	0.508381000
H	4.354901000	3.002767000	-0.415879000
H	-1.938555000	-2.337376000	-0.963558000
H	-0.781468000	-1.148657000	-1.568093000
H	0.530755000	-3.001764000	-0.666923000
H	-0.424513000	-3.032716000	0.817260000
H	1.603614000	-1.944809000	1.395531000
H	-2.728019000	1.817695000	0.805012000
H	-3.915241000	0.534016000	1.086702000

H	-4.975321000	2.498936000	-0.026296000
H	-5.021038000	1.084250000	-1.091474000
H	-3.832070000	2.364105000	-1.371201000

Sum of electronic and zero-point Energies= -708.588264
Sum of electronic and thermal Energies= -708.573463
Sum of electronic and thermal Enthalpies= -708.572519
Sum of electronic and thermal Free Energies= -708.631838

$2_{eq,eq,ax}$(B)

N	0.324506000	-1.943760000	-0.369230000
O	1.058171000	-0.752102000	-0.647576000
O	-2.426496000	0.265933000	0.149315000
C	-3.314167000	1.101624000	-0.608425000
C	1.664563000	-0.324495000	0.566670000
C	-3.901903000	2.120863000	0.335322000
O	-1.918877000	-0.875463000	-1.706102000
O	2.500939000	0.726817000	0.276723000
C	0.581734000	0.139015000	1.520242000
C	-0.467062000	-0.957916000	1.694473000
C	-0.879901000	-1.552185000	0.350083000
C	-1.781335000	-0.680854000	-0.528656000
C	3.671604000	0.373364000	-0.443122000
C	4.522641000	1.610827000	-0.599240000
H	0.061685000	-2.250075000	-1.300008000
H	-4.083119000	0.474793000	-1.063080000
H	-2.747709000	1.570406000	-1.414262000
H	2.220422000	-1.183824000	0.976383000
H	-3.118942000	2.735340000	0.780675000
H	-4.460354000	1.635325000	1.136251000
H	-4.582894000	2.774789000	-0.210901000
H	1.024260000	0.406558000	2.480608000

H	0.133192000	1.038231000	1.092742000
H	-1.337441000	-0.575779000	2.224672000
H	-0.047903000	-1.772638000	2.289269000
H	-1.446303000	-2.473304000	0.521947000
H	3.397625000	-0.036897000	-1.418784000
H	4.214217000	-0.405235000	0.109162000
H	5.434975000	1.370786000	-1.147341000
H	4.799108000	2.015317000	0.375201000
H	3.980696000	2.379593000	-1.150893000

Sum of electronic and zero-point Energies= -708.587874
Sum of electronic and thermal Energies= -708.573093
Sum of electronic and thermal Enthalpies= -708.572149
Sum of electronic and thermal Free Energies= -708.631491

$2_{eq,ax,ax}$

N	0.396414000	-0.357620000	-1.117367000
O	-0.720200000	-0.621347000	-0.311094000
O	2.720833000	-0.235838000	0.731917000
C	3.262048000	-0.932339000	-0.396018000
C	-1.728311000	0.392416000	-0.434878000
C	4.358350000	-1.832082000	0.121009000
O	1.481630000	1.333671000	1.610172000
O	-2.805428000	0.005059000	0.316771000
C	-1.202046000	1.718792000	0.059802000
C	0.088444000	2.073290000	-0.674338000
C	1.049125000	0.885775000	-0.706826000
C	1.754494000	0.682319000	0.642719000
C	-3.504265000	-1.130451000	-0.171423000
C	-4.718750000	-1.347059000	0.698787000
H	0.059360000	-0.257571000	-2.073443000
H	3.668989000	-0.206701000	-1.107281000

H	2.472824000	-1.499687000	-0.886232000
H	-1.997463000	0.446059000	-1.509297000
H	3.955747000	-2.554042000	0.831446000
H	5.136020000	-1.252733000	0.619008000
H	4.807813000	-2.377737000	-0.710118000
H	-1.959830000	2.487513000	-0.097503000
H	-1.017842000	1.630044000	1.129943000
H	0.565537000	2.934350000	-0.208562000
H	-0.138940000	2.343124000	-1.710938000
H	1.825720000	1.064148000	-1.457038000
H	-2.849520000	-2.005351000	-0.152508000
H	-3.799360000	-0.950663000	-1.214266000
H	-5.280397000	-2.213876000	0.347386000
H	-5.373100000	-0.475009000	0.673836000
H	-4.419668000	-1.524844000	1.732017000

Sum of electronic and zero-point Energies= -708.573709
Sum of electronic and thermal Energies= -708.558892
Sum of electronic and thermal Enthalpies= -708.557948
Sum of electronic and thermal Free Energies= -708.617137