

Supporting Information

Dynamics and thermochemistry of the negatively charged clusters in the 2-hydroxyethylhydrazinium
nitrate ionic liquid system

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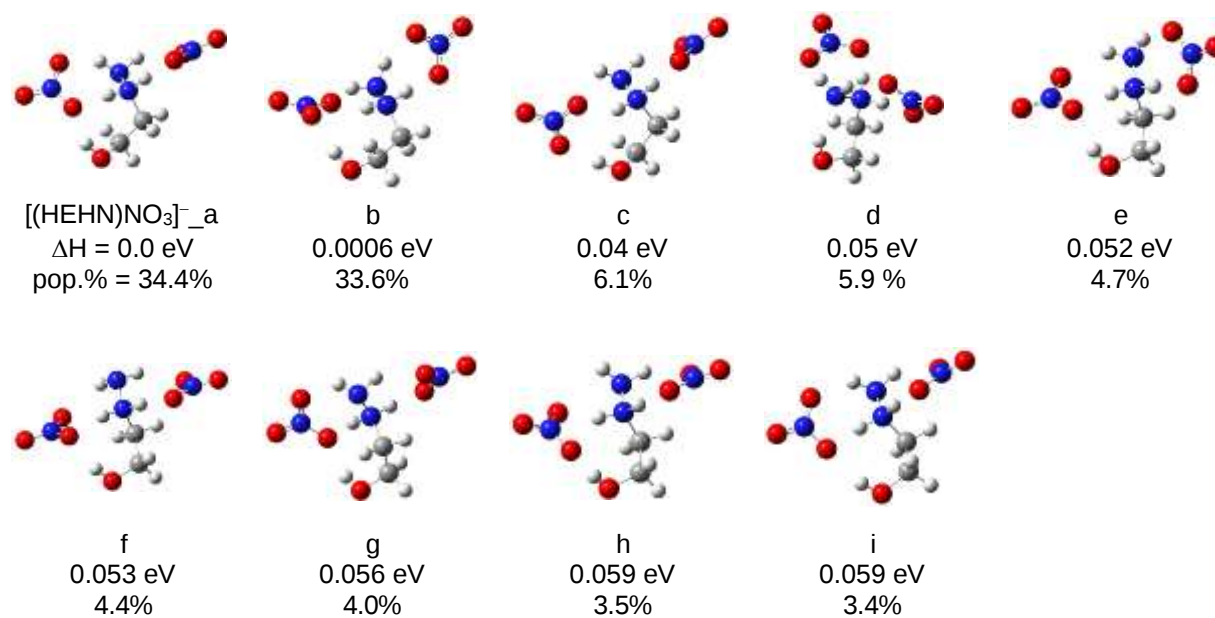


Figure S1 Probable conformations for $[(\text{HEHN})\text{NO}_3]^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the $\omega\text{B97XD}/6\text{-}31+\text{G}(\text{d},\text{p})$ level of theory.

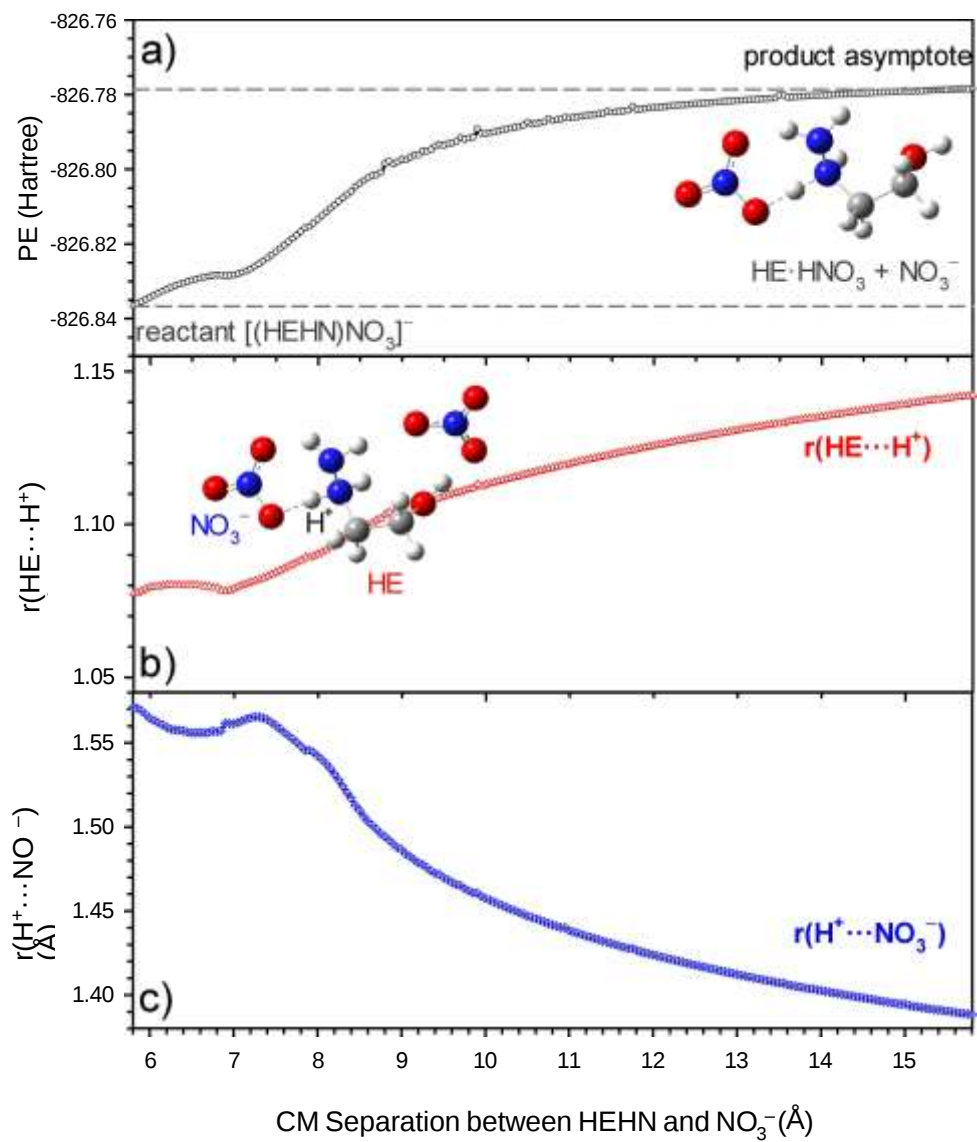


Figure S2 a) A relaxed PES scan for $[(\text{HEHN})\text{NO}_3]^-$ along the center-of-mass distance between HEHN and NO_3^- , calculated at the xB97XD/6-31+G(d,p) level of theory; and (b – c) the accompanying changes of H-bond lengths within the HEHN moiety.

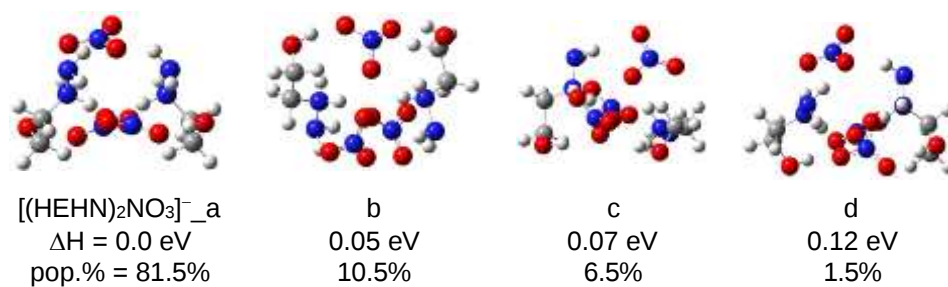


Figure S3 Probable confirmations for [(HEHN)₂NO₃]⁻, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

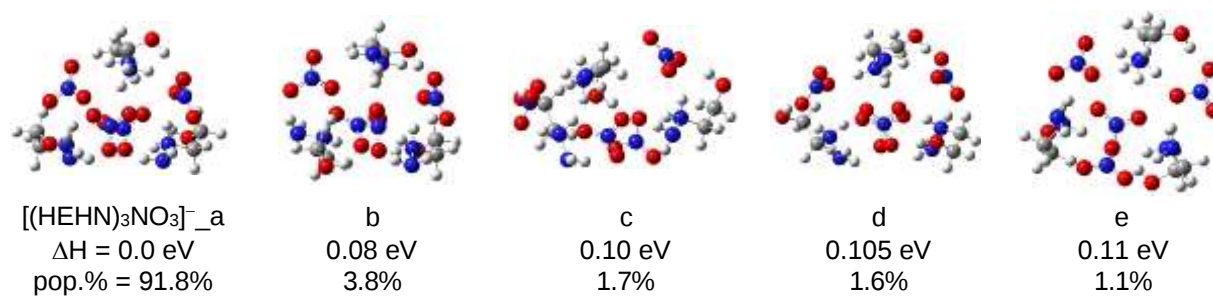


Figure S4 Probable conformations for [(HEHN)₃NO₃]⁻, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

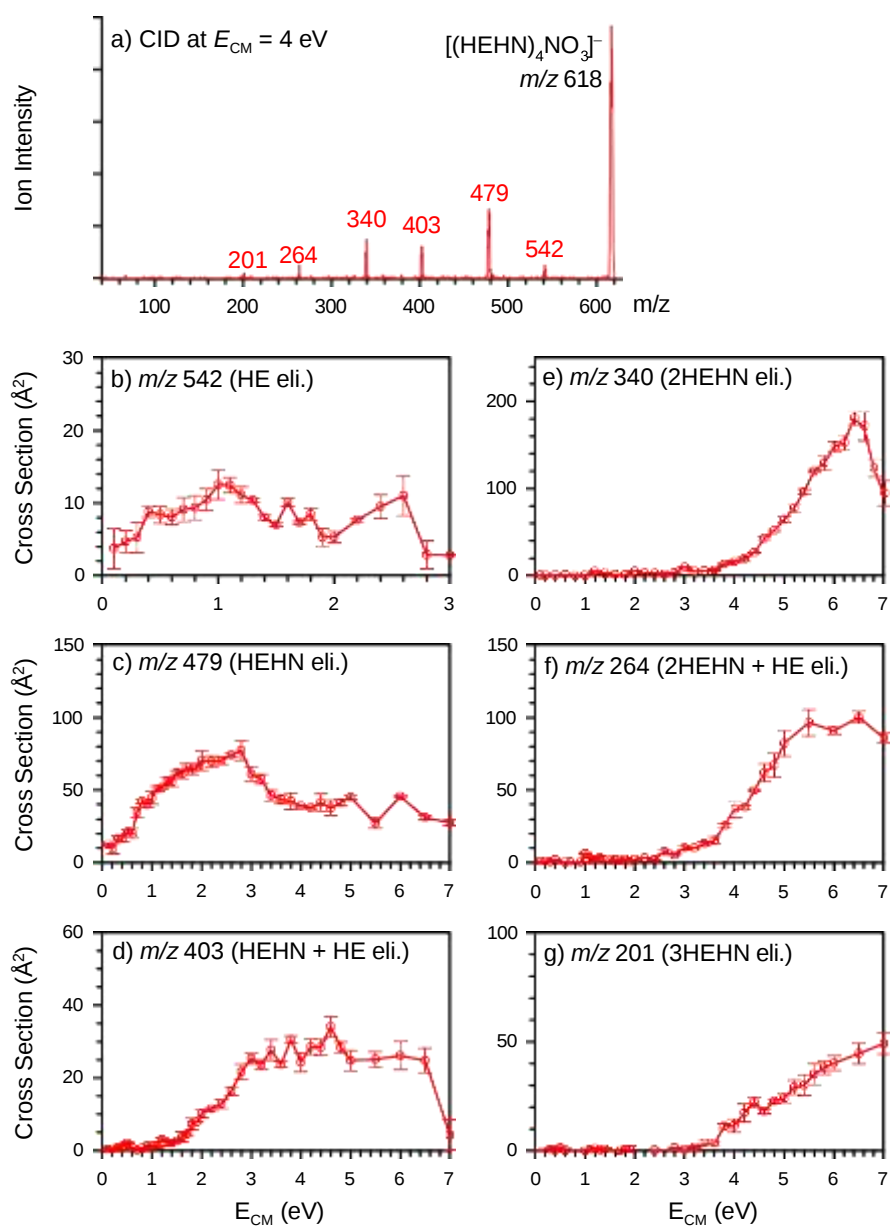


Figure S5 (a) A representative CID product ion mass spectrum for $[(\text{HEHN})_4\text{NO}_3]^-$; and (b – g) individual product ion cross sections as a function of E_{CM} .

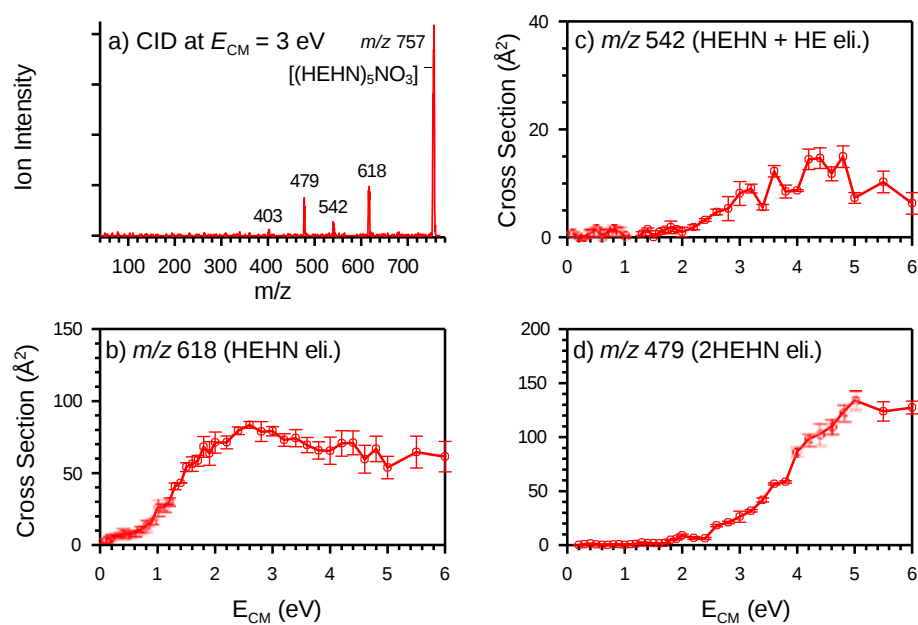


Figure S6 (a) A representative CID product ion mass spectrum for $[(\text{HEHN})_5\text{NO}_3]^-$; and (b – d) individual product ion cross sections as a function of E_{CM} .

