Supporting Information

Formation and Fragmentation of 2-Hydroxyethylhydrazinium Nitrate (HEHN) Cluster Ions: A Combined Electrospray Ionization Mass Spectrometry, Molecular Dynamics and Reaction Potential Surface Study

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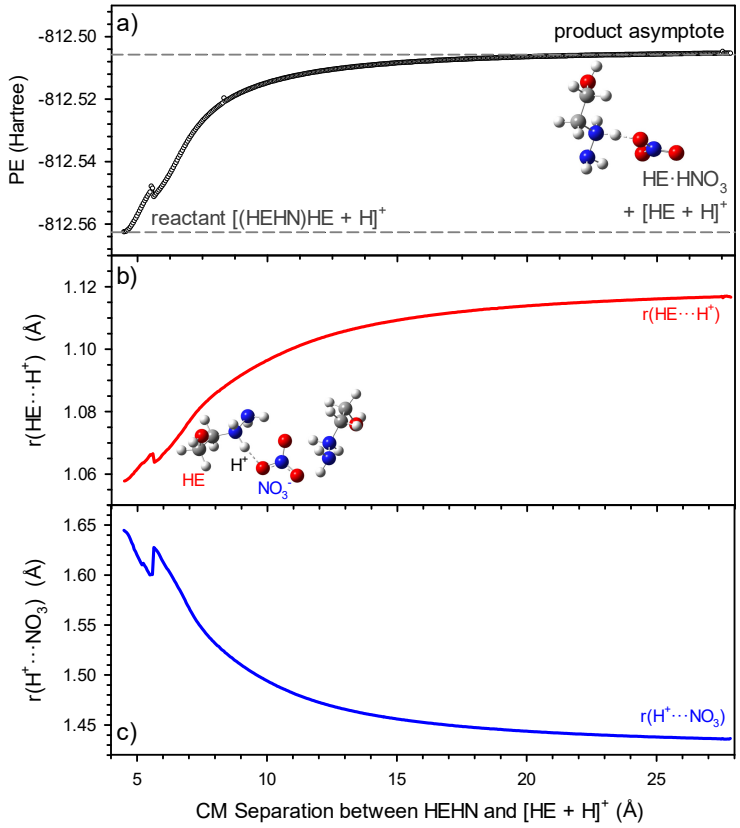

Figure S1 a) A relaxed PES scan for $[(HEHN)HE + H]^+$ along the center-of-mass distance between HEHN and $[HE + H]^+$, calculated at the ωB97XD/6-31+G(d,p) level of theory; and b – c) the accompanying changes of H-bond lengths within the HEHN moiety.

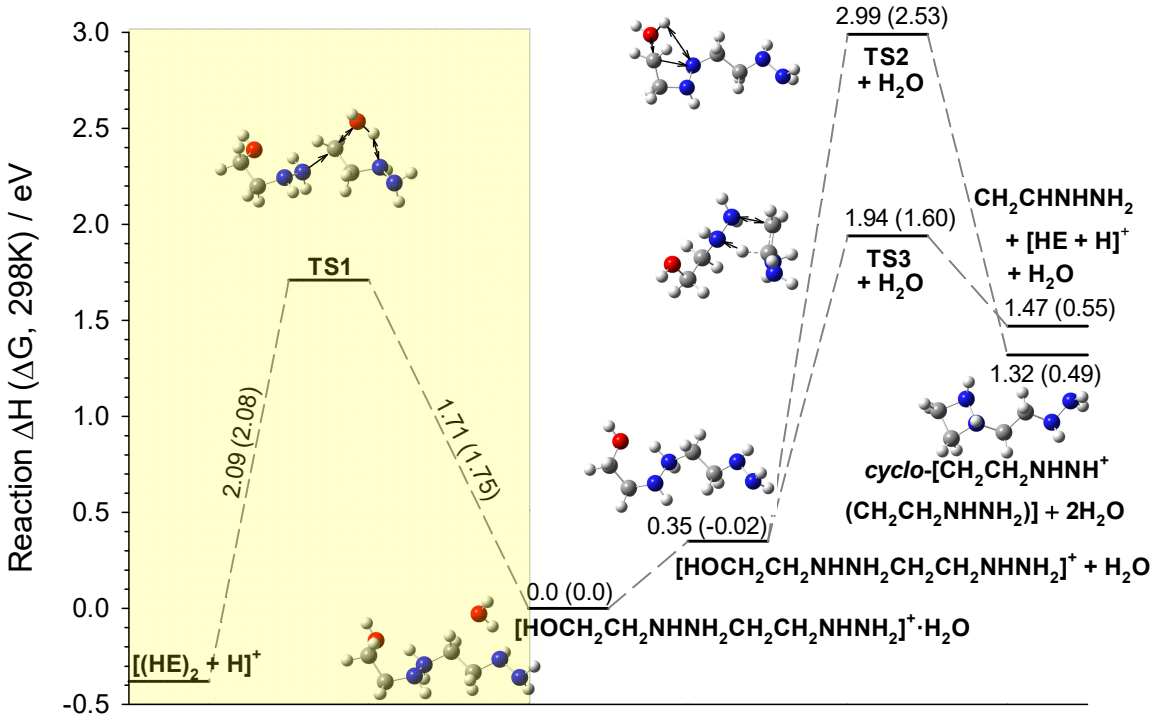

Figure S2 PES for the formation and dissociation pathways of $[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows a probable formation pathway of $[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$ from $[(HE)_2 + H]^+$ in the ion source. All reaction energies are referred to $[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$ as the zero energy point.

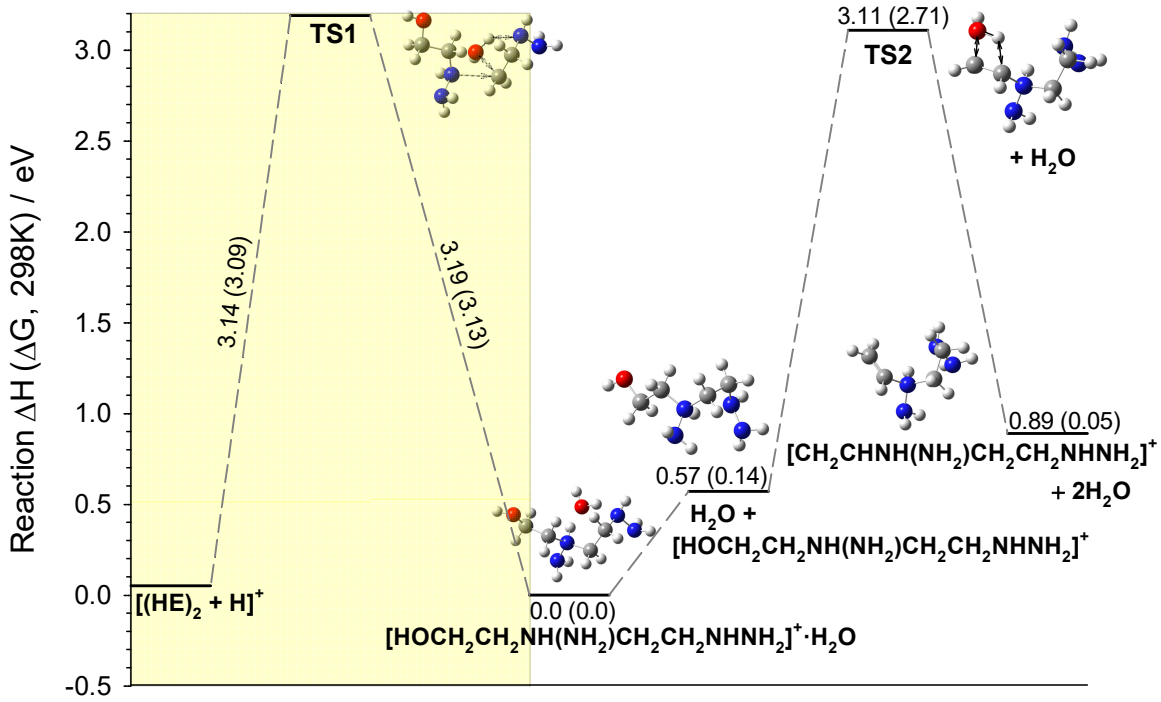

Figure S3 PES for the formation and dissociation pathways of $[HOCH_2CH_2NH(NH_2)CH_2CH_2NHNH_2]^+ \cdot H_2O$, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows a probable formation pathway of $[HOCH_2CH_2NH(NH_2)CH_2CH_2NHNH_2]^+ \cdot H_2O$ from $[(HE)_2 + H]^+$ in the ion source. All reaction energies are referred to $[HOCH_2CH_2NH(NH_2)CH_2CH_2NHNH_2]^+ \cdot H_2O$ as the zero energy point.

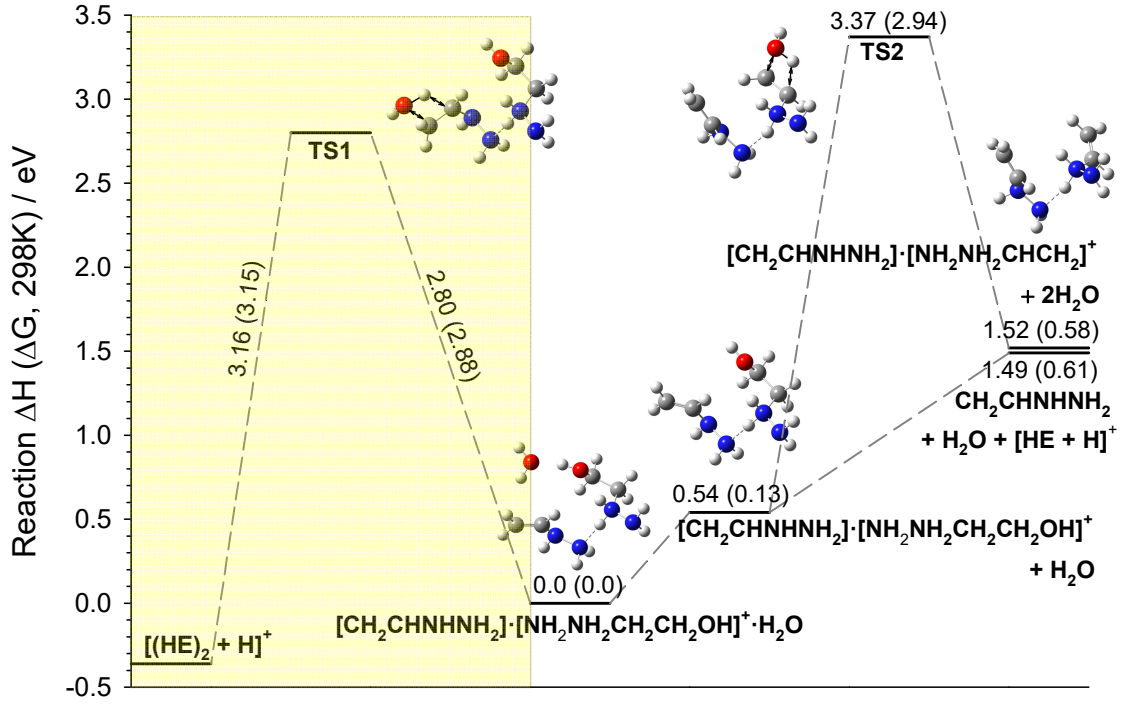

Figure S4 PES for the formation and dissociation pathways of $[CH_2CHNHNH_2]\cdot[NH_2NH_2CH_2CH_2OH]^+\cdot H_2O$, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows a probable formation pathway of $[CH_2CHNHNH_2]\cdot[NH_2NH_2CH_2CH_2OH]^+\cdot H_2O$ from $[(HE)_2 + H]^+$ in the ion source. All reaction energies are referred to $[CH_2CHNHNH_2]\cdot[NH_2NH_2CH_2CH_2OH]^+\cdot H_2O$ as the zero energy point.

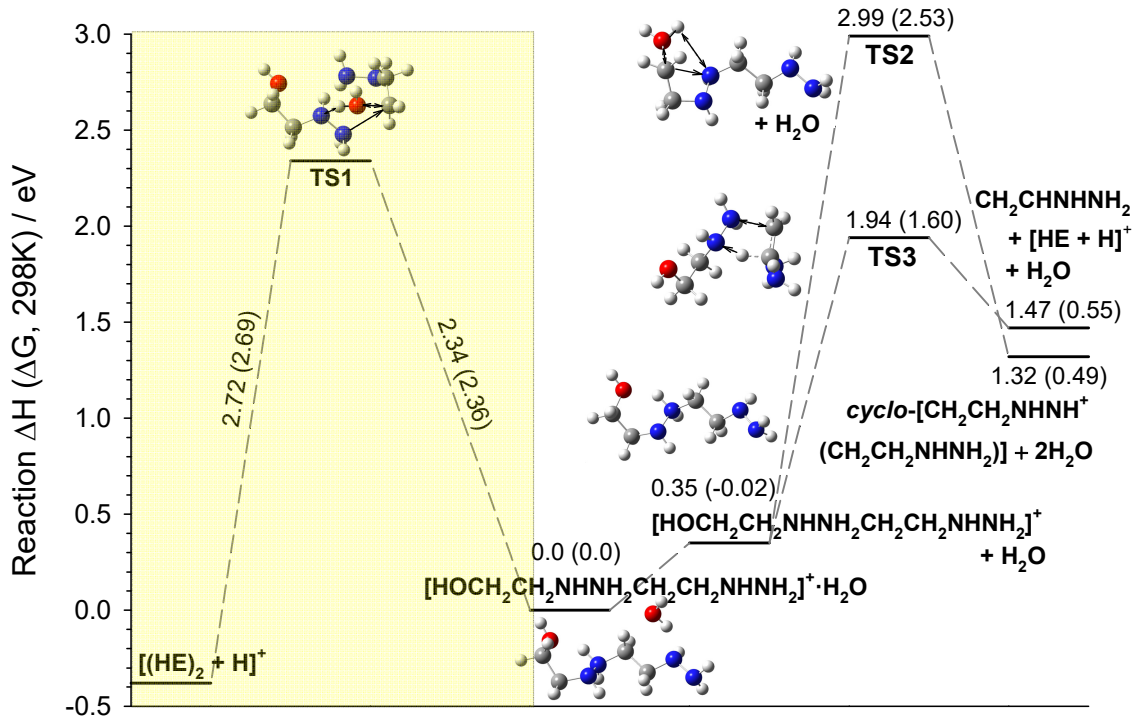

Figure S5 PES for another formation pathway of $[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$ and its dissociation, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows a probable formation pathway of $[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$ from $[(HE)_2 + H]^+$ in the ion source. All reaction energies are referred to $[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$ as the zero energy point.

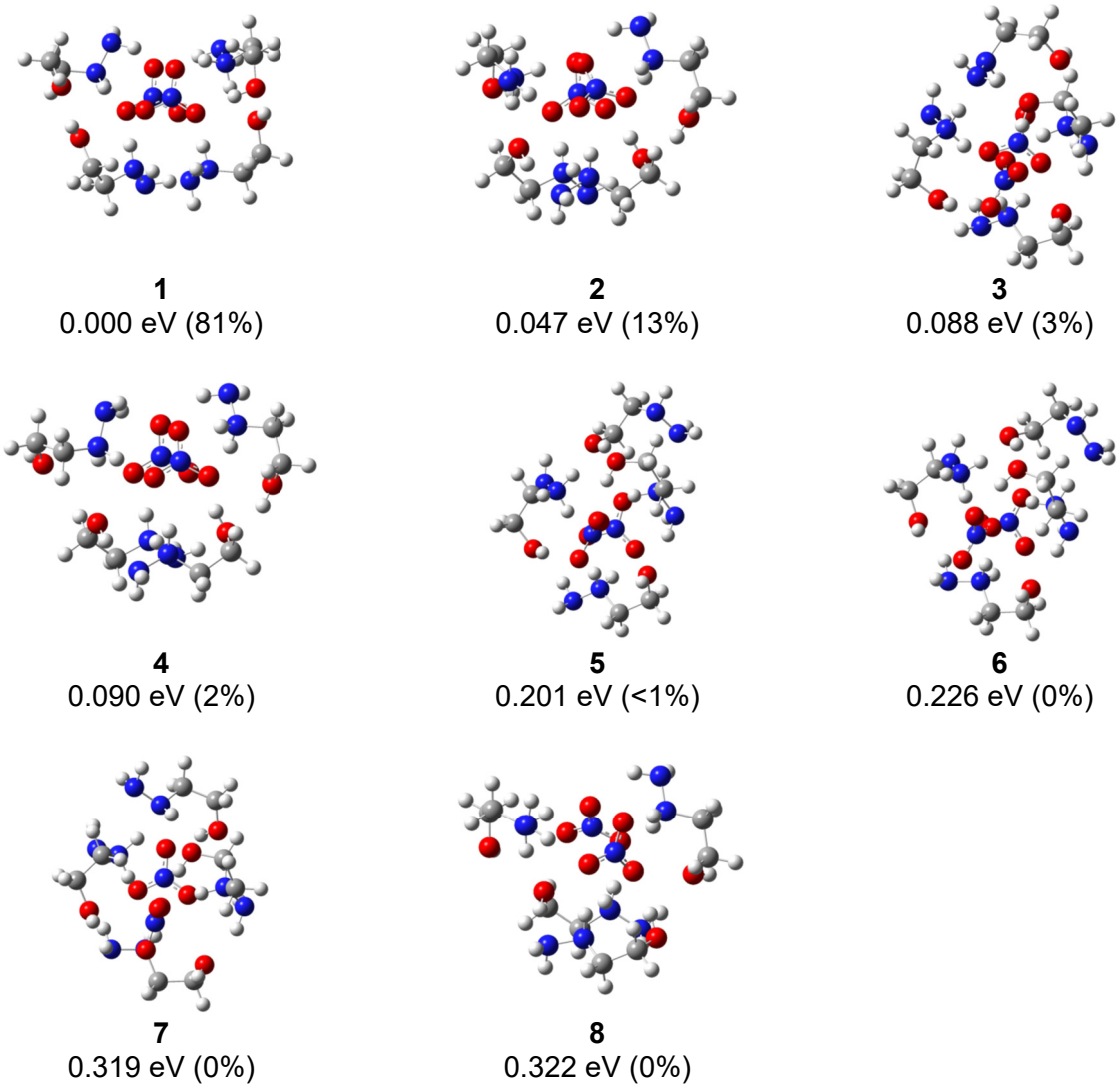

Figure S6 Different conformers of $[(HEHN)_2(HE)_2 + H]^+$ calculated at the ωB97XD/6-31+G(d,p) level of theory, with their relative enthalpies and thermal populations (in parentheses) indicated.

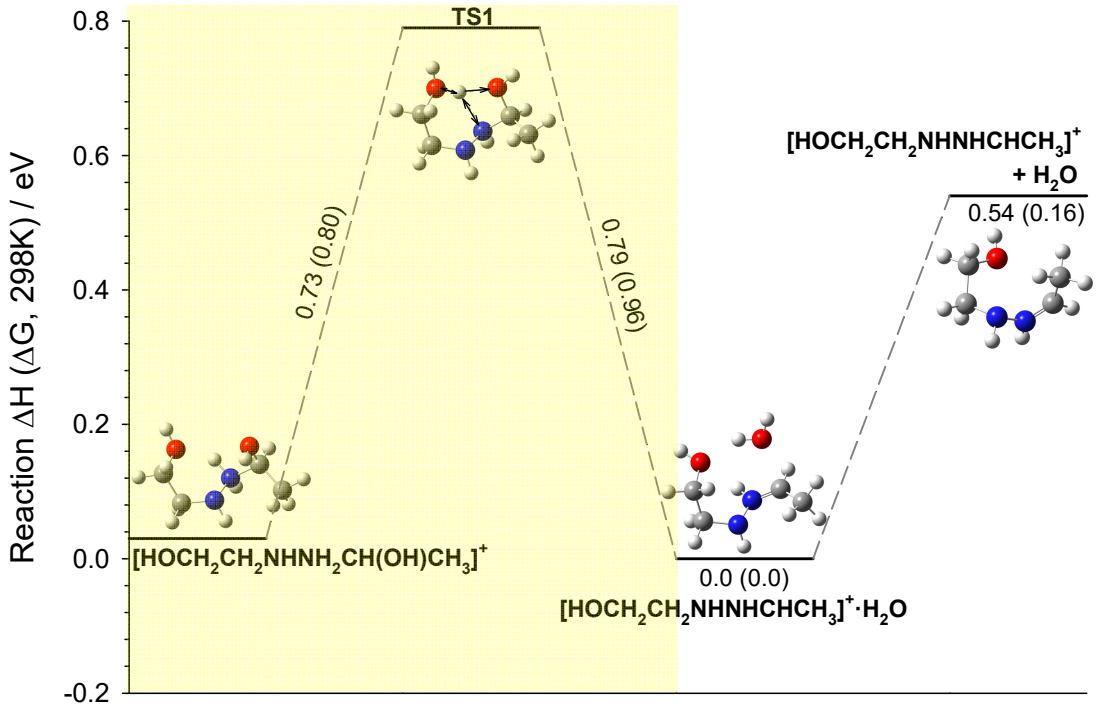

Figure S7 PES for the formation and dissoictaion pathways of $[HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows a probable formation pathway of $[HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$ from $[HOCH_2CH_2NHNH_2CH(OH)CH_3]^+$ in the ion source. All reaction energies are referred to $[HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$ as the zero energy point.

