Supporting Information

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

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[d] In-Space Propulsion Branch, Rocket Propulsion Division, Aerospace Systems Directorate, Air Force Research Laboratory, AFRL/RQRS, Edwards Air Force Base, California 93524, USA

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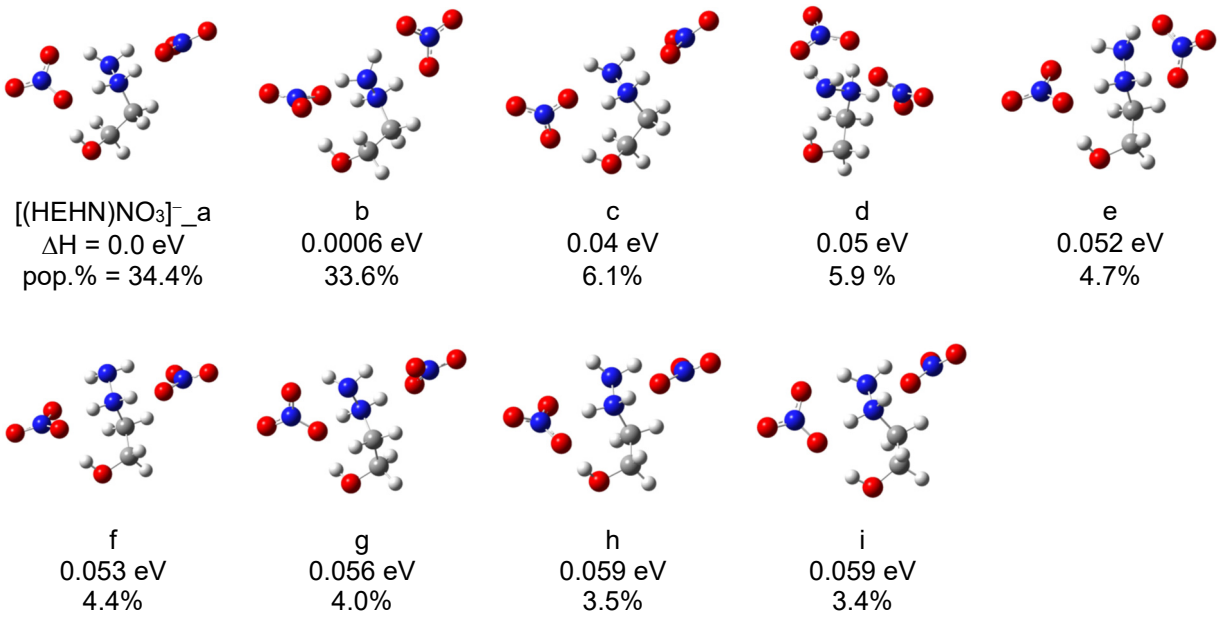


Figure S1 Probable conformations for $[(HEHN)NO_3]^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