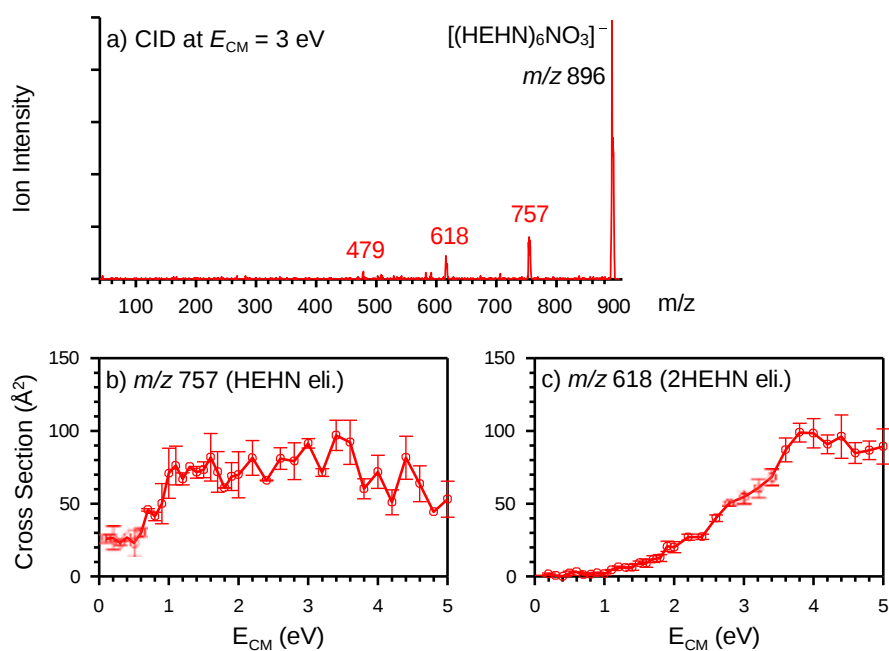


Figure S7 (a) A representative CID product ion mass spectrum for $[(\text{HEHN})_6\text{NO}_3]^-$; and (b – c) individual product ion cross sections as a function of E_{CM} .

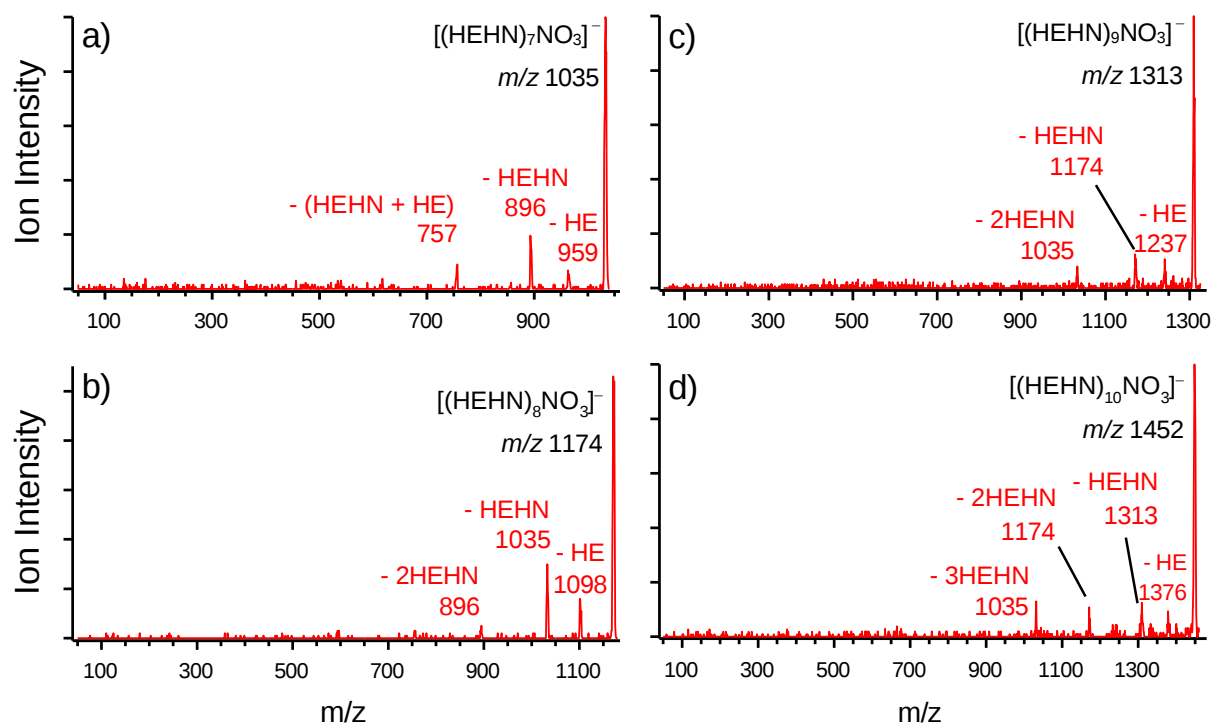


Figure S8 Representative CID product ion mass spectra for $[(\text{HEHN})_{7-10}\text{NO}_3]^-$, recorded at $E_{\text{CM}} = 4.0$ eV.

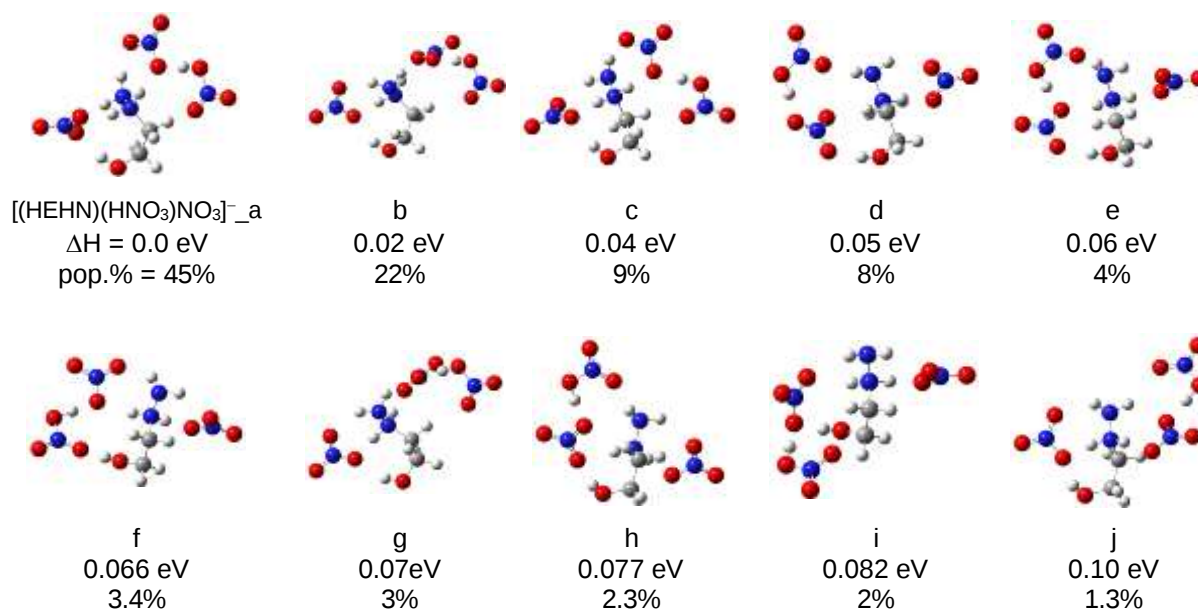


Figure S9 Probable conformations for $[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the $\omega\text{B97XD}/6\text{-}31\text{+G(d,p)}$ level of theory.

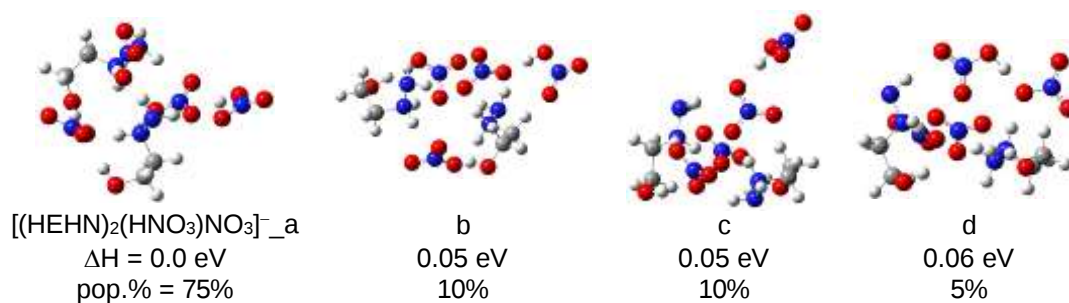


Figure S10 Probable conformations for [(HEHN)₂(HNO₃)NO₃]⁻, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

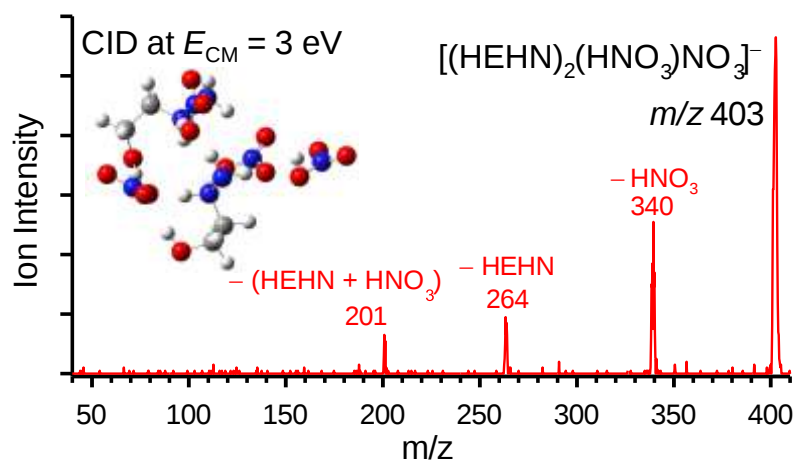


Figure S11 A representative CID product ion mass spectrum for $[(\text{HEHN})_2(\text{HNO}_3)\text{NO}_3]^-$.

**Cartesian coordinates for structures
in Rxns 2, calculated at ω B97XD/
6-31+G(d,p)**

[(HEHN)NO₃]⁻

O1 -1.930046 2.453198 -0.518864
C2 -0.907453 2.416567 0.449947
C3 0.353446 1.700097 -0.017862
N4 0.227760 0.221589 0.040200
N5 0.173226 -0.238402 1.402331
H6 -2.318338 1.566000 -0.613061
H7 -1.246919 1.960814 1.389550
H8 -0.643102 3.457902 0.658651
H9 1.215710 1.954853 0.603538
H10 0.571565 1.959937 -1.057554
H11 1.060926 -0.200481 -0.457136
H12 -0.667718 -0.077432 -0.418725
H13 1.134075 -0.498716 1.629132
H14 -0.436002 -1.057469 1.392277
N15 -2.860998 -1.218840 -0.142335
O16 -2.310930 -0.284800 -0.829781
O17 -2.131245 -1.928952 0.580237
O18 -4.074512 -1.391363 -0.218496
N19 3.419203 -0.514548 -0.220029
O20 4.601370 -0.692682 -0.511167
O21 3.074863 -0.153056 0.934542
O22 2.512939 -0.691593 -1.096514

[(HE)NO₃]⁻

O1 -1.028022 -1.875654 0.050845
C2 -1.852981 -0.976914 -0.657171
C3 -2.445064 0.116382 0.237253
N4 -1.498063 1.094327 0.755984
N5 -0.947216 1.868431 -0.318085
H6 -0.186661 -1.425824 0.267737
H7 -2.675186 -1.569548 -1.080162
H8 -1.307860 -0.516547 -1.493797
H9 -2.921840 -0.367398 1.100091
H10 -3.212455 0.667871 -0.320675
H11 -0.742028 0.596619 1.227867
H12 -0.654926 2.753626 0.079147
H13 -0.117470 1.408739 -0.703721
N14 2.042276 -0.066698 -0.005108
O15 3.260404 -0.002647 0.208240
O16 1.556867 0.303892 -1.101543
O17 1.264215 -0.507687 0.894144

HNO₃

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

[(HNO₃)NO₃]⁻

N1 1.970289 -0.022785 -0.069036
O2 1.592660 -0.644472 -1.065692
O3 3.123855 -0.062860 0.358715
O4 1.118301 0.719271 0.567062
H5 -0.079898 0.675145 0.071349
O6 -1.121155 0.860881 -0.336901
N7 -1.973478 -0.056088 0.065858
O8 -3.119530 0.046663 -0.352762
O9 -1.581354 -0.934862 0.823442

HE

N1 2.217126 -0.278438 -0.058113
H2 2.555479 0.648038 -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

NO₃⁻

N1 0.000022 -0.000012 0.000000
O2 -0.354908 -1.204016 0.000000
O3 -0.865281 0.909363 0.000000
O4 1.220170 0.294664 0.000000

HEHN

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 -0.120204 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 3, calculated at ω B97XD/
 6-31+G(d,p)**

$[(\text{HEHN})_2\text{NO}_3]^-$

O1 -3.961389 -0.368885 0.046089
 C2 -3.405553 0.324171 1.137942
 C3 -2.870935 1.658777 0.650401
 N4 -1.800070 1.451243 -0.351788
 N5 -1.517921 2.679674 -1.048532
 H6 -3.594252 -1.275876 0.038367
 H7 -2.598528 -0.254284 1.601247
 H8 -4.170937 0.526693 1.900277
 H9 -2.436179 2.248391 1.461298
 H10 -3.653727 2.233265 0.150327
 H11 -2.107020 0.747517 -1.028430
 H12 -0.933891 1.082662 0.119056
 H13 -0.838965 2.445658 -1.780715
 H14 -0.995811 3.234209 -0.367167
 O15 3.430587 -0.305573 1.586528
 C16 2.574323 -1.390951 1.830183
 C17 2.391998 -2.219510 0.568206
 N18 1.647658 -1.467195 -0.462972
 N19 1.527958 -2.232836 -1.675478
 H20 2.947686 0.524198 1.759462
 H21 1.597156 -1.053417 2.196667
 H22 3.013060 -2.050686 2.592226
 H23 1.817353 -3.127518 0.772758
 H24 3.356872 -2.485605 0.132016
 H25 2.122810 -0.579766 -0.724966
 H26 0.700179 -1.227152 -0.109060
 H27 0.796382 -2.918118 -1.472704
 H28 1.134954 -1.563307 -2.339760
 N29 1.242660 1.231137 -2.214522
 O30 0.263624 0.429624 -2.186450
 O31 2.383229 0.816106 -1.907822
 O32 1.057833 2.416970 -2.534162
 N33 -1.512857 -2.654115 0.021421
 O34 -0.721924 -3.592967 -0.186525
 O35 -2.740989 -2.859253 0.117572
 O36 -1.075291 -1.475637 0.139870
 N37 0.827280 1.939205 1.601279
 O38 1.894407 1.968327 2.236276
 O39 0.048094 2.910136 1.593610