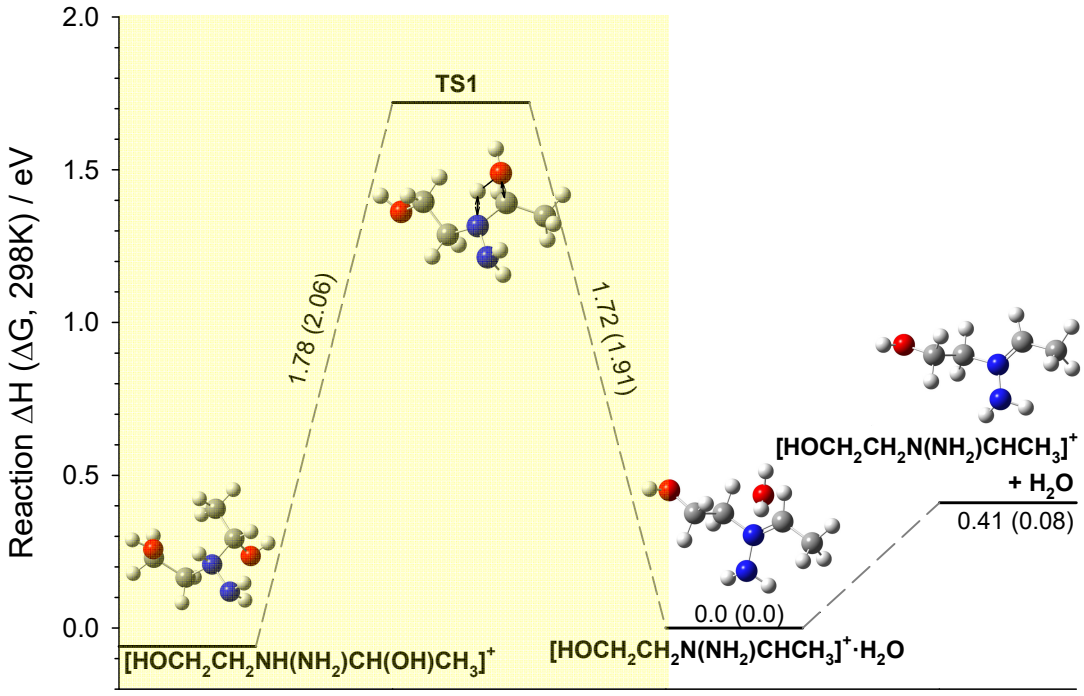

Figure S8 PES for the formation and dissociation pathways of $[HOCH_2CH_2N(NH_2)CHCH_3]^+ \cdot H_2O$, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows the probable formation of $[HOCH_2CH_2N(NH_2)CHCH_3]^+ \cdot H_2O$ from $[HOCH_2CH_2NH(NH_2)CH(OH)CH_3]^+$ in the ion source, before being selected by the first mass filter. All reaction energies are referred to $[HOCH_2CH_2N(NH_2)CHCH_3]^+ \cdot H_2O$ as the zero energy point.

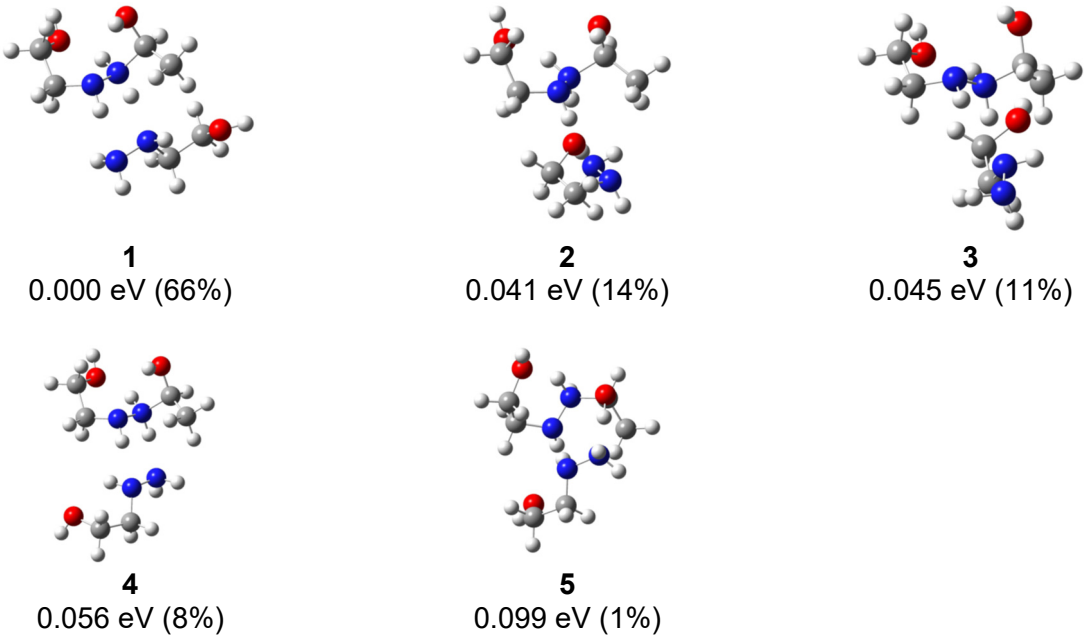

Figure S9 Different conformers of [HE][$HOCH_2CH_2NHNH_2CH(OH)CH_3$]$^+$ calculated at the ωB97XD/6-31+G(d,p) level of theory, with their relative enthalpies and thermal populations (in parentheses) indicated.

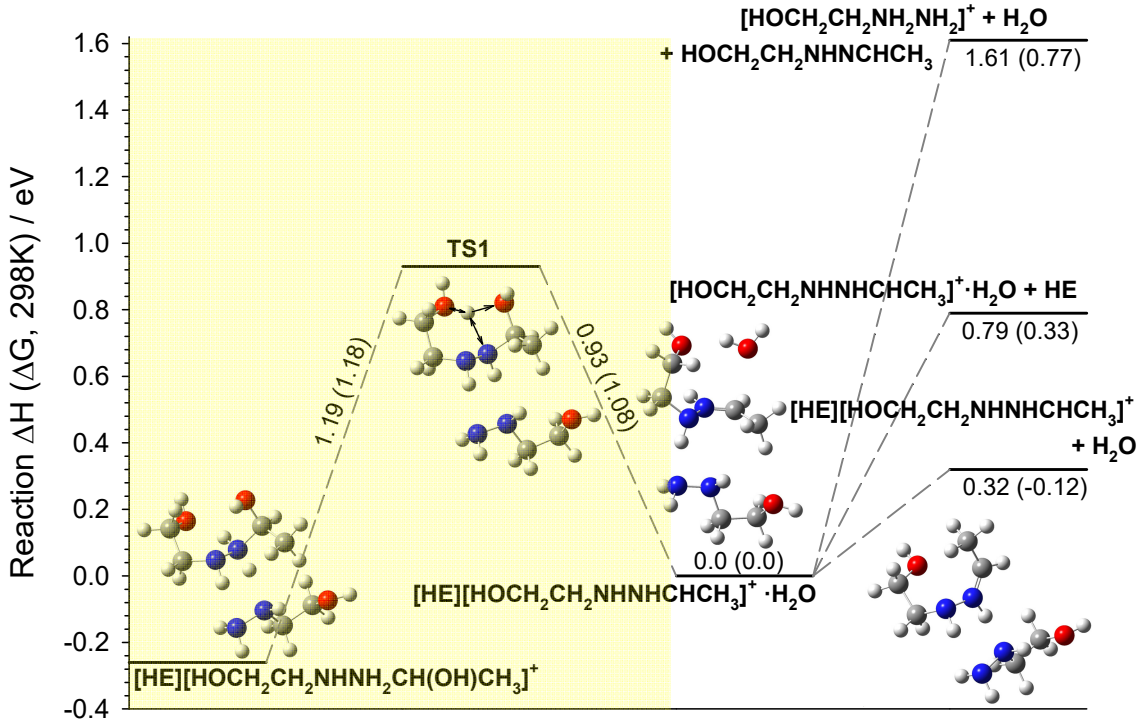

Figure S10 PES for the formation and dissociation pathways of $[HE][HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$, calculated at the ωB97XD/6-31+G(d,p) level of theory including thermal corrections at 298 K. The yellow-shaded portion shows the formation of $[HE][HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$ from $[HE][HOCH_2CH_2NHNH_2CH(OH)CH_3]^+$ in the ion source. All reaction energies are referred to $[HE][HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$ as the zero energy point.

Cartesian coordinates for structures in Rxns 2, calculated at ωB97XD/ 6-31+G(d,p)

$[HOCH_2CH_2NH_2NH_2]^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$[CH_3CH=NHNH_2]^+$
N1 1.815485 -0.185968 0.000015
N2 0.527035 0.363930 -0.000005
C3 -0.504084 -0.405376 0.000007
C4 -1.890145 0.086465 -0.000007
H5 -2.404664 -0.326675 -0.875469
H6 -1.972570 1.174366 -0.000151
H7 -2.404568 -0.326427 0.875640
H8 -0.279229 -1.471166 0.000044
H9 0.404570 1.378536 -0.000032
H10 2.312133 0.119662 0.833024
H11 2.312058 0.119433 -0.833125

TS_Rxn 2b.1
N1 2.356289 0.337700 -0.207243
N2 1.069390 0.270586 0.349501
C3 0.214312 -0.604765 -0.310986
C4 -1.078162 -0.918317 0.174552
H5 -1.719868 -1.519360 -0.460214
H6 -1.274057 -0.911398 1.242917
O7 -2.268713 0.735686 -0.140238
H8 -3.160221 0.820234 0.219461
H9 0.287115 -1.764377 0.000054
H10 0.372515 -0.618085 -1.389227
H11 1.002861 0.304362 1.362121
H12 -1.845122 1.600843 -0.086485
H13 3.030826 -0.220322 0.306959
H14 2.658997 1.303101 -0.250872

$[CH_2=NHNH_2]^+$
N1 1.160184 -0.168000 0.091487
N2 -0.075269 0.390765 -0.007371
C3 -1.205036 -0.211947 -0.015148
H4 -1.245151 -1.296104 -0.037387
H5 -0.060604 1.409682 0.041890
H6 1.176618 -1.159290 -0.121961
H7 1.871041 0.369606 -0.391792
H8 -2.106098 0.388434 0.011325

CH_3OH
C1 0.662528 -0.020652 -0.000009
H2 1.025131 -0.545268 -0.893777
H3 1.025040 -0.545584 0.893621
O4 -0.744790 0.122085 -0.000011
H5 -1.148737 -0.748814 0.000050
H6 1.081719 0.986894 0.000248

TS_Rxn 2c.1
N1 2.273413 0.213380 -0.282903
N2 1.104983 -0.525237 -0.039763
C3 0.102639 0.194505 0.740469
C4 -1.336889 0.601390 -0.229772
H5 -1.601304 1.504121 0.326920
H6 -1.176301 0.908543 -1.285145
O7 -2.164089 -0.484811 -0.068618
H8 -2.863939 -0.511108 -0.730771
H9 0.483391 1.149762 1.095330
H10 -0.421344 -0.414624 1.475348
H11 -0.150278 0.132177 -0.516268
H12 1.189731 -1.510860 0.190193
H13 2.614796 0.015959 -1.216250
H14 2.994690 0.012144 0.404064

$[CH_2=C=NH_2]^+$
N1 1.215366 0.000055 0.000013
C2 -0.044570 -0.000015 -0.000030
C3 -1.330027 -0.000001 -0.000002
H4 -1.874945 0.942584 0.001084
H5 -1.875027 -0.942570 -0.000990
H6 1.744982 0.000968 -0.872387
H7 1.745015 -0.001273 0.872392

$[NH=NH_2]^+$
N1 0.537312 0.029246 0.000007
N2 -0.672535 -0.156611 0.000011
H3 -1.187243 0.739794 -0.000076
H4 1.141362 -0.802986 -0.000068
H5 0.992443 0.954744 0.000013

CH_3CH_2OH
C1 1.220739 -0.222087 -0.000020
C2 -0.085312 0.547006 -0.000011
H3 -0.141047 1.192236 0.888831
H4 -0.141102 1.192231 -0.888851
O5 -1.148535 -0.394911 0.000022
H6 -1.987207 0.072942 -0.000074
H7 2.068970 0.469262 -0.000039
H8 1.288080 -0.858313 0.886739
H9 1.288020 -0.858584 -0.886603

TS_Rxn 2e.1
N1 -2.154637 -0.255452 -0.224448
N2 -1.132324 -0.113614 0.591813
C3 0.374979 1.101970 -0.255834
C4 1.601050 0.328351 0.110288
H5 2.425889 0.713068 -0.508184
H6 1.866980 0.484203 1.163516
O7 1.323625 -1.031695 -0.165221
H8 2.095506 -1.585735 -0.007533
H9 0.351793 2.143792 0.079152
H10 -0.014036 0.955415 -1.261277
H11 -0.687082 0.879591 0.742217
H12 -0.428422 -0.859959 0.544119
H13 -2.990988 0.273037 -0.026537
H14 -2.056085 -0.748319 -1.101984

$[N{=}NH_2]^+$
N1 0.000000 0.000000 -0.460036
N2 0.000000 0.000000 0.743267
H3 0.000000 0.895586 -0.991308
H4 0.000000 -0.895586 -0.991308

CH_3OH
C1 0.662528 -0.020652 -0.000009
H2 1.025131 -0.545268 -0.893777
H3 1.025040 -0.545584 0.893621
O4 -0.744790 0.122085 -0.000011
H5 -1.148737 -0.748814 0.000050
H6 1.081719 0.986894 0.000248

$^{\bullet}CH_3$
C1 0.000001 -0.000160 0.000425
H2 0.938463 -0.539219 -0.000850
H3 -0.936842 -0.542030 -0.000850
H4 -0.001626 1.082208 -0.000849

$[HOCH_2CH_2NHNH_3]^+$
H1 0.600796 -1.334643 0.017447
N2 1.449401 -0.731340 0.094710
N3 1.151569 0.637448 -0.279387
C4 -0.111105 1.078800 0.332515
C5 -1.359116 0.360200 -0.161649
H6 -2.228936 0.712238 0.401769
H7 -1.524725 0.557685 -1.227951
O8 -1.147440 -1.041158 0.048518
H9 -1.942602 -1.549278 -0.140968
H10 -0.185567 2.147692 0.119094
H11 -0.009280 0.976958 1.417982
H12 1.090926 0.651687 -1.295917
H13 1.772720 -0.728996 1.066230
H14 2.220714 -1.080836 -0.478293

$[CH_3CH{=}NNH_3]^+$
N1 -1.769795 0.063318 -0.000003
N2 -0.428499 -0.511355 -0.000004
C3 0.506536 0.359701 0.000015
C4 1.922602 -0.078233 -0.000012
H5 2.426519 0.334489 -0.880038
H6 2.003380 -1.165097 -0.000121
H7 2.426449 0.334233 0.880177
H8 0.301339 1.437783 0.000021
H9 -2.262084 -0.292412 0.826207
H10 -2.262404 -0.293366 -0.825609
H11 -1.819967 1.091821 -0.000602

TS_Rxn 2b.2
N1 -2.220751 0.325359 0.044854
N2 -0.837920 0.315126 -0.369670
C3 -0.157189 -0.698279 0.273464
C4 1.164085 -0.930539 -0.207329
H5 1.842872 -1.537786 0.381597
H6 1.331541 -0.830657 -1.274662
O7 2.035411 0.839560 0.194279
H8 2.839362 1.097558 -0.273356
H9 -0.189707 -1.813552 -0.205990
H10 -0.308348 -0.891606 1.347175
H11 1.336381 1.465885 -0.048919
H12 -2.781623 -0.442695 -0.345944
H13 -2.616424 1.192666 -0.322016
H14 -2.368022 0.333217 1.064785

$[CH_2{=}NHNH_2]^+$
N1 1.160184 -0.168000 0.091487
N2 -0.075269 0.390765 -0.007371
C3 -1.205036 -0.211947 -0.015148
H4 -1.245151 -1.296104 -0.037387
H5 -0.060604 1.409682 0.041890
H6 1.176618 -1.159290 -0.121961
H7 1.871041 0.369606 -0.391792

H8 -2.106098 0.388434 0.011325

CH_3OH
C1 0.662528 -0.020652 -0.000009
H2 1.025131 -0.545268 -0.893777
H3 1.025040 -0.545584 0.893621
O4 -0.744790 0.122085 -0.000011
H5 -1.148737 -0.748814 0.000050
H6 1.081719 0.986894 0.000248

TS_Rxn 2c.2
H1 -0.047821 -0.651101 -0.445824
N2 1.308165 -0.974656 0.034614
N3 1.531962 0.409941 0.045684
C4 0.332155 1.031117 0.270304
C5 -1.102611 0.047070 -0.625608
H6 -1.347829 1.037839 -1.029465
H7 -1.191405 -0.587439 -1.532652
O8 -1.917621 -0.363020 0.427233
H9 -2.848712 -0.209556 0.236779
H10 0.299077 2.073122 -0.039147
H11 -0.149358 0.821448 1.225495
H12 2.065775 0.724230 -0.756608
H13 1.280909 -1.345445 0.985290
H14 2.022178 -1.475052 -0.491995

$[CH_2=C=NH_2]^+$
N1 1.215366 0.000055 0.000013
C2 -0.044570 -0.000015 -0.000030
C3 -1.330027 -0.000001 -0.000002
H4 -1.874945 0.942584 0.001084
H5 -1.875027 -0.942570 -0.000990
H6 1.744982 0.000968 -0.872387
H7 1.745015 -0.001273 0.872392

$[N=NH_2]^+$
N1 0.000000 0.000000 -0.460036
N2 0.000000 0.000000 0.743267
H3 0.000000 0.895586 -0.991308
H4 0.000000 -0.895586 -0.991308

CH_3OH
C1 0.662528 -0.020652 -0.000009
H2 1.025131 -0.545268 -0.893777
H3 1.025040 -0.545584 0.893621
O4 -0.744790 0.122085 -0.000011
H5 -1.148737 -0.748814 0.000050
H6 1.081719 0.986894 0.000248

$^{\bullet}CH_3$
C1 0.000001 -0.000160 0.000425
H2 0.938463 -0.539219 -0.000850
H3 -0.936842 -0.542030 -0.000850
H4 -0.001626 1.082208 -0.000849

Cartesian coordinates for structures in Rxns 3, calculated at ωB97XD/ 6-31+G(d,p)

$[HOCH_2CH_2NHNH_2]\cdot[HOCH_2CH_2NH_2NH_2]^+$ (Structure I)
O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422
N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056
H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

$HOCH_2CH_2NHNH_2$ (HE)
N1 2.217126 -0.278438 -0.058113
H2 2.555479 0.648037 -0.315617
H3 2.270478 -0.880530 -0.871609
N4 0.873455 -0.241323 0.388914
H5 0.897688 -0.097285 1.393128
C6 0.020034 0.754971 -0.252602
C7 -1.423443 0.497918 0.161670
H8 0.309301 1.793594 -0.013848
H9 0.111177 0.617122 -1.335656

H10 -1.532872 0.659155 1.247005
H11 -2.091380 1.199932 -0.344256
O12 -1.830542 -0.804154 -0.193706
H13 -1.089154 -1.385805 0.020488

$[HOCH_2CH_2NH_2NH_2]^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$ (frist probable structure II for *m/z* 153)
O1 -1.982147 2.389763 -0.555460
C2 -0.534115 0.132705 0.738569
C3 -1.599759 -0.787719 0.148946
H4 -2.438283 3.114396 -0.989367
H5 -0.707053 0.320956 1.802770
H6 -1.518140 -1.799403 0.588564
N7 0.822449 -0.488639 0.653189
H8 1.533487 0.157260 1.060957
H9 0.860518 -1.360670 1.197838
N10 1.266626 -0.672672 -0.705608
H11 0.739896 -1.446476 -1.100939
C12 2.713060 -0.924185 -0.761944
C13 3.494546 0.342578 -0.462754
H14 3.027593 -1.731804 -0.083475
H15 2.924501 -1.241785 -1.785251
H16 4.566629 0.141119 -0.548314
H17 3.208829 1.131141 -1.166108
O18 3.163777 0.726560 0.878421
H19 3.607137 1.544553 1.123917
H20 -1.472889 -0.877334 -0.932830
N21 -2.915731 -0.196908 0.350222
H22 -3.134986 -0.134850 1.343192
N23 -3.894186 -0.940298 -0.361408
H24 -4.288043 -1.694353 0.195175
H25 -4.637694 -0.317130 -0.651434
H26 -2.630791 1.689171 -0.374104
H27 -0.490253 1.083968 0.204062