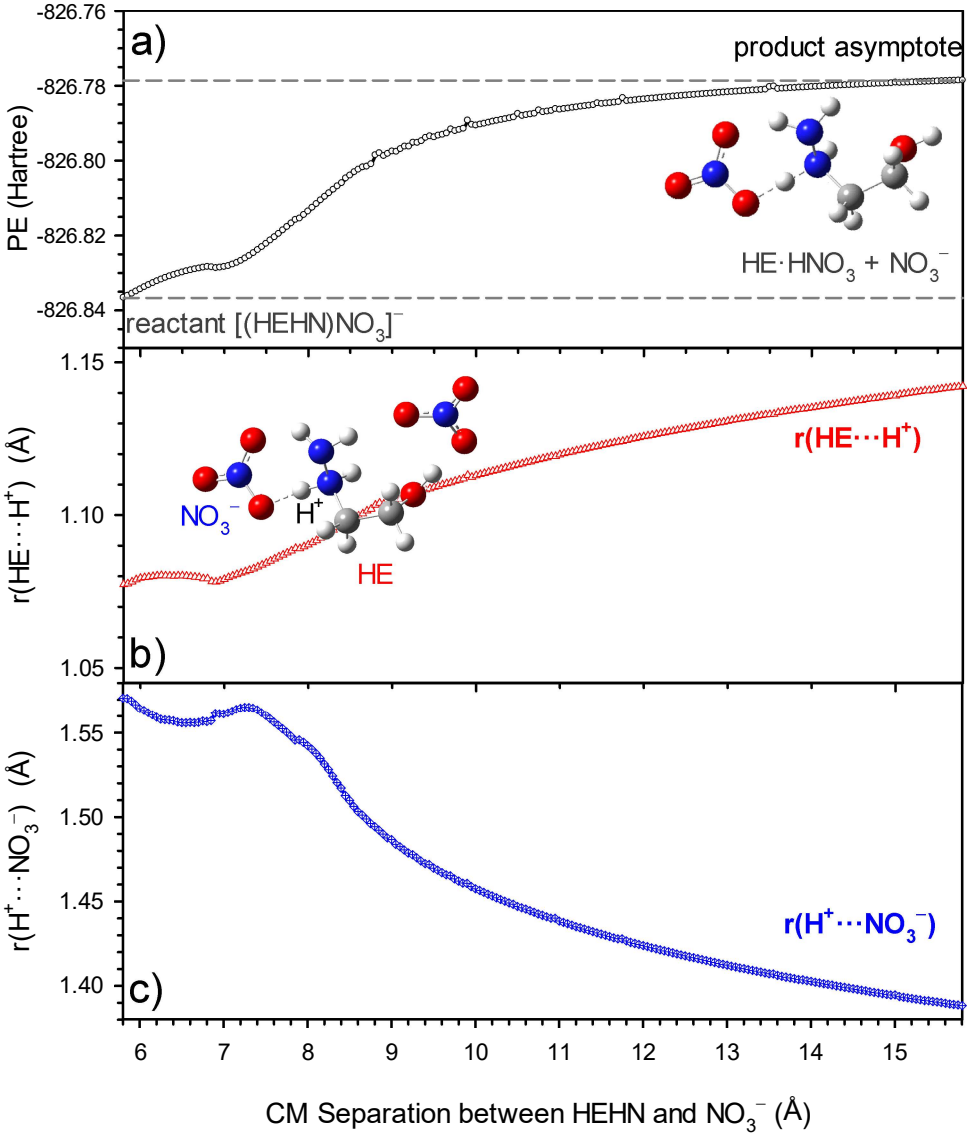
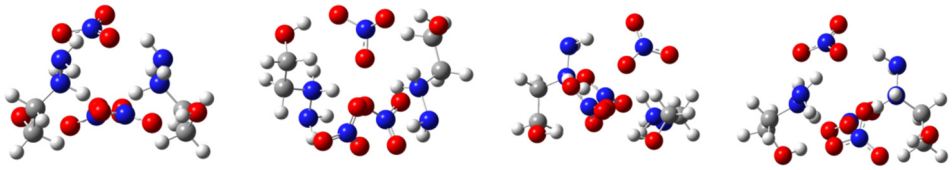


Figure S2 a) A relaxed PES scan for $[(HEHN)NO_3]^-$ along the center-of-mass distance between HEHN and NO_3^-, calculated at the ωB97XD/6-31+G(d,p) level of theory; and (b – c) the accompanying changes of H-bond lengths within the HEHN moiety.



[(HEHN)$_2$NO$_3$]$^-$_a	b	c	d
ΔH = 0.0 eV	0.05 eV	0.07 eV	0.12 eV
pop.% = 81.5%	10.5%	6.5%	1.5%

Figure S3 Probable confirmations for [(HEHN)$_2$NO$_3$]$^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

[(HEHN)$_3$NO$_3$]$^-$_a	b	c	d	e
ΔH = 0.0 eV	0.08 eV	0.10 eV	0.105 eV	0.11 eV
pop.% = 91.8%	3.8%	1.7%	1.6%	1.1%

Figure S4 Probable conformations for [(HEHN)$_3$NO$_3$]$^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