O40 0.521933 0.889704 0.956620

$[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-$

O1 2.666645 -2.480012 0.316107
 C2 1.680337 -2.275566 1.294408
 C3 0.455983 -1.538833 0.772889
 N4 0.736897 -0.124376 0.416347
 N5 1.238484 0.630139 1.536096
 H6 3.189798 -1.660342 0.233172
 H7 2.078633 -1.746586 2.170452
 H8 1.341727 -3.261592 1.630528
 H9 -0.333938 -1.517774 1.527255
 H10 0.072879 -2.017296 -0.131312
 H11 -0.167152 0.316533 0.138988
 H12 1.407802 -0.039517 -0.390273
 H13 0.816195 1.555632 1.448482
 H14 2.246849 0.702148 1.386502
 N15 3.736755 0.516027 -0.955159
 O16 3.841246 0.040992 0.222688
 O17 4.715127 0.966787 -1.537355
 O18 2.597438 0.509808 -1.499476
 N19 -1.755749 2.309248 0.371078
 O20 -0.702453 2.812922 0.781218
 O21 -2.806492 2.929307 0.262787
 O22 -1.734018 1.054057 0.042192
 H23 -3.064572 0.429831 -0.327217
 O24 -3.955430 -0.024997 -0.582290
 N25 -3.752241 -1.346800 -0.592550
 O26 -2.632454 -1.756887 -0.325815
 O27 -4.719003 -2.022517 -0.870185

HE

N1 2.217126 -0.278438 -0.058113
 H2 2.555479 0.648038 -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

$[(\text{HEHN})\text{NO}_3]^-$

O1 -1.930046 2.453198 -0.518864
 C2 -0.907453 2.416567 0.449947
 C3 0.353446 1.700097 -0.017862

N4 0.227760 0.221589 0.040200
 N5 0.173226 -0.238402 1.402331
 H6 -2.318338 1.566000 -0.613061
 H7 -1.246919 1.960814 1.389550
 H8 -0.643102 3.457902 0.658651
 H9 1.215710 1.954853 0.603538
 H10 0.571565 1.959937 -1.057554
 H11 1.060926 -0.200481 -0.457136
 H12 -0.667718 -0.077432 -0.418725
 H13 1.134075 -0.498716 1.629132
 H14 -0.436002 -1.057469 1.392277
 N15 -2.860998 -1.218840 -0.142335
 O16 -2.310930 -0.284800 -0.829781
 O17 -2.131245 -1.928952 0.580237
 O18 -4.074512 -1.391363 -0.218496
 N19 3.419203 -0.514548 -0.220029
 O20 4.601370 -0.692682 -0.511167
 O21 3.074863 -0.153056 0.934542
 O22 2.512939 -0.691593 -1.096514

HEHN

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 -0.120204 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

HNO₃

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

[(HNO₃)₂NO₃]⁻

N1 -0.000005 0.673338 0.000063
 O2 -0.000004 -0.555972 -0.000096

O3 -1.029982 1.329330 -0.319650
 O4 1.029970 1.329250 0.319942
 H5 2.246812 0.474249 0.599252
 O6 3.100122 0.009357 0.955529
 N7 3.845887 -0.379449 -0.084470
 O8 4.869302 -0.969064 0.203170
 O9 3.453855 -0.113439 -1.206078
 H10 -2.246829 0.474414 -0.599151
 O11 -3.100155 0.009621 -0.955522
 N12 -3.845879 -0.379473 0.084398
 O13 -4.869302 -0.969015 -0.203363
 O14 -3.453806 -0.113766 1.206064

[(HNO₃)NO₃]⁻

N1 1.970289 -0.022785 -0.069036
 O2 1.592660 -0.644472 -1.065692
 O3 3.123855 -0.062860 0.358715
 O4 1.118301 0.719271 0.567062
 H5 -0.079898 0.675145 0.071349
 O6 -1.121155 0.860881 -0.336901
 N7 -1.973478 -0.056088 0.065858
 O8 -3.119530 0.046663 -0.352762
 O9 -1.581354 -0.934862 0.823442

NO₃⁻

N1 0.000022 -0.000012 0.000000
 O2 -0.354908 -1.204016 0.000000
 O3 -0.865281 0.909363 0.000000
 O4 1.220170 0.294664 0.000000

(HEHN)₂

O1 -3.643688 -1.561259 1.771427
 C2 -3.318628 -0.183631 1.662105
 C3 -3.338090 0.143317 0.184607
 N4 -2.400367 -0.774344 -0.510190
 N5 -2.408698 -0.555295 -1.930556
 H6 -3.487173 -1.871229 2.666873
 H7 -2.326169 0.022601 2.084071
 H8 -4.051261 0.451032 2.173311
 H9 -3.012802 1.169913 -0.001980
 H10 -4.324099 -0.023950 -0.252766
 H11 -2.703720 -1.735620 -0.334821
 H12 -1.434292 -0.713980 -0.111263
 H13 -1.772494 -1.256608 -2.309339
 H14 -1.958690 0.356347 -2.044667
 O15 3.482614 -1.261059 1.446065
 C16 4.176844 -0.252194 0.756232
 C17 3.399779 1.058733 0.755109
 N18 2.107902 0.925757 0.042699
 N19 2.284573 0.752115 -1.374078

H20 2.915194 -1.742259 0.822259
 H21 4.418672 -0.551435 -0.272144
 H22 5.124894 -0.077966 1.273866
 H23 3.954895 1.859185 0.261429
 H24 3.160367 1.347147 1.781928
 H25 1.520777 1.795060 0.164009
 H26 1.539554 0.150299 0.437391
 H27 2.404640 -0.247072 -1.536874
 H28 1.386864 1.025657 -1.775574
 N29 -0.688727 2.508968 -0.223263
 O30 -0.576528 1.525213 -1.016366
 O31 0.355517 2.968885 0.310612
 O32 -1.793254 2.986976 0.029033
 N33 0.589501 -2.011517 -0.509832
 O34 1.809384 -2.216994 -0.667950
 O35 0.221090 -1.141270 0.346677
 O36 -0.263120 -2.609774 -1.174185

**Cartesian coordinates for structures
 in Rxns 4, calculated at ω B97XD/
 6-31+G(d,p)**

[(HEHN)₃NO₃]⁻

O1 -3.325544 -3.339695 1.256350
 C2 -4.029700 -2.366116 0.523603
 C3 -3.588489 -2.275076 -0.930436
 N4 -2.263050 -1.624986 -1.081137
 N5 -1.903466 -1.550230 -2.471918
 H6 -2.497076 -2.933860 1.561617
 H7 -3.962305 -1.375510 0.992175
 H8 -5.084357 -2.660160 0.522137
 H9 -4.287586 -1.658041 -1.500174
 H10 -3.509627 -3.265321 -1.382554
 H11 -1.510720 -2.156364 -0.597394
 H12 -2.305450 -0.685394 -0.637841
 H13 -0.917366 -1.271908 -2.489073
 H14 -2.431921 -0.753417 -2.828389
 O15 3.974520 0.844032 -2.928468
 C16 4.587675 0.699668 -1.671243
 C17 4.509000 -0.730888 -1.155252
 N18 3.105287 -1.109552 -0.879634
 N19 3.015196 -2.458337 -0.383145
 H20 3.053375 1.126381 -2.781987
 H21 4.150224 1.383606 -0.931363
 H22 5.648086 0.953816 -1.775632
 H23 5.048618 -0.831048 -0.210918
 H24 4.896041 -1.441198 -1.888661
 H25 2.533526 -1.038286 -1.736945
 H26 2.683219 -0.435807 -0.185166
 H27 3.284273 -2.385929 0.599456
 O44 3.753576 -0.352483 1.911609
 O45 2.407553 0.861839 3.104694
 O46 1.942060 0.445262 1.027341
 N47 0.667054 0.661889 -1.804413
 O48 -0.367626 0.780154 -1.122059

H28 2.014171 -2.679836 -0.358145
 O29 -2.005591 4.103671 0.855074
 C30 -0.655106 3.797545 0.604419
 C31 -0.102411 2.923769 1.719558
 N32 -0.645876 1.542516 1.630936
 N33 -0.601252 0.883394 2.908853
 H34 -2.572081 3.631164 0.215983
 H35 -0.071774 4.726396 0.593350
 H36 -0.516516 3.304646 -0.365950
 H37 -0.415190 3.315380 2.689246
 H38 0.985242 2.832291 1.684220
 H39 -0.101480 1.040738 0.912476
 H40 -1.624219 1.561009 1.295529
 H41 0.390449 0.876601 3.167089
 H42 -0.850442 -0.092505 2.724706
 N43 2.712569 0.313205 2.038173
 O49 0.877622 -0.412051 -2.437592
 O50 1.502515 1.584894 -1.859706
 N51 -3.392411 1.491171 -0.980083
 O52 -2.968549 0.924921 0.075017
 O53 -3.441777 2.730668 -1.041742
 O54 -3.758098 0.788198 -1.937894
 N55 0.019016 -2.263340 1.305952
 O56 0.054710 -2.699586 0.118976
 O57 1.009438 -2.307167 2.026733
 O58 -1.073109 -1.775279 1.724571

[(HEHN)₂(HNO₃)NO₃]⁻

O1 0.897618 3.691969 -1.407709
C2 -0.324442 3.034308 -1.628359
C3 -1.125093 2.787299 -0.355380
N4 -0.502349 1.742716 0.494193
N5 -1.347082 1.428161 1.611291
H6 1.541688 3.041222 -1.074888
H7 -0.185376 2.082664 -2.158096
H8 -0.931500 3.685305 -2.265815
H9 -2.125552 2.427362 -0.606897
H10 -1.196661 3.690773 0.252900
H11 0.406879 2.085978 0.884325
H12 -0.284902 0.914135 -0.080839
H13 -2.184085 0.994470 1.220446
H14 -0.857623 0.703731 2.142300
O15 3.962434 -0.397567 -1.488245
C16 4.142619 -1.211674 -0.350443
C17 3.315620 -2.481132 -0.502449

N18 1.924947 -2.103191 -0.825828
 N19 1.106228 -3.259008 -1.078175
 H20 3.575292 0.446699 -1.181429
 H21 3.855443 -0.675515 0.560308
 H22 5.197818 -1.494034 -0.247845
 H23 3.292833 -3.060721 0.423582
 H24 3.670393 -3.109693 -1.322484
 H25 1.934312 -1.513387 -1.662309
 H26 1.508018 -1.510214 -0.048496
 H27 0.248846 -2.911625 -1.517229
 H28 0.840471 -3.582904 -0.146119
 N29 2.792424 1.893048 0.874088
 O30 1.939354 2.471007 1.583855
 O31 2.485747 1.629106 -0.339837
 O32 3.895095 1.576609 1.312954
 N33 -1.290495 -0.858156 -1.587903
 O34 -0.141589 -0.394857 -1.725262
 O35 -1.563107 -2.025574 -1.890143
 O36 -2.187272 -0.095025 -1.109677
 N37 0.405743 -1.620765 2.033368
 O38 0.848587 -2.781048 1.916732
 O39 -0.310097 -1.276866 2.974718
 O40 0.705993 -0.759485 1.135992
 H41 -3.563642 -0.718071 -0.814531
 O42 -4.511323 -1.059377 -0.627208
 N43 -5.078593 -0.214378 0.245729
 O44 -6.227622 -0.457534 0.533545
 O45 -4.402647 0.712647 0.667232

HE

N1 2.217126 -0.278438 -0.058113
 H2 2.555479 0.648038 -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

[(HEHN)₂NO₃]⁻

O1 -3.961389 -0.368885 0.046089
 C2 -3.405553 0.324171 1.137942
 C3 -2.870935 1.658777 0.650401
 N4 -1.800070 1.451243 -0.351788
 N5 -1.517921 2.679674 -1.048532

H6 -3.594252 -1.275876 0.038367
 H7 -2.598528 -0.254284 1.601247
 H8 -4.170937 0.526693 1.900277
 H9 -2.436179 2.248391 1.461298
 H10 -3.653727 2.233265 0.150327
 H11 -2.107020 0.747517 -1.028430
 H12 -0.933891 1.082662 0.119056
 H13 -0.838965 2.445658 -1.780715
 H14 -0.995811 3.234209 -0.367167
 O15 3.430587 -0.305573 1.586528
 C16 2.574323 -1.390951 1.830183
 C17 2.391998 -2.219510 0.568206
 N18 1.647658 -1.467195 -0.462972
 N19 1.527958 -2.232836 -1.675478
 H20 2.947686 0.524198 1.759462
 H21 1.597156 -1.053417 2.196667
 H22 3.013060 -2.050686 2.592226
 H23 1.817353 -3.127518 0.772758
 H24 3.356872 -2.485605 0.132016
 H25 2.122810 -0.579766 -0.724966
 H26 0.700179 -1.227152 -0.109060
 H27 0.796382 -2.918118 -1.472704
 H28 1.134954 -1.563307 -2.339760
 N29 1.242660 1.231137 -2.214522
 O30 0.263624 0.429624 -2.186450
 O31 2.383229 0.816106 -1.907822
 O32 1.057833 2.416970 -2.534162
 N33 -1.512857 -2.654115 0.021421
 O34 -0.721924 -3.592967 -0.186525
 O35 -2.740989 -2.859253 0.117572
 O36 -1.075291 -1.475637 0.139870
 N37 0.827280 1.939205 1.601279
 O38 1.894407 1.968327 2.236276
 O39 0.048094 2.910136 1.593610
 O40 0.521933 0.889704 0.956620

HEHN

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 -0.120204 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

[(HEHN)(HNO₃)₂NO₃]⁻

O1 0.141260 3.233734 -0.507954
 C2 -0.922584 2.327628 -0.342492
 C3 -0.779743 1.074123 -1.197234
 N4 0.294534 0.192125 -0.669172
 N5 0.434674 -1.001883 -1.460319
 H6 0.882888 2.976126 0.065655
 H7 -1.838562 2.830337 -0.664714
 H8 -1.060960 2.046466 0.711052
 H9 -0.510194 1.324537 -2.224601
 H10 -1.705808 0.494421 -1.184822
 H11 0.056983 -0.050366 0.316356
 H12 1.210605 0.689160 -0.699916
 H13 1.296815 -1.444842 -1.141478
 H14 -0.344662 -1.594642 -1.167512
 N15 3.047020 1.534666 0.590043
 O16 4.081746 1.126870 1.179096
 O17 2.859430 1.211170 -0.609210
 O18 2.221404 2.234974 1.194021
 N19 -2.013272 -1.121209 1.228186
 O20 -3.065735 -1.098068 1.920889
 O21 -0.966803 -0.622271 1.690825
 O22 -2.034755 -1.628881 0.089805
 H23 -4.279347 -1.121162 0.989376
 O24 -5.146738 -1.130960 0.435868
 N25 -5.080581 -0.130485 -0.451889
 O26 -6.013558 -0.057168 -1.221927
 O27 -4.113740 0.612654 -0.409006
 N28 4.193744 -1.775991 -0.368243
 O29 3.066382 -1.635530 0.086653
 O30 4.575109 -2.685228 -1.070037
 O31 5.112356 -0.856914 -0.061675
 H32 4.642511 -0.076146 0.419941