$[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+$
C1 0.793598 -0.830484 0.009554
C2 1.932164 0.140869 0.307959
H3 0.964287 -1.804487 0.477258
H4 1.925259 0.419103 1.380168
N5 -0.511630 -0.339223 0.551165
H6 -1.272222 -1.022325 0.345386
H7 -0.460764 -0.245174 1.574660
N8 -0.955121 0.874261 -0.088801
H9 -0.351104 1.627170 0.229644
C10 -2.364773 1.151578 0.221981
C11 -3.281681 0.200764 -0.525890
H12 -2.571576 1.108346 1.301999
H13 -2.554355 2.172539 -0.116444
H14 -4.324318 0.438037 -0.293630
H15 -3.114184 0.290092 -1.603996
O16 -2.959446 -1.122831 -0.079504
H17 -3.518179 -1.779651 -0.506299
H18 1.818615 1.057110 -0.276597
N19 3.167325 -0.466094 -0.138855
H20 3.488753 -1.185206 0.503745
N21 4.159995 0.505537 -0.407948
H22 4.767750 0.678228 0.388172
H23 4.716714 0.194072 -1.194416
H24 0.661068 -0.962936 -1.064167

***cyclo*-$[CH_2CH_2NHNH^+(CH_2CH_2NHNH_2)]$**
C1 -0.169079 0.742094 -0.152305
C2 -1.318026 -0.103038 0.392871
H3 -0.255421 1.796089 0.131355
H4 -1.276137 -0.142708 1.498189
N5 1.133634 0.266051 0.389233
H6 1.117644 0.322996 1.414531
N7 1.550982 -1.045456 -0.089451
H8 1.356462 -1.777129 0.591313
C9 2.959925 -0.590921 -0.218882
C10 2.428421 0.847742 -0.148511
H11 3.598719 -0.857732 0.627827
H12 3.420511 -0.901849 -1.154916
H13 2.894295 1.552971 0.537091
H14 2.233287 1.306748 -1.116984
H15 -1.230176 -1.125335 0.016498
N16 -2.557010 0.426190 -0.134757
H17 -2.868010 1.246472 0.378074
N18 -3.557409 -0.569676 -0.230321
H19 -4.159942 -0.601216 0.587509
H20 -4.118145 -0.390869 -1.054364
H21 -0.111913 0.656541 -1.238093

TS_Rxn 3e.1

C1 -0.601876 0.567434 -0.308324
C2 -1.859838 -0.020643 0.339977
H3 -0.592883 1.659193 -0.211690
H4 -1.826245 0.142518 1.434006
N5 0.642661 0.084868 0.285738
H6 2.401363 2.313511 0.037822
H7 0.763818 0.413652 1.246198
N8 0.817957 -1.325001 0.169250
H9 0.373464 -1.845821 0.921660
C10 2.251043 -1.463845 0.125265
C11 2.676632 -0.424289 -0.811187
H12 2.765667 -1.328267 1.091101
H13 2.599191 -2.434150 -0.277699
H14 3.722751 -0.155372 -0.888985
H15 2.024698 -0.147624 -1.632812
O16 3.064308 1.662875 0.293271
H17 3.898886 2.141305 0.369166
H18 -1.897386 -1.098881 0.165282
N19 -3.032482 0.538747 -0.301268
H20 -3.164516 1.513585 -0.043101
N21 -4.184587 -0.242520 -0.039668
H22 -4.690771 0.065624 0.786443
H23 -4.797631 -0.201596 -0.844377
H24 -0.595483 0.314729 -1.371923

$[HE + H]^+$

O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$CH_2CHNHNH_2$

N1 -1.755825 -0.052331 0.174844
H2 -1.671786 -0.632683 1.005352
H3 -2.183407 -0.584515 -0.573705
N4 -0.507208 0.441293 -0.250666
H5 -0.379821 1.397234 0.051986
C6 0.617627 -0.368522 -0.132054
C7 1.863769 0.048432 0.122950
H8 0.409324 -1.419744 -0.323961
H9 2.091764 1.092294 0.319134
H10 2.686776 -0.654785 0.106578

TS_Rxn 3f.1

C1 1.973957 -1.258387 -0.555326
C2 1.532430 -0.057588 -1.124933
N3 1.815696 1.222175 -0.521369
N4 2.080327 1.127756 0.870206
H5 2.640776 -1.301029 0.296382
H6 1.831954 -2.183661 -1.103483
H7 1.446713 -0.008713 -2.210285
H8 2.533175 1.730204 -1.029738
H9 3.071596 0.992922 1.066413
H10 1.805352 2.005593 1.298150
N11 0.276552 -1.501547 0.821148
H12 0.652917 -0.969330 1.603202
H13 -0.041733 -2.424403 1.099744
N14 -0.669119 -0.754253 0.134448
H15 0.310290 -0.263690 -0.823803
C16 -1.362235 0.325420 0.862856
C17 -2.354454 0.953470 -0.098796
H18 -1.883686 -0.089319 1.732140
H19 -0.616797 1.053922 1.187478
H20 -2.963233 1.683787 0.445099
H21 -1.822173 1.467666 -0.909712
O22 -3.131988 -0.122050 -0.595555
H23 -3.818978 0.196399 -1.187689
H24 -1.352652 -1.350353 -0.333299

$[CH_2CHNHNH_2][NH_2NH_2CH_2CH_2OH]^+ \cdot H_2O$ (second probable structure II for *m/z* 153)

C1 2.966649 -1.094683 -0.735792
C2 1.672837 -1.052843 -0.404374
N3 1.123311 -1.593985 0.765411
N4 -0.178649 -2.149381 0.593966
H5 3.700420 -1.639271 -0.148727
H6 3.310154 -0.598624 -1.635817
H7 3.025422 2.860862 -0.064519
H8 1.758100 -2.232297 1.236701
H9 -0.143806 -3.032672 0.080778
H10 -0.543014 -2.350470 1.521573
N11 -3.095399 -0.753469 -0.946675
H12 -3.596747 -1.198779 -0.183259
H13 -3.687586 -0.030055 -1.346057
N14 -1.916116 -0.147434 -0.421224
H15 -1.275352 -0.929817 -0.089413
C16 -2.052723 0.883883 0.651110
C17 -0.676995 1.510297 0.836666
H18 -2.778601 1.621985 0.300853

H19 -2.424300 0.402456 1.558088
H20 -0.769954 2.396447 1.474057
H21 0.006398 0.800995 1.323996
O22 -0.235853 1.829078 -0.464910
H23 0.709330 2.079677 -0.423295
H24 -1.408565 0.314640 -1.187649
O25 2.396719 2.141524 0.040953
H26 2.883824 1.311413 -0.034526
H27 0.956708 -0.511353 -1.017134

$[CH_2CHNHNH_2][NH_2NH_2CH_2CH_2OH]^+$
C1 -3.336882 -0.549841 -0.645794
C2 -2.111831 -0.110760 -0.361606
N3 -1.782321 0.689666 0.752298
N4 -0.858678 1.735221 0.433553
H5 -4.208323 -0.256388 -0.067490
H6 -3.490893 -1.242478 -1.463753
H7 -2.615321 1.052490 1.209148
H8 -1.279218 2.434153 -0.183574
H9 -0.621557 2.202517 1.305172
N10 2.370343 1.511453 -0.872163
H11 2.572430 2.134341 -0.095177
H12 3.238801 1.084864 -1.184274
N13 1.483696 0.490472 -0.416650
H14 0.567257 0.982455 -0.137263
C15 1.947699 -0.405252 0.685524
C16 0.940288 -1.535053 0.832694
H17 2.929662 -0.792333 0.402134
H18 2.034809 0.185860 1.599638
H19 1.346621 -2.282425 1.522048
H20 -0.009275 -1.156362 1.233132
O21 0.777201 -2.048765 -0.479145
H22 0.191856 -2.811836 -0.479506
H23 1.252088 -0.108982 -1.216752
H24 -1.253469 -0.418001 -0.954496

$[CH_2CHNHNH_2][NH_2NH_2CHCH_2]^+$
C1 -2.306704 1.642000 0.308788
C2 -1.961539 0.355007 0.348262
N3 -1.759486 -0.423018 -0.822987
N4 -1.026757 -1.621340 -0.570145
H5 -2.443217 2.166806 -0.631981
H6 -2.511595 2.175905 1.228987
H7 -2.620006 -0.593915 -1.334003
H8 -1.575234 -2.314062 -0.056094
H9 -0.777861 -2.027174 -1.468586
N10 1.259414 -0.404116 1.786098
H11 1.592408 -1.361263 1.866380
H12 1.984036 0.222834 2.127962
N13 1.032085 -0.121825 0.397432
H14 0.318751 -0.864054 0.048679
C15 2.207369 -0.053650 -0.465420
C16 2.517453 1.048806 -1.130152
H17 2.770049 -0.980276 -0.498561
H18 3.390117 1.066077 -1.772385
H19 1.923353 1.956776 -1.068472
H20 0.496724 0.754322 0.357167
H21 -1.823794 -0.162853 1.299247

TS_Rxn 3e.2
C1 2.084884 1.600421 -1.232860
C2 2.106377 0.416067 -0.620687
N3 1.944223 0.255247 0.778091
N4 1.725452 -1.101095 1.157204
H5 1.939786 2.527946 -0.686215
H6 2.269380 1.665268 -2.298204
H7 2.687811 0.699685 1.308115
H8 2.578887 -1.659030 1.104324
H9 1.410300 -1.107697 2.122584
N10 -1.085115 -2.194366 -1.116851
H11 -1.192583 -2.952710 -0.447932
H12 -2.012278 -1.975074 -1.476980
N13 -0.644562 -1.039780 -0.387950
H14 0.224872 -1.317359 0.140603
C15 -1.650831 -0.389471 0.487694
C16 -1.376537 1.013568 0.798540
H17 -2.795918 0.582432 -0.208643
H18 -1.883658 -1.043607 1.324771
H19 -1.592744 1.334488 1.815605
H20 -0.481051 1.486789 0.397728
O21 -2.556674 1.644055 -0.099092
H22 -3.212009 2.199114 0.358513
H23 -0.311844 -0.370563 -1.087804
H24 2.261087 -0.505670 -1.183301

$[HE + H]^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$CH_2CHNHNH_2$

N1	-1.755825	-0.052331	0.174844
H2	-1.671786	-0.632683	1.005352
H3	-2.183407	-0.584515	-0.573705
N4	-0.507208	0.441293	-0.250666
H5	-0.379821	1.397234	0.051986
C6	0.617627	-0.368522	-0.132054
C7	1.863769	0.048432	0.122950
H8	0.409324	-1.419744	-0.323961
H9	2.091764	1.092294	0.319134
H10	2.686776	-0.654785	0.106578

Cartesian coordinates for structures in Rxns 4, calculated at ωB97XD/ 6-31+G(d,p)

$[(HE)_3 + H]^+$

O1	-0.294204	-0.059411	1.922145
C2	-0.506412	1.313952	2.140066
C3	-0.234573	2.144738	0.890482
N4	-1.013511	1.627343	-0.261022
N5	-0.801421	2.450294	-1.421461
H6	0.628080	-0.338031	2.109085
H7	0.115394	1.706322	2.953094
H8	-1.552246	1.435728	2.443721
H9	0.813134	2.097513	0.590336
H10	-0.514870	3.190896	1.032535
H11	-2.014295	1.605135	-0.033864
H12	-0.796326	0.609327	-0.459387
H13	-1.493423	2.177683	-2.114848
H14	0.122824	2.181896	-1.771282
N15	-0.079643	-1.424012	-2.100018
H16	-0.657747	-1.128980	-2.881978
H17	0.074234	-2.428203	-2.197016
N18	-0.764695	-1.111435	-0.888495
H19	-0.090135	-1.272116	-0.137801
C20	-2.005256	-1.868594	-0.681495
C21	-2.818767	-1.329223	0.482533
H22	-2.601013	-1.783404	-1.596334
H23	-1.805241	-2.937363	-0.509132
H24	-3.679024	-1.989656	0.629158
H25	-2.219114	-1.310771	1.398171
O26	-3.264773	0.001029	0.180304
H27	-4.131019	0.140003	0.571545
N28	2.093131	-1.472598	1.867948
H29	2.977860	-1.542229	2.374064
H30	1.606443	-2.356778	1.982977
N31	2.293043	-1.249699	0.465792
H32	2.895667	-1.975491	0.078592
C33	2.946095	0.046021	0.273177
C34	2.897136	0.497311	-1.180609
H35	2.412257	0.769856	0.894708
H36	3.994046	0.038220	0.616173
H37	3.454483	1.433235	-1.275003
H38	3.389655	-0.239975	-1.829404
O39	1.577661	0.741415	-1.624137
H40	1.163250	-0.111565	-1.878737

$[(HE)_2 + H]^+$

O1	-2.085492	-1.439869	-0.825220
C2	-2.746950	-0.188849	-0.809156
C3	-2.322517	0.497570	0.475819
N4	-0.842348	0.479701	0.568422
N5	-0.358036	1.214926	1.704249
H6	-2.424130	-1.993178	-1.534644
H7	-3.837279	-0.294666	-0.803188
H8	-2.462722	0.419097	-1.679388
H9	-2.713855	-0.033761	1.346803
H10	-2.645683	1.539156	0.511056
H11	-0.416173	0.961077	-0.260868
H12	-0.480002	-0.491371	0.564841
H13	-0.676331	0.729652	2.540380
H14	0.658704	1.116776	1.652618
N15	1.029514	1.810851	-1.045303
H16	1.351434	1.970206	-2.001242
H17	0.998046	2.714630	-0.579895
N18	1.921122	0.967849	-0.301135
H19	2.852323	1.376536	-0.264782
C20	1.993439	-0.372952	-0.894712
C21	2.241405	-1.432810	0.161945
H22	1.033767	-0.580668	-1.380274
H23	2.767037	-0.446213	-1.671270
H24	2.401136	-2.396464	-0.333871
H25	3.133202	-1.189893	0.752880
O26	1.093972	-1.493242	1.009789
H27	1.148661	-2.267080	1.577274

HE

N1	2.217126	-0.278438	-0.058113
H2	2.555479	0.648037	-0.315617
H3	2.270478	-0.880530	-0.871609
N4	0.873455	-0.241323	0.388914
H5	0.897688	-0.097285	1.393128
C6	0.020034	0.754971	-0.252602
C7	-1.423443	0.497918	0.161670
H8	0.309301	1.793594	-0.013848
H9	0.111177	0.617122	-1.335656
H10	-1.532872	0.659155	1.247005
H11	-2.091380	1.199932	-0.344256
O12	-1.830542	-0.804154	-0.193706

H13 -1.089154 -1.385805 0.020488

[HE + H]$^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

HE
N1 2.217126 -0.278438 -0.058113
H2 2.555479 0.648037 -0.315617
H3 2.270478 -0.880530 -0.871609
N4 0.873455 -0.241323 0.388914
H5 0.897688 -0.097285 1.393128
C6 0.020034 0.754971 -0.252602
C7 -1.423443 0.497918 0.161670
H8 0.309301 1.793594 -0.013848
H9 0.111177 0.617122 -1.335656
H10 -1.532872 0.659155 1.247005
H11 -2.091380 1.199932 -0.344256
O12 -1.830542 -0.804154 -0.193706
H13 -1.089154 -1.385805 0.020488

Cartesian coordinates for structures in Rxns 5, calculated at ωB97XD/ 6-31+G(d,p)

[(HEHN)HE + H]$^+$
O1 -4.480615 -0.321588 1.601512
C2 -4.808905 -0.364806 0.224733
C3 -4.105774 0.831683 -0.393786
N4 -2.677362 0.791194 0.012934
N5 -1.981922 2.011019 -0.298733
H6 -4.928385 -1.022135 2.083828
H7 -5.885604 -0.263813 0.052027
H8 -4.463021 -1.298614 -0.237225
H9 -4.516021 1.771881 -0.019882
H10 -4.157838 0.807294 -1.484500
H11 -2.176866 -0.034401 -0.419281
H12 -2.667414 0.676715 1.031538
H13 -2.110005 2.173066 -1.295993
H14 -0.994285 1.791892 -0.159454
N15 -0.014523 -0.973370 -0.842878
O16 0.856826 -1.749033 -1.230030
O17 -1.195085 -1.067770 -1.240081
O18 0.281847 -0.044554 -0.013575
O19 4.420198 1.283062 -0.834234
C20 3.943363 1.627468 0.451456
C21 3.782972 0.307351 1.185596
N22 2.979162 -0.611419 0.337587
N23 3.019012 -1.959992 0.831397
H24 4.642362 2.065538 -1.346165
H25 2.983490 2.158098 0.389484
H26 4.651668 2.250903 1.007613
H27 3.271652 0.435818 2.142037
H28 4.746882 -0.179060 1.344293
H29 3.411329 -0.612249 -0.592863
H30 1.991733 -0.270797 0.214716
H31 2.438678 -2.504330 0.193202
H32 2.555772 -1.958942 1.737757

[(HE)$_2$ + H]$^+$
O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422
N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056
H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

HNO_3
N1 0.000000 0.144358 0.000000
O2 1.175229 0.440613 0.000000
O3 -0.967887 0.848121 0.000000
O4 -0.281663 -1.211283 0.000000
H5 0.594568 -1.630119 0.000000

$[HE + H]^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$HE \cdot HNO_3$
O1 -1.172026 -1.995635 -0.598390
C2 -1.344870 -1.435904 0.689833
C3 -1.969873 -0.048665 0.601891
N4 -1.141460 0.810426 -0.257126
N5 -1.682866 2.128758 -0.337562
H6 -0.248609 -1.880244 -0.853309
H7 -0.388835 -1.384387 1.224925
H8 -2.012044 -2.087572 1.261950
H9 -2.024577 0.420859 1.587210
H10 -2.985503 -0.120205 0.191931
H11 -1.079782 0.365516 -1.174698
H12 0.207777 0.865168 0.222571
H13 -2.425363 2.170640 -1.030819
H14 -0.941363 2.764172 -0.611940
N15 2.001754 0.066496 -0.010221
O16 3.172594 0.061062 0.274492
O17 1.237529 0.964942 0.603843
O18 1.454999 -0.686156 -0.821671

Cartesian coordinates for structures in Rxns 6, calculated at ωB97XD/ 6-31+G(d,p)

$[(HEHN)_2HE + H]^+$
O1 -2.161562 -1.933708 -0.823146
C2 -1.864510 -3.259619 -0.413632
C3 -0.373571 -3.571428 -0.453699
N4 0.394183 -2.564231 0.322941
N5 1.775203 -2.939920 0.475529
H6 -1.672401 -1.716542 -1.636846
H7 -2.384429 -3.988712 -1.044638
H8 -2.251176 -3.359600 0.604282
H9 0.017473 -3.554424 -1.474263
H10 -0.167070 -4.549597 -0.016108
H11 -0.024567 -2.431888 1.259816
H12 0.293008 -1.625018 -0.122665
H13 2.080736 -2.494600 1.339059
H14 2.286982 -2.482413 -0.280542
N15 0.017508 -0.173713 2.262059
O16 -0.321096 1.029181 2.201564
O17 -0.859950 -1.066456 2.284231
O18 1.231656 -0.484603 2.251762
O19 -1.077379 2.870509 -0.646044
C20 -2.481366 2.800557 -0.812532
C21 -2.941910 1.348823 -0.860441
N22 -2.476390 0.633704 0.361080
N23 -3.290399 0.936089 1.502209
H24 -0.632613 2.572936 -1.453897
H25 -2.813978 3.311480 -1.722179
H26 -2.922681 3.303412 0.050112
H27 -2.510517 0.825017 -1.718399
H28 -4.029039 1.264145 -0.912860
H29 -1.527286 0.977330 0.584853
H30 -2.375019 -0.381107 0.163480
H31 -2.714059 0.737911 2.318988
H32 -4.079358 0.295326 1.499719
N33 0.136290 0.141917 -1.932171
O34 -0.292583 -0.791759 -2.622866
O35 0.128260 0.020098 -0.656505
O36 0.556669 1.198091 -2.418095
O37 3.029529 -0.607629 -1.084001
C38 3.856628 0.172067 -0.233130
C39 3.362456 1.603405 -0.070855
N40 2.020725 1.638812 0.561800
N41 1.631625 2.981537 0.896828
H42 3.224751 -0.409211 -2.005682
H43 4.889453 0.201147 -0.595433
H44 3.862319 -0.335405 0.736376
H45 3.279252 2.108385 -1.037029
H46 4.033553 2.177676 0.571432
H47 2.017990 1.086627 1.436459
H48 1.319768 1.147059 -0.034931
H49 0.798076 2.881409 1.475326
H50 1.324924 3.426662 0.034177