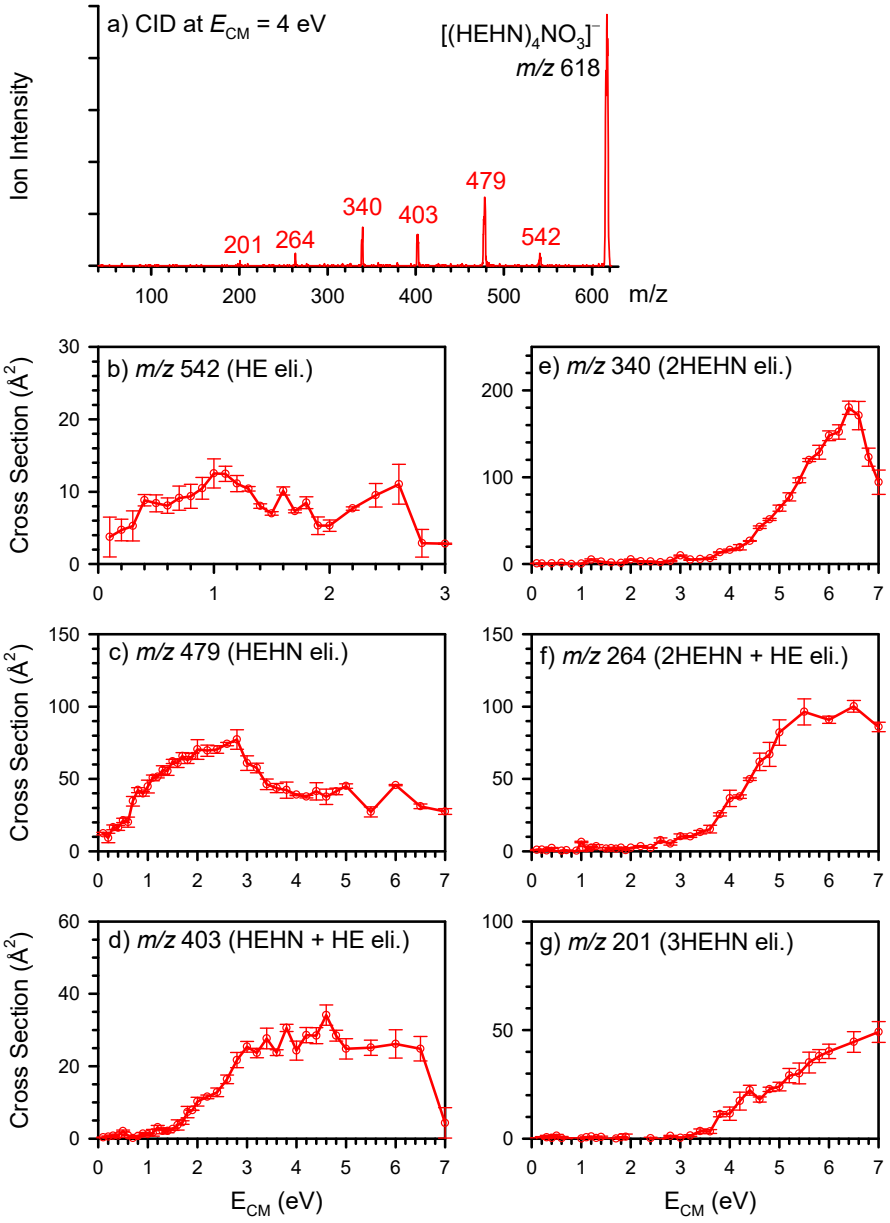


Figure S5 (a) A representative CID product ion mass spectrum for $[(HEHN)_4NO_3]^-$; and (b – g) individual product ion cross sections as a function of E_{CM}.