[(HEHN)(HNO₃)NO₃]⁻

O1 2.666645 -2.480012 0.316107
 C2 1.680337 -2.275566 1.294408
 C3 0.455983 -1.538833 0.772889
 N4 0.736897 -0.124376 0.416347
 N5 1.238484 0.630139 1.536096
 H6 3.189798 -1.660342 0.233172
 H7 2.078633 -1.746586 2.170452
 H8 1.341727 -3.261592 1.630528
 H9 -0.333938 -1.517774 1.527255

H10 0.072879 -2.017296 -0.131312
 H11 -0.167152 0.316533 0.138988
 H12 1.407802 -0.039517 -0.390273
 H13 0.816195 1.555632 1.448482
 H14 2.246849 0.702148 1.386502
 N15 3.736755 0.516027 -0.955159
 O16 3.841246 0.040992 0.222688
 O17 4.715127 0.966787 -1.537355
 O18 2.597438 0.509808 -1.499476
 N19 -1.755749 2.309248 0.371078
 O20 -0.702453 2.812922 0.781218
 O21 -2.806492 2.929307 0.262787
 O22 -1.734018 1.054057 0.042192
 H23 -3.064572 0.429831 -0.327217
 O24 -3.955430 -0.024997 -0.582290
 N25 -3.752241 -1.346800 -0.592550
 O26 -2.632454 -1.756887 -0.325815
 O27 -4.719003 -2.022517 -0.870185

[(HEHN)NO₃]⁻

O1 -1.930046 2.453198 -0.518864
 C2 -0.907453 2.416567 0.449947
 C3 0.353446 1.700097 -0.017862
 N4 0.227760 0.221589 0.040200
 N5 0.173226 -0.238402 1.402331
 H6 -2.318338 1.566000 -0.613061
 H7 -1.246919 1.960814 1.389550
 H8 -0.643102 3.457902 0.658651
 H9 1.215710 1.954853 0.603538
 H10 0.571565 1.959937 -1.057554
 H11 1.060926 -0.200481 -0.457136
 H12 -0.667718 -0.077432 -0.418725
 H13 1.134075 -0.498716 1.629132
 H14 -0.436002 -1.057469 1.392277
 N15 -2.860998 -1.218840 -0.142335
 O16 -2.310930 -0.284800 -0.829781
 O17 -2.131245 -1.928952 0.580237
 O18 -4.074512 -1.391363 -0.218496
 N19 3.419203 -0.514548 -0.220029
 O20 4.601370 -0.692682 -0.511167
 O21 3.074863 -0.153056 0.934542
 O22 2.512939 -0.691593 -1.096514

(HEHN)₂

O1 -3.643688 -1.561259 1.771427
 C2 -3.318628 -0.183631 1.662105
 C3 -3.338090 0.143317 0.184607
 N4 -2.400367 -0.774344 -0.510190
 N5 -2.408698 -0.555295 -1.930556
 H6 -3.487173 -1.871229 2.666873

H7 -2.326169 0.022601 2.084071
 H8 -4.051261 0.451032 2.173311
 H9 -3.012802 1.169913 -0.001980
 H10 -4.324099 -0.023950 -0.252766
 H11 -2.703720 -1.735620 -0.334821
 H12 -1.434292 -0.713980 -0.111263
 H13 -1.772494 -1.256608 -2.309339
 H14 -1.958690 0.356347 -2.044667
 O15 3.482614 -1.261059 1.446065
 C16 4.176844 -0.252194 0.756232
 C17 3.399779 1.058733 0.755109
 N18 2.107902 0.925757 0.042699
 N19 2.284573 0.752115 -1.374078
 H20 2.915194 -1.742259 0.822259
 H21 4.418672 -0.551435 -0.272144
 H22 5.124894 -0.077966 1.273866
 H23 3.954895 1.859185 0.261429
 H24 3.160367 1.347147 1.781928
 H25 1.520777 1.795060 0.164009
 H26 1.539554 0.150299 0.437391
 H27 2.404640 -0.247072 -1.536874
 H28 1.386864 1.025657 -1.775574
 N29 -0.688727 2.508968 -0.223263
 O30 -0.576528 1.525213 -1.016366
 O31 0.355517 2.968885 0.310612
 O32 -1.793254 2.986976 0.029033
 N33 0.589501 -2.011517 -0.509832
 O34 1.809384 -2.216994 -0.667950
 O35 0.221090 -1.141270 0.346677
 O36 -0.263120 -2.609774 -1.174185

HNO₃

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

[(HNO₃)NO₃]⁻

N1 1.970289 -0.022785 -0.069036
 O2 1.592660 -0.644472 -1.065692
 O3 3.123855 -0.062860 0.358715
 O4 1.118301 0.719271 0.567062
 H5 -0.079898 0.675145 0.071349
 O6 -1.121155 0.860881 -0.336901
 N7 -1.973478 -0.056088 0.065858
 O8 -3.119530 0.046663 -0.352762
 O9 -1.581354 -0.934862 0.823442

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

[(HNO₃)NO₃]⁻

N1 1.970289 -0.022785 -0.069036
 O2 1.592660 -0.644472 -1.065692
 O3 3.123855 -0.062860 0.358715
 O4 1.118301 0.719271 0.567062
 H5 -0.079898 0.675145 0.071349
 O6 -1.121155 0.860881 -0.336901
 N7 -1.973478 -0.056088 0.065858
 O8 -3.119530 0.046663 -0.352762
 O9 -1.581354 -0.934862 0.823442

HNO₃

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

NO₃⁻

N1 0.000022 -0.000012 0.000000
 O2 -0.354908 -1.204016 0.000000
 O3 -0.865281 0.909363 0.000000
 O4 1.220170 0.294664 0.000000

HE

N1 2.217126 -0.278438 -0.058113
 H2 2.555479 0.648038 -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 6, calculated at ω B97XD/
6-31+G(d,p)**

Reactions for $[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-$

$[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-$

O1 2.666645 -2.480012 0.316107
C2 1.680337 -2.275566 1.294408
C3 0.455983 -1.538833 0.772889
N4 0.736897 -0.124376 0.416347
N5 1.238484 0.630139 1.536096
H6 3.189798 -1.660342 0.233172
H7 2.078633 -1.746586 2.170452
H8 1.341727 -3.261592 1.630528
H9 -0.333938 -1.517774 1.527255
H10 0.072879 -2.017296 -0.131312
H11 -0.167152 0.316533 0.138988
H12 1.407802 -0.039517 -0.390273
H13 0.816195 1.555632 1.448482
H14 2.246849 0.702148 1.386502
N15 3.736755 0.516027 -0.955159
O16 3.841246 0.040992 0.222688
O17 4.715127 0.966787 -1.537355
O18 2.597438 0.509808 -1.499476
N19 -1.755749 2.309248 0.371078
O20 -0.702453 2.812922 0.781218
O21 -2.806492 2.929307 0.262787
O22 -1.734018 1.054057 0.042192
H23 -3.064572 0.429831 -0.327217
O24 -3.955430 -0.024997 -0.582290
N25 -3.752241 -1.346800 -0.592550
O26 -2.632454 -1.756887 -0.325815
O27 -4.719003 -2.022517 -0.870185

$[(\text{HEHN})\text{NO}_3]^-$

O1 -1.930046 2.453198 -0.518864
C2 -0.907453 2.416567 0.449947
C3 0.353446 1.700097 -0.017862
N4 0.227760 0.221589 0.040200
N5 0.173226 -0.238402 1.402331
H6 -2.318338 1.566000 -0.613061
H7 -1.246919 1.960814 1.389550
H8 -0.643102 3.457902 0.658651
H9 1.215710 1.954853 0.603538
H10 0.571565 1.959937 -1.057554
H11 1.060926 -0.200481 -0.457136
H12 -0.667718 -0.077432 -0.418725
H13 1.134075 -0.498716 1.629132
H14 -0.436002 -1.057469 1.392277

N15 -2.860998 -1.218840 -0.142335
O16 -2.310930 -0.284800 -0.829781
O17 -2.131245 -1.928952 0.580237
O18 -4.074512 -1.391363 -0.218496
N19 3.419203 -0.514548 -0.220029
O20 4.601370 -0.692682 -0.511167
O21 3.074863 -0.153056 0.934542
O22 2.512939 -0.691593 -1.096514

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

$[(\text{HNO}_3)_2\text{NO}_3]^-$

N1 -0.000005 0.673338 0.000063
O2 -0.000004 -0.555972 -0.000096
O3 -1.029982 1.329330 -0.319650
O4 1.029970 1.329250 0.319942
H5 2.246812 0.474249 0.599252
O6 3.100122 0.009357 0.955529
N7 3.845887 -0.379449 -0.084470
O8 4.869302 -0.969064 0.203170
O9 3.453855 -0.113439 -1.206078
H10 -2.246829 0.474414 -0.599151
O11 -3.100155 0.009621 -0.955522
N12 -3.845879 -0.379473 0.084398
O13 -4.869302 -0.969015 -0.203363
O14 -3.453806 -0.113766 1.206064

HE

N1 2.217126 -0.278438 -0.058113
H2 2.555479 0.648038 -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

$[(\text{HNO}_3)\text{NO}_3]^-$

N1 1.970289 -0.022785 -0.069036
O2 1.592660 -0.644472 -1.065692

O3 3.123855 -0.062860 0.358715
 O4 1.118301 0.719271 0.567062
 H5 -0.079898 0.675145 0.071349
 O6 -1.121155 0.860881 -0.336901
 N7 -1.973478 -0.056088 0.065858
 O8 -3.119530 0.046663 -0.352762
 O9 -1.581354 -0.934862 0.823442

HEHN

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 -0.120204 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

Reactions for [(HEHN)₂(HNO₃)NO₃]⁻

[(HEHN)₂(HNO₃)NO₃]⁻

O1 0.897618 3.691969 -1.407709
 C2 -0.324442 3.034308 -1.628359
 C3 -1.125093 2.787299 -0.355380
 N4 -0.502349 1.742716 0.494193
 N5 -1.347082 1.428161 1.611291
 H6 1.541688 3.041222 -1.074888
 H7 -0.185376 2.082664 -2.158096
 H8 -0.931500 3.685305 -2.265815
 H9 -2.125552 2.427362 -0.606897
 H10 -1.196661 3.690773 0.252900
 H11 0.406879 2.085978 0.884325
 H12 -0.284902 0.914135 -0.080839
 H13 -2.184085 0.994470 1.220446
 H14 -0.857623 0.703731 2.142300
 O15 3.962434 -0.397567 -1.488245
 C16 4.142619 -1.211674 -0.350443
 C17 3.315620 -2.481132 -0.502449
 N18 1.924947 -2.103191 -0.825828
 N19 1.106228 -3.259008 -1.078175

H20 3.575292 0.446699 -1.181429
 H21 3.855443 -0.675515 0.560308
 H22 5.197818 -1.494034 -0.247845
 H23 3.292833 -3.060721 0.423582
 H24 3.670393 -3.109693 -1.322484
 H25 1.934312 -1.513387 -1.662309
 H26 1.508018 -1.510214 -0.048496
 H27 0.248846 -2.911625 -1.517229
 H28 0.840471 -3.582904 -0.146119
 N29 2.792424 1.893048 0.874088
 O30 1.939354 2.471007 1.583855
 O31 2.485747 1.629106 -0.339837
 O32 3.895095 1.576609 1.312954
 N33 -1.290495 -0.858156 -1.587903
 O34 -0.141589 -0.394857 -1.725262
 O35 -1.563107 -2.025574 -1.890143
 O36 -2.187272 -0.095025 -1.109677
 N37 0.405743 -1.620765 2.033368
 O38 0.848587 -2.781048 1.916732
 O39 -0.310097 -1.276866 2.974718
 O40 0.705993 -0.759485 1.135992
 H41 -3.563642 -0.718071 -0.814531
 O42 -4.511323 -1.059377 -0.627208
 N43 -5.078593 -0.214378 0.245729
 O44 -6.227622 -0.457534 0.533545
 O45 -4.402647 0.712647 0.667232

[(HEHN)₂NO₃]⁻

O1 -3.961389 -0.368885 0.046089
 C2 -3.405553 0.324171 1.137942
 C3 -2.870935 1.658777 0.650401
 N4 -1.800070 1.451243 -0.351788
 N5 -1.517921 2.679674 -1.048532
 H6 -3.594252 -1.275876 0.038367
 H7 -2.598528 -0.254284 1.601247
 H8 -4.170937 0.526693 1.900277
 H9 -2.436179 2.248391 1.461298
 H10 -3.653727 2.233265 0.150327
 H11 -2.107020 0.747517 -1.028430
 H12 -0.933891 1.082662 0.119056
 H13 -0.838965 2.445658 -1.780715
 H14 -0.995811 3.234209 -0.367167
 O15 3.430587 -0.305573 1.586528
 C16 2.574323 -1.390951 1.830183
 C17 2.391998 -2.219510 0.568206
 N18 1.647658 -1.467195 -0.462972
 N19 1.527958 -2.232836 -1.675478
 H20 2.947686 0.524198 1.759462
 H21 1.597156 -1.053417 2.196667
 H22 3.013060 -2.050686 2.592226

H23 1.817353 -3.127518 0.772758
 H24 3.356872 -2.485605 0.132016
 H25 2.122810 -0.579766 -0.724966
 H26 0.700179 -1.227152 -0.109060
 H27 0.796382 -2.918118 -1.472704
 H28 1.134954 -1.563307 -2.339760
 N29 1.242660 1.231137 -2.214522
 O30 0.263624 0.429624 -2.186450
 O31 2.383229 0.816106 -1.907822
 O32 1.057833 2.416970 -2.534162
 N33 -1.512857 -2.654115 0.021421
 O34 -0.721924 -3.592967 -0.186525
 O35 -2.740989 -2.859253 0.117572
 O36 -1.075291 -1.475637 0.139870
 N37 0.827280 1.939205 1.601279
 O38 1.894407 1.968327 2.236276
 O39 0.048094 2.910136 1.593610
 O40 0.521933 0.889704 0.956620