$[(HEHN)(HE)_2 + H]^+$

O1	-1.856843	-1.963434	1.410265
C2	-2.701640	-2.688414	0.542843
C3	-3.878474	-1.805546	0.138900
N4	-3.339843	-0.483704	-0.269977
N5	-4.247542	0.262361	-1.095892
H6	-0.973419	-1.932792	1.011016
H7	-3.085598	-3.586416	1.037734
H8	-2.157573	-3.004426	-0.356252
H9	-4.562820	-1.637852	0.974373
H10	-4.428573	-2.221516	-0.707597
H11	-2.474088	-0.628461	-0.813923
H12	-3.053733	0.082056	0.576893
H13	-3.797747	1.162456	-1.264755
H14	-5.085271	0.436255	-0.544508
N15	-2.510751	1.581166	1.390035
H16	-3.230301	2.268869	1.593026
H17	-1.950055	1.464122	2.236940
N18	-1.736916	2.056670	0.289590
H19	-1.171929	1.272344	-0.029450
C20	-0.842736	3.168445	0.605906
C21	0.182966	3.333657	-0.503408
H22	-1.426989	4.090388	0.700394
H23	-0.312030	3.004479	1.558755
H24	-0.315165	3.446964	-1.471037
H25	0.784405	4.227087	-0.316656
O26	1.057480	2.204124	-0.528964
H27	0.956042	1.675894	-1.330508
N28	0.384602	-0.872137	-1.060720
O29	-0.717734	-0.365192	-1.342171
O30	1.417631	-0.446599	-1.630557
O31	0.480423	-1.781940	-0.204349
O32	2.994962	1.133357	1.086794
C33	4.071610	0.983791	0.185983
C34	4.526911	-0.473164	0.253313
N35	3.298908	-1.305865	0.191748
N36	3.550224	-2.708225	0.333461
H37	2.285662	1.633091	0.641923
H38	4.912312	1.630924	0.457666
H39	3.763014	1.233414	-0.836702
H40	5.022804	-0.710889	1.196065
H41	5.179882	-0.738879	-0.580832
H42	2.723742	-1.062742	-0.648417
H43	2.722750	-0.999299	0.984033
H44	4.084087	-3.007088	-0.479241
H45	2.640637	-3.164971	0.293970

$[(HE)_3 + H]^+$

O1	-0.294204	-0.059411	1.922145
C2	-0.506412	1.313952	2.140066
C3	-0.234573	2.144738	0.890482
N4	-1.013511	1.627343	-0.261022
N5	-0.801421	2.450294	-1.421461
H6	0.628080	-0.338031	2.109085
H7	0.115394	1.706322	2.953094
H8	-1.552246	1.435728	2.443721
H9	0.813134	2.097513	0.590336
H10	-0.514870	3.190896	1.032535
H11	-2.014295	1.605135	-0.033864
H12	-0.796326	0.609327	-0.459387
H13	-1.493423	2.177683	-2.114848
H14	0.122824	2.181896	-1.771282
N15	-0.079643	-1.424012	-2.100018
H16	-0.657747	-1.128980	-2.881978
H17	0.074234	-2.428203	-2.197016
N18	-0.764695	-1.111435	-0.888495
H19	-0.090135	-1.272116	-0.137801
C20	-2.005256	-1.868594	-0.681495
C21	-2.818767	-1.329223	0.482533
H22	-2.601013	-1.783404	-1.596334
H23	-1.805241	-2.937363	-0.509132
H24	-3.679024	-1.989656	0.629158
H25	-2.219114	-1.310771	1.398171
O26	-3.264773	0.001029	0.180304
H27	-4.131019	0.140003	0.571545
N28	2.093131	-1.472598	1.867948
H29	2.977860	-1.542229	2.374064
H30	1.606443	-2.356778	1.982977
N31	2.293043	-1.249699	0.465792
H32	2.895667	-1.975491	0.078592
C33	2.946095	0.046021	0.273177
C34	2.897136	0.497311	-1.180609
H35	2.412257	0.769856	0.894708
H36	3.994046	0.038220	0.616173
H37	3.454483	1.433235	-1.275003
H38	3.389655	-0.239975	-1.829404
O39	1.577661	0.741415	-1.624137
H40	1.163250	-0.111565	-1.878737

$[(HEHN)HE + H]^+$

O1	-4.480615	-0.321588	1.601512
C2	-4.808905	-0.364806	0.224733
C3	-4.105774	0.831683	-0.393786
N4	-2.677362	0.791194	0.012934
N5	-1.981922	2.011019	-0.298733
H6	-4.928385	-1.022135	2.083828
H7	-5.885604	-0.263813	0.052027
H8	-4.463021	-1.298614	-0.237225
H9	-4.516021	1.771881	-0.019882
H10	-4.157838	0.807294	-1.484500

H11 -2.176866 -0.034401 -0.419281
H12 -2.667414 0.676715 1.031538
H13 -2.110005 2.173066 -1.295993
H14 -0.994285 1.791892 -0.159454
N15 -0.014523 -0.973370 -0.842878
O16 0.856826 -1.749033 -1.230030
O17 -1.195085 -1.067770 -1.240081
O18 0.281847 -0.044554 -0.013575
O19 4.420198 1.283062 -0.834234
C20 3.943363 1.627468 0.451456
C21 3.782972 0.307351 1.185596
N22 2.979162 -0.611419 0.337587
N23 3.019012 -1.959992 0.831397
H24 4.642362 2.065538 -1.346165
H25 2.983490 2.158098 0.389484
H26 4.651668 2.250903 1.007613
H27 3.271652 0.435818 2.142037
H28 4.746882 -0.179060 1.344293
H29 3.411329 -0.612249 -0.592863
H30 1.991733 -0.270797 0.214716
H31 2.438678 -2.504330 0.193202
H32 2.555772 -1.958942 1.737757

HE·HNO$_3$
O1 -1.172026 -1.995635 -0.598390
C2 -1.344870 -1.435904 0.689833
C3 -1.969873 -0.048665 0.601891
N4 -1.141460 0.810426 -0.257126
N5 -1.682866 2.128758 -0.337562
H6 -0.248609 -1.880244 -0.853309
H7 -0.388835 -1.384387 1.224925
H8 -2.012044 -2.087572 1.261950
H9 -2.024577 0.420859 1.587210
H10 -2.985503 -0.120205 0.191931
H11 -1.079782 0.365516 -1.174698
H12 0.207777 0.865168 0.222571
H13 -2.425363 2.170640 -1.030819
H14 -0.941363 2.764172 -0.611940
N15 2.001754 0.066496 -0.010221
O16 3.172594 0.061062 0.274492
O17 1.237529 0.964942 0.603843
O18 1.454999 -0.686156 -0.821671

[(HE)$_2$ + H]$^+$
O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422
N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056
H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

Cartesian coordinates for structures in Rxns 7, calculated at ωB97XD/ 6-31+G(d,p)

[(HEHN)(HE)$_2$ + H]$^+$
O1 -1.856843 -1.963434 1.410265
C2 -2.701640 -2.688414 0.542843
C3 -3.878474 -1.805546 0.138900
N4 -3.339843 -0.483704 -0.269977
N5 -4.247542 0.262361 -1.095892
H6 -0.973419 -1.932792 1.011016
H7 -3.085598 -3.586416 1.037734
H8 -2.157573 -3.004426 -0.356252
H9 -4.562820 -1.637852 0.974373
H10 -4.428573 -2.221516 -0.707597
H11 -2.474088 -0.628461 -0.813923
H12 -3.053733 0.082056 0.576893
H13 -3.797747 1.162456 -1.264755
H14 -5.085271 0.436255 -0.544508
N15 -2.510751 1.581166 1.390035
H16 -3.230301 2.268869 1.593026
H17 -1.950055 1.464122 2.236940
N18 -1.736916 2.056670 0.289590
H19 -1.171929 1.272344 -0.029450
C20 -0.842736 3.168445 0.605906
C21 0.182966 3.333657 -0.503408
H22 -1.426989 4.090388 0.700394

H23 -0.312030 3.004479 1.558755
H24 -0.315165 3.446964 -1.471037
H25 0.784405 4.227087 -0.316656
O26 1.057480 2.204124 -0.528964
H27 0.956042 1.675894 -1.330508
N28 0.384602 -0.872137 -1.060720
O29 -0.717734 -0.365192 -1.342171
O30 1.417631 -0.446599 -1.630557
O31 0.480423 -1.781940 -0.204349
O32 2.994962 1.133357 1.086794
C33 4.071610 0.983791 0.185983
C34 4.526911 -0.473164 0.253313
N35 3.298908 -1.305865 0.191748
N36 3.550224 -2.708225 0.333461
H37 2.285662 1.633091 0.641923
H38 4.912312 1.630924 0.457666
H39 3.763014 1.233414 -0.836702
H40 5.022804 -0.710889 1.196065
H41 5.179882 -0.738879 -0.580832
H42 2.723742 -1.062742 -0.648417
H43 2.722750 -0.999299 0.984033
H44 4.084087 -3.007088 -0.479241
H45 2.640637 -3.164971 0.293970

Cartesian coordinates for structures in Rxns 8, calculated at ωB97XD/ 6-31+G(d,p)

$[(HEHN)_2(HE)_2 + H]^+$
N1 -1.470219 3.404237 -1.322582
H2 -1.596644 4.172478 -0.667839
H3 -1.431602 3.821613 -2.253819
N4 -0.238586 2.750075 -1.000659
H5 -0.161615 1.960365 -1.645851
C6 0.950737 3.604665 -1.049439
C7 2.215259 2.758690 -0.940526
H8 1.001497 4.183875 -1.984480
H9 0.894683 4.311498 -0.213703
H10 2.349649 2.162993 -1.849961
H11 3.077507 3.419582 -0.828342
O12 2.193037 1.893861 0.193815
H13 1.757097 1.066059 -0.065582
O14 4.338023 0.201533 0.924281
C15 4.703465 -0.292188 -0.344791
C16 4.434816 -1.789901 -0.368098
N17 3.005996 -2.023395 -0.046445
N18 2.666896 -3.417557 -0.026783
H19 3.756782 0.970138 0.817090
H20 5.770022 -0.128133 -0.535505
H21 4.137616 0.200649 -1.146278
H22 5.029623 -2.294747 0.397449
H23 4.636452 -2.240782 -1.341062
H24 2.413873 -1.565164 -0.766984
H25 2.751917 -1.525028 0.824563
H26 3.172258 -3.833029 0.753312
H27 1.676065 -3.446681 0.216841
O28 -3.240329 -1.719810 1.432493
C29 -3.182456 -2.877276 0.632317
C30 -3.670626 -2.516164 -0.760644
N31 -2.816208 -1.438856 -1.321393
N32 -3.242117 -1.053285 -2.638257
H33 -2.400112 -1.606673 1.909413
H34 -3.836287 -3.662152 1.030159
H35 -2.161243 -3.277608 0.589809
H36 -4.691991 -2.131977 -0.741782
H37 -3.619213 -3.376167 -1.434110
H38 -1.811708 -1.714779 -1.311761
H39 -2.892734 -0.583954 -0.732286
H40 -2.550388 -0.374188 -2.953527
H41 -3.146918 -1.872434 -3.235131
O42 -2.751533 1.145511 -0.167053
C43 -3.179431 1.519767 1.131607
C44 -2.155641 2.398541 1.853787
N45 -0.783149 1.888996 1.623946
N46 0.196079 2.664972 2.331094
H47 -2.579817 1.934140 -0.724411
H48 -3.335031 0.582707 1.667956
H49 -4.135351 2.054944 1.100450
H50 -2.353307 2.399655 2.928804
H51 -2.166772 3.435483 1.510998
H52 -0.557360 2.030883 0.599635
H53 -0.737508 0.870764 1.858228
H54 0.206333 2.342949 3.295919
H55 1.094619 2.425981 1.905440
N56 0.326324 -0.626368 -1.799515
O57 1.510731 -0.242400 -1.624413
O58 -0.006126 -1.777097 -1.444150
O59 -0.505466 0.147274 -2.311053
N60 0.199679 -1.300303 1.785274
O61 1.147706 -0.539742 1.473843
O62 0.252476 -2.516103 1.598824
O63 -0.834769 -0.779236 2.299450

Cartesian coordinates for structures in Rxns 9, calculated at B97XD/ 6-31+G(d,p)

$[HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$
O1 -0.990027 2.093525 -0.205134
C2 -1.667922 -0.248996 0.577808

C3 -2.480594 -0.613537 -0.593526
H4 -1.251622 2.966821 -0.508754
H5 -2.077198 0.373392 1.366739
H6 -3.110599 0.234917 -0.863141
H7 -3.142998 -1.444911 -0.319577
N8 -0.467808 -0.672220 0.786424
H9 -0.033603 2.112026 -0.045264
H10 0.052335 -0.319668 1.590332
N11 0.232681 -1.457110 -0.135172
H12 0.036934 -2.434725 0.064273
C13 1.674519 -1.186943 -0.130306
C14 1.992838 0.225651 -0.594365
H15 2.128530 -1.363007 0.856778
H16 2.105025 -1.905297 -0.832528
H17 3.064775 0.305031 -0.792107
H18 1.450626 0.448810 -1.518005
O19 1.591162 1.175164 0.401354
H20 2.355248 1.645182 0.746290
H21 -1.853688 -0.919832 -1.431224

$[HOCH_2CH_2NHNHCHCH_3]^+$
C1 1.694539 0.010182 -0.496752
C2 2.025786 0.719878 0.744145
H3 2.248434 0.223584 -1.408979
H4 1.828529 1.784424 0.567715
H5 3.100932 0.627772 0.930590
N6 0.768186 -0.873112 -0.625294
H7 0.581877 -1.258636 -1.552621
N8 -0.089538 -1.225613 0.426152
H9 0.007191 -2.227532 0.569274
C10 -1.488228 -0.856284 0.139200
C11 -1.738250 0.625022 0.350162
H12 -1.785410 -1.146958 -0.878975
H13 -2.096624 -1.427107 0.844705
H14 -2.803869 0.818653 0.184580
H15 -1.486864 0.899417 1.382200
O16 -0.934237 1.349625 -0.573221
H17 -1.279565 2.241257 -0.672566
H18 1.445641 0.366407 1.593307

$[HOCH_2CH_2N(NH_2)CHCH_3]^+ \cdot H_2O$
C1 2.744110 0.208195 0.191081
C2 1.356223 0.135052 0.702247
H3 1.094685 -0.505295 1.534840
O4 0.839375 -2.392876 -0.332959
H5 0.723387 -3.212294 0.158908
H6 2.763937 0.044762 -0.891819
H7 3.189095 1.189691 0.401411
H8 3.358289 -0.551084 0.671594
N9 0.546082 1.597009 -0.931603
N10 0.384057 0.813710 0.200535
C11 -1.011915 0.655053 0.643140
C12 -1.840324 -0.132667 -0.374650
H13 -1.891526 0.404656 -1.330446
H14 -1.364439 -1.107234 -0.542317
O15 -3.100502 -0.241045 0.237331
H16 -3.715833 -0.701013 -0.340667
H17 -1.436015 1.649709 0.807230
H18 -1.002397 0.126641 1.596395
H19 1.063973 -2.667695 -1.227618
H20 1.471371 2.011307 -0.970642
H21 -0.165054 2.320381 -0.955282

$[HOCH_2CH_2N(NH_2)CHCH_3]^+$
C1 -2.845633 -0.523973 0.314016
C2 -1.462502 -0.775374 -0.155328
H3 -1.121564 -1.774603 -0.404526
H4 -2.839486 -0.011119 1.283438
H5 -3.397845 0.100815 -0.400549
H6 -3.383777 -1.464628 0.419180
N7 -0.825258 1.458604 0.088992
N8 -0.578778 0.154556 -0.283947
C9 0.822473 -0.119798 -0.658702
C10 1.759381 -0.025752 0.549430
H11 1.728437 0.980738 0.985452
H12 1.437911 -0.745365 1.315598
O13 3.016348 -0.339131 0.015393
H14 3.698105 -0.274825 0.690756
H15 1.114850 0.595864 -1.431610
H16 0.866082 -1.120646 -1.088608
H17 -1.805878 1.705719 0.015218
H18 -0.241679 2.098357 -0.439303

Cartesian coordinates for structures in Rxns 10, calculated at ωB97XD/ 6-31+G(d,p)

$[HE][HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$
O1 -2.802667 2.427519 -0.301599
C2 -0.495420 1.178405 -0.519235
C3 0.139384 1.705103 0.696383
H4 -3.338506 3.217313 -0.194379
H5 -0.561876 1.793594 -1.410173
H6 -0.207830 2.730330 0.841222
H7 1.229440 1.735380 0.551676
N8 -0.992214 -0.003168 -0.640350
H9 -3.407681 1.669644 -0.340134
H10 -1.468848 -0.248577 -1.507863
N11 -0.986997 -0.949636 0.386072
H12 -0.131542 -1.523871 0.271353

C13 -2.189824 -1.779983 0.376463
C14 -3.451214 -0.987397 0.685243
H15 -2.322980 -2.315487 -0.577956
H16 -2.030301 -2.529185 1.156377
H17 -4.260525 -1.674359 0.946814
H18 -3.273841 -0.319724 1.533367
O19 -3.823236 -0.178733 -0.438174
H20 -4.638546 -0.502487 -0.829518
H21 -0.091733 1.090530 1.566293
H22 1.936828 -0.403701 0.698609
N23 2.166032 -0.834493 -0.192679
N24 1.634998 -2.157417 -0.145794
H25 1.655618 -2.536117 -1.088140
H26 2.201331 -2.775234 0.439744
C27 4.039790 0.694336 -0.372249
H28 5.132707 0.756728 -0.404420
H29 3.631552 1.190460 -1.262124
C30 3.617322 -0.763680 -0.357279
H31 3.887458 -1.225292 -1.312844
H32 4.147864 -1.299233 0.446952
O33 3.520831 1.303902 0.806681
H34 4.039019 2.080082 1.033167

[HE][$HOCH_2CH_2NHNHCHCH_3$]$^+$
C1 -1.037594 1.641605 0.422406
C2 -2.352293 2.185302 0.806221
H3 -0.283844 2.298758 -0.007924
H4 -2.913886 2.366632 -0.117362
H5 -2.218315 3.147761 1.306133
N6 -0.666856 0.421814 0.541543
H7 0.324351 0.112314 0.278879
N8 -1.517044 -0.568743 1.072469
H9 -0.914631 -1.112111 1.690262
C10 -2.032529 -1.467958 0.023264
C11 -3.181072 -0.876925 -0.770740
H12 -1.241121 -1.785422 -0.671316
H13 -2.396136 -2.351354 0.554595
H14 -3.617910 -1.675699 -1.381465
H15 -3.950502 -0.503495 -0.082518
O16 -2.681138 0.171100 -1.591281
H17 -3.315218 0.362781 -2.287524
H18 -2.907323 1.487565 1.431885
H19 2.227265 -0.082031 1.156610
N20 1.842406 -0.640986 0.396164
N21 1.410371 -1.876370 0.978942
H22 1.020824 -2.448248 0.233924
H23 2.202769 -2.393903 1.361232
C24 3.316058 0.622661 -1.071258
H25 4.163545 0.535727 -1.760048
H26 2.490837 1.122434 -1.598651
C27 2.887991 -0.765523 -0.629563
H28 2.482636 -1.318723 -1.482647
H29 3.753669 -1.315390 -0.234574
O30 3.660538 1.335002 0.105674
H31 4.172290 2.118616 -0.110451

[$HOCH_2CH_2NHNHCHCH_3$]$^+$·H_2O
O1 -0.990027 2.093525 -0.205134
C2 -1.667922 -0.248996 0.577808
C3 -2.480594 -0.613537 -0.593526
H4 -1.251622 2.966821 -0.508754
H5 -2.077198 0.373392 1.366739
H6 -3.110599 0.234917 -0.863141
H7 -3.142998 -1.444911 -0.319577
N8 -0.467808 -0.672220 0.786424
H9 -0.033603 2.112026 -0.045264
H10 0.052335 -0.319668 1.590332
N11 0.232681 -1.457110 -0.135172
H12 0.036934 -2.434725 0.064273
C13 1.674519 -1.186943 -0.130306
C14 1.992838 0.225651 -0.594365
H15 2.128530 -1.363007 0.856778
H16 2.105025 -1.905297 -0.832528
H17 3.064775 0.305031 -0.792107
H18 1.450626 0.448810 -1.518005
O19 1.591162 1.175164 0.401354
H20 2.355248 1.645182 0.746290
H21 -1.853688 -0.919832 -1.431224