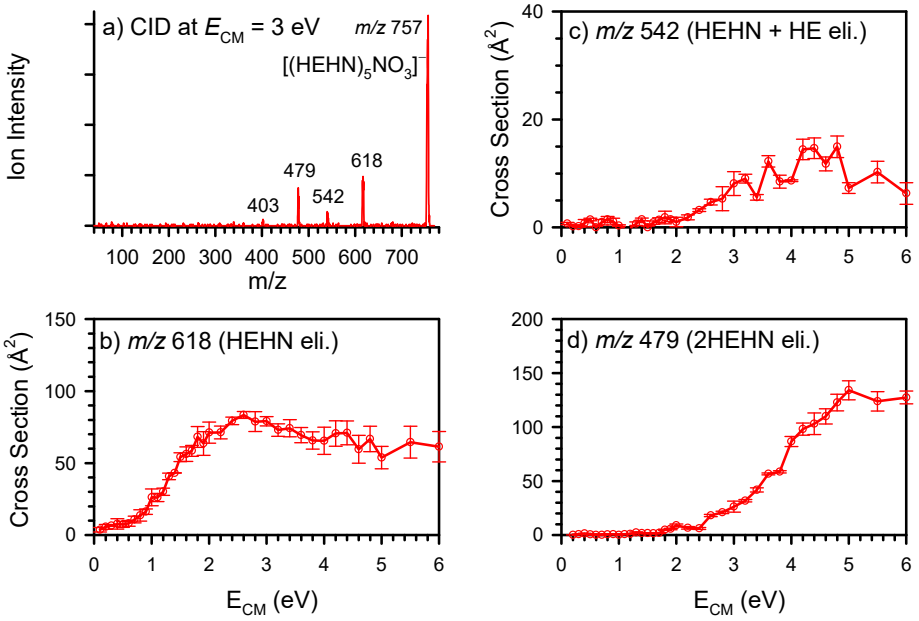


Figure S6 (a) A representative CID product ion mass spectrum for $[(HEHN)_5NO_3]^-$; and (b – d) individual product ion cross sections as a function of E_{CM}.

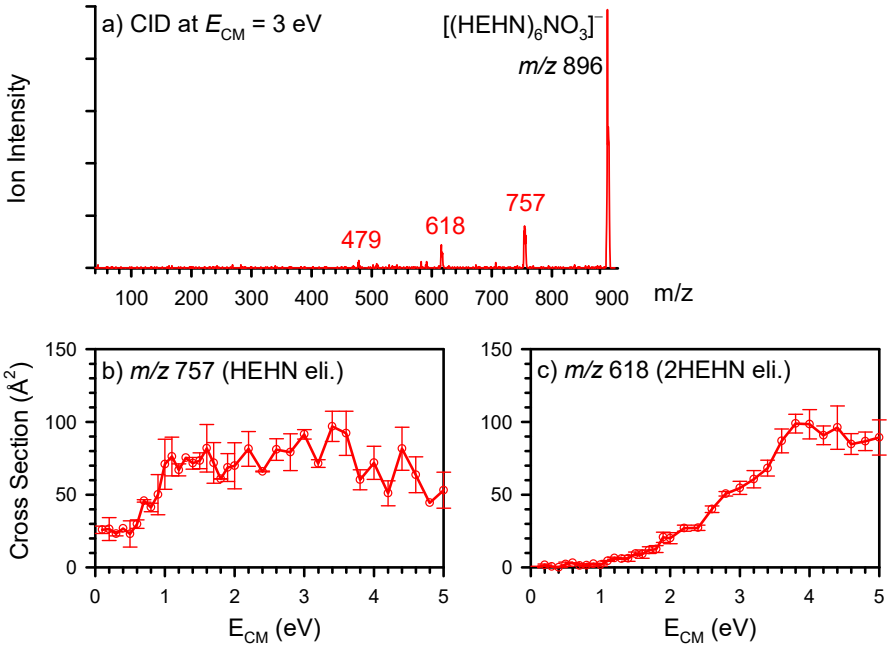


Figure S7 (a) A representative CID product ion mass spectrum for $[(HEHN)_6NO_3]^-$; and (b – c) individual product ion cross sections as a function of E_{CM}.