HNO₃

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

[(HEHN)(HNO₃)NO₃]⁻

O1 2.666645 -2.480012 0.316107
 C2 1.680337 -2.275566 1.294408
 C3 0.455983 -1.538833 0.772889
 N4 0.736897 -0.124376 0.416347
 N5 1.238484 0.630139 1.536096
 H6 3.189798 -1.660342 0.233172
 H7 2.078633 -1.746586 2.170452
 H8 1.341727 -3.261592 1.630528
 H9 -0.333938 -1.517774 1.527255
 H10 0.072879 -2.017296 -0.131312
 H11 -0.167152 0.316533 0.138988
 H12 1.407802 -0.039517 -0.390273
 H13 0.816195 1.555632 1.448482
 H14 2.246849 0.702148 1.386502
 N15 3.736755 0.516027 -0.955159
 O16 3.841246 0.040992 0.222688
 O17 4.715127 0.966787 -1.537355
 O18 2.597438 0.509808 -1.499476
 N19 -1.755749 2.309248 0.371078
 O20 -0.702453 2.812922 0.781218
 O21 -2.806492 2.929307 0.262787
 O22 -1.734018 1.054057 0.042192
 H23 -3.064572 0.429831 -0.327217

O24 -3.955430 -0.024997 -0.582290
 N25 -3.752241 -1.346800 -0.592550
 O26 -2.632454 -1.756887 -0.325815
 O27 -4.719003 -2.022517 -0.870185

HEHN

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 -0.120204 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

N1 2.217126 -0.278438 -0.058113
 H2 2.555479 0.648038 -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

[(HEHN)NO₃]⁻

O1 -1.930046 2.453198 -0.518864
 C2 -0.907453 2.416567 0.449947
 C3 0.353446 1.700097 -0.017862
 N4 0.227760 0.221589 0.040200
 N5 0.173226 -0.238402 1.402331
 H6 -2.318338 1.566000 -0.613061
 H7 -1.246919 1.960814 1.389550
 H8 -0.643102 3.457902 0.658651
 H9 1.215710 1.954853 0.603538

H10	0.571565	1.959937	-1.057554
H11	1.060926	-0.200481	-0.457136
H12	-0.667718	-0.077432	-0.418725
H13	1.134075	-0.498716	1.629132
H14	-0.436002	-1.057469	1.392277
N15	-2.860998	-1.218840	-0.142335
O16	-2.310930	-0.284800	-0.829781
O17	-2.131245	-1.928952	0.580237
O18	-4.074512	-1.391363	-0.218496
N19	3.419203	-0.514548	-0.220029
O20	4.601370	-0.692682	-0.511167
O21	3.074863	-0.153056	0.934542
O22	2.512939	-0.691593	-1.096514

**Cartesian coordinates for structures
in Figure S1, calculated at ω B97XD/
6-31+G(d,p)**

[(HEHN)NO₃]⁻_a

O1 -1.930046 2.453198 -0.518864
C2 -0.907453 2.416567 0.449947
C3 0.353446 1.700097 -0.017862
N4 0.227760 0.221589 0.040200
N5 0.173226 -0.238402 1.402331
H6 -2.318338 1.566000 -0.613061
H7 -1.246919 1.960814 1.389550
H8 -0.643102 3.457902 0.658651
H9 1.215710 1.954853 0.603538
H10 0.571565 1.959937 -1.057554
H11 1.060926 -0.200481 -0.457136
H12 -0.667718 -0.077432 -0.418725
H13 1.134075 -0.498716 1.629132
H14 -0.436002 -1.057469 1.392277
N15 -2.860998 -1.218840 -0.142335
O16 -2.310930 -0.284800 -0.829781
O17 -2.131245 -1.928952 0.580237
O18 -4.074512 -1.391363 -0.218496
N19 3.419203 -0.514548 -0.220029
O20 4.601370 -0.692682 -0.511167
O21 3.074863 -0.153056 0.934542
O22 2.512939 -0.691593 -1.096514

[(HEHN)NO₃]⁻_b

O1 2.479842 1.931973 -0.435205
C2 1.362448 2.486687 0.209318
C3 0.036291 1.980409 -0.338524
N4 -0.219862 0.551185 -0.039771
N5 -0.215648 0.288673 1.374190
H6 2.641444 1.046533 -0.055214
H7 1.392535 3.569168 0.041266
H8 1.391401 2.316979 1.293654
H9 0.010495 2.081569 -1.427298
H10 -0.797135 2.538387 0.097123
H11 0.465334 -0.081772 -0.517764
H12 -1.197428 0.332966 -0.401979
H13 0.661150 -0.196102 1.567608
H14 -1.010977 -0.334242 1.529257
N15 2.487508 -1.477074 -0.147026
O16 3.291914 -2.400788 -0.204746
O17 2.594736 -0.577659 0.749159
O18 1.532861 -1.389636 -0.966411
N19 -3.419200 -0.464505 -0.084537
O20 -4.616428 -0.654251 -0.294819
O21 -2.748041 0.280100 -0.875195

O22 -2.832239 -0.985243 0.893290
O22 2.512939 -0.691593 -1.096514

[(HEHN)NO₃]⁻_c

O1 -1.843542 2.158133 -0.747335
C2 -0.897858 2.351290 0.272853
C3 0.421742 1.676133 -0.065051
N4 0.308359 0.199448 -0.017218
N5 0.227316 -0.272014 1.340660
H6 -2.423341 1.406636 -0.498317
H7 -1.260645 1.973833 1.237663
H8 -0.709709 3.426791 0.377839
H9 1.222893 1.949980 0.625815
H10 0.721810 1.932337 -1.084796
H11 1.158077 -0.217923 -0.492230
H12 -0.565956 -0.136165 -0.480473
H13 -0.307041 -1.136934 1.298703
H14 1.195851 -0.475701 1.598821
N15 -3.027228 -1.095695 -0.089433
O16 -3.809358 -2.024139 0.107908
O17 -3.361586 0.093372 0.156444
O18 -1.863687 -1.327031 -0.540363
N19 3.510836 -0.514727 -0.134450
O20 3.121293 -0.139180 1.001915
O21 4.703991 -0.684354 -0.379086
O22 2.639111 -0.715111 -1.040327

[(HEHN)NO₃]⁻_d

O1 0.565437 3.124691 -0.663763
C2 0.721594 2.549437 0.614730
C3 -0.335578 1.495585 0.925443
N4 -0.077713 0.222549 0.214700
N5 -0.019094 0.409967 -1.214532
H6 0.466687 2.371826 -1.271330
H7 0.625311 3.359077 1.344785
H8 1.719665 2.103016 0.736941
H9 -1.331840 1.839924 0.635186
H10 -0.337355 1.251169 1.992074
H11 -0.851938 -0.456992 0.458246
H12 0.865958 -0.159372 0.519070
H13 0.653834 -0.288298 -1.539669
H14 -0.961794 0.189602 -1.545016
N15 -3.171219 -0.875150 0.038721
O16 -2.877849 -0.056012 -0.870411
O17 -4.325564 -1.268693 0.198746
O18 -2.243358 -1.291850 0.804116
N19 2.942724 -1.198059 0.005492
O20 2.392223 -0.545777 0.954780
O21 2.288813 -1.390727 -1.048001
O22 4.089358 -1.621038 0.139282

[(HEHN)NO₃]⁻_e

O1 -1.834801 2.369011 -0.422513
 C2 -0.533962 2.424341 0.111446
 C3 -0.249591 1.373468 1.184911
 N4 0.186735 0.092120 0.582438
 N5 0.375241 -0.923056 1.581419
 H6 -1.990782 1.494749 -0.821928
 H7 -0.437321 3.410530 0.574509
 H8 0.234521 2.359413 -0.674043
 H9 -1.147573 1.177354 1.775458
 H10 0.558971 1.689512 1.848457
 H11 1.124384 0.255782 0.109253
 H12 -0.525930 -0.206217 -0.124846
 H13 -0.471790 -1.490158 1.548899
 H14 1.175292 -1.466614 1.252052
 N15 -2.797158 -1.024873 -0.397469
 O16 -1.949536 -0.365249 -1.099702
 O17 -3.935120 -1.199205 -0.822753
 O18 -2.426414 -1.471504 0.710998
 N19 3.339197 -0.386395 -0.408254
 O20 2.846887 -1.451423 0.035049
 O21 4.496911 -0.331617 -0.820057
 O22 2.608753 0.660517 -0.427633

[(HEHN)NO₃]⁻_f

O1 -1.401932 -2.394556 -0.215364
 C2 -0.065769 -2.028160 -0.464654
 C3 0.110228 -0.623559 -1.039560
 N4 0.143845 0.396998 0.046926
 N5 0.237490 1.757826 -0.372439
 H6 -1.829984 -1.722668 0.343950
 H7 0.313371 -2.741895 -1.201518
 H8 0.561545 -2.130247 0.434494
 H9 -0.722657 -0.371841 -1.700778
 H10 1.065007 -0.530997 -1.563437
 H11 1.007169 0.210801 0.624761
 H12 -0.734522 0.312750 0.607219
 H13 1.107225 1.829627 -0.898380
 H14 -0.584242 1.940944 -0.943644
 N15 3.411387 0.214919 0.273044
 O16 2.561590 -0.148556 1.148082
 O17 2.994529 0.741929 -0.790728
 O18 4.613316 0.042471 0.473673
 N19 -3.153656 0.543982 0.274352
 O20 -2.653401 1.115956 -0.719417
 O21 -4.361479 0.553831 0.492017
 O22 -2.368013 -0.071355 1.082915

[(HEHN)NO₃]⁻_g

O1 1.563618 2.629495 -0.047113

C2 0.171637 2.415182 -0.031891
 C3 -0.283100 1.389164 1.003957
 N4 -0.137423 0.005262 0.491621
 N5 -0.231377 -0.966061 1.545113
 H6 2.017059 1.832810 -0.371525
 H7 -0.209872 2.132517 -1.024676
 H8 -0.283122 3.375971 0.225440
 H9 -1.339206 1.517764 1.257437
 H10 0.320372 1.466202 1.910082
 H11 0.793243 -0.098364 0.012188
 H12 -0.901422 -0.153889 -0.222906
 H13 0.439124 -1.694940 1.306904
 H14 -1.189496 -1.315436 1.506122
 N15 2.978745 -0.945025 -0.348589
 O16 2.421520 -1.814248 0.354242
 O17 4.174766 -0.988706 -0.622083
 O18 2.258482 0.016831 -0.798734
 N19 -3.263000 -0.496546 -0.430048
 O20 -3.059870 -0.710619 0.792382
 O21 -4.397873 -0.512984 -0.905415
 O22 -2.261457 -0.253784 -1.178047

[(HEHN)NO₃]⁻_h

O1 -1.593825 2.360626 -0.429197
 C2 -0.195662 2.239037 -0.449804
 C3 0.366872 1.588620 0.809401
 N4 0.153169 0.124380 0.791751
 N5 0.593330 -0.474718 2.024624
 H6 -1.994639 1.505037 -0.683003
 H7 0.218887 3.250979 -0.508652
 H8 0.155343 1.690960 -1.336608
 H9 -0.126755 1.981045 1.700444
 H10 1.447504 1.740757 0.885849
 H11 0.713126 -0.273188 -0.007253
 H12 -0.866643 -0.128296 0.691922
 H13 0.124101 -1.375448 2.077364
 H14 1.596278 -0.632424 1.886659
 N15 -2.942578 -0.917761 -0.251491
 O16 -2.556874 -0.121616 -1.149074
 O17 -2.310943 -0.936923 0.851598
 O18 -3.900799 -1.663990 -0.429409
 N19 3.111723 -0.613604 -0.506542
 O20 1.969922 -0.773920 -1.040116
 O21 3.170223 -0.261723 0.702847
 O22 4.134299 -0.796635 -1.165736

[(HEHN)NO₃]⁻_i

O1 1.210784 2.826911 0.338892
 C2 -0.143764 2.441774 0.270489
 C3 -0.467037 1.538705 -0.915802

N4 -0.057363 0.144327 -0.632658
N5 -0.159493 -0.692635 -1.795728
H6 1.773204 2.064585 0.537527
H7 -0.713483 3.367896 0.155765
H8 -0.482071 1.962083 1.200369
H9 0.066021 1.865141 -1.810832
H10 -1.542197 1.513009 -1.113361
H11 -0.684971 -0.213518 0.135896
H12 0.943426 0.128762 -0.308582
H13 -1.117520 -1.047684 -1.775566
H14 0.494721 -1.454892 -1.618751
N15 2.933999 -0.964509 0.279202
O16 2.477662 0.226362 0.380752
O17 2.250315 -1.805549 -0.345829
O18 4.015259 -1.248368 0.787899
N19 -3.040191 -0.696565 0.460312
O20 -2.938345 -0.653718 -0.793971
O21 -1.986321 -0.566638 1.159987
O22 -4.130729 -0.854324 1.008709

**Cartesian coordinates for structures
in Figure S3, calculated at ω B97XD/
6-31+G(d,p)**

$[(\text{HEHN})_2\text{NO}_3]^-$ _a

O1 -3.961389 -0.368885 0.046089
C2 -3.405553 0.324171 1.137942
C3 -2.870935 1.658777 0.650401
N4 -1.800070 1.451243 -0.351788
N5 -1.517921 2.679674 -1.048532
H6 -3.594252 -1.275876 0.038367
H7 -2.598528 -0.254284 1.601247
H8 -4.170937 0.526693 1.900277
H9 -2.436179 2.248391 1.461298
H10 -3.653727 2.233265 0.150327
H11 -2.107020 0.747517 -1.028430
H12 -0.933891 1.082662 0.119056
H13 -0.838965 2.445658 -1.780715
H14 -0.995811 3.234209 -0.367167
O15 3.430587 -0.305573 1.586528
C16 2.574323 -1.390951 1.830183
C17 2.391998 -2.219510 0.568206
N18 1.647658 -1.467195 -0.462972
N19 1.527958 -2.232836 -1.675478
H20 2.947686 0.524198 1.759462
H21 1.597156 -1.053417 2.196667
H22 3.013060 -2.050686 2.592226
H23 1.817353 -3.127518 0.772758
H24 3.356872 -2.485605 0.132016
H25 2.122810 -0.579766 -0.724966
H26 0.700179 -1.227152 -0.109060
H27 0.796382 -2.918118 -1.472704
H28 1.134954 -1.563307 -2.339760
N29 1.242660 1.231137 -2.214522
O30 0.263624 0.429624 -2.186450
O31 2.383229 0.816106 -1.907822
O32 1.057833 2.416970 -2.534162
N33 -1.512857 -2.654115 0.021421
O34 -0.721924 -3.592967 -0.186525
O35 -2.740989 -2.859253 0.117572
O36 -1.075291 -1.475637 0.139870
N37 0.827280 1.939205 1.601279
O38 1.894407 1.968327 2.236276
O39 0.048094 2.910136 1.593610
O40 0.521933 0.889704 0.956620