HE
N1 2.217126 -0.278438 -0.058113
H2 2.555479 0.648037 -0.315617
H3 2.270478 -0.880530 -0.871609
N4 0.873455 -0.241323 0.388914
H5 0.897688 -0.097285 1.393128
C6 0.020034 0.754971 -0.252602
C7 -1.423443 0.497918 0.161670
H8 0.309301 1.793594 -0.013848
H9 0.111177 0.617122 -1.335656
H10 -1.532872 0.659155 1.247005
H11 -2.091380 1.199932 -0.344256
O12 -1.830542 -0.804154 -0.193706
H13 -1.089154 -1.385805 0.020488

[HE + H]$^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662

H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$HOCH_2CH_2NHNCHCH_3$
C1 -1.853222 0.598223 -0.477424
C2 -2.500830 -0.702877 -0.104237
H3 -2.362266 1.225927 -1.208253
H4 -2.197834 -1.514969 -0.776056
H5 -3.587164 -0.608608 -0.181500
N6 -0.785110 1.113795 -0.001905
N7 -0.087323 0.361681 0.963072
H8 0.620657 0.994410 1.320583
C9 0.616982 -0.816384 0.453651
C10 1.642949 -0.511155 -0.630192
H11 1.129314 -1.265490 1.310843
H12 -0.096469 -1.555500 0.080420
H13 2.089291 -1.451138 -0.985087
H14 1.151156 -0.015418 -1.476681
O15 2.632718 0.328550 -0.054497
H16 3.093714 0.807237 -0.746348
H17 -2.230384 -0.980021 0.919102

Cartesian coordinates for structures in Figure S2, calculated at ωB97XD/ 6-31+G(d,p)

$[(HE)_2 + H]^+$

O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422
N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056
H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

TS1

O1 -2.214971 1.961461 -0.523720
C2 -0.917237 0.752235 0.075947
C3 -1.805682 -0.488294 0.006376
H4 -2.215946 2.125017 -1.475410
H5 -0.835831 1.312486 0.996763
H6 -1.362485 -1.289401 0.604000
N7 0.916929 -0.260528 0.693484
H8 1.525315 0.506967 0.987225
H9 0.952976 -0.958218 1.443748
N10 1.488970 -0.754708 -0.520276
H11 0.937570 -1.555209 -0.811575
C12 2.902056 -1.129787 -0.395119
C13 3.804327 0.090774 -0.418053
H14 3.090402 -1.713975 0.519363
H15 3.149339 -1.757998 -1.255783
H16 4.848681 -0.235416 -0.349247
H17 3.658458 0.635213 -1.358616
O18 3.459894 0.915002 0.693831
H19 4.069721 1.655026 0.757865
H20 -1.879498 -0.834476 -1.026551
N21 -3.175813 -0.171616 0.430749
H22 -3.238413 -0.130348 1.447244
N23 -4.103716 -1.089389 -0.129114
H24 -4.206203 -1.924059 0.442166
H25 -5.004961 -0.634464 -0.213822
H26 -2.999268 1.385555 -0.278206
H27 -0.234625 0.985710 -0.728861

$[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$

O1 -1.982147 2.389763 -0.555460
C2 -0.534115 0.132705 0.738569
C3 -1.599759 -0.787719 0.148946
H4 -2.438283 3.114396 -0.989367
H5 -0.707053 0.320956 1.802770
H6 -1.518140 -1.799403 0.588564
N7 0.822449 -0.488639 0.653189
H8 1.533487 0.157260 1.060957
H9 0.860518 -1.360670 1.197838
N10 1.266626 -0.672672 -0.705608
H11 0.739896 -1.446476 -1.100939
C12 2.713060 -0.924185 -0.761944
C13 3.494546 0.342578 -0.462754
H14 3.027593 -1.731804 -0.083475
H15 2.924501 -1.241785 -1.785251
H16 4.566629 0.141119 -0.548314
H17 3.208829 1.131141 -1.166108
O18 3.163777 0.726560 0.878421
H19 3.607137 1.544553 1.123917
H20 -1.472889 -0.877334 -0.932830
N21 -2.915731 -0.196908 0.350222
H22 -3.134986 -0.134850 1.343192
N23 -3.894186 -0.940298 -0.361408
H24 -4.288043 -1.694353 0.195175
H25 -4.637694 -0.317130 -0.651434
H26 -2.630791 1.689171 -0.374104
H27 -0.490253 1.083968 0.204062

$[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+$

C1 0.793598 -0.830484 0.009554
C2 1.932164 0.140869 0.307959
H3 0.964287 -1.804487 0.477258
H4 1.925259 0.419103 1.380168
N5 -0.511630 -0.339223 0.551165
H6 -1.272222 -1.022325 0.345386
H7 -0.460764 -0.245174 1.574660
N8 -0.955121 0.874261 -0.088801

H9 -0.351104 1.627170 0.229644
C10 -2.364773 1.151578 0.221981
C11 -3.281681 0.200764 -0.525890
H12 -2.571576 1.108346 1.301999
H13 -2.554355 2.172539 -0.116444
H14 -4.324318 0.438037 -0.293630
H15 -3.114184 0.290092 -1.603996
O16 -2.959446 -1.122831 -0.079504
H17 -3.518179 -1.779651 -0.506299
H18 1.818615 1.057110 -0.276597
N19 3.167325 -0.466094 -0.138855
H20 3.488753 -1.185206 0.503745
N21 4.159995 0.505537 -0.407948
H22 4.767750 0.678228 0.388172
H23 4.716714 0.194072 -1.194416
H24 0.661068 -0.962936 -1.064167

TS2
C1 -0.601876 0.567434 -0.308324
C2 -1.859838 -0.020643 0.339977
H3 -0.592883 1.659193 -0.211690
H4 -1.826245 0.142518 1.434006
N5 0.642661 0.084868 0.285738
H6 2.401363 2.313511 0.037822
H7 0.763818 0.413652 1.246198
N8 0.817957 -1.325001 0.169250
H9 0.373464 -1.845821 0.921660
C10 2.251043 -1.463845 0.125265
C11 2.676632 -0.424289 -0.811187
H12 2.765667 -1.328267 1.091101
H13 2.599191 -2.434150 -0.277699
H14 3.722751 -0.155372 -0.888985
H15 2.024698 -0.147624 -1.632812
O16 3.064308 1.662875 0.293271
H17 3.898886 2.141305 0.369166
H18 -1.897386 -1.098881 0.165282
N19 -3.032482 0.538747 -0.301268
H20 -3.164516 1.513585 -0.043101
N21 -4.184587 -0.242520 -0.039668
H22 -4.690771 0.065624 0.786443
H23 -4.797631 -0.201596 -0.844377
H24 -0.595483 0.314729 -1.371923

***cyclo*-[$CH_2CH_2NHNH^+(CH_2CH_2NHNH_2)$]**
C1 -0.169079 0.742094 -0.152305
C2 -1.318026 -0.103038 0.392871
H3 -0.255421 1.796089 0.131355
H4 -1.276137 -0.142708 1.498189
N5 1.133634 0.266051 0.389233
H6 1.117644 0.322996 1.414531
N7 1.550982 -1.045456 -0.089451
H8 1.356462 -1.777129 0.591313
C9 2.959925 -0.590921 -0.218882
C10 2.428421 0.847742 -0.148511
H11 3.598719 -0.857732 0.627827
H12 3.420511 -0.901849 -1.154916
H13 2.894295 1.552971 0.537091
H14 2.233287 1.306748 -1.116984
H15 -1.230176 -1.125335 0.016498
N16 -2.557010 0.426190 -0.134757
H17 -2.868010 1.246472 0.378074
N18 -3.557409 -0.569676 -0.230321
H19 -4.159942 -0.601216 0.587509
H20 -4.118145 -0.390869 -1.054364
H21 -0.111913 0.656541 -1.238093

TS3
C1 1.973957 -1.258387 -0.555326
C2 1.532430 -0.057588 -1.124933
N3 1.815696 1.222175 -0.521369
N4 2.080327 1.127756 0.870206
H5 2.640776 -1.301029 0.296382
H6 1.831954 -2.183661 -1.103483
H7 1.446713 -0.008713 -2.210285
H8 2.533175 1.730204 -1.029738
H9 3.071596 0.992922 1.066413
H10 1.805352 2.005593 1.298150
N11 0.276552 -1.501547 0.821148
H12 0.652917 -0.969330 1.603202
H13 -0.041733 -2.424403 1.099744
N14 -0.669119 -0.754253 0.134448
H15 0.310290 -0.263690 -0.823803
C16 -1.362235 0.325420 0.862856
C17 -2.354454 0.953470 -0.098796
H18 -1.883686 -0.089319 1.732140
H19 -0.616797 1.053922 1.187478
H20 -2.963233 1.683787 0.445099
H21 -1.822173 1.467666 -0.909712
O22 -3.131988 -0.122050 -0.595555
H23 -3.818978 0.196399 -1.187689
H24 -1.352652 -1.350353 -0.333299

$[HE + H]^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256

H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$CH_2CHNHNH_2$
N1 -1.755825 -0.052331 0.174844
H2 -1.671786 -0.632683 1.005352
H3 -2.183407 -0.584515 -0.573705
N4 -0.507208 0.441293 -0.250666
H5 -0.379821 1.397234 0.051986
C6 0.617627 -0.368522 -0.132054
C7 1.863769 0.048432 0.122950
H8 0.409324 -1.419744 -0.323961
H9 2.091764 1.092294 0.319134
H10 2.686776 -0.654785 0.106578

H_2O
O1 0.000000 0.000000 0.115787
H2 0.000000 0.765916 -0.463148
H3 0.000000 -0.765916 -0.463148

Cartesian coordinates for structures in Figure S3, calculated at ωB97XD/ 6-31+G(d,p)

$[(HE)_2 + H]^+$
O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422
N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056
H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

TS1
N1 2.638775 -1.029993 -0.218089
C2 1.746040 -0.166869 -0.973252
C3 1.461288 1.105310 -0.292996
H4 0.723255 1.762186 -0.725906
H5 1.449077 0.573230 2.381549
H6 0.827847 -0.707755 -1.219013
H7 2.177435 0.170739 -1.940681
N8 -1.124122 1.048996 0.198357
N9 -1.948532 2.077257 -0.378253
H10 -1.570041 2.980908 -0.106710
H11 -1.873791 2.008593 -1.391447
C12 -1.618856 -0.271593 -0.175015
H13 -1.486742 -0.405110 -1.257215
H14 -0.989752 -1.007297 0.334066
C15 -3.077816 -0.557168 0.179520
H16 -3.745158 0.102422 -0.385656
H17 -3.237720 -0.370027 1.251766
O18 -3.274411 -1.916507 -0.145746
H19 -4.202649 -2.146645 -0.052279
H20 -1.198433 1.149172 1.207371
N21 3.910333 -0.416223 -0.054861
H22 4.348578 -0.781211 0.782886
H23 4.525385 -0.595476 -0.846126
H24 1.644373 -0.602499 1.360865
H25 2.690451 -1.948563 -0.652105
H26 2.256102 1.555638 0.290192
O27 1.057246 0.146925 1.609351

$[HOCH_2CH_2NH(NH_2)CH_2CH_2NHNH_2]^+ \cdot H_2O$
N1 -2.376905 0.555190 -0.719462
C2 -1.525251 -0.526874 -1.230549
C3 -0.784157 -1.254303 -0.112748
H4 -0.416817 -2.222147 -0.464171
H5 -0.445111 2.783615 1.020949
H6 -0.843994 -0.096513 -1.970438
H7 -2.120501 -1.290034 -1.750348
N8 0.405197 -0.523244 0.454864
N9 0.830119 -1.019471 1.732000
H10 0.108283 -0.797381 2.413031
H11 0.929080 -2.030678 1.670606
C12 1.576492 -0.502728 -0.468564

H13 1.896510 -1.534900 -0.635374
H14 1.242724 -0.083305 -1.419115
C15 2.716695 0.356641 0.067302
H16 3.231165 -0.154550 0.886398
H17 2.315608 1.305046 0.455607
O18 3.548682 0.560723 -1.049202
H19 4.402687 0.902523 -0.770465
H20 0.126380 0.477194 0.642455
N21 -3.395769 0.018289 0.119536
H22 -3.692002 0.726408 0.780931
H23 -4.203716 -0.293877 -0.414177
H24 -1.400483 1.706553 0.319865
H25 -2.769199 1.059515 -1.512957
H26 -1.483009 -1.412744 0.712049
O27 -0.676029 1.852215 0.973443

$[HOCH_2CH_2NH(NH_2)CH_2CH_2NHNH_2]^+$
N1 -1.924314 -0.940644 -0.628201
C2 -1.753115 -0.984426 0.820472
C3 -0.979434 0.267026 1.253422
H4 -0.511861 0.152305 2.232466
H5 -1.200725 -1.898762 1.056089
H6 -2.699096 -1.011044 1.377144
N7 0.081611 0.530905 0.218509
N8 0.256372 1.894812 -0.180952
H9 -0.641141 2.226537 -0.529014
H10 0.511858 2.437737 0.641432
C11 1.398731 -0.080699 0.560051
H12 1.795096 0.436508 1.437815
H13 1.207648 -1.123292 0.825665
C14 2.378824 -0.034888 -0.606956
H15 2.737498 0.986270 -0.769606
H16 1.878195 -0.373042 -1.527607
O17 3.406821 -0.912443 -0.220772
H18 4.168299 -0.811618 -0.798818
H19 -0.293440 0.024763 -0.614177
N20 -2.728656 0.174945 -1.009297
H21 -2.639445 0.302695 -2.011784
H22 -3.714486 0.020087 -0.799015
H23 -2.281671 -1.827730 -0.974881
H24 -1.636421 1.135923 1.258125

TS2
N1 -1.692205 -1.126726 -0.262268
C2 -1.547276 -0.592444 1.090722
C3 -0.951747 0.810613 1.006154
H4 -0.565611 1.155793 1.966084
H5 -0.882378 -1.261401 1.642136
H6 -2.499700 -0.526402 1.634585
N7 0.170176 0.791739 0.009414
N8 0.372435 2.023335 -0.718242
H9 -0.525150 2.327865 -1.092676
H10 0.703010 2.717979 -0.051551
C11 1.420042 0.278741 0.607950
H12 1.692231 0.889224 1.466413
H13 1.706221 -1.361473 0.537171
C14 2.483982 -0.011574 -0.356965
H15 3.492556 0.291260 -0.090116
H16 2.275031 0.139369 -1.416537
O17 2.538740 -1.592233 -0.125095
H18 2.349463 -2.158023 -0.892580
H19 -0.156679 0.095831 -0.681720
N20 -2.644430 -0.363090 -1.000743
H21 -2.536825 -0.575870 -1.986005
H22 -3.602128 -0.583195 -0.729687
H23 -1.934445 -2.113991 -0.220557
H24 -1.697343 1.512086 0.631506

$[CH_2CHNH(NH_2)CH_2CH_2NHNH_2]^+$
N1 -1.558579 -0.769727 -0.464506
C2 -1.107959 -0.860263 0.921459
C3 -0.179256 0.322429 1.204465
H4 0.438775 0.167755 2.090131
H5 -0.579419 -1.811518 1.032925
H6 -1.923832 -0.837034 1.655797
N7 0.710384 0.492468 -0.003573
N8 1.004318 1.841526 -0.399105
H9 0.113201 2.309702 -0.554693
H10 1.487353 2.302159 0.369435
C11 1.950200 -0.282158 0.094931
H12 2.644109 0.108040 0.831865
C13 2.152903 -1.354243 -0.651648
H14 3.074805 -1.913855 -0.547716
H15 1.428879 -1.702105 -1.382622
H16 0.133342 0.072750 -0.764482
N17 -2.331081 0.411808 -0.670546
H18 -2.419715 0.565308 -1.669301
H19 -3.268792 0.325093 -0.279708
H20 -2.049081 -1.618618 -0.736284
H21 -0.750242 1.245212 1.303521

Cartesian coordinates for structures in Figure S4, calculated at ωB97XD/ 6-31+G(d,p)

$[(HE)_2 + H]^+$
O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422

N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056
H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

TS1
C1 2.712564 0.434629 0.794381
C2 1.625954 -0.162533 0.035676
N3 1.098918 0.473796 -1.140799
N4 0.317094 1.662188 -0.848132
H5 3.146955 1.376494 0.454592
H6 2.736910 0.319298 1.874601
H7 2.947878 -1.010738 -0.197115
H8 1.836551 0.711525 -1.798313
H9 0.873552 2.384329 -0.383814
H10 -0.003834 2.049697 -1.733843
N11 -2.539118 1.595080 1.078493
H12 -2.832978 2.238518 0.349134
H13 -3.366289 1.203975 1.521671
N14 -1.787775 0.543749 0.474257
H15 -0.928850 1.019646 -0.002505
C16 -2.488647 -0.346666 -0.496653
C17 -1.614566 -1.563684 -0.748748
H18 -3.440671 -0.642155 -0.047846
H19 -2.674331 0.217629 -1.413239
H20 -2.170903 -2.270970 -1.373159
H21 -0.689114 -1.269770 -1.260581
O22 -1.344814 -2.091603 0.541160
H23 -0.766373 -2.857077 0.479076
H24 -1.416323 -0.051094 1.222571
O25 3.869065 -0.708898 0.379858
H26 4.641885 -0.408984 -0.127524
H27 0.876258 -0.700483 0.613486

$[CH_2CHNHNH_2][NH_2NH_2CH_2CH_2OH]^+ \cdot H_2O$
C1 2.966649 -1.094683 -0.735792
C2 1.672837 -1.052843 -0.404374
N3 1.123311 -1.593985 0.765411
N4 -0.178649 -2.149381 0.593966
H5 3.700420 -1.639271 -0.148727
H6 3.310154 -0.598624 -1.635817
H7 3.025422 2.860862 -0.064519
H8 1.758100 -2.232297 1.236701
H9 -0.143806 -3.032672 0.080778
H10 -0.543014 -2.350470 1.521573
N11 -3.095399 -0.753469 -0.946675
H12 -3.596747 -1.198779 -0.183259
H13 -3.687586 -0.030055 -1.346057
N14 -1.916116 -0.147434 -0.421224
H15 -1.275352 -0.929817 -0.089413
C16 -2.052723 0.883883 0.651110
C17 -0.676995 1.510297 0.836666
H18 -2.778601 1.621985 0.300853
H19 -2.424300 0.402456 1.558088
H20 -0.769954 2.396447 1.474057
H21 0.006398 0.800995 1.323996
O22 -0.235853 1.829078 -0.464910
H23 0.709330 2.079677 -0.423295
H24 -1.408565 0.314640 -1.187649
O25 2.396719 2.141524 0.040953
H26 2.883824 1.311413 -0.034526
H27 0.956708 -0.511353 -1.017134

$[CH_2CHNHNH_2][NH_2NH_2CH_2CH_2OH]^+$
C1 -3.336882 -0.549841 -0.645794
C2 -2.111831 -0.110760 -0.361606
N3 -1.782321 0.689666 0.752298
N4 -0.858678 1.735221 0.433553
H5 -4.208323 -0.256388 -0.067490
H6 -3.490893 -1.242478 -1.463753
H7 -2.615321 1.052490 1.209148
H8 -1.279218 2.434153 -0.183574
H9 -0.621557 2.202517 1.305172
N10 2.370343 1.511453 -0.872163
H11 2.572430 2.134341 -0.095177
H12 3.238801 1.084864 -1.184274
N13 1.483696 0.490472 -0.416650
H14 0.567257 0.982455 -0.137263
C15 1.947699 -0.405252 0.685524
C16 0.940288 -1.535053 0.832694
H17 2.929662 -0.792333 0.402134

H18 2.034809 0.185860 1.599638
H19 1.346621 -2.282425 1.522048
H20 -0.009275 -1.156362 1.233132
O21 0.777201 -2.048765 -0.479145
H22 0.191856 -2.811836 -0.479506
H23 1.252088 -0.108982 -1.216752
H24 -1.253469 -0.418001 -0.954496

TS2
C1 2.084884 1.600421 -1.232860
C2 2.106377 0.416067 -0.620687
N3 1.944223 0.255247 0.778091
N4 1.725452 -1.101095 1.157204
H5 1.939786 2.527946 -0.686215
H6 2.269380 1.665268 -2.298204
H7 2.687811 0.699685 1.308115
H8 2.578887 -1.659030 1.104324
H9 1.410300 -1.107697 2.122584
N10 -1.085115 -2.194366 -1.116851
H11 -1.192583 -2.952710 -0.447932
H12 -2.012278 -1.975074 -1.476980
N13 -0.644562 -1.039780 -0.387950
H14 0.224872 -1.317359 0.140603
C15 -1.650831 -0.389471 0.487694
C16 -1.376537 1.013568 0.798540
H17 -2.795918 0.582432 -0.208643
H18 -1.883658 -1.043607 1.324771
H19 -1.592744 1.334488 1.815605
H20 -0.481051 1.486789 0.397728
O21 -2.556674 1.644055 -0.099092
H22 -3.212009 2.199114 0.358513
H23 -0.311844 -0.370563 -1.087804
H24 2.261087 -0.505670 -1.183301