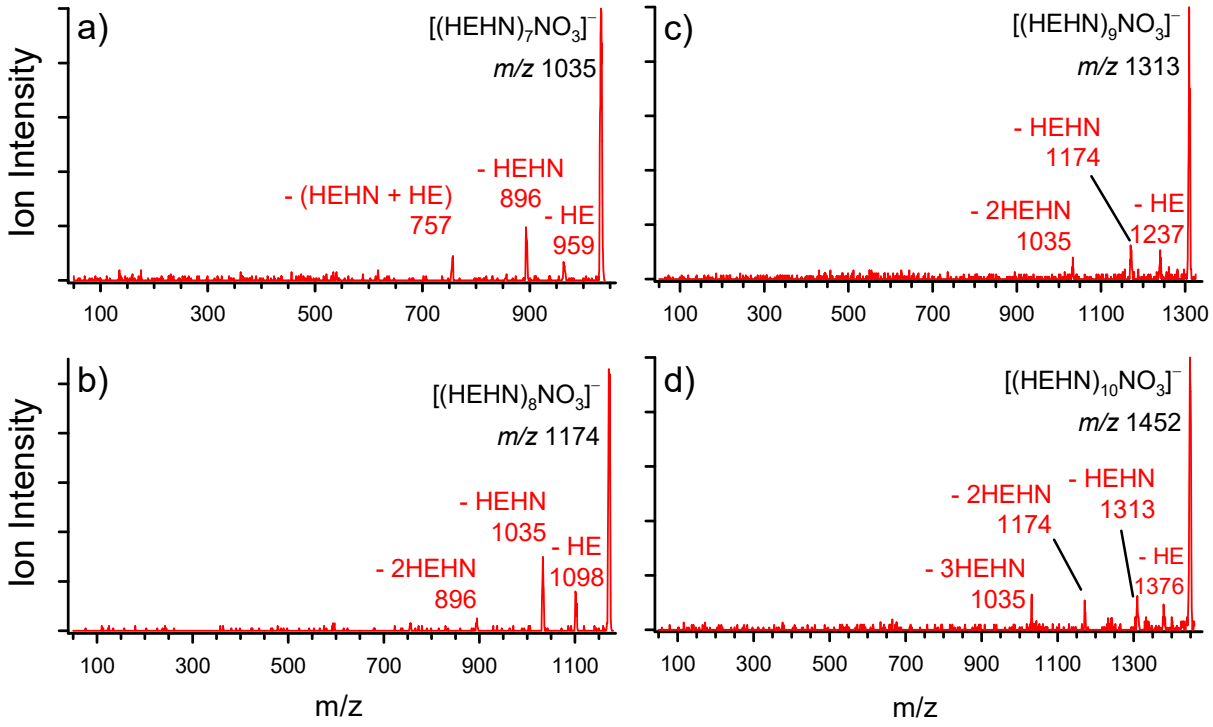


Figure S8 Representative CID product ion mass spectra for $[(HEHN)_{7\text{-}10}NO_3]^-$, recorded at E_{CM} = 4.0 eV.

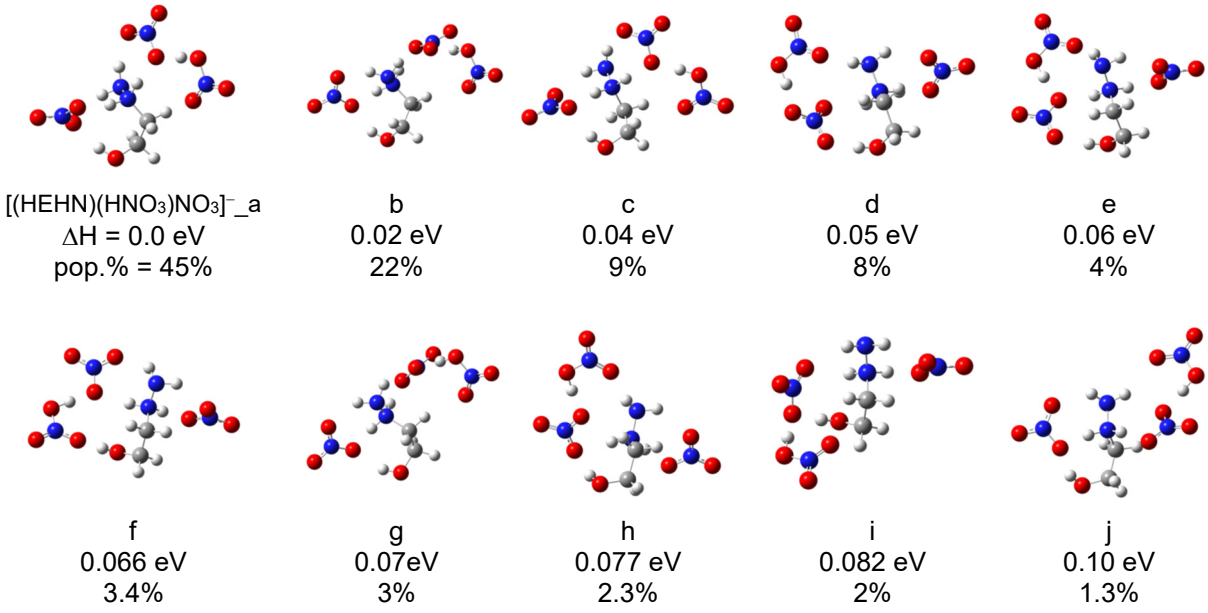


Figure S9 Probable conformations for $[(HEHN)(HNO_3)NO_3]^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