$[(\text{HEHN})_2\text{NO}_3]^-$ _b

O1 2.843392 3.199237 -0.417047
C2 3.044000 1.909487 -0.948380
C3 3.285490 0.847155 0.117556

N4 2.020581 0.377265 0.737093
N5 2.300185 -0.486657 1.854128
H6 1.978424 3.221174 0.025238
H7 3.945984 1.965026 -1.564797
H8 2.211356 1.602672 -1.595250
H9 3.914387 1.237582 0.920078
H10 3.746179 -0.043670 -0.317480
H11 1.473130 -0.120237 -0.005560
H12 1.454700 1.179852 1.059403
H13 2.626560 -1.354039 1.423611
H14 1.392182 -0.707575 2.270065
O15 -3.598365 1.800307 -1.047519
C16 -3.828683 0.810585 -0.073268
C17 -3.478105 -0.559358 -0.629384
N18 -2.036452 -0.622499 -0.953414
N19 -1.726448 -1.816273 -1.698164
H20 -2.894414 2.386271 -0.708462
H21 -4.890476 0.798588 0.204921
H22 -3.246576 1.008310 0.836011
H23 -4.019725 -0.757052 -1.556940
H24 -3.672367 -1.349879 0.099720
H25 -1.475779 -0.560506 -0.056636
H26 -1.781835 0.198967 -1.511860
H27 -1.814026 -2.568191 -1.013023
H28 -0.720840 -1.750606 -1.893901
N29 -0.903523 -1.757784 1.887512
O30 -0.213748 -2.134416 2.839272
O31 -0.683173 -0.603864 1.382713
O32 -1.804582 -2.465624 1.395973
N33 1.739909 -2.243286 -1.299784
O34 2.753037 -2.299012 -0.572382
O35 1.363938 -3.202494 -1.976629
O36 1.072225 -1.152961 -1.340066
N37 -0.523439 2.524248 0.214137
O38 0.429277 2.787381 0.999050
O39 -1.625051 3.080413 0.375858
O40 -0.344295 1.708659 -0.714827

$[(\text{HEHN})_2\text{NO}_3]^-$ _c

O1 1.713300 -3.201246 1.111820
C2 2.705260 -2.205162 1.069010
C3 2.980447 -1.663670 -0.329326
N4 1.843018 -0.862502 -0.842425
N5 2.222895 -0.145135 -2.031174
H6 0.842395 -2.776490 1.023838
H7 3.633126 -2.664097 1.425373
H8 2.467295 -1.367988 1.738693
H9 3.165793 -2.466474 -1.045915
H10 3.839265 -0.988916 -0.294345
H11 1.532273 -0.208156 -0.086083

H12	1.045952	-1.485975	-1.083086	H20	-3.982489	1.109041	0.164996
H13	1.357548	0.263604	-2.391042	H21	-2.987366	0.440152	-1.566633
H14	2.776532	0.640361	-1.685367	H22	-4.427459	-0.508570	-1.976817
N15	2.390849	1.733725	1.159880	H23	-2.554020	-2.056003	-1.643417
O16	1.430543	0.890350	1.250528	H24	-3.727427	-2.258070	-0.303970
O17	3.305294	1.502942	0.341967	H25	-2.300501	-0.662283	0.921943
O18	2.384326	2.733837	1.876484	H26	-1.167535	-0.798397	-0.276870
O19	-3.858977	-1.064492	1.142838	H27	-0.996936	-3.019673	0.075178
C20	-3.922492	0.018095	0.244447	H28	-0.759817	-2.236389	1.477932
C21	-3.224383	1.227862	0.842073	N29	0.565011	-1.065344	-1.943983
N22	-1.792342	0.928978	1.062403	O30	1.598904	-0.863208	-2.600623
N23	-1.160002	1.979162	1.821559	O31	-0.051484	-2.137843	-2.011078
H24	-3.343869	-1.771621	0.709537	O32	0.121601	-0.141155	-1.183653
H25	-4.969310	0.289469	0.056797	N33	1.810454	-1.936256	1.676243
H26	-3.464924	-0.241539	-0.718410	O34	1.764843	-3.164108	1.723642
H27	-3.648366	1.487005	1.814623	O35	0.809419	-1.237761	2.007579
H28	-3.266412	2.087367	0.168408	O36	2.854151	-1.337501	1.285024
H29	-1.316045	0.786018	0.124355	N37	-1.857046	2.323414	0.750113
H30	-1.712072	0.044403	1.574773	O38	-2.959890	2.545603	0.196999
H31	-1.142107	2.770583	1.176059	O39	-0.961453	3.188208	0.731731
H32	-0.176100	1.691417	1.903873	O40	-1.655335	1.222124	1.322966
N33	-0.561931	1.924833	-1.780522				
O34	-0.586120	0.726998	-1.333137				
O35	-1.250946	2.792408	-1.206783				
O36	0.141980	2.182596	-2.759519				
N37	-1.155488	-2.318629	-0.475420				
O38	-2.366169	-2.580506	-0.593992				
O39	-0.359632	-2.550176	-1.404501				
O40	-0.723967	-1.812053	0.603119				

[(HEHN)₂NO₃]⁻_d

O1	2.757604	1.638067	-2.281563
C2	3.602724	1.424155	-1.181349
C3	3.021152	1.991521	0.108323
N4	1.926826	1.143991	0.630031
N5	1.364236	1.698085	1.832254
H6	2.261325	0.817685	-2.460890
H7	4.551112	1.942365	-1.367625
H8	3.830790	0.357011	-1.048414
H9	2.614176	2.989813	-0.068476
H10	3.771208	2.042513	0.901383
H11	2.317784	0.198623	0.887956
H12	1.217702	0.956437	-0.101522
H13	0.894714	0.905233	2.271300
H14	0.616483	2.334600	1.535171
O15	-4.405226	0.254979	-0.066839
C16	-3.719145	-0.276954	-1.170595
C17	-3.024382	-1.573394	-0.782873
N18	-1.950813	-1.307810	0.200855
N19	-1.492799	-2.525408	0.817952

**Cartesian coordinates for structures
in Figure S4, calculated at ω B97XD/
6-31+G(d,p)**

[(HEHN)₃NO₃]⁻_a

O1 -3.325544 -3.339695 1.256350
C2 -4.029700 -2.366116 0.523603
C3 -3.588489 -2.275076 -0.930436
N4 -2.263050 -1.624986 -1.081137
N5 -1.903466 -1.550230 -2.471918
H6 -2.497076 -2.933860 1.561617
H7 -3.962305 -1.375510 0.992175
H8 -5.084357 -2.660160 0.522137
H9 -4.287586 -1.658041 -1.500174
H10 -3.509627 -3.265321 -1.382554
H11 -1.510720 -2.156364 -0.597394
H12 -2.305450 -0.685394 -0.637841
H13 -0.917366 -1.271908 -2.489073
H14 -2.431921 -0.753417 -2.828389
O15 3.974520 0.844032 -2.928468
C16 4.587675 0.699668 -1.671243
C17 4.509000 -0.730888 -1.155252
N18 3.105287 -1.109552 -0.879634
N19 3.015196 -2.458337 -0.383145
H20 3.053375 1.126381 -2.781987
H21 4.150224 1.383606 -0.931363
H22 5.648086 0.953816 -1.775632
H23 5.048618 -0.831048 -0.210918
H24 4.896041 -1.441198 -1.888661
H25 2.533526 -1.038286 -1.736945
H26 2.683219 -0.435807 -0.185166
H27 3.284273 -2.385929 0.599456
H28 2.014171 -2.679836 -0.358145
O29 -2.005591 4.103671 0.855074
C30 -0.655106 3.797545 0.604419
C31 -0.102411 2.923769 1.719558
N32 -0.645876 1.542516 1.630936
N33 -0.601252 0.883394 2.908853
H34 -2.572081 3.631164 0.215983
H35 -0.071774 4.726396 0.593350
H36 -0.516516 3.304646 -0.365950
H37 -0.415190 3.315380 2.689246
H38 0.985242 2.832291 1.684220
H39 -0.101480 1.040738 0.912476
H40 -1.624219 1.561009 1.295529
H41 0.390449 0.876601 3.167089
H42 -0.850442 -0.092505 2.724706
N43 2.712569 0.313205 2.038173
O44 3.753576 -0.352483 1.911609
O45 2.407553 0.861839 3.104694

O46 1.942060 0.445262 1.027341
N47 0.667054 0.661889 -1.804413
O48 -0.367626 0.780154 -1.122059
O49 0.877622 -0.412051 -2.437592
O50 1.502515 1.584894 -1.859706
N51 -3.392411 1.491171 -0.980083
O52 -2.968549 0.924921 0.075017
O53 -3.441777 2.730668 -1.041742
O54 -3.758098 0.788198 -1.937894
N55 0.019016 -2.263340 1.305952
O56 0.054710 -2.699586 0.118976
O57 1.009438 -2.307167 2.026733
O58 -1.073109 -1.775279 1.724571

[(HEHN)₃NO₃]⁻_b

O1 1.922446 2.978000 -1.955797
C2 0.735309 2.320229 -2.325937
C3 -0.497907 2.949278 -1.693809
N4 -0.562104 2.696024 -0.233847
N5 -1.685769 3.380310 0.352944
H6 2.240974 2.570919 -1.131661
H7 0.777981 1.246769 -2.098075
H8 0.625455 2.411413 -3.410835
H9 -1.412089 2.529975 -2.118394
H10 -0.487239 4.033397 -1.822590
H11 0.289389 3.046220 0.240085
H12 -0.606578 1.677099 -0.035904
H13 -2.507647 3.007058 -0.134619
H14 -1.736694 3.008637 1.302561
O15 4.420589 -2.183788 -1.294326
C16 4.642203 -1.075919 -0.458045
C17 4.043441 -1.280330 0.926113
N18 2.562643 -1.206777 0.899072
N19 2.020863 -1.590938 2.176753
H20 3.621480 -2.007468 -1.821897
H21 4.254911 -0.148784 -0.900590
H22 5.723278 -0.954114 -0.329723
H23 4.373113 -0.498153 1.616060
H24 4.306039 -2.263288 1.321240
H25 2.161953 -1.833475 0.176372
H26 2.304654 -0.228371 0.637729
H27 1.004426 -1.509298 2.094873
H28 2.279188 -0.827668 2.803722
O29 -3.340413 -2.271266 2.757918
C30 -3.295564 -1.963176 1.383961
C31 -2.089511 -2.644459 0.732461
N32 -1.778741 -2.086756 -0.602879
N33 -2.639598 -2.588283 -1.642419
H34 -2.622161 -1.775245 3.179573
H35 -3.239678 -0.878458 1.218255

H36 -4.229485 -2.313918 0.938524
H37 -2.240955 -3.718195 0.612221
H38 -1.209890 -2.460569 1.352656
H39 -0.796468 -2.329808 -0.839928
H40 -1.838460 -1.040912 -0.587871
H41 -3.418828 -1.924055 -1.685578
H42 -2.100235 -2.464358 -2.498472
N43 2.225665 2.026787 1.484615
O44 2.668084 1.438149 2.479062
O45 1.638670 3.117372 1.567440
O46 2.369845 1.491783 0.332423
N47 1.034896 -1.787797 -2.221920
O48 2.125039 -1.296007 -2.562698
O49 0.026096 -1.681294 -2.928257
O50 0.951905 -2.408075 -1.107770
N51 -3.567963 0.802577 -1.161203
O52 -2.337583 0.570176 -0.935965
O53 -4.347471 -0.150809 -1.339792
O54 -3.957938 1.979626 -1.193435
N55 -0.882184 0.193420 2.157284
O56 -0.235135 0.135627 1.068895
O57 -0.818546 -0.786983 2.939537
O58 -1.565365 1.185106 2.432142

[(HEHN)₃NO₃]⁻_c

O1 -4.599900 -0.835842 -2.457939
C2 -3.332095 -1.420002 -2.623597
C3 -2.973256 -2.393678 -1.507718
N4 -2.797670 -1.690650 -0.212768
N5 -2.479020 -2.618988 0.841991
H6 -4.506207 -0.071460 -1.862098
H7 -2.542602 -0.662725 -2.710908
H8 -3.350072 -1.991135 -3.557480
H9 -2.022547 -2.889255 -1.721621
H10 -3.758327 -3.137792 -1.360521
H11 -3.677444 -1.212093 0.060287
H12 -2.073007 -0.954727 -0.337424
H13 -2.340663 -2.030074 1.664878
H14 -1.550806 -2.981966 0.611791
O15 5.984030 0.292793 -0.838494
C16 5.470836 -0.995421 -0.624591
C17 4.828846 -1.145292 0.748361
N18 3.559034 -0.392318 0.836497
N19 3.010007 -0.466242 2.164462
H20 5.268832 0.836561 -1.224238
H21 6.303355 -1.705905 -0.674347
H22 4.749284 -1.276841 -1.404819
H23 5.486435 -0.758806 1.529196
H24 4.584507 -2.191757 0.951469
H25 2.874904 -0.770279 0.142425

H26 3.672046 0.616802 0.590390
H27 2.573228 -1.386149 2.233330
H28 2.228856 0.195473 2.199721
O29 -0.745112 0.029672 -1.081458
C30 -0.543204 1.329143 -1.603213
C31 -0.359656 2.363211 -0.501190
N32 -1.511162 2.283928 0.428552
N33 -1.453539 3.284255 1.457719
H34 0.103736 -0.460612 -0.985267
H35 -1.429373 1.574363 -2.201136
H36 0.334192 1.369420 -2.255982
H37 -0.313852 3.374186 -0.908204
H38 0.547042 2.180298 0.079047
H39 -1.547159 1.333719 0.867887
H40 -2.400973 2.382810 -0.083069
H41 -0.731254 2.948263 2.096671
H42 -2.346452 3.201620 1.943424
N43 -4.367684 1.090773 0.494047
O44 -4.333356 2.049578 1.274988
O45 -4.873331 -0.002929 0.809893
O46 -3.845346 1.214752 -0.665232
N47 -0.422609 -0.157692 2.270338
O48 -1.636031 -0.016020 1.926926
O49 0.004109 -1.270590 2.587502
O50 0.319258 0.854990 2.266607
N51 3.026137 2.214853 -1.253883
O52 3.734318 1.410703 -1.913942
O53 2.285041 3.017937 -1.827465
O54 3.069357 2.177641 0.010833
N55 1.236032 -2.542561 -0.213383
O56 0.154247 -3.079333 -0.495154
O57 1.478164 -1.368832 -0.664578
O58 2.094405 -3.099171 0.479172