$[CH_2CHNHNH_2][NH_2NH_2CHCH_2]^+$
C1 -2.306704 1.642000 0.308788
C2 -1.961539 0.355007 0.348262
N3 -1.759486 -0.423018 -0.822987
N4 -1.026757 -1.621340 -0.570145
H5 -2.443217 2.166806 -0.631981
H6 -2.511595 2.175905 1.228987
H7 -2.620006 -0.593915 -1.334003
H8 -1.575234 -2.314062 -0.056094
H9 -0.777861 -2.027174 -1.468586
N10 1.259414 -0.404116 1.786098
H11 1.592408 -1.361263 1.866380
H12 1.984036 0.222834 2.127962
N13 1.032085 -0.121825 0.397432
H14 0.318751 -0.864054 0.048679
C15 2.207369 -0.053650 -0.465420
C16 2.517453 1.048806 -1.130152
H17 2.770049 -0.980276 -0.498561
H18 3.390117 1.066077 -1.772385
H19 1.923353 1.956776 -1.068472
H20 0.496724 0.754322 0.357167
H21 -1.823794 -0.162853 1.299247

$[HE + H]^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$CH_2CHNHNH_2$
N1 -1.755825 -0.052331 0.174844
H2 -1.671786 -0.632683 1.005352
H3 -2.183407 -0.584515 -0.573705
N4 -0.507208 0.441293 -0.250666
H5 -0.379821 1.397234 0.051986
C6 0.617627 -0.368522 -0.132054
C7 1.863769 0.048432 0.122950
H8 0.409324 -1.419744 -0.323961
H9 2.091764 1.092294 0.319134
H10 2.686776 -0.654785 0.106578

Cartesian coordinates for structures in Figure S5, calculated at ωB97XD/ 6-31+G(d,p)

$[(HE)_2 + H]^+$
O1 -2.085492 -1.439869 -0.825220
C2 -2.746950 -0.188849 -0.809156
C3 -2.322517 0.497570 0.475819
N4 -0.842348 0.479701 0.568422
N5 -0.358036 1.214926 1.704249
H6 -2.424130 -1.993178 -1.534644
H7 -3.837279 -0.294666 -0.803188
H8 -2.462722 0.419097 -1.679388
H9 -2.713855 -0.033761 1.346803
H10 -2.645683 1.539156 0.511056

H11 -0.416173 0.961077 -0.260868
H12 -0.480002 -0.491371 0.564841
H13 -0.676331 0.729652 2.540380
H14 0.658704 1.116776 1.652618
N15 1.029514 1.810851 -1.045303
H16 1.351434 1.970206 -2.001242
H17 0.998046 2.714630 -0.579895
N18 1.921122 0.967849 -0.301135
H19 2.852323 1.376536 -0.264782
C20 1.993439 -0.372952 -0.894712
C21 2.241405 -1.432810 0.161945
H22 1.033767 -0.580668 -1.380274
H23 2.767037 -0.446213 -1.671270
H24 2.401136 -2.396464 -0.333871
H25 3.133202 -1.189893 0.752880
O26 1.093972 -1.493242 1.009789
H27 1.148661 -2.267080 1.577274

TS1
N1 -0.078724 -1.039014 1.285532
N2 0.818902 -0.650958 0.249946
C3 2.233101 -0.673067 0.636438
C4 3.055698 0.010851 -0.437617
H5 4.111633 -0.010378 -0.144456
H6 2.945877 -0.520331 -1.392412
O7 2.573143 1.343233 -0.545933
H8 3.144881 1.846754 -1.131453
H9 2.562597 -1.710821 0.751430
H10 2.387066 -0.152530 1.593938
H11 -0.086119 -1.607048 -0.862526
H12 0.542954 0.308189 0.011140
H13 0.025588 -2.036332 1.454851
H14 0.113068 -0.544718 2.159142
O15 -0.947058 -2.057192 -1.085128
C16 -2.498737 -0.816053 0.196261
H17 -2.926500 -1.681909 -0.290878
H18 -2.352398 -0.845312 1.267246
C19 -2.538397 0.480606 -0.476177
H20 -2.109700 0.412986 -1.487144
H21 -3.633433 0.571069 -0.646145
N22 -2.102816 1.602145 0.319322
N23 -0.726970 1.889512 0.122593
H24 -0.566071 2.513022 -0.666839
H25 -0.372014 2.341467 0.958411
H26 -0.984152 -2.208871 -2.034706
H27 -2.694682 2.410620 0.153714

$[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+ \cdot H_2O$
O1 -1.982147 2.389763 -0.555460
C2 -0.534115 0.132705 0.738569
C3 -1.599759 -0.787719 0.148946
H4 -2.438283 3.114396 -0.989367
H5 -0.707053 0.320956 1.802770
H6 -1.518140 -1.799403 0.588564
N7 0.822449 -0.488639 0.653189
H8 1.533487 0.157260 1.060957
H9 0.860518 -1.360670 1.197838
N10 1.266626 -0.672672 -0.705608
H11 0.739896 -1.446476 -1.100939
C12 2.713060 -0.924185 -0.761944
C13 3.494546 0.342578 -0.462754
H14 3.027593 -1.731804 -0.083475
H15 2.924501 -1.241785 -1.785251
H16 4.566629 0.141119 -0.548314
H17 3.208829 1.131141 -1.166108
O18 3.163777 0.726560 0.878421
H19 3.607137 1.544553 1.123917
H20 -1.472889 -0.877334 -0.932830
N21 -2.915731 -0.196908 0.350222
H22 -3.134986 -0.134850 1.343192
N23 -3.894186 -0.940298 -0.361408
H24 -4.288043 -1.694353 0.195175
H25 -4.637694 -0.317130 -0.651434
H26 -2.630791 1.689171 -0.374104
H27 -0.490253 1.083968 0.204062

$[HOCH_2CH_2NHNH_2CH_2CH_2NHNH_2]^+$
C1 0.793598 -0.830484 0.009554
C2 1.932164 0.140869 0.307959
H3 0.964287 -1.804487 0.477258
H4 1.925259 0.419103 1.380168
N5 -0.511630 -0.339223 0.551165
H6 -1.272222 -1.022325 0.345386
H7 -0.460764 -0.245174 1.574660
N8 -0.955121 0.874261 -0.088801
H9 -0.351104 1.627170 0.229644
C10 -2.364773 1.151578 0.221981
C11 -3.281681 0.200764 -0.525890
H12 -2.571576 1.108346 1.301999
H13 -2.554355 2.172539 -0.116444
H14 -4.324318 0.438037 -0.293630
H15 -3.114184 0.290092 -1.603996
O16 -2.959446 -1.122831 -0.079504
H17 -3.518179 -1.779651 -0.506299
H18 1.818615 1.057110 -0.276597
N19 3.167325 -0.466094 -0.138855
H20 3.488753 -1.185206 0.503745
N21 4.159995 0.505537 -0.407948
H22 4.767750 0.678228 0.388172
H23 4.716714 0.194072 -1.194416

H24 0.661068 -0.962936 -1.064167

TS2
C1 -0.601876 0.567434 -0.308324
C2 -1.859838 -0.020643 0.339977
H3 -0.592883 1.659193 -0.211690
H4 -1.826245 0.142518 1.434006
N5 0.642661 0.084868 0.285738
H6 2.401363 2.313511 0.037822
H7 0.763818 0.413652 1.246198
N8 0.817957 -1.325001 0.169250
H9 0.373464 -1.845821 0.921660
C10 2.251043 -1.463845 0.125265
C11 2.676632 -0.424289 -0.811187
H12 2.765667 -1.328267 1.091101
H13 2.599191 -2.434150 -0.277699
H14 3.722751 -0.155372 -0.888985
H15 2.024698 -0.147624 -1.632812
O16 3.064308 1.662875 0.293271
H17 3.898886 2.141305 0.369166
H18 -1.897386 -1.098881 0.165282
N19 -3.032482 0.538747 -0.301268
H20 -3.164516 1.513585 -0.043101
N21 -4.184587 -0.242520 -0.039668
H22 -4.690771 0.065624 0.786443
H23 -4.797631 -0.201596 -0.844377
H24 -0.595483 0.314729 -1.371923

***cyclo*-[$CH_2CH_2NHNH^+(CH_2CH_2NHNH_2)$]**
C1 -0.169079 0.742094 -0.152305
C2 -1.318026 -0.103038 0.392871
H3 -0.255421 1.796089 0.131355
H4 -1.276137 -0.142708 1.498189
N5 1.133634 0.266051 0.389233
H6 1.117644 0.322996 1.414531
N7 1.550982 -1.045456 -0.089451
H8 1.356462 -1.777129 0.591313
C9 2.959925 -0.590921 -0.218882
C10 2.428421 0.847742 -0.148511
H11 3.598719 -0.857732 0.627827
H12 3.420511 -0.901849 -1.154916
H13 2.894295 1.552971 0.537091
H14 2.233287 1.306748 -1.116984
H15 -1.230176 -1.125335 0.016498
N16 -2.557010 0.426190 -0.134757
H17 -2.868010 1.246472 0.378074
N18 -3.557409 -0.569676 -0.230321
H19 -4.159942 -0.601216 0.587509
H20 -4.118145 -0.390869 -1.054364
H21 -0.111913 0.656541 -1.238093

TS3
C1 1.973957 -1.258387 -0.555326
C2 1.532430 -0.057588 -1.124933
N3 1.815696 1.222175 -0.521369
N4 2.080327 1.127756 0.870206
H5 2.640776 -1.301029 0.296382
H6 1.831954 -2.183661 -1.103483
H7 1.446713 -0.008713 -2.210285
H8 2.533175 1.730204 -1.029738
H9 3.071596 0.992922 1.066413
H10 1.805352 2.005593 1.298150
N11 0.276552 -1.501547 0.821148
H12 0.652917 -0.969330 1.603202
H13 -0.041733 -2.424403 1.099744
N14 -0.669119 -0.754253 0.134448
H15 0.310290 -0.263690 -0.823803
C16 -1.362235 0.325420 0.862856
C17 -2.354454 0.953470 -0.098796
H18 -1.883686 -0.089319 1.732140
H19 -0.616797 1.053922 1.187478
H20 -2.963233 1.683787 0.445099
H21 -1.822173 1.467666 -0.909712
O22 -3.131988 -0.122050 -0.595555
H23 -3.818978 0.196399 -1.187689
H24 -1.352652 -1.350353 -0.333299

[HE + H]$^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$CH_2CHNHNH_2$
N1 -1.755825 -0.052331 0.174844
H2 -1.671786 -0.632683 1.005352
H3 -2.183407 -0.584515 -0.573705
N4 -0.507208 0.441293 -0.250666
H5 -0.379821 1.397234 0.051986
C6 0.617627 -0.368522 -0.132054
C7 1.863769 0.048432 0.122950

H8 0.409324 -1.419744 -0.323961
H9 2.091764 1.092294 0.319134
H10 2.686776 -0.654785 0.106578

Cartesian coordinates for structures in Figure S6, calculated at B97XD/ 6-31+G(d,p)

$[(HEHN)_2(HE)_2 + H]^+$
Conformer_1
O1 3.568984 -0.975171 -1.965970
C2 3.496172 -2.360423 -1.687022
C3 3.679304 -2.660052 -0.204183
N4 2.672322 -1.952436 0.638092
N5 2.658179 -2.493671 1.969685
H6 2.659268 -0.630657 -2.053051
H7 4.301232 -2.866474 -2.227301
H8 2.542946 -2.769308 -2.039013
H9 4.662913 -2.338672 0.147721
H10 3.560014 -3.726127 -0.003075
H11 1.730336 -2.057533 0.224535
H12 2.871370 -0.931334 0.639488
H13 1.777908 -2.183016 2.386251
H14 3.428922 -2.060279 2.472265
N15 0.102761 -0.532871 -1.332641
O16 0.284356 -1.722249 -0.955462
O17 1.045478 0.105977 -1.842463
O18 -1.011559 0.001960 -1.188293
O19 -4.643758 -0.988175 -1.677755
C20 -4.972050 -2.004338 -0.734110
C21 -4.338558 -1.606230 0.581942
N22 -2.863508 -1.499653 0.440738
N23 -2.253483 -2.781521 0.208168
H24 -4.850362 -1.280648 -2.569510
H25 -4.578712 -2.972290 -1.059562
H26 -6.055813 -2.078036 -0.594498
H27 -4.548829 -2.349926 1.352849
H28 -4.693130 -0.627610 0.913160
H29 -2.443404 -0.992635 1.248492
H30 -2.622737 -0.893959 -0.361409
H31 -1.353531 -2.580707 -0.238451
H32 -2.041825 -3.169902 1.124584
N33 -0.191270 -0.452242 1.943629
O34 0.822668 0.180592 1.601693
O35 -1.310814 0.142814 1.999881
O36 -0.138503 -1.663389 2.216026
O37 -3.636201 1.241534 -0.350284
C38 -3.169051 2.475129 -0.861403
C39 -2.460204 3.212735 0.255356
N40 -1.174842 2.558557 0.598294
N41 -0.520664 3.240596 1.682207
H42 -4.085936 0.739957 -1.048141
H43 -4.002255 3.101035 -1.203120
H44 -2.484553 2.313287 -1.705362
H45 -3.078780 3.232482 1.155564
H46 -2.226208 4.239799 -0.030788
H47 -0.505567 2.628421 -0.223386
H48 -1.313070 1.558730 0.832484
H49 -0.786770 2.760408 2.538624
H50 0.481898 3.094657 1.540989
N51 0.962582 2.968855 -1.090690
H52 1.108645 3.962287 -1.246628
H53 1.088542 2.470325 -1.974392
N54 1.905997 2.534200 -0.107796
H55 1.678880 1.561674 0.090901
C56 3.296280 2.625211 -0.547535
C57 4.206858 1.855936 0.397228
H58 3.423896 2.235196 -1.572746
H59 3.594797 3.679822 -0.555920
H60 5.253016 2.093215 0.174245
H61 4.003535 2.135111 1.433640
O62 3.998748 0.451324 0.310722
H63 4.149139 0.144455 -0.603631

Conformer_2
N1 -1.470219 3.404237 -1.322582
H2 -1.596644 4.172478 -0.667839
H3 -1.431602 3.821613 -2.253819
N4 -0.238586 2.750075 -1.000659
H5 -0.161615 1.960365 -1.645851
C6 0.950737 3.604665 -1.049439
C7 2.215259 2.758690 -0.940526
H8 1.001497 4.183875 -1.984480
H9 0.894683 4.311498 -0.213703
H10 2.349649 2.162993 -1.849961
H11 3.077507 3.419582 -0.828342
O12 2.193037 1.893861 0.193815
H13 1.757097 1.066059 -0.065582
O14 4.338023 0.201533 0.924281
C15 4.703465 -0.292188 -0.344791
C16 4.434816 -1.789901 -0.368098
N17 3.005996 -2.023395 -0.046445
N18 2.666896 -3.417557 -0.026783
H19 3.756782 0.970138 0.817090
H20 5.770022 -0.128133 -0.535505
H21 4.137616 0.200649 -1.146278
H22 5.029623 -2.294747 0.397449
H23 4.636452 -2.240782 -1.341062
H24 2.413873 -1.565164 -0.766984
H25 2.751917 -1.525028 0.824563

H26 3.172258 -3.833029 0.753312
H27 1.676065 -3.446681 0.216841
O28 -3.240329 -1.719810 1.432493
C29 -3.182456 -2.877276 0.632317
C30 -3.670626 -2.516164 -0.760644
N31 -2.816208 -1.438856 -1.321393
N32 -3.242117 -1.053285 -2.638257
H33 -2.400112 -1.606673 1.909413
H34 -3.836287 -3.662152 1.030159
H35 -2.161243 -3.277608 0.589809
H36 -4.691991 -2.131977 -0.741782
H37 -3.619213 -3.376167 -1.434110
H38 -1.811708 -1.714779 -1.311761
H39 -2.892734 -0.583954 -0.732286
H40 -2.550388 -0.374188 -2.953527
H41 -3.146918 -1.872434 -3.235131
O42 -2.751533 1.145511 -0.167053
C43 -3.179431 1.519767 1.131607
C44 -2.155641 2.398541 1.853787
N45 -0.783149 1.888996 1.623946
N46 0.196079 2.664972 2.331094
H47 -2.579817 1.934140 -0.724411
H48 -3.335031 0.582707 1.667956
H49 -4.135351 2.054944 1.100450
H50 -2.353307 2.399655 2.928804
H51 -2.166772 3.435483 1.510998
H52 -0.557360 2.030883 0.599635
H53 -0.737508 0.870764 1.858228
H54 0.206333 2.342949 3.295919
H55 1.094619 2.425981 1.905440
N56 0.326324 -0.626368 -1.799515
O57 1.510731 -0.242400 -1.624413
O58 -0.006126 -1.777097 -1.444150
O59 -0.505466 0.147274 -2.311053
N60 0.199679 -1.300303 1.785274
O61 1.147706 -0.539742 1.473843
O62 0.252476 -2.516103 1.598824
O63 -0.834769 -0.779236 2.299450

Conformer_3

O1 2.424804 -0.874907 2.083098
C2 2.853311 -2.196188 1.814356
C3 1.853609 -2.956281 0.951335
N4 1.392548 -2.104593 -0.174876
N5 0.650761 -2.892935 -1.121867
H6 1.537896 -0.906365 2.482369
H7 3.023089 -2.760251 2.738479
H8 3.810312 -2.111921 1.293484
H9 0.963716 -3.238011 1.519093
H10 2.301207 -3.851699 0.516915
H11 2.213412 -1.689718 -0.658202
H12 0.833274 -1.311211 0.193384
H13 0.387703 -2.258637 -1.878453
H14 -0.219123 -3.142768 -0.646720
N15 -0.351816 0.211106 -2.198545
O16 -0.988090 1.261968 -1.952582
O17 0.879324 0.154641 -2.043335
O18 -0.981388 -0.810407 -2.576718
O19 -2.810951 2.172512 0.918452
C20 -2.192640 3.373560 1.341941
C21 -0.706936 3.166438 1.588459
N22 -0.026568 2.651414 0.374899
N23 0.123042 3.661447 -0.639585
H24 -2.711927 1.481243 1.593486
H25 -2.654536 3.764601 2.255463
H26 -2.340966 4.103236 0.543052
H27 -0.542399 2.423990 2.376957
H28 -0.217988 4.100538 1.871250
H29 -0.568631 1.864113 -0.010862
H30 0.934453 2.257244 0.642033
H31 -0.196836 3.232730 -1.506780
H32 1.124759 3.816741 -0.746059
N33 -1.032399 -0.566284 1.831174
O34 -0.351136 -1.225963 2.627107
O35 -0.517072 -0.149701 0.748782
O36 -2.231790 -0.313079 2.063169
O37 -2.063615 -2.831626 0.342468
C38 -3.162473 -2.847836 -0.554904
C39 -3.972647 -1.558774 -0.544877
N40 -3.131148 -0.390753 -0.918504
N41 -3.928897 0.719004 -1.369617
H42 -2.373780 -2.937484 1.248509
H43 -3.839148 -3.683005 -0.344196
H44 -2.734674 -3.011753 -1.548667
H45 -4.407096 -1.355075 0.436811
H46 -4.773755 -1.609881 -1.284611
H47 -2.481641 -0.645279 -1.695229
H48 -2.508613 -0.136133 -0.135008
H49 -3.299333 1.269470 -1.952812
H50 -4.109894 1.297546 -0.549358
H51 3.758811 -0.836573 -2.209683
H52 4.978369 2.115861 -0.458891
H53 5.622446 -0.197526 -0.902945
C54 4.249806 1.468532 -0.962068
H55 4.372623 1.638571 -2.038032
H56 2.211591 1.391023 -1.150847
N57 2.552031 1.814894 0.756758
H58 2.707439 0.883026 1.155619
N59 2.904932 1.922773 -0.625664
C60 4.584202 0.017032 -0.625229