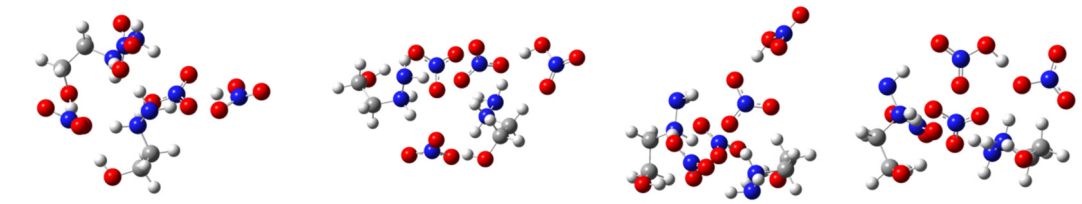


Figure S10 Probable conformations for $[(HEHN)_2(HNO_3)NO_3]^-$, with 298 K enthalpies (relative to global minimum) and thermal populations calculated at the ωB97XD/6-31+G(d,p) level of theory.

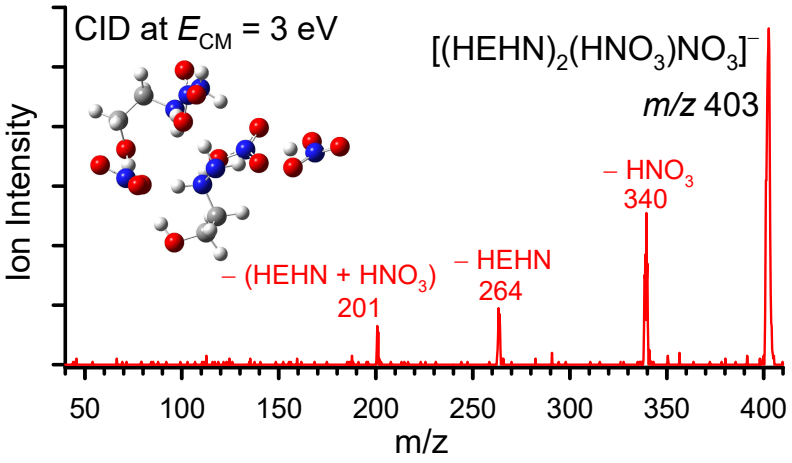


Figure S11 A representative CID product ion mass spectrum for $[(HEHN)_2(HNO_3)NO_3]^-$.

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

$[(HEHN)NO_3]^-$

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

$[(HE)NO_3]^-$

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

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

$[(HNO_3)NO_3]^-$

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

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

NO_3^-

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 ωB97XD/ 6-31+G(d,p)

$[(HEHN)_2NO_3]^-$
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

$[(HEHN)(HNO_3)NO_3]^-$
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

$[(HEHN)NO_3]^-$
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

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

$[(HNO_3)_2NO_3]^-$
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

$[(HNO_3)NO_3]^-$
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

NO_3^-
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 ωB97XD/ 6-31+G(d,p)

$[(HEHN)_3NO_3]^-$
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

$[(HEHN)_2(HNO_3)NO_3]^-$
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

$[(HEHN)_2NO_3]^-$

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

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

$[(HEHN)(HNO_3)_2NO_3]^-$
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

$[(HEHN)(HNO_3)NO_3]^-$
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

$[(HEHN)NO_3]^-$
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

$(HEHN)_2$
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

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

$[(HNO_3)NO_3]^-$
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

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

$[(HNO_3)NO_3]^-$
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

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

NO_3^-
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 ωB97XD/ 6-31+G(d,p)