[(HEHN)₃NO₃]⁻_d

O1 -5.746735 -0.269658 -0.894135
C2 -4.703598 -0.627461 -1.768558
C3 -3.943263 -1.863777 -1.300370
N4 -3.069624 -1.548413 -0.143553
N5 -2.529424 -2.748683 0.440804
H6 -5.366610 0.137846 -0.096676
H7 -4.002020 0.201545 -1.923595
H8 -5.164879 -0.869777 -2.730528
H9 -3.284738 -2.245022 -2.086266
H10 -4.631702 -2.647338 -0.978589
H11 -3.603693 -1.028354 0.578308
H12 -2.319544 -0.906876 -0.489316
H13 -2.060314 -2.437618 1.292611
H14 -1.775504 -3.018992 -0.193998
O15 3.208097 -2.153165 2.724080

C16 4.015735 -2.727145 1.728153
 C17 4.338571 -1.773032 0.586395
 N18 3.153082 -1.419365 -0.226461
 N19 2.535130 -2.572305 -0.823742
 H20 2.278680 -2.175163 2.439348
 H21 3.575001 -3.648483 1.323622
 H22 4.964554 -3.000532 2.201095
 H23 5.062359 -2.227435 -0.095445
 H24 4.733739 -0.829781 0.972126
 H25 3.475343 -0.764328 -0.987288
 H26 2.469781 -0.865790 0.331179
 H27 1.799959 -2.868351 -0.181174
 H28 2.040567 -2.216370 -1.644054
 O29 2.150858 3.834449 0.688478
 C30 1.214386 3.324463 1.605415
 C31 -0.188825 3.199973 1.027982
 N32 -0.295330 2.148772 -0.018790
 N33 0.095549 2.605987 -1.326967
 H34 2.626429 3.083443 0.284395
 H35 1.150237 4.020344 2.450501
 H36 1.533836 2.350976 2.002084
 H37 -0.511562 4.133224 0.561746
 H38 -0.903864 2.919911 1.806643
 H39 -1.295566 1.871103 -0.073269
 H40 0.225422 1.305277 0.289028
 H41 1.075293 2.884858 -1.275881
 H42 0.044938 1.777424 -1.920047
 N43 -3.476007 1.313216 1.294134
 O44 -4.330288 0.398650 1.504691
 O45 -2.998939 1.408576 0.128444
 O46 -3.130206 2.072618 2.193137
 N47 -0.213675 -1.007546 -1.848480
 O48 -1.103536 -0.167947 -1.532024
 O49 -0.428979 -2.228850 -1.671559
 O50 0.862639 -0.610944 -2.320253
 N51 0.181264 -0.992939 1.507752
 O52 0.552362 -2.179195 1.690536
 O53 1.009724 -0.160016 1.039551
 O54 -0.970285 -0.634438 1.770915
 N55 3.425343 1.462865 -1.551152
 O56 3.122986 1.451958 -0.320043
 O57 3.972825 0.436785 -2.036827
 O58 3.182185 2.448051 -2.246924

[(HEHN)₃NO₃]⁻_e

O1 -4.652432 -2.226885 1.442118
 C2 -3.395703 -2.851459 1.413600
 C3 -2.851395 -3.095978 0.004467
 N4 -1.951817 -1.997839 -0.429888
 N5 -1.713561 -2.041049 -1.848978

H6 -4.642071 -1.390351 0.942378
 H7 -3.528079 -3.820098 1.902790
 H8 -2.649179 -2.294518 2.002736
 H9 -3.667475 -3.147705 -0.718486
 H10 -2.254027 -4.009175 -0.048230
 H11 -1.057322 -2.080020 0.104319
 H12 -2.369003 -1.069825 -0.202695
 H13 -1.202669 -1.175551 -2.043541
 H14 -1.048173 -2.803957 -1.979636
 O15 4.182013 -0.964681 -1.905908
 C16 4.461982 0.023726 -0.946014
 C17 4.418025 -0.525794 0.474131
 N18 3.049638 -0.983327 0.812171
 N19 2.971029 -1.450464 2.168855
 H20 3.222495 -0.960226 -2.067147
 H21 3.773953 0.873581 -1.043290
 H22 5.478247 0.392717 -1.122434
 H23 4.682496 0.247022 1.199684
 H24 5.074253 -1.390366 0.590592
 H25 2.784505 -1.797824 0.220263
 H26 2.371848 -0.211256 0.659458
 H27 2.909350 -0.602051 2.733563
 H28 2.076793 -1.940539 2.214186
 O29 0.671600 3.846531 -1.723837
 C30 -0.733252 3.845827 -1.720995
 C31 -1.284318 3.904223 -0.304586
 N32 -1.055377 2.628788 0.416213
 N33 -1.488644 2.723058 1.783899
 H34 1.003494 2.943937 -1.892057
 H35 -1.139624 2.971490 -2.244422
 H36 -1.086246 4.743822 -2.242454
 H37 -2.363386 4.067296 -0.291477
 H38 -0.778890 4.685471 0.266916
 H39 -0.063577 2.322703 0.382156
 H40 -1.612428 1.867658 -0.012809
 H41 -0.635440 2.833325 2.335391
 H42 -1.918935 1.826698 1.998106
 N43 0.965403 -3.377442 -0.048839
 O44 2.197389 -3.445210 -0.205688
 O45 0.496509 -2.550277 0.797554
 O46 0.189099 -4.092307 -0.701675
 N47 -3.941294 0.891484 -0.152331
 O48 -2.823242 0.489333 0.341595
 O49 -4.024687 2.044275 -0.574220
 O50 -4.890137 0.092689 -0.184297
 N51 0.901759 0.363973 -1.819830
 O52 1.673621 1.302935 -2.101694
 O53 1.345986 -0.803925 -1.728285
 O54 -0.317977 0.582084 -1.628712
 N55 1.891533 1.932224 2.076072

O56 1.348969 2.965636 2.498773
O57 2.935129 1.490838 2.587796
O58 1.361458 1.305042 1.102870

**Cartesian coordinates for structures
in Figure S9, calculated at ω B97XD/
6-31+G(d,p)**

$[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-_{\text{a}}$

O1 2.666645 -2.480012 0.316107
C2 1.680337 -2.275566 1.294408
C3 0.455983 -1.538833 0.772889
N4 0.736897 -0.124376 0.416347
N5 1.238484 0.630139 1.536096
H6 3.189798 -1.660342 0.233172
H7 2.078633 -1.746586 2.170452
H8 1.341727 -3.261592 1.630528
H9 -0.333938 -1.517774 1.527255
H10 0.072879 -2.017296 -0.131312
H11 -0.167152 0.316533 0.138988
H12 1.407802 -0.039517 -0.390273
H13 0.816195 1.555632 1.448482
H14 2.246849 0.702148 1.386502
N15 3.736755 0.516027 -0.955159
O16 3.841246 0.040992 0.222688
O17 4.715127 0.966787 -1.537355
O18 2.597438 0.509808 -1.499476
N19 -1.755749 2.309248 0.371078
O20 -0.702453 2.812922 0.781218
O21 -2.806492 2.929307 0.262787
O22 -1.734018 1.054057 0.042192
H23 -3.064572 0.429831 -0.327217
O24 -3.955430 -0.024997 -0.582290
N25 -3.752241 -1.346800 -0.592550
O26 -2.632454 -1.756887 -0.325815
O27 -4.719003 -2.022517 -0.870185

$[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-_{\text{b}}$

O1 -2.330813 -2.440696 -1.254444
C2 -1.160355 -2.299018 -0.481698
C3 -0.372716 -1.032647 -0.789268
N4 -0.988867 0.177751 -0.178734
N5 -0.870375 0.157884 1.253544
H6 -3.002354 -1.806426 -0.953956
H7 -0.520285 -3.150758 -0.728694
H8 -1.370415 -2.337261 0.595134
H9 -0.340743 -0.860739 -1.868679
H10 0.649052 -1.092012 -0.406498
H11 -2.023172 0.203269 -0.393190
H12 -0.525398 1.021387 -0.574574
H13 -1.691609 0.654979 1.602865
H14 -0.017498 0.673226 1.464462
N15 -4.294373 0.410961 0.485411
O16 -3.659058 1.110917 1.302704

O17 -3.655272 -0.086335 -0.512004
O18 -5.495444 0.194797 0.601961
N19 1.742463 1.993100 -0.660796
O20 2.795104 2.422475 -1.113720
O21 0.634612 2.241856 -1.183365
O22 1.748210 1.254204 0.390442
H23 3.078190 0.606544 0.705650
O24 3.940990 0.161811 1.055515
N25 4.051487 -1.045508 0.487783
O26 3.169954 -1.402945 -0.277189
O27 5.036756 -1.678777 0.799203

$[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-_{\text{c}}$

O1 1.810503 -2.585158 -0.595097
C2 0.564794 -2.149061 -0.105101
C3 0.660452 -1.163298 1.058062
N4 0.863004 0.224243 0.568754
N5 1.118008 1.138407 1.650429
H6 2.312154 -1.827646 -0.941794
H7 0.044017 -3.038904 0.255616
H8 -0.061249 -1.719098 -0.901556
H9 1.510065 -1.411691 1.697688
H10 -0.258730 -1.154867 1.646790
H11 -0.016330 0.539244 0.106256
H12 1.658645 0.232261 -0.121226
H13 2.136471 1.198789 1.699790
H14 0.749778 2.035058 1.331890
N15 4.055327 0.107899 -0.346008
O16 3.017503 -0.066237 -1.083346
O17 5.170845 -0.093914 -0.811361
O18 3.884526 0.481152 0.836322
N19 -1.664203 2.382421 -0.308716
O20 -2.717831 2.940046 -0.588883
O21 -0.626230 2.987843 -0.009395
O22 -1.616761 1.085819 -0.322535
H23 -2.953609 0.373842 -0.417668
O24 -3.854492 -0.125259 -0.481163
N25 -3.680842 -1.356915 0.009939
O26 -2.564938 -1.667085 0.399750
O27 -4.667094 -2.060360 0.018917

$[(\text{HEHN})(\text{HNO}_3)\text{NO}_3]^-_{\text{d}}$

O1 0.972081 -2.860024 -0.304844
C2 1.556643 -2.143960 0.755838
C3 1.018996 -0.718061 0.855253
N4 1.101559 -0.079467 -0.483341
N5 0.601206 1.254811 -0.585114
H6 0.008432 -2.916800 -0.156556
H7 2.632270 -2.113600 0.558403
H8 1.400138 -2.637240 1.725803

H9 1.619808 -0.109569 1.535007
 H10 -0.030290 -0.699760 1.160372
 H11 0.574078 -0.663623 -1.138869
 H12 2.129910 -0.038383 -0.764780
 H13 -0.326288 1.273272 -0.162164
 H14 1.248291 1.822540 -0.038055
 N15 4.137203 0.983336 -0.049307
 O16 5.333854 1.245148 0.042513
 O17 3.280712 1.547042 0.678362
 O18 3.738370 0.114930 -0.894871
 N19 -2.240369 -1.658881 -0.175702
 O20 -3.405713 -1.315299 0.179720
 O21 -1.762348 -2.715113 0.275923
 O22 -1.598437 -0.935109 -0.958031
 H23 -3.676047 0.105451 -0.139231
 O24 -4.008396 1.071357 -0.348448
 N25 -3.143402 1.939865 0.171920
 O26 -2.207302 1.497378 0.827551
 O27 -3.371261 3.108713 -0.047332

[(HEHN)(HNO₃)NO₃]⁻_e

O1 -0.682364 -2.544322 1.314114
 C2 -1.705727 -2.433153 0.356298
 C3 -1.328612 -1.532494 -0.813722
 N4 -0.844304 -0.226106 -0.309889
 N5 -0.585469 0.670515 -1.405538
 H6 0.156717 -2.756031 0.867050
 H7 -2.575298 -2.017623 0.874316
 H8 -1.992834 -3.411922 -0.057427
 H9 -2.199244 -1.329814 -1.441320
 H10 -0.523671 -1.955846 -1.418457
 H11 0.051107 -0.386981 0.180544
 H12 -1.579957 0.184155 0.334499
 H13 0.021311 1.398764 -1.033504
 H14 -1.500962 1.080378 -1.608356
 N15 -3.817679 1.056976 0.116590
 O16 -3.488893 0.900921 -1.089546
 O17 -4.950868 1.415371 0.429372
 O18 -2.948178 0.828857 1.017768
 N19 2.427818 -1.815293 -0.130021
 O20 3.608733 -1.827242 -0.453945
 O21 1.893992 -0.710202 0.266703
 O22 1.709227 -2.830082 -0.165992
 H23 2.811036 0.472868 0.209130
 O24 3.436515 1.301215 0.199486
 N25 2.679453 2.397365 0.239584
 O26 1.462072 2.256338 0.264687
 O27 3.274649 3.450613 0.250228

[(HEHN)(HNO₃)NO₃]⁻_f

O1 -0.218715 -1.728594 -1.356456
 C2 0.747023 -2.155568 -0.422668
 C3 0.854518 -1.218854 0.773303
 N4 1.084581 0.165787 0.305771
 N5 1.279695 1.055223 1.418637
 H6 -1.081711 -1.689017 -0.920411
 H7 1.700150 -2.182977 -0.958504
 H8 0.537065 -3.167171 -0.046768
 H9 1.703180 -1.490738 1.405351
 H10 -0.061129 -1.205202 1.369682
 H11 0.234428 0.481231 -0.193499
 H12 1.933097 0.176134 -0.327506
 H13 1.010726 1.977722 1.078968
 H14 2.286777 1.025623 1.592596
 N15 4.316615 -0.132064 -0.118305
 O16 3.444957 0.067963 -1.024180
 O17 3.950591 -0.094275 1.086134
 O18 5.484661 -0.361529 -0.425601
 N19 -1.539114 2.348276 -0.284512
 O20 -2.609892 2.938037 -0.366106
 O21 -0.444630 2.918845 -0.207149
 O22 -1.534638 1.049582 -0.280258
 H23 -2.850816 0.462936 -0.202694
 O24 -3.819184 0.044539 -0.130487
 N25 -3.725006 -1.228542 0.221136
 O26 -2.602956 -1.725276 0.321594
 O27 -4.767494 -1.809638 0.419993