O61 3.702587 -0.915712 -1.251641
H62 3.107307 2.487296 1.278783
H63 4.485757 -0.167161 0.447973

Conformer_4
N1 -1.296654 3.613423 -1.327330
H2 -1.451403 4.361986 -0.656135
H3 -1.212207 4.057318 -2.242990
N4 -0.083623 2.948006 -0.964500
H5 0.027633 2.162526 -1.608020
C6 1.095873 3.818098 -0.916391
C7 2.381013 3.006288 -0.786203
H8 1.174394 4.447549 -1.816243
H9 0.980624 4.480583 -0.050599
H10 2.606113 2.504261 -1.733742
H11 3.205007 3.683284 -0.550408
O12 2.308553 2.033996 0.253297
H13 1.933416 1.231826 -0.154348
O14 4.265542 0.108477 0.938256
C15 4.679231 -0.413698 -0.307075
C16 4.462031 -1.917833 -0.250606
N17 3.045164 -2.194342 0.100090
N18 2.840749 -3.564050 0.483919
H19 3.812879 0.956465 0.810154
H20 5.744955 -0.227003 -0.483947
H21 4.106668 0.017721 -1.134944
H22 5.075384 -2.350246 0.543914
H23 4.688294 -2.418722 -1.192482
H24 2.419121 -2.026654 -0.708009
H25 2.734332 -1.524561 0.827355
H26 3.392809 -3.719983 1.324800
H27 1.856754 -3.619193 0.754888
O28 -4.638454 -1.426472 0.799225
C29 -4.844382 -2.028284 -0.471413
C30 -3.833527 -1.394730 -1.404542
N31 -2.468082 -1.584253 -0.847822
N32 -2.060392 -2.964856 -0.890227
H33 -5.062232 -1.951613 1.483024
H34 -5.852170 -1.827883 -0.852307
H35 -4.683368 -3.110329 -0.425086
H36 -3.981942 -0.315427 -1.473069
H37 -3.864112 -1.848588 -2.396420
H38 -2.476488 -1.300027 0.143318
H39 -1.782353 -0.950067 -1.308488
H40 -1.500212 -3.074117 -1.732286
H41 -1.421125 -3.101623 -0.104619
O42 -2.736197 1.360358 -0.349344
C43 -3.152452 1.635853 0.970997
C44 -2.093928 2.381170 1.787698
N45 -0.743699 1.828439 1.520086
N46 0.240605 2.410186 2.387178
H47 -2.483053 2.181223 -0.818868
H48 -3.369004 0.666639 1.427056
H49 -4.079634 2.222321 0.995416
H50 -2.301763 2.284004 2.856208
H51 -2.045415 3.447335 1.554055
H52 -0.467187 2.120483 0.538367
H53 -0.774626 0.787057 1.560195
H54 0.232524 1.887274 3.259032
H55 1.142479 2.257399 1.930501
N56 0.692877 -0.564982 -1.685510
O57 1.751502 0.092902 -1.555687
O58 0.724444 -1.807003 -1.588110
O59 -0.387512 0.031870 -1.894642
N60 0.011010 -1.480445 1.467889
O61 1.033106 -0.764891 1.552010
O62 0.086104 -2.702357 1.273669
O63 -1.123830 -0.932166 1.570515

Conformer_5
O1 2.302988 -0.301285 2.146531
C2 2.797241 -1.619032 2.013871
C3 1.901956 -2.473090 1.121979
N4 1.588674 -1.766088 -0.146318
N5 0.833740 -2.623340 -1.019860
H6 1.399268 -0.336365 2.513348
H7 2.886135 -2.112294 2.988365
H8 3.794472 -1.511684 1.582825
H9 0.945820 -2.681495 1.608886
H10 2.377344 -3.420813 0.860311
H11 2.485683 -1.523106 -0.636788
H12 1.066799 -0.902875 0.083322
H13 0.583942 -2.051303 -1.827937
H14 -0.045363 -2.816759 -0.533193
N15 -0.757115 0.194281 -2.152351
O16 -1.490310 1.182878 -1.905361
O17 0.479217 0.295455 -2.079961
O18 -1.289224 -0.906025 -2.438302
O19 -2.736033 2.388829 0.803373
C20 -1.975976 3.501012 1.232863
C21 -0.493056 3.160773 1.299571
N22 -0.029974 2.622775 -0.004844
N23 0.024204 3.639051 -1.015640
H24 -2.701753 1.681467 1.464572
H25 -2.301646 3.866632 2.213381
H26 -2.141117 4.289626 0.496511
H27 -0.293077 2.383389 2.043232
H28 0.110852 4.037926 1.541715
H29 -0.714799 1.921617 -0.341386
H30 0.892030 2.137471 0.104554

H31 -0.190655 3.174601 -1.896161
H32 0.975604 3.993376 -1.049807
N33 -1.071100 -0.339445 1.837949
O34 -0.386380 -0.703824 2.803401
O35 -0.532437 -0.079717 0.728223
O36 -2.314834 -0.214288 1.947359
O37 -1.951388 -2.913782 0.408626
C38 -2.993238 -3.102063 -0.539247
C39 -4.035817 -1.992007 -0.486276
N40 -3.382633 -0.673268 -0.662310
N41 -4.335546 0.377252 -0.882777
H42 -2.263825 -3.131845 1.292877
H43 -3.493486 -4.066249 -0.401116
H44 -2.507602 -3.111597 -1.518224
H45 -4.562296 -1.975799 0.472596
H46 -4.766978 -2.103725 -1.289742
H47 -2.752203 -0.712055 -1.492840
H48 -2.783090 -0.482285 0.162165
H49 -3.777756 1.201979 -1.106777
H50 -4.785157 0.566508 0.010881
H51 4.622991 -1.285864 -2.077218
H52 5.175095 1.703454 -0.229611
H53 5.818649 -0.476379 -0.162509
C54 4.638009 0.997871 -0.869647
H55 5.080827 1.055596 -1.880006
H56 2.615660 0.678148 -1.563547
O57 2.548391 1.673343 0.257594
H58 2.645856 0.926445 0.885144
C59 3.183764 1.415119 -0.988310
N60 4.818636 -0.325269 -0.276275
N61 4.266708 -1.352780 -1.119667
H62 4.589740 -2.246106 -0.755860
H63 3.147644 2.354007 -1.547994

Conformer_6

O1 -2.073241 -0.076479 2.075881
C2 -2.399143 1.273962 2.324500
C3 -1.503929 2.226981 1.537504
N4 -1.410334 1.809342 0.117258
N5 -0.702091 2.794869 -0.653067
H6 -1.160697 -0.262364 2.379552
H7 -2.313598 1.517005 3.389522
H8 -3.443909 1.384373 2.026042
H9 -0.484192 2.231571 1.931486
H10 -1.889346 3.248888 1.554428
H11 -2.378981 1.737017 -0.288859
H12 -0.949769 0.887791 0.077752
H13 -0.544528 2.373381 -1.569499
H14 0.221061 2.889548 -0.220656
N15 0.666547 0.081372 -2.247439
O16 1.382653 -0.948243 -2.163779
O17 -0.556068 0.006358 -2.011435
O18 1.192990 1.179026 -2.531050
O19 2.426537 -2.716847 0.836369
C20 1.519464 -3.804880 0.919026
C21 0.082214 -3.308365 0.907131
N22 -0.185421 -2.527526 -0.330454
N23 -0.155293 -3.355860 -1.502599
H24 2.600724 -2.362883 1.715761
H25 1.684343 -4.405183 1.819298
H26 1.700932 -4.433391 0.045132
H27 -0.111946 -2.634278 1.746551
H28 -0.630512 -4.135326 0.938809
H29 0.547654 -1.810647 -0.446332
H30 -1.102787 -2.025981 -0.249072
H31 0.177588 -2.756263 -2.256779
H32 -1.111345 -3.637510 -1.700352
N33 1.322699 -0.095409 1.828623
O34 0.562590 -0.419712 2.760361
O35 0.843597 0.097680 0.667834
O36 2.543175 0.025364 2.005914
O37 2.126756 2.973249 0.560218
C38 3.205901 3.112512 -0.353292
C39 4.086491 1.871677 -0.385464
N40 3.280158 0.690554 -0.768786
N41 4.071349 -0.506393 -0.791636
H42 2.460085 2.981595 1.463436
H43 3.824367 3.983769 -0.113028
H44 2.747702 3.283528 -1.331067
H45 4.517754 1.662415 0.597074
H46 4.895437 1.970667 -1.111907
H47 2.867605 0.829826 -1.707178
H48 2.462547 0.600935 -0.133017
H49 3.490190 -1.203345 -1.255791
H50 4.153986 -0.807644 0.177903
H51 -4.384845 2.631932 -0.022648
H52 -5.368028 -1.249544 -0.429872
H53 -3.471510 -1.779881 -1.964019
H54 -2.746061 -0.956530 0.678875
H55 -5.746646 0.881545 0.237465
C56 -4.778368 -0.464847 -0.912088
H57 -5.263088 -0.221571 -1.874112
N58 -4.179107 1.831995 -0.616482
N59 -4.778455 0.677524 -0.000143
C60 -3.386265 -0.987364 -1.216045
O61 -2.743328 -1.566436 -0.087904
H62 -2.762688 -0.200289 -1.651523
H63 -4.601333 2.033845 -1.527197

Conformer_7

O1 1.786038 -0.910884 2.035642
C2 1.663101 -2.276123 2.371697
C3 0.370289 -2.900307 1.855426
N4 0.150011 -2.548367 0.428609
N5 -0.725134 -3.488773 -0.216166
H6 1.028552 -0.415450 2.398669
H7 1.718058 -2.436218 3.455035
H8 2.521017 -2.782790 1.919754
H9 -0.500342 -2.553628 2.418844
H10 0.415112 -3.989277 1.914720
H11 1.060590 -2.530708 -0.095144
H12 -0.206014 -1.578047 0.374972
H13 -0.643939 -3.292998 -1.212446
H14 -1.674918 -3.228116 0.056783
N15 -0.105387 -0.121359 -2.396633
O16 -0.743527 0.945406 -2.587174
O17 1.143316 -0.094781 -2.447874
O18 -0.719820 -1.171974 -2.130648
O19 -1.168327 3.171400 1.195163
C20 0.098862 3.815909 1.209482
C21 1.224053 2.806973 1.048145
N22 1.080627 2.038003 -0.221565
N23 1.083474 2.901957 -1.369514
H24 -1.478871 3.030532 2.095054
H25 0.258332 4.368657 2.140206
H26 0.109944 4.524104 0.379428
H27 1.216665 2.065674 1.851294
H28 2.204774 3.286038 1.031134
H29 0.173695 1.551618 -0.180528
H30 1.835921 1.293574 -0.281786
H31 0.709985 2.349563 -2.144025
H32 2.054551 3.123198 -1.571305
N33 -1.358915 0.378042 1.816133
O34 -0.598887 0.342336 2.794836
O35 -0.882507 0.113100 0.652136
O36 -2.552206 0.667316 1.917896
O37 -3.250191 -1.962084 0.408221
C38 -4.123187 -1.635611 -0.664068
C39 -4.309674 -0.132601 -0.809358
N40 -3.004840 0.520211 -1.062923
N41 -3.110737 1.953316 -1.026856
H42 -3.642129 -1.684887 1.243797
H43 -5.104903 -2.104204 -0.536427
H44 -3.662407 -2.057692 -1.561560
H45 -4.707825 0.308523 0.107351
H46 -4.980057 0.116276 -1.634217
H47 -2.614271 0.263712 -1.978197
H48 -2.291485 0.184524 -0.378751
H49 -2.350254 2.304733 -1.604905
H50 -2.903103 2.239811 -0.069625
H51 4.326465 2.103904 -0.692020
H52 4.000980 -0.151899 -2.017312
H53 4.285066 -2.550126 -1.511535
H54 1.949530 -1.486856 -1.761843
H55 3.169289 -0.002103 0.787652
C56 4.122277 -0.490619 -0.981379
H57 5.200082 -0.477208 -0.756335
O58 2.297505 -2.152498 -1.131387
C59 3.667539 -1.935445 -0.846217
N60 3.404992 0.442467 -0.101725
N61 4.137479 1.636522 0.190826
H62 5.048254 1.415753 0.596823
H63 3.841961 -2.283885 0.178296

Conformer_8

N1 -0.230409 -3.897926 0.270523
H2 -0.158447 -4.487299 -0.555379
H3 -0.343429 -4.527138 1.068306
N4 0.962667 -3.120530 0.372643
H5 0.801040 -2.456904 1.131366
C6 2.179355 -3.894673 0.610727
C7 3.311933 -2.975408 1.057762
H8 2.035066 -4.667074 1.385068
H9 2.454881 -4.403151 -0.321228
H10 3.105146 -2.598245 2.068611
H11 4.240329 -3.549954 1.104285
O12 3.520376 -1.893102 0.166909
H13 2.931635 -1.174780 0.442929
O14 3.115167 1.789974 -1.572701
C15 3.698078 2.227800 -0.351394
C16 2.948115 3.427804 0.207206
N17 1.523656 3.087787 0.434455
N18 0.764413 4.253050 0.795741
H19 3.462906 2.298037 -2.311847
H20 4.751982 2.492226 -0.480762
H21 3.637646 1.384618 0.338472
H22 2.974453 4.263267 -0.498857
H23 3.367880 3.763713 1.157475
H24 1.422880 2.420170 1.230234
H25 1.110497 2.596038 -0.388219
H26 0.691793 4.834233 -0.036889
H27 -0.172637 3.907321 1.001251
O28 -4.628958 -0.490279 -1.110813
C29 -5.025490 0.562611 -0.253377
C30 -4.550135 0.199918 1.137746
N31 -3.069200 0.086852 1.167340
N32 -2.614455 -0.349783 2.457638
H33 -4.719499 -0.205554 -2.024090

H34 -6.116653 0.670483 -0.222586
H35 -4.583780 1.514812 -0.570805
H36 -4.943455 -0.766582 1.457010
H37 -4.845796 0.964143 1.860770
H38 -2.620269 0.975714 0.869035
H39 -2.750386 -0.632061 0.478283
H40 -1.611894 -0.545239 2.386018
H41 -2.723437 0.430382 3.101280
O42 -1.595896 -1.625615 -0.407506
C43 -1.602447 -1.650186 -1.824376
C44 -0.193734 -1.781652 -2.396147
N45 0.722937 -0.809963 -1.751997
N46 2.055438 -0.921643 -2.280718
H47 -1.290728 -2.506710 -0.067951
H48 -2.055652 -0.711057 -2.146284
H49 -2.215380 -2.474205 -2.207370
H50 -0.177589 -1.587870 -3.469898
H51 0.240346 -2.764976 -2.208753
H52 0.715299 -0.959440 -0.729215
H53 0.397984 0.161642 -1.903175
H54 2.529757 -0.047394 -2.040998
H55 2.517975 -1.657025 -1.740211
N56 0.895967 0.177687 1.821600
O57 1.598467 0.115718 0.768175
O58 0.796609 1.263197 2.416748
O59 0.309508 -0.838558 2.232933
N60 -1.261562 1.848783 -0.951533
O61 -0.129352 1.918054 -1.515084
O62 -1.353504 2.167580 0.265351
O63 -2.245003 1.451579 -1.573335

Cartesian coordinates for structures in Figure S7, calculated at ωB97XD/ 6-31+G(d,p)

$[HOCH_2CH_2NHNH_2CH(OH)CH_3]^+$
O1 -1.422685 1.331854 -0.721052
C2 -1.690981 0.459453 0.301883
C3 -2.715911 -0.614000 -0.001142
H4 -1.368898 0.862515 -1.562413
H5 -1.980829 1.056900 1.171121
H6 -3.675232 -0.128614 -0.188213
H7 -2.847056 -1.299190 0.841844
N8 -0.358050 -0.172317 0.729160
H9 0.342154 0.600120 0.834246
H10 -0.449428 -0.640782 1.639464
N11 0.192171 -1.022249 -0.292635
H12 -0.267849 -1.925952 -0.223606
C13 1.650985 -1.168571 -0.150273
C14 2.371590 0.132207 -0.453161
H15 1.937391 -1.530107 0.847879
H16 1.947878 -1.922498 -0.882540
H17 3.452215 -0.033311 -0.409095
H18 2.095519 0.495056 -1.448840
O19 1.970000 1.070596 0.551889
H20 2.349570 1.939811 0.388187
H21 -2.446910 -1.186128 -0.894246

TS1
O1 1.035749 1.437940 0.148097
C2 1.602486 0.233285 -0.395230
C3 2.477443 -0.478701 0.617946
H4 1.700853 1.993212 0.568223
H5 2.174308 0.489590 -1.294488
H6 3.331484 0.147802 0.890343
H7 2.875645 -1.401551 0.186427
N8 0.431321 -0.483544 -0.861759
H9 -0.609637 1.148546 -0.458137
H10 0.589833 -0.956883 -1.746462
N11 -0.220225 -1.287822 0.103129
H12 0.071440 -2.258964 0.056377
C13 -1.663034 -1.149487 0.015717
C14 -2.110744 0.176459 0.590265
H15 -2.058773 -1.268408 -1.003285
H16 -2.120134 -1.921814 0.642568
H17 -3.193056 0.296829 0.580748
H18 -1.682343 0.351917 1.577887
O19 -1.604004 1.269173 -0.304188
H20 -1.756742 2.152124 0.069005
H21 1.908587 -0.719080 1.517737

$[HOCH_2CH_2NHNHCHCH_3]^+ \cdot H_2O$
O1 -0.990027 2.093525 -0.205134
C2 -1.667922 -0.248996 0.577808
C3 -2.480594 -0.613537 -0.593526
H4 -1.251622 2.966821 -0.508754
H5 -2.077198 0.373392 1.366739
H6 -3.110599 0.234917 -0.863141
H7 -3.142998 -1.444911 -0.319577
N8 -0.467808 -0.672220 0.786424
H9 -0.033603 2.112026 -0.045264
H10 0.052335 -0.319668 1.590332
N11 0.232681 -1.457110 -0.135172
H12 0.036934 -2.434725 0.064273
C13 1.674519 -1.186943 -0.130306
C14 1.992838 0.225651 -0.594365
H15 2.128530 -1.363007 0.856778
H16 2.105025 -1.905297 -0.832528
H17 3.064775 0.305031 -0.792107
H18 1.450626 0.448810 -1.518005

O19 1.591162 1.175164 0.401354
H20 2.355248 1.645182 0.746290
H21 -1.853688 -0.919832 -1.431224

$[HOCH_2CH_2NHNHCHCH_3]^+$
C1 1.694539 0.010182 -0.496752
C2 2.025786 0.719878 0.744145
H3 2.248434 0.223584 -1.408979
H4 1.828529 1.784424 0.567715
H5 3.100932 0.627772 0.930590
N6 0.768186 -0.873112 -0.625294
H7 0.581877 -1.258636 -1.552621
N8 -0.089538 -1.225613 0.426152
H9 0.007191 -2.227532 0.569274
C10 -1.488228 -0.856284 0.139200
C11 -1.738250 0.625022 0.350162
H12 -1.785410 -1.146958 -0.878975
H13 -2.096624 -1.427107 0.844705
H14 -2.803869 0.818653 0.184580
H15 -1.486864 0.899417 1.382200
O16 -0.934237 1.349625 -0.573221
H17 -1.279565 2.241257 -0.672566
H18 1.445641 0.366407 1.593307

Cartesian coordinates for structures in Figure S8, calculated at ωB97XD/ 6-31+G(d,p)

$[HOCH_2CH_2NH(NH_2)CH(OH)CH_3]^+$
C1 -0.728874 1.864990 -0.349062
C2 -1.259064 0.447011 -0.396829
H3 -1.733282 0.243853 -1.366530
O4 -2.097183 0.113036 0.664593
H5 -2.914314 0.621375 0.638915
H6 -0.375996 2.118807 0.652095
H7 0.069114 2.020175 -1.080753
H8 -1.543912 2.547645 -0.601398
N9 -0.648156 -1.939006 -0.437483
N10 -0.160672 -0.595144 -0.298204
C11 0.703818 -0.516177 0.941686
C12 1.939046 0.344645 0.663055
H13 1.746470 1.409166 0.826279
H14 2.729819 0.025528 1.348666
O15 2.278728 0.095674 -0.690262
H16 3.134680 0.469210 -0.919499
H17 0.995028 -1.548515 1.129723
H18 0.099414 -0.145329 1.769674
H19 0.513634 -0.444514 -1.067404
H20 -1.042171 -2.039733 -1.370425
H21 -1.398610 -2.051121 0.242713

TS1
C1 -2.396805 0.247430 1.015717
C2 -1.077500 0.562475 0.382537
H3 -0.405765 1.127725 1.030172
O4 -1.273769 1.368807 -0.888438
H5 -0.953612 2.286491 -0.878612
H6 -3.090513 -0.210876 0.309590
H7 -2.233324 -0.433768 1.856535
H8 -2.845563 1.161185 1.409520
N9 -0.988801 -1.738572 -0.563293
N10 -0.338916 -0.508159 -0.324274
C11 1.041850 -0.732744 0.175517
C12 1.990976 0.388676 -0.237555
H13 2.161119 0.338027 -1.321976
H14 1.559379 1.380921 -0.010427
O15 3.162198 0.175831 0.499709
H16 3.895410 0.677409 0.132026
H17 1.372776 -1.675595 -0.256755
H18 1.041078 -0.834542 1.267283
H19 -0.606688 0.564909 -1.299609
H20 -1.745942 -1.629953 -1.226956
H21 -1.312900 -2.176937 0.294717