Reactions for $[(HEHN)(HNO_3)NO_3]^-$

$[(HEHN)(HNO_3)NO_3]^-$

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

$[(HEHN)NO_3]^-$

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

$[(HNO_3)_2NO_3]^-$

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

$[(HNO_3)NO_3]^-$

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 $[(HEHN)_2(HNO_3)NO_3]^-$

$[(HEHN)_2(HNO_3)NO_3]^-$
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

$[(HEHN)_2NO_3]^-$
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

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

$[(HEHN)(HNO_3)NO_3]^-$
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

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

$[(HEHN)NO_3]^-$
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

Cartesian coordinates for structures in Figure S1, calculated at ωB97XD/ 6-31+G(d,p)

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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

$[(HEHN)NO_3]^-$ _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 ωB97XD/ 6-31+G(d,p)

$[(HEHN)_2NO_3]^-$ _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

$[(HEHN)_2NO_3]^-$ _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

$[(HEHN)_2NO_3]^-$ _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
H13 1.357548 0.263604 -2.391042
H14 2.776532 0.640361 -1.685367
N15 2.390849 1.733725 1.159880
O16 1.430543 0.890350 1.250528
O17 3.305294 1.502942 0.341967
O18 2.384326 2.733837 1.876484
O19 -3.858977 -1.064492 1.142838
C20 -3.922492 0.018095 0.244447
C21 -3.224383 1.227862 0.842073
N22 -1.792342 0.928978 1.062403
N23 -1.160002 1.979162 1.821559
H24 -3.343869 -1.771621 0.709537
H25 -4.969310 0.289469 0.056797
H26 -3.464924 -0.241539 -0.718410
H27 -3.648366 1.487005 1.814623
H28 -3.266412 2.087367 0.168408
H29 -1.316045 0.786018 0.124355
H30 -1.712072 0.044403 1.574773
H31 -1.142107 2.770583 1.176059
H32 -0.176100 1.691417 1.903873
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

$[(HEHN)_2NO_3]^-$_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
H20 -3.982489 1.109041 0.164996
H21 -2.987366 0.440152 -1.566633
H22 -4.427459 -0.508570 -1.976817
H23 -2.554020 -2.056003 -1.643417
H24 -3.727427 -2.258070 -0.303970
H25 -2.300501 -0.662283 0.921943
H26 -1.167535 -0.798397 -0.276870
H27 -0.996936 -3.019673 0.075178
H28 -0.759817 -2.236389 1.477932
N29 0.565011 -1.065344 -1.943983
O30 1.598904 -0.863208 -2.600623
O31 -0.051484 -2.137843 -2.011078
O32 0.121601 -0.141155 -1.183653
N33 1.810454 -1.936256 1.676243
O34 1.764843 -3.164108 1.723642
O35 0.809419 -1.237761 2.007579
O36 2.854151 -1.337501 1.285024
N37 -1.857046 2.323414 0.750113
O38 -2.959890 2.545603 0.196999
O39 -0.961453 3.188208 0.731731
O40 -1.655335 1.222124 1.322966

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

$[(HEHN)_3NO_3]^-$ _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

$[(HEHN)_3NO_3]^-$ _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

$[(HEHN)_3NO_3]^-$ _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

$[(HEHN)_3NO_3]^-$ _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

$[(HEHN)_3NO_3]^-$_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 ωB97XD/ 6-31+G(d,p)

[(HEHN)(HNO$_3$)NO$_3$]$^-$_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

[(HEHN)(HNO$_3$)NO$_3$]$^-$_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

[(HEHN)(HNO$_3$)NO$_3$]$^-$_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

[(HEHN)(HNO$_3$)NO$_3$]$^-$_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)(HNO$_3$)NO$_3$]$^-$_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)(HNO$_3$)NO$_3$]$^-$_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)(HNO$_3$)NO$_3$]$^-$_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)(HNO$_3$)NO$_3$]$^-$_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)(HNO$_3$)NO$_3$]$^-$_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)(HNO$_3$)NO$_3$]$^-$_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 ωB97XD/ 6-31+G(d,p)

$[(HEHN)_2(HNO_3)NO_3]^-$ _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

$[(HEHN)_2(HNO_3)NO_3]^-$ _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

$[(HEHN)_2(HNO_3)NO_3]^-$ _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

$[(HEHN)_2(HNO_3)NO_3]^-$ _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
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