[(HEHN)(HNO₃)NO₃]⁻_g

O1 -2.093202 -2.590135 -0.994708
 C2 -0.842786 -1.953567 -1.124546
 C3 -0.374374 -1.248493 0.145372
 N4 -1.004978 0.091228 0.278454
 N5 -0.855746 0.630126 1.599688
 H6 -2.796327 -1.929347 -0.889874
 H7 -0.831368 -1.248033 -1.969442
 H8 -0.118348 -2.739485 -1.352196
 H9 0.708343 -1.096871 0.142298
 H10 -0.660182 -1.822393 1.028375
 H11 -2.037596 0.023954 0.055325
 H12 -0.574988 0.728905 -0.424384
 H13 -1.707347 1.162166 1.774994
 H14 -0.043169 1.242631 1.563029
 N15 -4.337780 0.361866 0.373027
 O16 -5.550717 0.199827 0.302116
 O17 -3.808691 1.098219 1.232889
 O18 -3.566870 -0.232468 -0.464558
 N19 1.615402 1.688444 -0.983443
 O20 2.625147 1.968336 -1.614750

O21 0.477437 1.686470 -1.500386
 O22 1.700029 1.378707 0.261792
 H23 3.052824 0.820500 0.637185
 O24 3.939020 0.446319 1.011330
 N25 4.071584 -0.813655 0.578545
 O26 3.173896 -1.283892 -0.102071
 O27 5.090416 -1.375849 0.916576

[(HEHN)(HNO₃)NO₃]⁻_h

O1 0.606107 -2.586796 1.682126
 C2 1.567515 -1.556073 1.680346
 C3 1.042080 -0.205249 1.201985
 N4 1.047656 -0.119555 -0.285712
 N5 0.518610 1.083440 -0.845144
 H6 0.236395 -2.696665 0.792378
 H7 2.458703 -1.829135 1.095191
 H8 1.887324 -1.439445 2.719183
 H9 1.688724 0.606447 1.544703
 H10 0.014916 -0.049204 1.539362
 H11 0.508665 -0.906376 -0.679617
 H12 2.062668 -0.173810 -0.602775
 H13 1.161773 1.820524 -0.557893
 H14 -0.406785 1.228927 -0.444657
 N15 4.096629 1.015415 -0.388556
 O16 3.259828 1.834232 0.068686
 O17 3.673602 -0.109947 -0.816664
 O18 5.297473 1.272565 -0.424524
 N19 -1.753874 -1.892931 -0.786780
 O20 -2.781575 -2.427477 -1.173192
 O21 -0.622631 -2.424621 -0.933026
 O22 -1.784190 -0.752918 -0.211308
 H23 -3.075001 0.013025 -0.155120
 O24 -3.926077 0.594099 -0.078048
 N25 -3.552275 1.828189 0.275821
 O26 -4.451343 2.624723 0.425592
 O27 -2.357718 2.050108 0.418838

[(HEHN)(HNO₃)NO₃]⁻_i

O1 0.089478 0.162213 2.227607
 C2 -0.378486 -0.867849 1.384648
 C3 -0.733202 -0.335509 -0.000844
 N4 -1.595374 0.864449 0.165017
 N5 -1.832535 1.660960 -0.995317
 H6 0.914462 0.525639 1.851173
 H7 -1.269630 -1.283797 1.864002
 H8 0.359318 -1.670284 1.261345
 H9 -1.296519 -1.060975 -0.591555
 H10 0.164667 -0.034916 -0.543771
 H11 -1.159411 1.460600 0.874448
 H12 -2.555263 0.533269 0.503552

H13 -2.358825 1.062434 -1.630685
 H14 -0.923581 1.915126 -1.376875
 N15 -4.397869 -0.698540 -0.266362
 O16 -3.693304 -0.613162 -1.303275
 O17 -5.478918 -1.280565 -0.266196
 O18 -3.962409 -0.165920 0.809930
 N19 1.966357 1.869567 -0.149795
 O20 0.860212 2.430374 -0.083882
 O21 2.721977 1.994108 -1.108513
 O22 2.320123 1.116657 0.836492
 H23 3.356902 0.096853 0.436351
 O24 4.076168 -0.628132 0.277798
 N25 3.505644 -1.636404 -0.391152
 O26 2.313952 -1.554256 -0.646315
 O27 4.242027 -2.554321 -0.679589

[(HEHN)(HNO₃)NO₃]⁻_j

O1 3.395786 -1.678352 1.580559
 C2 2.070973 -2.078688 1.324058
 C3 1.043813 -0.962912 1.507839
 N4 0.961017 -0.097368 0.303736
 N5 0.283241 1.135343 0.580024
 H6 3.694236 -1.058647 0.893765
 H7 1.842040 -2.862853 2.051263
 H8 1.962762 -2.523494 0.323355
 H9 1.322924 -0.318777 2.343043
 H10 0.040432 -1.364176 1.673948
 H11 0.484233 -0.646148 -0.439628
 H12 1.938160 0.118727 -0.042402
 H13 0.743009 1.841167 0.007504
 H14 -0.689850 1.017031 0.301964
 N15 3.753457 1.441830 -0.703059
 O16 3.509791 0.195861 -0.498298
 O17 2.784472 2.228243 -0.723107
 O18 4.908848 1.812455 -0.876885
 N19 -1.618413 -1.707170 -1.102334
 O20 -0.424595 -1.907417 -1.410492
 O21 -2.546757 -2.316173 -1.617466
 O22 -1.847591 -0.820220 -0.201051
 H23 -3.268490 -0.341642 -0.044290
 O24 -4.225409 0.010498 0.119723
 N25 -4.141812 1.314721 0.411865
 O26 -5.197530 1.868197 0.629783
 O27 -3.034589 1.829022 0.435796

**Cartesian coordinates for structures
in Figure S10, calculated at ω B97XD/
6-31+G(d,p)**

$[(\text{HEHN})_2(\text{HNO}_3)\text{NO}_3]^-$ _a

O1 0.897618 3.691969 -1.407709
C2 -0.324442 3.034308 -1.628359
C3 -1.125093 2.787299 -0.355380
N4 -0.502349 1.742716 0.494193
N5 -1.347082 1.428161 1.611291
H6 1.541688 3.041222 -1.074888
H7 -0.185376 2.082664 -2.158096
H8 -0.931500 3.685305 -2.265815
H9 -2.125552 2.427362 -0.606897
H10 -1.196661 3.690773 0.252900
H11 0.406879 2.085978 0.884325
H12 -0.284902 0.914135 -0.080839
H13 -2.184085 0.994470 1.220446
H14 -0.857623 0.703731 2.142300
O15 3.962434 -0.397567 -1.488245
C16 4.142619 -1.211674 -0.350443
C17 3.315620 -2.481132 -0.502449
N18 1.924947 -2.103191 -0.825828
N19 1.106228 -3.259008 -1.078175
H20 3.575292 0.446699 -1.181429
H21 3.855443 -0.675515 0.560308
H22 5.197818 -1.494034 -0.247845
H23 3.292833 -3.060721 0.423582
H24 3.670393 -3.109693 -1.322484
H25 1.934312 -1.513387 -1.662309
H26 1.508018 -1.510214 -0.048496
H27 0.248846 -2.911625 -1.517229
H28 0.840471 -3.582904 -0.146119
N29 2.792424 1.893048 0.874088
O30 1.939354 2.471007 1.583855
O31 2.485747 1.629106 -0.339837
O32 3.895095 1.576609 1.312954
N33 -1.290495 -0.858156 -1.587903
O34 -0.141589 -0.394857 -1.725262
O35 -1.563107 -2.025574 -1.890143
O36 -2.187272 -0.095025 -1.109677
N37 0.405743 -1.620765 2.033368
O38 0.848587 -2.781048 1.916732
O39 -0.310097 -1.276866 2.974718
O40 0.705993 -0.759485 1.135992
H41 -3.563642 -0.718071 -0.814531
O42 -4.511323 -1.059377 -0.627208
N43 -5.078593 -0.214378 0.245729
O44 -6.227622 -0.457534 0.533545
O45 -4.402647 0.712647 0.667232

$[(\text{HEHN})_2(\text{HNO}_3)\text{NO}_3]^-$ _b

O1 -5.064115 -1.551328 0.350906
C2 -5.018609 -1.367778 -1.039379
C3 -4.259891 -0.113704 -1.455247
N4 -2.813149 -0.201030 -1.142645
N5 -2.162928 -1.256758 -1.877903
H6 -4.213863 -1.920201 0.652398
H7 -6.050485 -1.247996 -1.385308
H8 -4.604859 -2.246201 -1.554500
H9 -4.631999 0.760432 -0.917466
H10 -4.340556 0.044417 -2.533823
H11 -2.646496 -0.309967 -0.110354
H12 -2.347659 0.700541 -1.365588
H13 -1.162292 -1.042188 -1.852072
H14 -2.260420 -2.087238 -1.291797
O15 1.178816 3.492333 -0.835787
C16 2.080269 2.439538 -0.596117
C17 2.050442 1.918173 0.835127
N18 0.768171 1.230293 1.136128
N19 0.839882 0.515769 2.383288
H20 0.283394 3.122036 -0.917114
H21 3.087614 2.824605 -0.775856
H22 1.920655 1.604674 -1.292358
H23 2.162516 2.724724 1.562021
H24 2.845515 1.181473 0.964817
H25 0.534784 0.585044 0.352907
H26 0.001799 1.930334 1.209237
H27 1.419067 -0.299526 2.179151
H28 -0.101296 0.142888 2.526249
N29 -1.740710 -1.767581 1.570946
O30 -1.825460 -0.513941 1.384612
O31 -0.958323 -2.216462 2.401640
O32 -2.476271 -2.525784 0.879357
N33 1.584134 -1.343907 -0.849685
O34 1.904288 -2.133864 -1.725592
O35 0.526055 -0.665838 -0.920858
O36 2.318457 -1.166103 0.175922
N37 -2.043138 2.584541 0.122047
O38 -1.459240 2.971227 1.153850
O39 -3.269706 2.609844 0.013567
O40 -1.334830 2.128628 -0.844830
H41 3.800577 -1.557421 -0.001416
O42 4.789832 -1.821185 -0.011461
N43 5.510231 -0.716326 -0.257163
O44 6.707706 -0.881878 -0.318075
O45 4.911953 0.339001 -0.392067

$[(\text{HEHN})_2(\text{HNO}_3)\text{NO}_3]^-$ _c

O1 -4.539869 -1.630160 0.134533
C2 -4.128442 -0.935955 1.283106

C3 -2.961344 -1.590999 2.013094
 N4 -1.694683 -1.466508 1.252006
 N5 -0.580712 -1.899415 2.051131
 H6 -3.903785 -1.438487 -0.579253
 H7 -4.975144 -0.927239 1.977240
 H8 -3.874378 0.109780 1.058388
 H9 -3.138811 -2.655385 2.178037
 H10 -2.796531 -1.088756 2.969620
 H11 -1.581099 -0.475524 0.949895
 H12 -1.722440 -2.058654 0.391134
 H13 0.225060 -1.922857 1.423389
 H14 -0.412473 -1.130512 2.700790
 O15 -0.645746 4.085391 -0.349562
 C16 0.578659 3.472931 -0.678271
 C17 0.413448 2.718495 -1.987409
 N18 -0.594244 1.646359 -1.806196
 N19 -1.117225 1.176461 -3.062648
 H20 -0.900106 3.797191 0.549012
 H21 0.911881 2.785030 0.107835
 H22 1.364283 4.226529 -0.815894
 H23 1.348084 2.248589 -2.299189
 H24 0.028630 3.377395 -2.768432
 H25 -1.364632 2.035637 -1.249884
 H26 -0.187561 0.860593 -1.241190
 H27 -0.357174 0.655902 -3.498324
 H28 -1.805845 0.458177 -2.806118
 N29 -1.268509 1.775911 2.016276
 O30 -1.057696 2.995370 2.158415
 O31 -1.508068 1.319880 0.856381
 O32 -1.246762 1.000311 2.985365
 N33 -1.797013 -1.938996 -1.981432
 O34 -1.311973 -1.976441 -3.110638
 O35 -1.640056 -2.868978 -1.159875
 O36 -2.481700 -0.920769 -1.618036
 N37 1.661556 -0.342858 -0.158796
 O38 2.318984 0.587085 -0.635133
 O39 2.160609 -1.116759 0.703431
 O40 0.470547 -0.539687 -0.507900
 N41 5.510859 -0.991097 0.346086
 O42 5.067156 -1.497394 -0.666161
 O43 6.674063 -0.763713 0.601183
 O44 4.638718 -0.641188 1.309542
 H45 3.702255 -0.826837 0.962472

H6 -1.998659 -2.969982 -0.648532
 H7 -4.247766 -2.712252 1.001009
 H8 -3.571107 -1.520163 -0.110124
 H9 -2.184571 -2.432997 2.455887
 H10 -3.271080 -1.008695 2.378573
 H11 -1.897775 0.023570 0.864505
 H12 -0.846897 -1.293373 0.707102
 H13 -0.241399 -1.067249 2.894754
 H14 -0.026115 0.362752 2.148204
 O15 3.136900 -2.874072 -0.002387
 C16 3.734366 -1.770239 0.632268
 C17 4.070382 -0.628593 -0.319166
 N18 2.848142 0.064541 -0.792742
 N19 3.196662 1.224625 -1.569875
 H20 2.193114 -2.678984 -0.131203
 H21 4.676485 -2.119375 1.066561
 H22 3.111927 -1.386895 1.452710
 H23 4.606897 -0.986803 -1.199865
 H24 4.665581 0.127299 0.199506
 H25 2.277357 0.337340 0.048396
 H26 2.276170 -0.562734 -1.390031
 H27 3.414045 1.936288 -0.869169
 H28 2.338876 1.519649 -2.039663
 N29 -4.028912 1.429999 0.202131
 O30 -4.589342 2.284544 -0.473749
 O31 -4.580757 0.773281 1.086057
 O32 -2.768248 1.189870 -0.024708
 N33 0.167599 -1.781847 -1.522092
 O34 1.037605 -1.468262 -2.350484
 O35 0.499426 -1.914406 -0.297358
 O36 -1.011988 -1.959797 -1.855408
 N37 2.525836 1.772877 2.019701
 O38 3.485820 2.130148 1.300246
 O39 2.327518 2.250674 3.132080
 O40 1.738874 0.868901 1.566974
 N41 -0.328085 1.835218 -1.821953
 O42 0.456632 2.244183 -2.658221
 O43 -0.055469 1.058827 -0.916046
 O44 -1.566867 2.288863 -1.916924
 H45 -2.121919 1.862971 -1.133487

[(HEHN)₂(HNO₃)NO₃]⁻_d

O1 -2.566660 -3.337901 0.049978
 C2 -3.310109 -2.290917 0.625626
 C3 -2.598004 -1.652591 1.810938
 N4 -1.473517 -0.789517 1.369172
 N5 -0.747798 -0.278063 2.499440