$[HOCH_2CH_2N(NH_2)CHCH_3]^+ \cdot H_2O$
C1 2.744110 0.208195 0.191081
C2 1.356223 0.135052 0.702247
H3 1.094685 -0.505295 1.534840
O4 0.839375 -2.392876 -0.332959
H5 0.723387 -3.212294 0.158908
H6 2.763937 0.044762 -0.891819
H7 3.189095 1.189691 0.401411
H8 3.358289 -0.551084 0.671594
N9 0.546082 1.597009 -0.931603
N10 0.384057 0.813710 0.200535
C11 -1.011915 0.655053 0.643140
C12 -1.840324 -0.132667 -0.374650
H13 -1.891526 0.404656 -1.330446
H14 -1.364439 -1.107234 -0.542317
O15 -3.100502 -0.241045 0.237331
H16 -3.715833 -0.701013 -0.340667
H17 -1.436015 1.649709 0.807230
H18 -1.002397 0.126641 1.596395
H19 1.063973 -2.667695 -1.227618
H20 1.471371 2.011307 -0.970642
H21 -0.165054 2.320381 -0.955282

$[HOCH_2CH_2N(NH_2)CHCH_3]^+$
C1 -2.845633 -0.523973 0.314016
C2 -1.462502 -0.775374 -0.155328
H3 -1.121564 -1.774603 -0.404526

H4 -2.839486 -0.011119 1.283438
H5 -3.397845 0.100815 -0.400549
H6 -3.383777 -1.464628 0.419180
N7 -0.825258 1.458604 0.088992
N8 -0.578778 0.154556 -0.283947
C9 0.822473 -0.119798 -0.658702
C10 1.759381 -0.025752 0.549430
H11 1.728437 0.980738 0.985452
H12 1.437911 -0.745365 1.315598
O13 3.016348 -0.339131 0.015393
H14 3.698105 -0.274825 0.690756
H15 1.114850 0.595864 -1.431610
H16 0.866082 -1.120646 -1.088608
H17 -1.805878 1.705719 0.015218
H18 -0.241679 2.098357 -0.439303

Cartesian coordinates for structures in Figure S9, calculated at ωB97XD/ 6-31+G(d,p)

[HE][$HOCH_2CH_2NHNH_2CH(OH)CH_3$]$^+$
Conformer_1
O1 1.964084 2.240880 0.017149
C2 0.673328 1.766516 0.131338
C3 -0.269649 2.209231 -0.969251
H4 2.272449 2.090468 -0.885403
H5 0.306043 2.075926 1.113764
H6 -0.238453 3.298710 -1.029348
H7 -1.300206 1.911523 -0.751568
N8 0.733119 0.249605 0.205794
H9 1.322715 0.005193 1.024261
H10 -0.240668 -0.165001 0.286021
N11 1.389170 -0.295533 -0.965151
H12 0.644185 -0.700643 -1.534428
C13 2.323025 -1.376805 -0.615951
C14 3.447497 -0.913310 0.290370
H15 1.815558 -2.230340 -0.142713
H16 2.741519 -1.719497 -1.565083
H17 4.209560 -1.696429 0.352676
H18 3.899815 0.003866 -0.102573
O19 2.872537 -0.679374 1.580787
H20 3.516182 -0.270283 2.167306
H21 0.037251 1.804202 -1.938643
H22 -2.011696 -0.234705 -1.005019
N23 -1.742229 -0.935312 -0.316748
N24 -1.211066 -2.036460 -1.059517
H25 -0.845027 -2.714166 -0.396614
H26 -1.943679 -2.508112 -1.591573
C27 -3.427034 0.061123 1.118780
H28 -4.391366 -0.116013 1.606088
H29 -2.710890 0.402793 1.879109
C30 -2.940264 -1.229502 0.481843
H31 -2.681684 -1.955193 1.259056
H32 -3.731531 -1.659872 -0.148419
O33 -3.532999 1.021455 0.076549
H34 -4.123420 1.734263 0.333806

Conformer_2
O1 -2.410073 -1.954199 -0.123182
C2 -1.280347 -1.765561 0.640985
C3 -0.083911 -2.603236 0.235671
H4 -2.176342 -1.856450 -1.055553
H5 -1.561017 -1.954967 1.680539
H6 -0.371936 -3.655166 0.272576
H7 0.745084 -2.456644 0.934748
N8 -0.932969 -0.283245 0.600486
H9 -1.773873 0.238017 0.920013
N10 -0.688532 0.143715 -0.758676
H11 0.333193 0.080044 -0.895929
C12 -1.141795 1.520007 -0.985080
C13 -2.647510 1.666444 -0.866611
H14 -0.661394 2.242322 -0.307080
H15 -0.838345 1.763804 -2.006097
H16 -2.944001 2.670198 -1.187851
H17 -3.149914 0.920448 -1.492226
O18 -2.976677 1.471407 0.512971
H19 -3.930590 1.442295 0.634186
H20 0.246680 -2.370702 -0.781332
H21 2.151772 -1.000974 -0.068317
N22 2.277916 -0.188792 -0.663739
N23 2.870343 -0.675189 -1.859700
H24 2.710014 -0.005525 -2.603377
H25 3.874952 -0.812541 -1.758194
C26 2.176416 1.416985 1.162631
H27 2.759222 2.060897 1.826235
H28 1.394315 2.027884 0.701527
C29 3.056194 0.804197 0.083682
H30 3.365355 1.596058 -0.606104
H31 3.966861 0.366978 0.520948
O32 1.502776 0.392938 1.911557
H33 1.899192 0.281823 2.779651
H34 -0.129025 -0.067401 1.224598

Conformer_3
O1 2.067063 -1.612891 -1.427631
C2 0.818984 -1.646201 -0.838678
C3 0.547146 -2.863341 0.026646
H4 2.743539 -1.809976 -0.768543
H5 0.083490 -1.557751 -1.642458
H6 0.543420 -3.750568 -0.608320

H7 -0.423426 -2.790306 0.528699
N8 0.619272 -0.379235 -0.040698
H9 0.871051 0.418127 -0.648431
N10 1.504179 -0.310612 1.094822
H11 1.083529 -0.886350 1.820241
C12 1.638092 1.071150 1.576579
C13 2.460392 1.922980 0.628445
H14 0.661712 1.550140 1.746355
H15 2.156269 1.009182 2.536468
H16 2.641121 2.901499 1.086009
H17 3.419063 1.432775 0.426591
O18 1.704630 2.069431 -0.577159
H19 2.230763 2.512794 -1.249317
H20 1.326549 -2.996599 0.783603
H21 -2.266519 -1.061440 -0.177957
N22 -2.098961 -0.359069 0.538785
N23 -2.485043 -0.956314 1.772263
H24 -2.151578 -0.372366 2.531872
H25 -3.499461 -1.020607 1.852220
C26 -2.057178 1.546185 -0.982551
H27 -2.692605 2.302069 -1.453987
H28 -1.164503 2.048078 -0.584345
C29 -2.823057 0.861569 0.142887
H30 -2.869355 1.531909 1.006563
H31 -3.851438 0.628963 -0.163989
O32 -1.659059 0.540439 -1.912260
H33 -1.614314 0.905668 -2.799420
H34 -0.410774 -0.288519 0.238369

Conformer_4
O1 3.311341 1.017812 -0.545593
C2 2.186120 1.537787 0.058530
C3 1.428259 2.548775 -0.779483
H4 3.085559 0.724637 -1.437435
H5 2.506559 1.970201 1.010269
H6 2.093548 3.385586 -0.997795
H7 0.555505 2.934653 -0.246383
N8 1.282383 0.383013 0.448118
H9 1.859941 -0.294888 0.983422
N10 0.821135 -0.322470 -0.729416
H11 -0.091703 0.086275 -0.940443
C12 0.642390 -1.757480 -0.464749
C13 1.956743 -2.459936 -0.184286
H14 -0.051044 -1.950757 0.367459
H15 0.195111 -2.171494 -1.371185
H16 1.790482 -3.541145 -0.143122
H17 2.682640 -2.232960 -0.973012
O18 2.421870 -1.981501 1.081915
H19 3.304285 -2.315629 1.269414
H20 1.100416 2.110599 -1.726108
H21 -1.792509 -0.422544 0.621027
N22 -1.871838 0.565799 0.388182
N23 -1.237048 1.286135 1.450728
H24 -1.279939 2.275064 1.216867
H25 -1.739982 1.178235 2.335114
C26 -3.846193 -0.171174 -0.782377
H27 -4.926504 -0.042898 -0.896394
H28 -3.378844 -0.004232 -1.757780
C29 -3.302382 0.833861 0.225395
H30 -3.440321 1.853032 -0.151322
H31 -3.839347 0.741659 1.183616
O32 -3.505656 -1.490634 -0.373201
H33 -4.276944 -1.944288 -0.025382
H34 0.470593 0.717141 1.032731

Conformer_5
O1 1.706285 -1.528575 0.908616
C2 2.010088 -1.469870 -0.412399
C3 1.128480 -2.278376 -1.345795
H4 0.724845 -1.632925 1.085558
H5 3.066764 -1.729444 -0.544584
H6 1.245973 -3.334539 -1.097346
H7 1.419726 -2.146606 -2.392562
N8 1.984223 0.023813 -0.832091
H9 2.438428 0.551394 -0.049326
H10 2.528785 0.180351 -1.688053
N11 0.655480 0.556467 -0.909628
H12 0.278975 0.379158 -1.836162
C13 0.590650 1.984596 -0.567320
C14 0.935590 2.211114 0.892284
H15 1.237764 2.600589 -1.207995
H16 -0.450931 2.264197 -0.742503
H17 0.769542 3.262224 1.147569
H18 0.309380 1.571073 1.523776
O19 2.322581 1.878721 1.047140
H20 2.561787 1.838884 1.978311
H21 0.074774 -2.011681 -1.230003
H22 -0.937019 -0.185314 0.191024
N23 -1.533486 -0.490484 0.955312
N24 -0.969726 -1.709965 1.432435
H25 -1.155513 -1.787117 2.428555
H26 -1.397706 -2.523420 0.983716
C27 -3.315453 0.664918 -0.225027
H28 -4.350564 0.566532 -0.567224
H29 -3.250172 1.513619 0.466763
C30 -2.905410 -0.611871 0.481851
H31 -3.574222 -0.776503 1.333854
H32 -3.027898 -1.459162 -0.216139
O33 -2.434788 0.873084 -1.335576
H34 -2.884447 1.410964 -1.992427

Cartesian coordinates for structures in Figure S10, calculated at ωB97XD/ 6-31+G(d,p)

[HE][$HOCH_2CH_2NHNH_2CH(OH)CH_3$]$^+$
Conformer_1
O1 1.964084 2.240880 0.017149
C2 0.673328 1.766516 0.131338
C3 -0.269649 2.209231 -0.969251
H4 2.272449 2.090468 -0.885403
H5 0.306043 2.075926 1.113764
H6 -0.238453 3.298710 -1.029348
H7 -1.300206 1.911523 -0.751568
N8 0.733119 0.249605 0.205794
H9 1.322715 0.005193 1.024261
H10 -0.240668 -0.165001 0.286021
N11 1.389170 -0.295533 -0.965151
H12 0.644185 -0.700643 -1.534428
C13 2.323025 -1.376805 -0.615951
C14 3.447497 -0.913310 0.290370
H15 1.815558 -2.230340 -0.142713
H16 2.741519 -1.719497 -1.565083
H17 4.209560 -1.696429 0.352676
H18 3.899815 0.003866 -0.102573
O19 2.872537 -0.679374 1.580787
H20 3.516182 -0.270283 2.167306
H21 0.037251 1.804202 -1.938643
H22 -2.011696 -0.234705 -1.005019
N23 -1.742229 -0.935312 -0.316748
N24 -1.211066 -2.036460 -1.059517
H25 -0.845027 -2.714166 -0.396614
H26 -1.943679 -2.508112 -1.591573
C27 -3.427034 0.061123 1.118780
H28 -4.391366 -0.116013 1.606088
H29 -2.710890 0.402793 1.879109
C30 -2.940264 -1.229502 0.481843
H31 -2.681684 -1.955193 1.259056
H32 -3.731531 -1.659872 -0.148419
O33 -3.532999 1.021455 0.076549
H34 -4.123420 1.734263 0.333806

TS1
O1 2.093326 2.051431 0.155778
C2 0.734825 1.581690 0.093894
C3 0.068791 1.960610 -1.215356
H4 2.355833 2.432525 -0.688130
H5 0.208099 2.042025 0.935416
H6 0.137753 3.040525 -1.375590
H7 -0.995651 1.712219 -1.173438
N8 0.816154 0.168060 0.418442
H9 2.661964 0.544884 0.901372
H10 -0.071805 -0.162385 0.807060
N11 1.206955 -0.661867 -0.680619
H12 0.383886 -1.138116 -1.057798
C13 2.149849 -1.668848 -0.222693
C14 3.529912 -1.080187 -0.036403
H15 1.833603 -2.172531 0.702386
H16 2.245318 -2.430899 -1.003207
H17 4.263924 -1.810222 0.301883
H18 3.862872 -0.547850 -0.928712
O19 3.454083 -0.074966 1.070686
H20 4.259685 0.460244 1.145063
H21 0.530388 1.436310 -2.056405
H22 -1.895609 -0.232835 -0.742918
N23 -1.955844 -0.958369 -0.033972
N24 -1.493482 -2.158183 -0.652841
H25 -1.336700 -2.846319 0.077275
H26 -2.194922 -2.546503 -1.286490
C27 -3.740254 0.389988 0.905472
H28 -4.804981 0.392483 1.164360
H29 -3.158992 0.657255 1.798143
C30 -3.345437 -0.993865 0.422873
H31 -3.433857 -1.708881 1.247384
H32 -4.026566 -1.311085 -0.383140
O33 -3.463192 1.297128 -0.155809
H34 -3.900588 2.136599 0.006457

[HE][$HOCH_2CH_2NHNHCHCH_3$]$^+$·H_2O
O1 -2.802667 2.427519 -0.301599
C2 -0.495420 1.178405 -0.519235
C3 0.139384 1.705103 0.696383
H4 -3.338506 3.217313 -0.194379
H5 -0.561876 1.793594 -1.410173
H6 -0.207830 2.730330 0.841222
H7 1.229440 1.735380 0.551676
N8 -0.992214 -0.003168 -0.640350
H9 -3.407681 1.669644 -0.340134
H10 -1.468848 -0.248577 -1.507863
N11 -0.986997 -0.949636 0.386072
H12 -0.131542 -1.523871 0.271353
C13 -2.189824 -1.779983 0.376463
C14 -3.451214 -0.987397 0.685243
H15 -2.322980 -2.315487 -0.577956
H16 -2.030301 -2.529185 1.156377
H17 -4.260525 -1.674359 0.946814
H18 -3.273841 -0.319724 1.533367
O19 -3.823236 -0.178733 -0.438174
H20 -4.638546 -0.502487 -0.829518
H21 -0.091733 1.090530 1.566293
H22 1.936828 -0.403701 0.698609

N23 2.166032 -0.834493 -0.192679
N24 1.634998 -2.157417 -0.145794
H25 1.655618 -2.536117 -1.088140
H26 2.201331 -2.775234 0.439744
C27 4.039790 0.694336 -0.372249
H28 5.132707 0.756728 -0.404420
H29 3.631552 1.190460 -1.262124
C30 3.617322 -0.763680 -0.357279
H31 3.887458 -1.225292 -1.312844
H32 4.147864 -1.299233 0.446952
O33 3.520831 1.303902 0.806681
H34 4.039019 2.080082 1.033167

[HE][$HOCH_2CH_2NHNHCHCH_3$]$^+$
C1 -1.037594 1.641605 0.422406
C2 -2.352293 2.185302 0.806221
H3 -0.283844 2.298758 -0.007924
H4 -2.913886 2.366632 -0.117362
H5 -2.218315 3.147761 1.306133
N6 -0.666856 0.421814 0.541543
H7 0.324351 0.112314 0.278879
N8 -1.517044 -0.568743 1.072469
H9 -0.914631 -1.112111 1.690262
C10 -2.032529 -1.467958 0.023264
C11 -3.181072 -0.876925 -0.770740
H12 -1.241121 -1.785422 -0.671316
H13 -2.396136 -2.351354 0.554595
H14 -3.617910 -1.675699 -1.381465
H15 -3.950502 -0.503495 -0.082518
O16 -2.681138 0.171100 -1.591281
H17 -3.315218 0.362781 -2.287524
H18 -2.907323 1.487565 1.431885
H19 2.227265 -0.082031 1.156610
N20 1.842406 -0.640986 0.396164
N21 1.410371 -1.876370 0.978942
H22 1.020824 -2.448248 0.233924
H23 2.202769 -2.393903 1.361232
C24 3.316058 0.622661 -1.071258
H25 4.163545 0.535727 -1.760048
H26 2.490837 1.122434 -1.598651
C27 2.887991 -0.765523 -0.629563
H28 2.482636 -1.318723 -1.482647
H29 3.753669 -1.315390 -0.234574
O30 3.660538 1.335002 0.105674
H31 4.172290 2.118616 -0.110451

[$HOCH_2CH_2NHNHCHCH_3$]$^+$·H_2O
O1 -0.990027 2.093525 -0.205134
C2 -1.667922 -0.248996 0.577808
C3 -2.480594 -0.613537 -0.593526
H4 -1.251622 2.966821 -0.508754
H5 -2.077198 0.373392 1.366739
H6 -3.110599 0.234917 -0.863141
H7 -3.142998 -1.444911 -0.319577
N8 -0.467808 -0.672220 0.786424
H9 -0.033603 2.112026 -0.045264
H10 0.052335 -0.319668 1.590332
N11 0.232681 -1.457110 -0.135172
H12 0.036934 -2.434725 0.064273
C13 1.674519 -1.186943 -0.130306
C14 1.992838 0.225651 -0.594365
H15 2.128530 -1.363007 0.856778
H16 2.105025 -1.905297 -0.832528
H17 3.064775 0.305031 -0.792107
H18 1.450626 0.448810 -1.518005
O19 1.591162 1.175164 0.401354
H20 2.355248 1.645182 0.746290
H21 -1.853688 -0.919832 -1.431224

$OHCH_2CH_2NHNH_2$ (HE)
N1 2.217126 -0.278438 -0.058113
H2 2.555479 0.648037 -0.315617
H3 2.270478 -0.880530 -0.871609
N4 0.873455 -0.241323 0.388914
H5 0.897688 -0.097285 1.393128
C6 0.020034 0.754971 -0.252602
C7 -1.423443 0.497918 0.161670
H8 0.309301 1.793594 -0.013848
H9 0.111177 0.617122 -1.335656
H10 -1.532872 0.659155 1.247005
H11 -2.091380 1.199932 -0.344256
O12 -1.830542 -0.804154 -0.193706
H13 -1.089154 -1.385805 0.020488

[HE + H]$^+$
O1 1.353141 -0.806526 -0.426858
C2 1.223684 0.234158 0.526470
C3 0.084362 1.102238 0.008007
N4 -0.990024 0.202679 -0.535109
N5 -1.626194 -0.558328 0.504662
H6 2.172580 -1.296881 -0.310192
H7 2.124798 0.850458 0.599256
H8 0.995926 -0.164393 1.522043
H9 0.409620 1.716766 -0.834684
H10 -0.363482 1.720944 0.785656
H11 -0.542720 -0.392386 -1.248824
H12 -1.706814 0.777787 -0.982576
H13 -2.465640 -0.986219 0.120515
H14 -0.984150 -1.302694 0.769940

$HOCH_2CH_2NHNCHCH_3$

C1	-1.853222	0.598223	-0.477424
C2	-2.500830	-0.702877	-0.104237
H3	-2.362266	1.225927	-1.208253
H4	-2.197834	-1.514969	-0.776056
H5	-3.587164	-0.608608	-0.181500
N6	-0.785110	1.113795	-0.001905
N7	-0.087323	0.361681	0.963072
H8	0.620657	0.994410	1.320583
C9	0.616982	-0.816384	0.453651
C10	1.642949	-0.511155	-0.630192
H11	1.129314	-1.265490	1.310843
H12	-0.096469	-1.555500	0.080420
H13	2.089291	-1.451138	-0.985087
H14	1.151156	-0.015418	-1.476681
O15	2.632718	0.328550	-0.054497
H16	3.093714	0.807237	-0.746348
H17	-2.230384	-0.980021	0.919102